SOFTWARE VALIDATION REPORT FOR MINTEQA2 FOR WINDOWS VERSION 1.5

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1 SCOPE OF THE VALIDATION

This document reports the results of the validation testing for the geochemical equilibrium speciation code MINTEQA2 for Windows® Version 1.5 (Allison Geoscience Consultants, Inc. and HydroGeoLogic, Inc.,2003) performed under the Software Validation Test Plan (Myers, 2005). MINTEQA2 for Windows Version 1.5 is a commercially acquired code that uses the same computational algorithms and thermodynamic databases as the DOS version originally developed for the U.S. Environmental Protection Agency (Allison, et al., 1991). Staff at the Center for Nuclear Waste Regulatory Analyses (CNWRA) use the software to provide technical assistance to the U.S. Nuclear Regulatory Commission (NRC) in its high-level waste program.

As stated in Technical Operating Procedure (TOP)–018 (CNWRA, 2007), one purpose of software validation is to develop confidence that the software is correctly implementing numerical algorithms intended to represent the theory that is the basis for the code. One means of developing this confidence is benchmarking the software against hand calculations and similar software packages, and in this case, former versions of the same software package. Benchmarking is used in the validation results reported here and is described in the approved software validation test plan for MINTEQA2 for Windows Version 1.5 (Myers, 2005). The DOS program MINTEQA2 Version 4.02 will be used as a benchmark for the results of MINTEQA2 for Windows Version 1.5.

MINTEQA2 for Windows Version 1.5 includes a number of capabilities that are not planned for use in CNWRA applications and therefore, were not tested at this time. These capabilities include

- Ion Exchange
- Freundlich Isotherm
- Langmuir Isotherm
- Triple-Layer Model
- Constant Capacitance Model
- Composite Organic Liquid Model

If a decision is made to use these code capabilities, the software validation test plan will be modified as necessary and the report supplemented.

2 THERMODYNAMIC DATA USED IN TESTING

Historically, the MINTEQA2 databases provided with the code have been modified to include extensive thermodynamic data for various toxic elements and potentially important radioelements. MINTEQA2 for Windows Version 1.5 is not compatible with the former Version 4.02 databases; therefore, the original Version 4.02 database was reformatted to run with the current Windows version. At this time, the Themo database for the MINTEQA2 for Windows Version 1.5 model was not modified to include toxic elements or potentially important radioelements, and CNWRA have no plans to do so at this time.

3 TEST CASES

The test cases to be used in the validation testing have been identified previously (Myers, 2005). The following sections are intended to report the results of the testing. When using the same input data, we anticipated that differences between MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 would be small. In most cases this was true, but in some cases, differences were larger than expected. Possible reasons for the differences are discussed below. The MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 input files are included in the appendix. Key model results are summarized in tables or figures for each of the test cases. Output files for MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 are quite extensive and are included in electronic form on the compact disc accompanying this report.

3.1 Installation Check—Results

The installation of MINTEQA2 for Windows Version 1.5 software was checked as part of bringing the code into configuration management under TOP–018 (CNWRA, 2007). The results indicate that the code was installed correctly on the personal computer platform and produced the correct results for 11 different example problems provided with MINTEQA2 for Windows Version 1.5. The results are documented in the configuration management package for MINTEQA2 for Windows Version 1.5 stored in the CNWRA quality assurance records room.

3.2 Validation Check—Results

Benchmarking is the major method that has been used in validating the MINTEQA2 for Windows Version 1.5 geochemical speciation code. MINTEQA2 for Windows Version 1.5 results for simple systems reported in geochemical text books (Richardson and McSween, 1989; Stumm and Morgan, 1996; Langmuir, 1997) and for more complicated geochemical systems are checked against computer simulations using the geochemical speciation code MINTEQA2 Version 4.02 (Allison, et al., 1991; EPA, 1999a,b). MINTEQA2 Version 4.02 is currently under CNWRA TOP–018 configuration management (CNWRA, 2007).

3.2.1 Aqueous Speciation

Parkhurst and Appelo (1999) provide an example to calculate the distribution of aqueous species in seawater and the saturation state of seawater at 25 °C [77 °F] relative to a set of minerals. Representative calculated speciation results for this problem generated by MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 are reported in Table 3-1.

As originally posed in the PHREEQC Version 2.4.2 user's manual (Parkhurst and Appelo, 1999), the speciation problem specified thermodynamic equilibrium constants for the uranium aqueous speciation in the input file. With the update to MINTEQA2 Version 4.02 to include data from the Nuclear Energy Agency thermodynamic databases (Grenthe, et al., 1992; Silva, et al.,

Table 3-1. Comparison of MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 Calculated Concentrations of Selected Component Species, Carbonate Species, and Redox Sensitive Species T = 25 °C [77 °F]		
Species	**Aqueous Concentration (molal) MINTEQA2 for Windows Version 1.5**	**Aqueous Concentration (molal) MINTEQA2 Version 4.02**
Non-Redox/Non-Carbonate Species		
K^+	1.033×10^{-2}	1.033×10^{-2}
Na^+	4.766×10^{-1}	4.766×10^{-1}
Cl^-	5.656×10^{-1}	5.656×10^{-1}
Carbonate Species		
CO_3^{2-}	3.024×10^{-5}	3.024×10^{-5}
HCO_3^-	1.613×10^{-3}	1.613×10^{-3}
$Na\ HCO_3$	8.289×10^{-5}	2.058×10^{-4}
UO_2CO_3	5.079×10^{-12}	1.242×10^{-12}
Redox-Sensitive Species		
$U(IV)_{total}$	2.054×10^{-63}	1.419×10^{-37}
$U(V)_{total}$	1.670×10^{-26}	5.437×10^{-28}
$U(VI)_{total}$	1.630×10^{-16}	1.267×10^{-8}
$U^{V}O_2(CO_3)_3^{5-}$	0	1.071×10^{-21}
$U^{VI}O_2(CO_3)_3^{4-}$	1.124×10^{-8}	1.180×10^{-8}
Saturation Indices (SI) With Respect to Solid Phases		
Anhydrite	−0.68	−0.68
Calcite	0.88	0.88
Halite	−2.43	−2.43
Schoepite	−5.88	−4.88
Uraninite	−27.20	−27.37

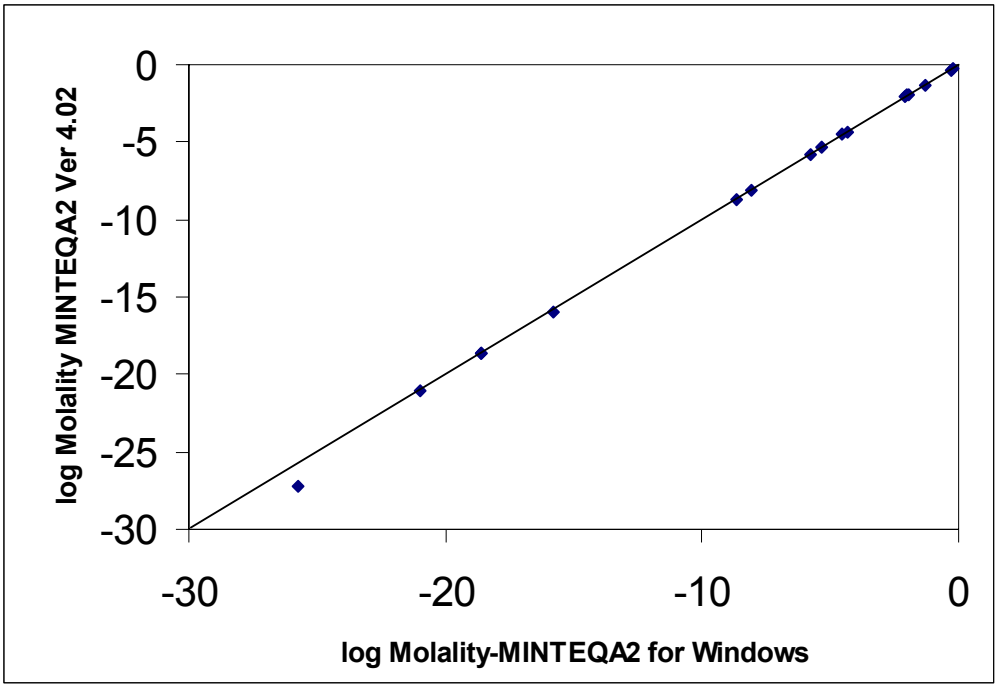
1995; Rard, et al., 1999; Lemire, et al., 2001), we used the values from the database for uranium speciation and then specified thermodynamic data in the input files for the MINTEQA2 for Windows Version 1.5. The original formulation of the example in the PHREEQC Version 2.4.2 user's manual (Parkhurst and Appelo, 1999) also used the NO_3^-/NH_4^+ redox couple to control the oxidation state of uranium while controlling the distribution of the other redox sensitive elements (iron, manganese) by the overall redox equilibrium with atmospheric oxygen.

