

FRIENDS OF FREZCHEM (Version 12.2)

Attached is a "beta" version of the FREZCHEM model that includes chloride, bromide, nitrate, sulfate, and bicarbonate-carbonate salts, strong acid chemistry, ferrous and ferric iron chemistry, aluminum and silicon chemistries, and gas hydrate chemistry. This version includes both temperature and pressure dependencies. This folder includes a FORTRAN program listing (which you can download directly), a list of chemical species in the model (Table 1), instructions for model input (Table 2), and two examples of model outputs (Tables 3 and 4).

This model is very much a work in progress. I will be mainly adding new chemistries to the model in the next few years. I have not spend much time debugging the model or making it user-friendly. A user-friendly version (10.2) is available at <http://frezchem.dri.edu>. In addition, there are convergence problems, at times, with the model. My version of the model was created with Absoft's ProFortran for the Macintosh. Porting this code to another FORTRAN compiler is always problematic. If you have problems, contact me via e-mail (giles.marion@dri.edu). Indicate the FREZCHEM version you are using (e.g., FREZCHEM12.2) and your model input.

The model is an equilibrium chemical thermodynamic model, meaning it will always select the most stable minerals. There are a few minerals (e.g., aragonite and vaterite) that are always metastable with respect to other minerals (e.g., calcite). To explicitly include a metastable mineral in your calculations necessitates removing the stable mineral from the minerals database. This is most simply done by assigning the stable mineral an arbitrary high K_{sp} . See the comments at the end of the "Parameter" subroutine on how to do this. The # of the K_{sp} for a specific mineral in the FORTRAN program is the same as the solid phase # in Table 1 (e.g., K_{52} is the solubility product for calcite). If you are using the model to calculate pH, then you should make sure that the initial solution is charge-balanced. Otherwise, the model will force a charge balance by changing the bicarbonate-carbonate or acid concentrations, which could lead to a serious error in calculated pH if the solution is badly charge-balanced. If necessary, force a charge-balance in the initial solution by changing a major constituent that minimizes the effect on pH (e.g., Na or Cl). If you input Fe, Al, or Si, then you will have four options on how to deal with pH (see Table 2).

The validation of this model is discussed in 12 publications: (1) Spencer et al. (1990) The prediction of mineral solubilities in natural waters: A chemical equilibrium model for the Na-K-Ca-Mg-Cl-SO₄-H₂O system. *Geochim. Cosmochim. Acta*, 54:575-590; (2) Marion and Farren (1999) Mineral solubilities in the Na-K-Mg-Ca-Cl-SO₄-H₂O system: A re-evaluation of the sulfate chemistry in the Spencer-Møller-Weare model. *Geochim. Cosmochim. Acta*, 63:1305-1318; (3) Marion (2001) Carbonate mineral solubility at low temperatures in the Na-K-Mg-Ca-H-Cl-SO₄-OH-HCO₃-CO₃-CO₂-H₂O system. *Geochim. Cosmochim. Acta*, 65:1883-

1896; (4) Marion (2002) A molal-based model for strong acid chemistry at low temperatures (<200 to 298 K). *Geochim. Cosmochim. Acta*, 66:2499-2516; (5) Marion et al. (2003) Modeling aqueous ferrous iron chemistry at low temperatures with application to Mars. *Geochim. Cosmochim. Acta*, 67:4251-4266; (6) Marion et al. (2005) Effects of pressure on aqueous chemical equilibria at subzero temperatures with applications to Europa. *Geochim. Cosmochim. Acta*, 69:259-274; (7) Marion et al. (2006) Modeling gas hydrate equilibria in electrolyte solutions. *CALPHAD*, 30:248-259; (8) Marion (2007) Adapting molar data (without density) for molal models. *Computers & Geosciences*, 33:829-834. (9) Marion and Kargel (2008) *Cold Aqueous Planetary Geochemistry with FREZCHEM: From Modeling to the Search for Life at the Limits*. Springer; (10) Marion et al. (2008) Modeling ferrous-ferric iron chemistry with application to Martian surface geochemistry. *Geochim. Cosmochim. Acta*, 72:242-266; (11) Marion et al., (in press) Br/Cl partitioning in chloride minerals in the Burns formation on Mars. *Icarus*; and (12) Marion et al. (in submission) Modeling aluminum-silicon chemistries and application to Australian playa lakes as analogues for Mars. *Geochim. Cosmochim. Acta*.

Compared to Version 11.2, this version of the FREZCHEM model contains new parameterizations dealing with Br, Al, and Si chemistries. The last two papers mentioned above contain descriptions of these chemistries. In addition, Version 12.2 has an option for estimating molal concentrations [moles/kg(H₂O)] from molar concentrations (moles/liter) even for cases where the solution density is unknown (see 2007 paper cited above and Table 4 example). Instructions for inputting these new chemistries are discussed in Table 2.