MINTEQA2 for Windows Version 1.5 does not allow the user to specify individual redox controls, so the entire problem was formulated to control all redox reactions, including uranium speciation, only by atmospheric oxygen. In MINTEQA2 for Windows Version 1.5, the redox couples were selected for manganese, iron, and uranium species. The problem was further defined by the atmospheric oxygen and a fixed equilibrium pH of 7. Because the electron activity (pe) was not specified, a small arbitrary value ($1E^{-6}$) for U^{+4}, UO_2^{+1}, Fe^{+2}, and Mn^{+3} was added to allow the system to equilibrate. For the MINTEQA2 for Windows Version 1.5 program, the intent was to update the database with the Nuclear Energy Agency thermodynamic databases; however, update of the database wasn't completed at the time of this validation exercise. As PHREEQC authors suggested, the log K values for various uranium species and redox reactions were updated in the input file. A few select uranium species were also added to the database. Because of the large number of aqueous species in a multicomponent solution like seawater, only a few representative species concentrations are included in Table 3-1. The speciation results for two versions of MINTEQA2 models are very similar. Differences in calculated concentrations for manganese, iron, and uranium species are most likely due to the arbitrary initial concentration added to allow the problem to equilibrate. A graphical comparison of the calculated concentration of aqueous species (Figure 3-1a) and the calculated activity coefficients (Figure 3-1b) shows a reasonable, although not perfect, correlation between the two MINTEQA2 versions. Most calculated values agree within a factor of two. Calculated mineral saturations (Table 3-1) also show reasonable agreement of the predictions of saturation and undersaturation between the two MINTEQA2 versions. The discrepancies between the two codes appear to be due to differences in the thermodynamic databases; for example, not all the uranium species that had been added to MINTEQA2 Version 4.02 were updated in MINTEQA2 for Windows Version 1.5.

3.2.2 Mineral Solubility

Richardson and McSween (1989) presented two worked problems to investigate the solubility of barite ($BaSO_4$) at 24.85 °C [76.73 °F] in pure water (Worked Problem 3-7) and in a 0.2 m NaCl solution (Worked Problem 3-8). Using an iterative solution of the congruent barite dissolution reaction, Richardson and McSween (1989) demonstrated that barite solubility increases with ionic strength. The concentrations of Ba^2+ and SO_4^{2-} MINTEQA2 for Windows Version 1.5 calculated in pure water and in a 0.2 m NaCl solution are identical to the results obtained from MINTEQA2 Version 4.02 (Table 3-2). The concentrations of Ba^2+ and SO_4^{2-} reported in Richardson and McSween (1989) differ slightly from the results MINTEQA2 for Windows Version 1.5 (Table 3-2) calculated. The results differ by less than two percent and are likely due to slight differences in the activity coefficient formulation and a more complete handling of the geochemical system in MINTEQA2 for Windows Version 1.5. MINTEQA2 for Windows Version 1.5 allows the user to choose between the Davies and extended Debye-Hückel equation for a correction of activity coefficient. In this example, the extended Debye-Hückel is used in MINTEQA2 (Allison, et al., 1991), versus the Debye-Hückel formulation used in Richardson and McSween (1989). MINTEQA2 for Windows Version 1.5 also includes the dissociation products of water (H^+ and OH^-) in the geochemical system, resulting in small changes in calculated ionic strength. Reevaluating the Richardson and McSween (1989) calculations using the activity coefficients MINTEQA2 for Windows Version 1.5 calculated shows excellent agreement between the two sets of results (Table 3-2). Both the MINTEQA2 for Windows Version 1.5 and Richardson and McSween (1989) solubility calculations are in good agreement with the experimental data of Blount (1977) as reported in Richardson and McSween (1989).

(a)



(b)

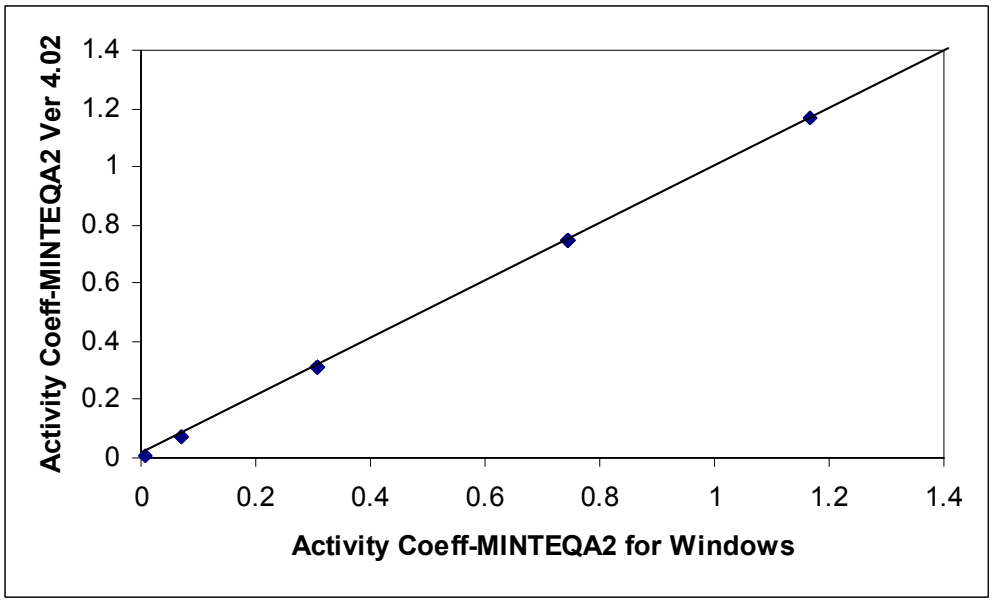


Figure 3-1. Comparison of Aqueous Speciation of Seawater From MINTEQA2 Version 4.02 and MINTEQA2 for Windows Version 1.5 (a) Comparison of Concentration (log Molality) of Aqueous Species; (b) Comparison of the Calculated Activity Coefficents Used by the Two Computer Codes. The Solid Line Indicates a One-to-One Perfect Correlation Between Model Results.

Table 3-2. Comparison of Barite Solubility Results for Richardson and McSween (1989), MINTEQA2 for Windows Version 1.5, and MINTEQA2 Version 4.02				
	mBa^{2+} (molal)	**mSO_4^{2-} (molal)**	**γ Ba^{2+}**	**γ SO_4^{2-}**
Problem 3-7 (pure H_2O)				
MINTEQA2 for Windows Version 1.5	1.055×10^{-5}	1.055×10^{-5}	0.97018	0.97011
MINTEQA2 Version 4.02	1.055×10^{-5}	1.055×10^{-5}	0.97018	0.97011
Richardson and McSween (1989)	1.051×10^{-5}	1.051×10^{-5}	0.9704	0.9704
Richardson and McSween (1989) calculations with MINTEQA2 activity coefficients	1.055×10^{-5}	1.055×10^{-5}	0.97018	0.97011
Blount (1977)	1.06×10^{-5}	1.06×10^{-5}	N/R*	N/R
Problem 3-8 (0.2 m NaCl)				
MINTEQA2 for Windows Version 1.5	3.675×10^{-5}	3.675×10^{-5}	0.29726	0.26082
MINTEQA2 Version 4.02	3.675×10^{-5}	3.675×10^{-5}	0.29726	0.26082
Richardson and McSween (1989)	3.611×10^{-5}	3.611×10^{-5}	0.2987	0.2671
Richardson & McSween (1989) calculations with MINTEQA2 activity coefficients	3.675×10^{-5}	3.675×10^{-5}	0.29726	0.26082
Blount (1977)	3.7×10^{-5}	3.7×10^{-5}	N/R	N/R
*Note: N/R—Not Reported				

3.2.3 Aqueous and Gas Phase Carbonate Chemistry

Stumm and Morgan (1996) present several hand calculations of aqueous carbonate speciation, including is Example 7.8, where calcite ($CaCO_3$) is equilibrated in seawater at 25 °C [77 °F] and open to atmosphere (fixed $P_{CO2} = 3.55 \times 10^{-4}$ atm). The seawater composition is not specified in the example problem, but a representative composition is provided in Table 15.2 of Stumm and Morgan (1996) and reproduced in Table 3-3 of this report. As indicated in the problem formulation, initial Ca^{2+}, HCO_3^-, and B were omitted. Results from Stumm and Morgan (1996), MINTEQA2 Version 4.02, and MINTEQA2 for Windows Version 1.5 are compared in Table 3-4.

The model results between the two versions agree very well for pH and HCO_3^- and agree within less than a factor of two for Ca^{2+}, H_2CO_3(aq), and CO_3^{2-} concentrations. The difference between the two versions of MINTEQA2 is attributed to the slight variation of the log K values for the carbonate species. The modeled results vary more when compared to Stumm and Morgan (1996) by about a factor of 2 to 10—most notably for species HCO_{3-} and CO_3^{2-}. The differences in HCO_3^- and CO_3^{2-} are likely due to uncertainty in starting composition and slight differences in thermodynamic data for the aqueous carbonate system. Stumm and Morgan (1996) do not indicate the precise starting composition of the seawater used in their

Table 3-3. Representative Seawater Composition (Stumm and Morgan, 1996; Table 15.2)	
Constituent	**Concentration (mg/L)**
Na^+	10770
Mg^{2+}	1290
Ca^{2+}	412.1
K^+	399
Sr^{2+}	7.9
Cl^-	19354
SO_4^{2-}	2712
HCO_3^-	142.4
Br^-	67.3
F^-	1.3
B	4.5

Table 3-4. Seawater in Equilibrium With Calcite at 25 °C [77 °F] and Open to Atmosphere (Fixed P_{CO2} = 3.55 × 10^{-4} atm). All Concentrations in Molarity.					
	pH	**Ca^{2+} (total)**	**HCO_3^- (total)**	**CO_3^{2-} (total)**	**H_2CO_3(aq) (total)**
Problem 7.8					
MINTEQA2 for Windows Version 1.5	8.35	9.765 × 10^{-4}	1.418 × 10^{-3}	3.652 × 10^{-5}	9.030 × 10^{-6}
MINTEQA2 Version 4.02	8.32	1.007 × 10^{-3}	1.490 × 10^{-3}	3.541 × 10^{-5}	1.025 × 10^{-5}
Stumm and Morgan (1996)	8.34	1.51 × 10^{-3}	2.77 × 10^{-3}	3.80 × 10^{-4}	1.05 × 10^{-5}

calculations. As noted previously, there are also likely to be differences due to the thermodynamic data for aqueous speciation and different activity coefficient models. Because the details of the model inputs are not presented in Stumm and Morgan (1996), it is not possible to evaluate these differences in more detail.

Alternatively, Langmuir (1997) presents results for calcite solubility in fresh water at 25 °C [77 °F] and under variable fixed P_{CO2}. These results are easier to interpret due to the simpler geochemical system. Between the two MINTEQA2 model versions, the results are the same (Table 3-5). Again, there are slight differences between MINTEQA2 for Windows Version 1.5 and the Langmuir (1997) example due to differences in thermodynamic data or activity coefficient models. However, at all three P_{CO2} values covering two orders of magnitude, the agreement between modeled results is within three percent (Table 3-5). The overall excellent

Table 3-5. Fresh Water in Equilibrium with Calcite at 25 °C [77 °F] and Variable P_{CO_2}			
	pH	**Ca^{2+} (mg/L)**	**HCO_3^- (mg/L)**
$P_{CO_2} = 10^{-3.5}$ bar = $10^{-3.51}$ atm			
MINTEQA2 for Windows Version 1.5	8.284	19.4	58.1
MINTEQA2 Version 4.02	8.284	19.4	58.1
Langmuir (1997); Table 6.3	8.29	20	58
$P_{CO_2} = 10^{-2.5}$ bar = $10^{-2.51}$ atm			
MINTEQA2 for Windows Version 1.5	7.628	42.9	131.3
MINTEQA2 Version 4.02	7.628	42.9	131.3
Langmuir (1997); Table 6.3	7.62	44	131
$P_{CO_2} = 10^{-1.5}$ bar = $10^{-1.51}$ atm			
MINTEQA2 for Windows Version 1.5	6.976	96.9	300.4
MINTEQA2 Version 4.02	6.976	96.9	300.4
Langmuir (1997); Table 6.3	6.97	100	298

agreement indicates that MINTEQA2 for Windows Version 1.5 is correctly implementing carbonate equilibria in aqueous speciation calculations.

3.2.4 Sorption—Surface Complexation Modeling

Parkhurst and Appelo (1999) provide an example to calculate Zn^{2+} sorption on ferrihydrite (HFO) using the diffuse-layer surface complexation model and parameters described in Dzombak and Morel (1990). Sorption at 25 °C [77 °F] is investigated for two Zn^{2+} concentrations (10^{-4} and 10^{-7} molal), and the results are presented in terms of dissolved and sorbed Zn^{2+} molality as a function of pH. In addition, the species $ZnNO_3^+$ and $Zn(NO_3)_2(aq)$ are excluded from the run because they were not included in the database at the time MINTEQA2 Version 4.02 was validated. Model results are given in Table 3-6 (percent sorbed) and shown in Figure 3-2 (surface complex concentration).

The results from MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 show excellent agreement, indicating that the surface complexation modeling subroutines are performing as expected.

Table 3-6. Comparison of MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 Results for Zinc Sorption on Ferrihydrite (Percent Sorbed). DLM Constants from Dzombak and Morel (1990).				
	$Zn_T = 1 \times 10^{-4}$ molal		$Zn_T = 1 \times 10^{-7}$ molal	
pH	MINTEQA2 for Windows Version 1.5 (% sorbed)	MINTEQA2 Version 4.02 (% sorbed)	MINTEQA2 for Windows Version 1.5 (% sorbed)	MINTEQA2 Version 4.02 (% sorbed)
5.00	0.3	0.3	0.3	0.3
5.25	0.8	0.8	0.9	0.9
5.50	1.7	1.7	2.4	2.4
5.75	3.0	3.0	6.2	6.2
6.00	4.5	4.5	15.3	15.3
6.25	6.2	6.2	33.0	33.0
6.50	9.2	9.2	57.3	57.3
6.75	15.1	15.1	78.7	78.7
7.00	24.9	24.8	91.1	91.1
7.25	37.4	37.4	96.6	96.6
7.50	50.5	50.4	98.8	98.8
7.75	62.5	62.4	99.6	99.6
8.00	72.7	72.3	99.8	99.8

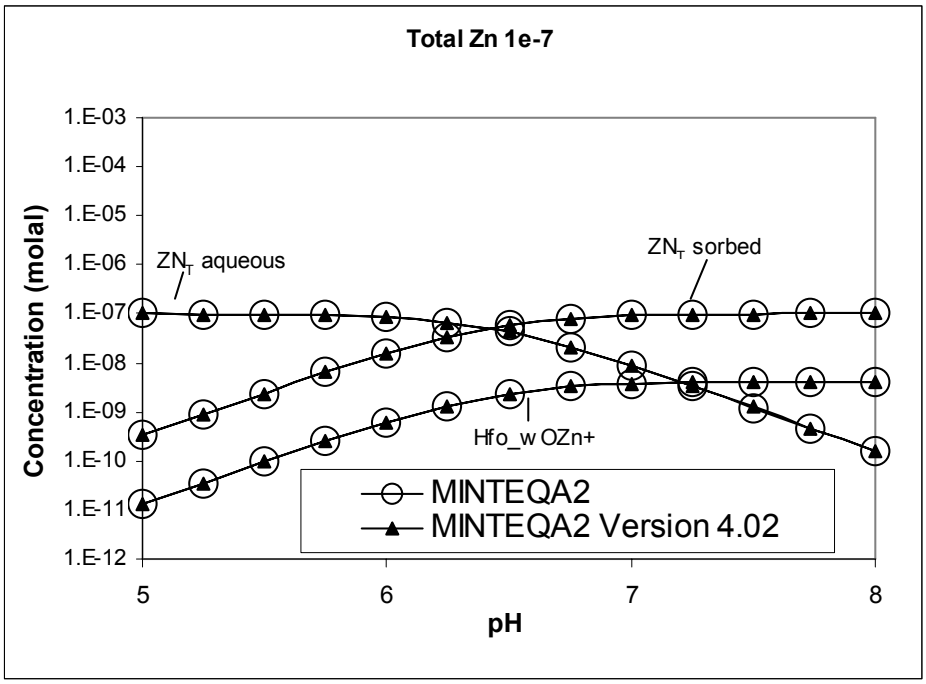
3.2.5 Redox Equilibria

Stumm and Morgan (1996) present a number of relatively simple calculations to determine redox equilibrium and equilibrium distribution in the SO_4^{2-}/HS^- system. MINTEQA2 for Windows Version 1.5 uses electron activity (pe) as a master variable to control redox potential. Example 8.2 from Stumm and Morgan (1996) presents three different geochemical problems to calculate pe for iron and manganese systems open to atmosphere. Simple thermodynamic calculations can be used to calculate pe.

Example 8.2(a). An acid solution with $\{Fe^{3+}\} = 10^{-5}$ M; $\{Fe^{2+}\} = 10^{-3}$ M

$$pe = \log K + \log \frac{\{Fe^{3+}\}}{\{Fe^{2+}\}} \tag{3-1}$$

(a)



(b)

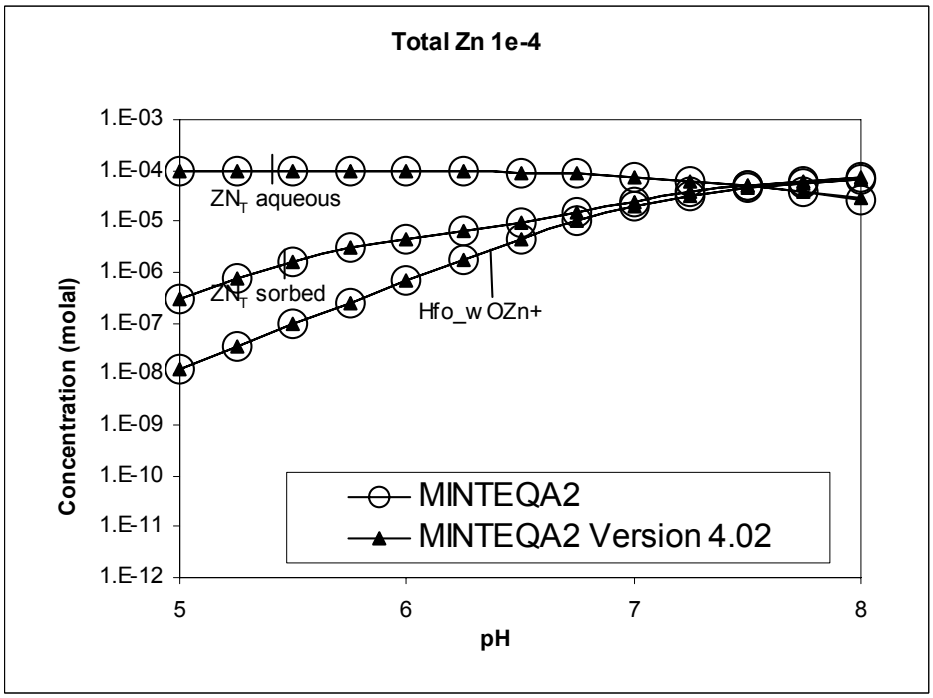


Figure 3-2. Comparison of Zinc-Ferrihydrite Sorption Results for MINTEQA2 for Windows Version 1.5 (Open Circles) and MINTEQA2 Version 4.02 (Triangles) for Total Zinc Concentration of (a) 10^{-7} molal and (b) 10^{-4} molal

Example 8.2(b). Natural water with pH = 7.5 in equilibrium with atmosphere (P_{O2} = 0.22 atm)

$$pe = \frac{1}{2}\log K + \frac{1}{4}\log P_{O2} - pH \tag{3-2}$$

Example 8.2(c). Natural water with pH = 8 in equilibrium with γ–MnO_2

$$pe = \frac{1}{2}\log K - 2pH - \frac{1}{2}\log \left\{Mn^{2+}\right\} \tag{3-3}$$

Equilibrium constants (log K) were modified in the MINTEQA2 for Windows Version 1.5 input files and in the database (iron redox couple) to match the values provided in Stumm and Morgan (1996). Formation of ferric- and ferrous-hydroxy species was suppressed in the MINTEQA2 for Windows Version 1.5 simulation of Example 8.2(a) to match the geochemical equilibrium model used in Stumm and Morgan (1996). Also, a dilute NaCl (10^{-3} M) solution was added to the natural water in Example 8.2(b) to avoid problems with creating a singular matrix in the MINTEQA2 for Windows Version 1.5 simulation. Comparison of model results in Table 3-7 shows that there are slight differences in calculated pe values. In Stumm and Morgan (1996), the assumption is that the activity coefficients for all of the components are unity (γ = 1.0), while the Davies equation was selected for use in MINTEQA2 for Windows Version 1.5 to correct for ionic strength effects. Incorporating activity coefficients calculated with the Davies equation improves the agreement significantly. Both MINTEQA2 versions are combined in one column in Table 3-7 because they predicted the same concentration values. A difference among the two MINTEQA2 versions is that the new Windows version cannot have more than one problem in a single input file; therefore for Stumm and Morgan (1996, Example 8.2), MINTEQA2 for Windows Version 1.5 has three separate input files.

Example 8.4 in Stumm and Morgan (1996) calls for a simple calculation of the speciation of HS^- and SO_4^{2-} as a function of pe, with pH = 10 and $\{HS^-\} + \{SO_4^{2-}\} = 10^{-4}$ M. Based on the redox equilibrium reaction

$$SO_4^{2-} + 9H^+ + 8e^- = HS^- + 4H_2O \tag{3-4}$$

pe can be expressed in terms of pH and component activity

$$pe = \frac{1}{8}\left(\log K + pH + \log [SO_4^{2-}] + \log [HS^-]\right) \tag{3-5}$$

Aqueous speciation log K values for the reaction in Eq. (3-5) were modified in the MINTEQA2 for Windows Version 1.5 input file to match the values (log K = 34.02) provided in Stumm and Morgan (1996). The results from MINTEQA2 for Windows Version 1.5 are compared with hand calculations using Eq. (3-5) in Table 3-8.

Comparison of the results in Table 3-8 shows that there is very good agreement. MINTEQA2 for Windows Version 1.5 correctly predicts the crossover point (pe = –7.0) where the concentrations of HS^- and SO_4^{2-} are equal. There is a slight discrepancy when unity activity

Table 3-7. Calculated Electron Activity (pe) for Example 8.2 in Stumm and Morgan (1996)			
	pe Calculated		
Geochemical System	MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02	Hand Calculation ($\gamma = 1.0$)	Hand Calculation (γ From Davies Equation)
$\{Fe^{2+}\} = 10^{-3}$ M $\{Fe^{3+}\} = 10^{-5}$ M	10.891	11.01	10.89
pH = 7.5 $P_{O2} = 0.22$ atm	13.106	12.94	13.106
$\{Mn^{2+}\} = 10^{-5}$ M Equilibrium with γ–MnO_2	6.925	6.92	6.925
Note: MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 share a single column because results were identical.			

Table 3-8. Calculated HS^-/SO_4^{2-} Speciation as a Function of Electron Activity (pe) for Example 8.4 in Stumm and Morgan (1996)						
	MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02		Hand Calculation ($\gamma = 1.0$)		Hand Calculation (γ From Davies Equation)	
pe	mHS^-(molal)	mSO_4^{2-}(molal)	mHS^-(molal)	mSO_4^{2-}(molal)	mHS^-(molal)	mSO_4^{2-}(molal)
−9.0	9.99×10^{-5}	9.88×10^{-21}	1.00×10^{-4}	9.55×10^{-21}	1.00×10^{-4}	9.89×10^{-21}
−8.8	9.99×10^{-5}	3.93×10^{-19}	1.00×10^{-4}	3.80×10^{-19}	1.00×10^{-4}	3.94×10^{-19}
−8.6	9.99×10^{-5}	1.57×10^{-17}	1.00×10^{-4}	1.51×10^{-17}	1.00×10^{-4}	1.57×10^{-17}
−8.4	9.99×10^{-5}	6.24×10^{-16}	1.00×10^{-4}	6.03×10^{-16}	1.00×10^{-4}	6.24×10^{-16}
−8.2	9.99×10^{-5}	2.48×10^{-14}	1.00×10^{-4}	2.40×10^{-14}	1.00×10^{-4}	2.48×10^{-14}
−8.0	9.99×10^{-5}	9.88×10^{-13}	1.00×10^{-4}	9.55×10^{-13}	1.00×10^{-4}	9.89×10^{-13}
−7.8	9.99×10^{-5}	3.93×10^{-11}	1.00×10^{-4}	3.80×10^{-11}	1.00×10^{-4}	3.94×10^{-11}
−7.6	9.99×10^{-5}	1.57×10^{-9}	1.00×10^{-4}	1.51×10^{-9}	1.00×10^{-4}	1.57×10^{-9}
−7.4	9.99×10^{-5}	6.23×10^{-8}	9.99×10^{-4}	6.02×10^{-8}	9.99×10^{-4}	6.24×10^{-8}
−7.2	9.75×10^{-5}	2.42×10^{-6}	9.77×10^{-5}	2.34×10^{-6}	9.76×10^{-5}	2.43×10^{-6}
−7.0	5.00×10^{-5}	5.00×10^{-5}	5.12×10^{-5}	4.88×10^{-5}	5.00×10^{-5}	5.00×10^{-5}
−6.8	2.43×10^{-6}	9.76×10^{-5}	2.56×10^{-6}	9.74×10^{-5}	2.43×10^{-6}	9.76×10^{-5}
−6.6	6.25×10^{-8}	9.99×10^{-5}	6.60×10^{-8}	9.99×10^{-5}	6.25×10^{-8}	9.99×10^{-5}
−6.4	1.57×10^{-9}	1.00×10^{-4}	1.66×10^{-9}	1.00×10^{-4}	1.57×10^{-9}	1.00×10^{-4}

Table 3-8. Calculated HS^-/SO_4^{2-} Speciation as a Function of Electron Activity (pe) for Example 8.4 in Stumm and Morgan (1996) (continued)						
	MINTEQA2 for Windows Version 1.5, MINTEQA2 Version 4.02		Hand Calculation ($\gamma = 1.0$)		Hand Calculation (γ From Davies Equation)	
pe	mHS^-(molal)	mSO_4^{2-}(molal)	mHS^-(molal)	mSO_4^{2-}(molal)	mHS^-(molal)	mSO_4^{2-}(molal)
−6.2	3.95×10^{-11}	1.00×10^{-4}	4.17×10^{-11}	1.00×10^{-4}	$3.95E \times 10^{-11}$	1.00×10^{-4}
−6.0	9.91×10^{-13}	1.00×10^{-4}	1.05×10^{-12}	1.00×10^{-4}	9.91×10^{-13}	1.00×10^{-4}
−5.4	1.57×10^{-17}	1.00×10^{-4}	1.66×10^{-17}	1.00×10^{-4}	1.57×10^{-17}	1.00×10^{-4}
−5.2	3.95×10^{-17}	1.00×10^{-4}	4.17×10^{-17}	1.00×10^{-4}	3.95×10^{-17}	1.00×10^{-4}
−5.0	9.91×10^{-21}	1.00×10^{-4}	1.05×10^{-20}	1.00×10^{-4}	9.91×10^{-21}	1.00×10^{-4}
Note: MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 share a single column because results were identical.						

coefficients ($\gamma = 1$) were assumed for the hand calculations. Performing the hand calculations with the activity coefficients MINTEQA2 for Windows Version 1.5 derived for each pe value using the Davies equation results in a match to the HS^- and SO_4^{2-} concentrations MINTEQA2 for Windows Version 1.5 predicted to at least three significant figures (Table 3-8). Both MINTEQA2 versions are combined in one column in Table 3-8 because they predicted the same concentration values. Concentration-pe plots comparing MINTEQA2 for Windows Version 1.5 and hand calculation results (Figure 3-3) demonstrate the excellent agreement, indicating that MINTEQA2 for Windows Version 1.5 correctly implements redox equilibria reactions.

3.2.6 Temperature Effects

Parkhurst and Appelo (1999) provide an example of the use of MINTEQA2 to calculate the solubility of gypsum and anhydrite in pure water over a range in temperature from 25 to 75 °C (77 to 167 °F). Only the pH and temperature are used to define a pure water solution. Gypsum and anhydrite are allowed to react to equilibrium, and the initial phase assemblage has 1 mol of each mineral. Each mineral will react either to equilibrium or until it is exhausted in the assemblage. For both MINTEQA2 versions (Windows and 4.02), the degree of saturation with respect to a given mineral is indicated by the saturation index (SI), such that

$$SI = \log \frac{IAP}{K} \tag{3-6}$$

where IAP is the ion activity product and K is the equilibrium constant. When a solution is undersaturated with respect to a given mineral, SI < 0. Under supersaturated conditions, SI > 0, and SI = 0 at equilibrium.

As a default, both MINTEQA2 Version 4.02 and MINTEQA2 for Windows Version 1.5 use the Van't Hoff relationship and enthalpies of reaction ($\Delta H_r°$) to correct equilibrium constants for the effects of temperature. If data are available, both MINTEQA2 versions will employ a polynomial expression to correct equilibrium constants for the effects of temperature:

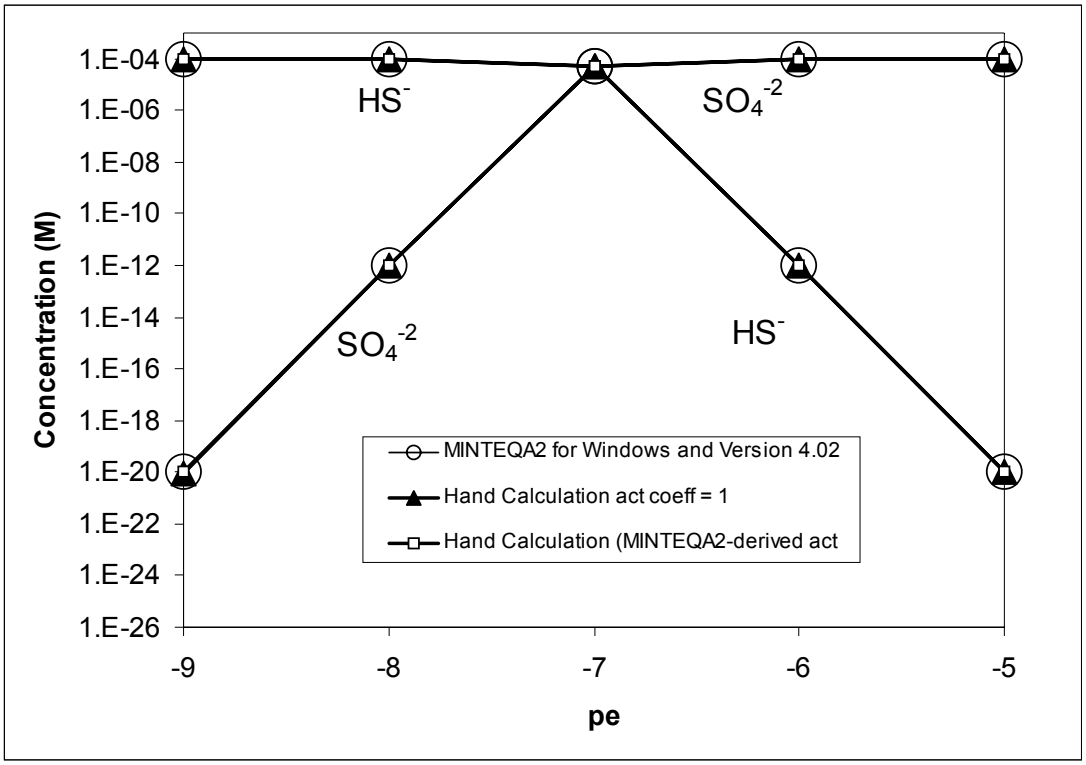


Figure 3-3. Calculated HS^-/SO_4^{2-} Speciation as a Function of Electron Activity (pe) for Example 8.4 in Stumm and Morgan (1996)

$$\text{Log } K_T = A_1 + A_2T + \frac{A_3}{T} + A_4\text{Log}(T) + A_5T^2 + \frac{A_6}{T2} + A_7\sqrt{T} \qquad (3\text{-}7)$$

where K_T is the equilibrium constant at a given temperature T in Kelvin.

If the same thermodynamic data and polynomial expressions are used, both codes should produce similar results. PHREEQC Version 2.12.5 provides a polynomial expression in the *phreeqc.dat* database for both anhydrite and gypsum. In conducting this validation exercise, the same thermodynamic constants and polynomial expressions were used for anhydrite and gypsum (Appendix, Validation Test Case 7b). These values were extracted from the PHREEQC database. This is the same approach used to validate MINTEQA2 Version 4.02.

To update MINTEQA2 for Windows Version 1.5, the user needs to update the database file named ANALYT.DBS. The procedure for updating this file is not mentioned in either user manual and will briefly be discussed here. The file should be opened in a text editor program (e.g., Textpad, Wordpad). The program reads “110 read (lun07,9070) idt,at,bt,ct,dt,et,ft,gt,”; this line of code reads a “record.” The relationship between the parameters in the ANALYT.DBS and Eq. (3-7) are listed in Table 3-9. MINTEQA2 identifier, idt, occupies the first 7 spaces, then it skips a space and reads the next 7 variables (at,bt,ct,dt,et,ft,gt) as decimal numbers, each occupying 10 spaces with 1 space after each number. Each entry will be stored with three digits to the right of the decimal point (this occurs whether the decimal point is specified or not; if

Table 3-9. Parameter Equivalents From Equation 3-7 and MINTEQA2 for Windows Version 1.5 ANAYLT.DBS	
Parameters From Equation 3-7	**Parameters From ANAYLT.DBS**
A_1	at
A_2	bt
A_3	ct
A_4	dt
A_5	et
A_6	ft
A_7	gt

more than three digits to the right are specified, they are ignored). If the constants are being added for a mineral or an aqueous species, they are added to the top or bottom, respectively, of the file that is separated by a single 0 character. Note that if the polynomial constants are taken from PHREEQC, they must be multiplied by (−1) before they are entered into the MINTEQA2 database. MINTEQA2 (all versions) assumes solid phase reactions in its database are written as formation reactions, but the solid phase reactions in the PHREEQC database are written as solubility products.

Comparing results between the two versions of MINTEQA2 in Table 3-10 and Figure 3-4(a) shows a slight discrepancy between the SI values calculated by MINTEQA2 Version 4.02 and MINTEQA2 for Windows Version 1.5; this is likely due to an accumulation of rounding errors. For the most part, the output is comparable. In Figure 3-4(b), gypsum or anhydrite was assigned to be present in an infinite amount. Once again, the values are comparable and vary only in the third decimal place due to rounding.

3.2.7 Modified Database

In this section of the test plan, the main code function to be checked ensures that the MINTEQA2 for Windows Version 1.5 database modified to include Nuclear Energy Agency radionuclide thermodynamic data is correct and produces reasonable results. If thermodynamic data are the same, different geochemical equilibrium speciation codes should produce similar results.

The MINTEQA2 Version 4.02 modified database is not compatible with Windows Version 1.5, and the radionuclides of interest (neptunium, selenium, etc.) have not yet been added to the Windows Version 1.5 database. Therefore, the modified database was not tested at this time. If the modified database becomes available in the future, validation testing will be performed at that time.

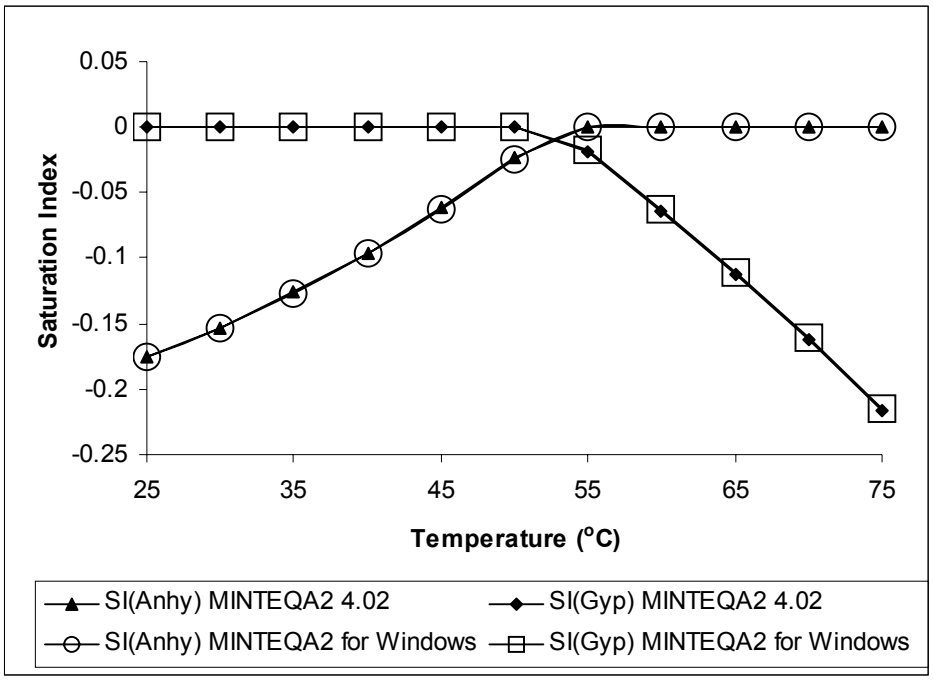
Table 3-10. Comparison of Saturation Indexes (SI) Calculated by MINTEQA2 for Windows Version 1.5 and MINTEQA2 Version 4.02 for Anhydrite and Gypsum as a Function of Temperature						
	MINTEQA2 Version 4.02			MINTEQA2 for Windows Version 1.5		
T(°C)	pH	SI(Anhy)	SI(Gyp)	pH	SI(Anhy)	SI(Gyp)
25	7.08	−0.175	0.000	7.08	−0.175	0.000
30	7.01	−0.153	0.000	7.01	−0.154	0.000
35	6.94	−0.126	0.000	6.94	−0.127	0.000
40	6.88	−0.096	0.000	6.88	−0.096	0.000
45	6.82	−0.061	0.000	6.82	−0.062	0.000
50	6.76	−0.023	0.000	6.76	−0.024	0.000
55	6.70	0.000	−0.019	6.70	0.000	-0.018
60	6.65	0.000	−0.064	6.65	0.000	−0.063
65	6.59	0.000	−0.112	6.59	0.000	−0.111
70	6.54	0.000	−0.162	6.54	0.000	−0.161
75	6.49	0.000	−0.216	6.49	0.000	-0.215

4 SUMMARY AND CONCLUSIONS

Comparisons for a variety of geochemical problems (solubility, gas chemistry, redox, sorption) show that MINTEQA2 for Windows Version 1.5 produces results that are consistent with those produced by other methods such as hand calculations, experiments, and other computer codes. For the simplest systems, the MINTEQA2 for Windows Version 1.5 results agree well with those calculated by other methods. For more complicated systems, however, there are differences in how the problems are formulated in the different codes, especially activity coefficient corrections, that lead to differences in the results. Typically, when combined with slight differences in the thermodynamic databases used by the two codes, these differences have a relatively small effect, but some can lead to large variance between the calculated results produced by the two codes, particularly for highly charged aqueous species.

Overall, the agreement of trends and results between MINTEQA2 for Windows Version 1.5 and the various calculational methods used in the model validation exercise indicates that the code is correctly and consistently applying mass action and mass balance constraints to calculating geochemical equilibrium. As has been demonstrated for the geochemical systems considered in this validation exercise, the observed differences in calculated results are generally small, but in some cases, they can be larger than might otherwise be expected. However, in most instances, the results for the previously validated MINTEQA2 Version 4.02 and those of

(a)



(b)

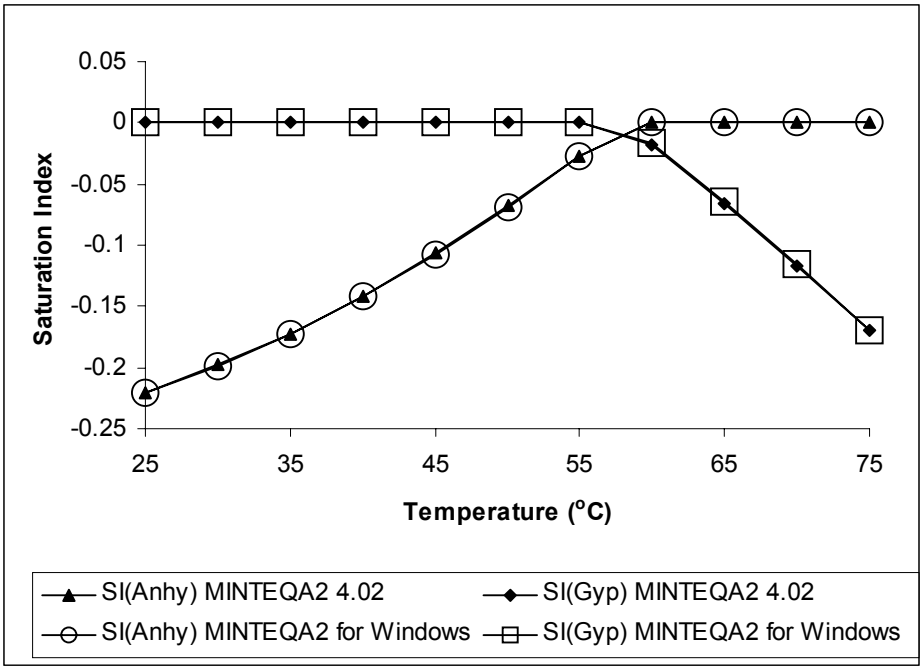


Figure 3-4. Comparison of Saturation Indexes (SI) Calculated by MINTEQA2 Version 4.02 and MINTEQA2 for Windows Version 1.5 for Anhydrite and Gypsum as a Function of Temperature. (a) 1.0 mole anhydrite + 1.0 mole gypsum; (b) Infinite Gypsum (25–55 °C), Infinite Anhydrite (60–75 °C).

MINTEQA2 for Windows Version 1.5 are identical. For the purposes of this validation, the differences in results do not seem to represent errors in the formulation of MINTEQA2 for Windows Version 1.5, but instead reflect different approaches to geochemical equilibrium calculations used by different calculation methods (hand calculations and computer code simulations), differences in computational approach, and minor differences in thermodynamic databases that are beyond the scope of this model validation. These types of variations are often observed among geochemical speciation codes (Morrey, et al., 1986; Emren, et al., 1999) and indicate that the code user should pay careful attention to interpreting the results of any geochemical speciation calculations.

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APPENDIX

MINTEQA2 for Windows® Version 1.5 and MINTEQA2 Version 4.02 Input Files

Validation Test Case 1

The installation of MINTEQA2 for Windows® Version 1.5 software was checked as part of bringing the code into configuration management under Technical Operating Procedure (TOP)–018 for the Center for Nuclear Waste Requlatory Analyses (CNWRA). The results indicate that the code was installed correctly on the PC platform and produced the correct results for 12 different example problems provided with MINTEQA2 for Windows Version 1.5. The results are documented in the configuration management package for MINTEQA2 for Windows Version 1.5 stored in the CNWRA Quality Assurance Records Room.

Validation Test Case 2a—Aqueous Speciation. PHREEQC, Version 2.4.2 input file for seawater speciation check (from Parkhurst and Appelo, 1999).

```
TITLE Modified Example 1.--Add uranium and speciate seawater.
SOLUTION 1  SEAWATER FROM (Nordstrom et al., 1979)
              units       ppm
              pH          8.22
              pe          8.451
              density     1.000
              temp        25.0
              redox       O(0)/O(-2)
              Ca              412.3
              Mg              1291.8
              Na              10768.0
              K               399.1
              Fe              0.002
              Mn              0.0002
              Si              4.28
              Cl              19353.0
              C(4)            141.682 as HCO3
              S(6)            2712.0
              N(5)            0.29    gfw   62.0
              N(-3)           0.03    as    NH4
              U               3.3     ppb
              O(0)            1.0     O2(g) -0.66
END
```

Validation Test Case 2b—Aqueous Speciation. MINTEQA2 for Windows, Version 1.5 input file for seawater speciation check (from Parkhurst and Appelo, 1999).

```
Valid 62  Add U and speciate seawater (Nordstrom et al., 1979)
Modified PHREEQC 2.4.2 Ex.  1 (Parkhurst and Appelo, 1999)
 25.0 mg/L  0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -8.22 Y                    /H+1
    150  4.123E+02   -1.99 Y                    /Ca+2
    460  1.292E+03   -1.27 Y                    /Mg+2
    500  1.077E+04   -0.33 Y                    /Na+1
    410  3.991E+02   -1.99 Y                    /K+1
    280  1.000E-06  -11.75 Y                    /Fe+2
    281  2.000E-03   -7.45 Y                    /Fe+3
    470  2.000E-04   -8.44 Y                    /Mn+2
    471  1.000E-06  -11.74 Y                    /Mn+3
    770  4.280E+00   -3.82 Y                    /H4SiO4
    180  1.935E+04   -0.26 Y                    /Cl-1
    140  1.393E+02   -2.63 Y                    /CO3-2
    732  2.712E+03   -1.55 Y                    /SO4-2
    492  2.900E-01   -5.33 Y                    /NO3-1
    490  3.000E-02   -5.78 Y                    /NH4+1
    891  1.000E-06  -12.43 Y                    /U+4
    892  1.000E-06  -12.43 Y                    /UO2+1
    893  3.300E-03   -7.80 Y                    /UO2+2
    001  0.000E+00    0.00 Y                    /E-1

  2   6
8913303    -8.5380   103.5958                   /U(OH)4 (aq)
8913304   -13.1470   115.3738                   /U(OH)5-
8933301    -5.6260    41.8200                   /(UO2)2(OH)2+2
8933302   -15.6410   108.0500                   /(UO2)3(OH)5+
8931402    21.3970   -40.0000                   /UO2(CO3)3-4
8933300    -5.7820    47.8100                   /UO2OH+
  3   6
3300021   -82.4295   571.6600                   /O2 (g)
2802810    13.0320   -42.7000                   /Fe+2/Fe+3
4704710    25.3500  -107.8000                   /Mn+2/Mn+3
8918930     9.2160  -144.1000                   /U+4/UO2+2
8928930     2.7850   -13.8000                   /UO2+/UO2+2
    330     8.2200     0.0000                   /H+1
```

```
  6   1
    001     0.0000     0.0000                    /E-1
```

Validation Test Case 3a—Mineral Solubility. MINTEQA2 for Windows Version 1.5 input file. Barite solubility in pure H_2O comparison to Richardson and McSween (1989) (Worked Problem 3-7).

```
 valid 63a Validation for Barite (BaSO4) solubility Solubility
comparison to Richardson & McSween (1989)
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 0 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    100  0.000E+00   -6.00 Y                    /Ba+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   1
6010000     9.9800   -23.0000   9.980E+00       /BARITE
  6   2
1003300   -13.3570    60.8100                   /BaOH+
3307320     1.9900    22.0000                   /HSO4-
```

Note: HSO_4^- and $BaOH^+$ are aqueous species included in the MINTEQA2 for Windows Version 1.5 database, but excluded in this calculation for direct comparison to the results of Richardson and McSween (1989). Also, although the Davies equation is the MINTEQA2 for Windows Version 1.5 default, a flag is set to use the extended Debye-Hückel approach to calculate activity coefficients as a more direct comparison to Richardson and McSween (1989).

Validation Test Case 3b—Mineral Solubility. MINTEQA2 for Windows Version 1.5 input file. Barite solubility in 0.2 m NaCl comparison to Richardson and McSween (1989) (Worked Problem 3-8).

```
 valid 63b Validation for Barite solubility in 0.2m NaCl solution
           Solubility comparison to Richardson & McSween (1989)
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 0 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    100  0.000E+00   -6.00 Y                    /Ba+2
    732  0.000E+00   -6.00 Y                    /SO4-2
    500  2.000E-01   -0.70 Y                    /Na+1
    180  2.000E-01   -0.70 Y                    /Cl-1

  3   1
6010000     9.9800   -23.0000                   /BARITE
  6   3
3307320     1.9900    22.0000                   /HSO4-
1003300   -13.3570    60.8100                   /BaOH+
5007320     0.7300     1.0000                   /NaSO4-
```

Note: HSO_4^-, $BaOH^+$, and $NaOH^+$ are aqueous species included in the MINTEQA2 for Windows Version 1.5 database, but excluded in this calculation for direct comparison to the results of Richardson and McSween (1989). Also, although the Davies equation is the MINTEQA2 for Windows Version 1.5 default, a flag is set to use the extended Debye-Hückel approach to calculate activity coefficients as a more direct comparison to Richardson and McSween (1989).

Validation Test Case 4a—Gas Chemistry. MINTEQA2 for Windows Version 1.5 input file. Aqueous speciation of seawater in equilibrium with calcite at 25 °C and open to atmosphere (fixed P_{CO_2} = 3.55 × 10^{-4} atm) (Stumm and Morgan, 1996; Example 7.8).

```
 valid 64a Calcite-Seawater with PCO2 = 1E-3.5 atm
            Example 7.8; Stumm&Morgan(1996); Seawater from Table 15.2
 25.0 mg/L  0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    500  1.077E+04   -0.33 Y                    /Na+1
    460  1.290E+03   -1.28 Y                    /Mg+2
    410  3.990E+02   -1.99 Y                    /K+1
    800  7.900E+00   -4.04 Y                    /Sr+2
    180  1.935E+04   -0.26 Y                    /Cl-1
    732  2.712E+03   -1.55 Y                    /SO4-2
    270  1.300E+00   -4.16 Y                    /F-1
    130  6.730E+01   -3.07 Y                    /Br-1
    140  0.000E+00   -6.00 Y                    /CO3-2
    150  0.000E+00   -6.00 Y                    /Ca+2

  3   2
5015001     8.4800     8.0000                   /CALCITE
3301403    21.6530    -4.0600                   /CO2 (g)
```

Note: The data from Table 15.2 in Stumm and Morgan (1996) are reported in g/L. These values are converted to molality by MINTEQA2, assuming that the density of water ~1 g/mL. This assumption is slightly inaccurate for seawater, where the density of water is slightly greater than 1g/mL.

Validation Test Case 4b—Gas Chemistry. MINTEQA2 for Windows Version 1.5 input file. Aqueous speciation of fresh water in equilibrium with calcite at 25 °C and variable P_{CO_2} (Langmuir, 1997; Table 6.3).

```
 valid 64a Calcite solubility in fresh water, 25C with
PCO2=1e-3.5 bar    Langmuir (1997), Calculated values in Table 6.3
 25.0 mg/L  0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    140  0.000E+00   -6.00 Y                    /CO3-2
    150  0.000E+00   -6.00 Y                    /Ca+2

  3   2
5015001     8.4800     8.0000                   /CALCITE
3301403    21.6756    -4.0600                   /CO2 (g)


 valid 64a Calcite solubility in fresh water, 25C with
PCO2=1e-3.5 bar    Langmuir (1997), Calculated values in Table 6.3
 25.0 mg/L  0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    140  0.000E+00   -6.00 Y                    /CO3-2
    150  0.000E+00   -6.00 Y                    /Ca+2

  3   2
5015001     8.4800     8.0000                   /CALCITE
3301403    20.6476    -4.0600                   /CO2 (g)
```

```
 valid 64a Calcite solubility in fresh water, 25C with
PCO2=1e-3.5 bar    Langmuir (1997), Calculated values in Table 6.3
 25.0 mg/L  0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    140  0.000E+00   -6.00 Y                    /CO3-2
    150  0.000E+00   -6.00 Y                    /Ca+2

  3   2
5015001     8.4800     8.0000                   /CALCITE
3301403    19.6530    -4.0600                   /CO2 (g)
```

Note: The partial pressures in Langmuir (1997) are presented in terms of bars, while MINTEQA2 reads pressures in terms of atmospheres. For conversion, 1 bar = 0.98692 atm.

Validation Test Case 5—Surface Complexation (Double Diffuse-Layer Model). PHREEQC Version 2.4.2 input files for zinc sorption on ferrihydrite, using the parameters of Dzombak and Morel (1990). This input file is from Example 8 in the MINTEQA2 Version 4.02 installation test problems (Parkhurst and Appelo, 1999).

```
TITLE Example 8.--Sorption of zinc on hydrous
                  iron oxides.
SURFACE_SPECIES
        Hfo_sOH  + H+ = Hfo_sOH2+
        log_k  7.18

        Hfo_sOH = Hfo_sO- + H+
        log_k  -8.82

        Hfo_sOH + Zn+2 = Hfo_sOZn+ + H+
        log_k  0.66

        Hfo_wOH  + H+ = Hfo_wOH2+
        log_k  7.18

        Hfo_wOH = Hfo_wO- + H+
        log_k  -8.82

        Hfo_wOH + Zn+2 = Hfo_wOZn+ + H+
        log_k  -2.32
SURFACE 1
        Hfo_sOH        5e-6    600.    0.09
        Hfo_wOH        2e-4
SOLUTION 1
        -units  mmol/kgw
        pH      8.0
        Zn      0.0001
        Na      100.    charge
        N(5)    100.
SOLUTION 2
        -units  mmol/kgw
        pH      8.0
        Zn      0.1
        Na      100.    charge
        N(5)    100.
USE solution none
#
# Model definitions
#
PHASES
        Fix_H+
        H+ = H+
        log_k  0.0
END
```

```
#
#   Zn = 1e-7
#
SELECTED_OUTPUT
        -file ex8.sel
        -molalities     Zn+2    Hfo_wOZn+      Hfo_sOZn+
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.0   NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.25  NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.5   NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.75  NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.0   NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.25  NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.5   NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.75  NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.0   NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.25  NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.5   NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.75  NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
```

```
        Fix_H+   -8.0   NaOH    10.0
END
#
#   Zn = 1e-4
#
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.0   NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.25  NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.5   NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.75  NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.0   NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.25  NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.5   NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -6.75  NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.0   NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.25  NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.5   NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -7.75  NaOH    10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -8.0   NaOH    10.0
```

```
END
```

Validation Test Case 5—Surface Complexation (Double Diffuse-Layer Model). MINTEQA2 for Windows Version 1.5 input file for zinc sorption on ferrihydrite, using the parameters of Dzombak and Morel (1990). This input file is constructed to match Example 8 in the MINTEQA2 Version 4.02 installation test problems (Parkhurst and Appelo, 1999).

```
valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -5.00 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     5.0000     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

```
 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -5.25 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     5.2500     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -5.50 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
```

```
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     5.5000     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -5.75 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     5.7500     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
```

```
    813     0.0000     0.0000                    /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -6.00 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     6.0000     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
```

```
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -6.25 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     6.2500     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

```
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -6.50 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     6.5000     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
```

```
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -6.75 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     6.7500     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
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 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -7.00 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     7.0000     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -7.25 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
```

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    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     7.2500     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -7.50 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     7.5000     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1
```

```
  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

 valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -7.75 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     7.7500     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
```

```
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0


valid65 Zn-HFO sorption, Double Diffuse-Layer Model
          Example 8; PHREEQC, Version 2.4.2 installation test files
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -8.00 Y                    /H+1
    500  1.000E-01   -1.00 Y                    /Na+1
    492  1.000E-01   -1.00 Y                    /NO3-1
    950  1.000E-07   -7.00 Y                    /Zn+2
    811  5.000E-06   -5.30 N                    /Site 1-1
    812  2.000E-04   -3.70 N                    /Site 1-2
    813  0.000E+00    0.00 N                    /EStat1-1

  3   1
    330     8.0000     0.0000                   /H+1
  6   3
9504921     0.4000    -4.6000                   /ZnNO3+
9504922    -0.3000     0.0000                   /Zn(NO3)2 (aq)
    813     0.0000     0.0000                   /EStat1-1

  2   6
8110001 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110002  Hfo_sO-        0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110003  Hfo_sOZn+      0.0000    0.6600   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

```
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120001 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120002 Hfo_wO-         0.0000   -8.8200   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8120003 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

Validation Test Case 6a—Redox Equilibria. MINTEQA2 for Windows Version 1.5 input file for redox Example 8.2 in Stumm and Morgan (1996). The simulation is intended to determine electron activity (pe).

```
valid66a  Calculate electron activity (pe) for 10-5 M Fe(III)
and 10-3 M Fe(II) Example 8.2 from Stumm and Morgan (1996)
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    281  1.000E-05   -5.00 Y                    /Fe+3
    280  1.000E-03   -3.00 Y                    /Fe+2
    001  0.000E+00   -7.00 Y                    /E-1

  3   1
2802810    13.0320   -42.7000                   /Fe+2/Fe+3
  6  10
2813300    -2.1870    41.8100                   /FeOH+2
2813301    -4.5940     0.0000                   /Fe(OH)2+
2813302   -12.5600   103.8000                   /Fe(OH)3 (aq)
2813303   -21.5880     0.0000                   /Fe(OH)4-
2813304    -2.8540    57.6200                   /Fe2(OH)2+4
2813305    -6.2880    65.2400                   /Fe3(OH)4+5
2803300    -9.3970    55.8100                   /FeOH+
2803301   -28.9910   126.4300                   /Fe(OH)3-
2803302   -20.4940   119.6200                   /Fe(OH)2 (aq)
    001     0.0000     0.0000                   /E-1


Valid66a2 Calculate electron activity (pe) for pH=7.5, pO2=0.22
atm          Example 8.2 from Stumm and Morgan (1996)
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.50 Y                    /H+1
    500  1.000E-03   -3.00 Y                    /Na+1
    180  1.000E-03   -3.00 Y                    /Cl-1
    001  0.000E+00   -5.00 Y                    /E-1

  3   2
3300021   -82.4117   571.6600                   /O2 (g)
    330     7.5000     0.0000                   /H+1
  6   1
    001     0.0000     0.0000                   /E-1


valid66a3 Calculate electron activity (pe) for 10-5 M Mn(II) and
pyrolusite Example 8.2 from Stumm and Morgan (1996)
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -8.00 Y                    /H+1
    470  1.000E-05   -5.00 Y                    /Mn+2
    001  0.000E+00    0.00 Y                    /E-1

  3   2
2047000   -40.8400   272.0000                   /PYROLUSITE
    330     8.0000     0.0000                   /H+1
  6   1
    001     0.0000     0.0000                   /E-1
```

Validation Test Case 6b—Redox Equilibria. MINTEQA2 for Windows Version 1.5 input file for redox Example 8.4 in Stumm and Morgan (1996). The simulation is intended to determine HS^{-}–SO_4^{2-} speciation as a function of electron activity (pe).

```
 valid66b Redox equilbria test; 10-4 M SO4-2/HS- system
           Based on Example 8.4 from Stumm and Morgan (1996)
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00  -10.00 Y                    /H+1
    730  1.000E-04   -4.00 Y                    /HS-1
    732  0.000E+00   -6.00 Y                    /SO4-2
    001  0.000E+00    9.00 Y                    /E-1

  3   3
7307320    33.6600   -60.1400                   /HS-/SO4-2
    330    10.0000     0.0000                   /H+1
    001    -9.0000     0.0000                   /E-1
  6   3
3307320     1.9900    22.0000                   /HSO4-
3307301   -17.3000    49.4000                   /S-2
3307300     7.0200   -22.0000                   /H2S (aq)
```

Validation Test Case 7a—Temperature Effects. PHREEQC Version 2.4.2 input file for temperature effects on saturation of gypsum and anhydrite. Pure water with 1.0 moles of anhydrite and 1.0 moles of gypsum. This input file is from Example 2 in the MINTEQA2 Version 4.02 installation test problems (Parkhurst and Appelo, 1999).

```
TITLE Example 2.--Temperature dependence of solubility
                  of gypsum and anhydrite
SOLUTION 1 Pure water
        pH      7.0
        temp    25.0
EQUILIBRIUM_PHASES 1
        Gypsum          0.0     1.0
        Anhydrite       0.0     1.0
REACTION_TEMPERATURE 1
        25.0 75.0 in 51 steps
SELECTED_OUTPUT
        -file   ex2.sel
        -si     anhydrite  gypsum
END
```

Validation Test Case 7a—Temperature Effects. MINTEQA2 for Windows Version 1.5 input file for temperature effects on saturation of gypsum and anhydrite. Pure water with 1.0 moles of anhydrite and 1.0 moles of gypsum based on Example 2 in the MINTEQA2 Version 4.02 installation test problems (Parkhurst and Appelo, 1999).

```
SENS 0 Temperature
valid 67a Anhydrite/Gypsum solubility as function of temperature
           Test Example 2 for PHREEQC, Version 2.4.2
25.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM
```

```
 30.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM



 35.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM



 40.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM



 45.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM



 50.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM
```

```
 55.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM



 60.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM



 65.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM



 70.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM



 75.0 mol/L 0.000E+00 0.000E+00
0 0 1 0 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  4   2
6015000     4.3600     7.2000   1.000E+00       /ANHYDRITE
```

```
6015001     4.6100    -1.0000   1.000E+00       /GYPSUM
```

Validation Test Case 7b—Temperature Effects. MINTEQA2 for Windows Version 1.5 input file for temperature effects on saturation of gypsum and anhydrite. Pure water assuming infinite gypsum and infinite anhydrite.

```
SENS 0 Temperature                                11 1   25.0000    5.0000
Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 30.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 35.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 40.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 45.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
```

```
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 50.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 55.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 60.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 65.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM


Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 70.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM
```

```
Valid67b1 Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2 with
 75.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015001     4.6100    -1.0000                   /GYPSUM
```

Validation Test Case 7b—Temperature Effects, Part 2.

```
SENS 0 Temperature                                11 1   25.0000    5.0000
Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 25.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 30.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 35.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE
```

```
Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 40.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 45.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 50.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 55.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 60.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 65.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
```

```
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 70.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE


Valid67b2. Anhydrite/Gypsum solubility as function of
temperature.      Test Example 2 for PHREEQC, Version 2.4.2  with
 75.0 mol/L 0.000E+00 0.000E+00
0 0 1 1 2 1 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 Y                    /H+1
    150  0.000E+00   -6.00 Y                    /Ca+2
    732  0.000E+00   -6.00 Y                    /SO4-2

  3   1
6015000     4.3600     7.2000                   /ANHYDRITE
```