Table 1. A listing of chemical species in the FREZCHEM model (Version 12.2).

A. Solution and Atmospheric Species							
#	Species	#	Species	#	Species	#	Species
1	Na ⁺ (aq)	11	Cl ⁻ (aq)	21	CO ₂ (aq)	151	O ₂ (g)
2	K ⁺ (aq)	12	SO ₄ ²⁻ (aq)	22	FeCO ₃ ^o (aq)	152	O ₂ (aq)
3	Ca ²⁺ (aq)	13	OH ⁻ (aq)	23	HCl(g)	153	H ₂ (g)
4	Mg ²⁺ (aq)	14	HCO ₃ ⁻ (aq)	24	CaCO ₃ ^o (aq)	154	CH ₄ (g)
5	H ⁺ (aq)	15	CO ₃ ²⁻ (aq)	25	MgCO ₃ ^o (aq)	155	CH ₄ (aq)
6	MgOH ⁺ (aq)	16	HSO ₄ ⁻ (aq)	26	HNO ₃ (g)	156	Fe(OH) ₂ ⁰ (aq)
7	Fe ²⁺ (aq)	17	NO ₃ ⁻ (aq)	27	H ₂ SO ₄ (g)	157	Fe(OH) ₃ ⁻ (aq)
8	FeOH ⁺ (aq)	18	Br ⁻ (aq)	28	H ₂ O(g)	158	FeOH ²⁺ (aq)
9	Fe ³⁺ (aq)	19		29	CO ₂ (g)	159	Fe(OH) ₂ ⁺ (aq)
10	Al ³⁺ (aq)	20		30	H ₂ O(l)	160	Fe(OH) ₃ ⁰ (aq)
B. Solid Phase Species							
#	Species	#	Species	#	Species	#	Species
31	H ₂ O(cr,l)	51	Na ₂ SO ₄ •3K ₂ SO ₄ (cr)	71	H ₂ SO ₄ •4H ₂ O(cr)	91	FeCl ₃ •2KCl•H ₂ O(cr)
32	NaCl•2H ₂ O(cr)	52	CaCO ₃ (cr,calcite)	72	HCl•6H ₂ O(cr)	92	Fe ₂ (SO ₄) ₃ (cr)
33	NaCl(cr)	53	MgCO ₃ (cr)	73	NaNO ₃ •Na ₂ SO ₄ •2H ₂ O(cr)	93	Fe ₂ (SO ₄) ₃ •2K ₂ SO ₄ •14H ₂ O(cr)
34	KCl(cr)	54	MgCO ₃ •3H ₂ O(cr)	74	Na ₃ H(SO ₄) ₂ (cr)	94	K ₂ SO ₄ •FeSO ₄ •6H ₂ O(cr)
35	CaCl ₂ •6H ₂ O(cr)	55	MgCO ₃ •5H ₂ O(cr)	75	NaHSO ₄ •H ₂ O(cr)	95	Na ₂ SO ₄ •FeSO ₄ •4H ₂ O(cr)
36	MgCl ₂ •6H ₂ O(cr)	56	CaCO ₃ •6H ₂ O(cr)	76	K ₃ H(SO ₄) ₂ (cr)	96	Fe ₂ (SO ₄) ₃ •9H ₂ O(cr)
37	MgCl ₂ •8H ₂ O(cr)	57	NaHCO ₃ (cr)	77	K ₅ H ₃ (SO ₄) ₄ (cr)	97	Fe ₂ (SO ₄) ₃ •H ₂ SO ₄ •8H ₂ O(cr)
38	MgCl ₂ •12H ₂ O(cr)	58	Na ₂ CO ₃ •10H ₂ O(cr)	78	K ₈ H ₆ (SO ₄) ₇ •H ₂ O(cr)	98	KFe ₃ (SO ₄) ₂ (OH) ₆ (cr)
39	KMgCl ₃ •6H ₂ O(cr)	59	NaHCO ₃ •Na ₂ CO ₃ •2H ₂ O(cr)	79	KHSO ₄ (cr)	99	NaFe ₃ (SO ₄) ₂ (OH) ₆ (cr)
40	CaCl ₂ •2MgCl ₂ •12H ₂ O(cr)	60	3MgCO ₃ •Mg(OH) ₂ •3H ₂ O(cr)	80	MgSO ₄ •H ₂ O(cr)	100	H ₃ OFe ₃ (SO ₄) ₂ (OH) ₆ (cr)
41	Na ₂ SO ₄ •10H ₂ O(cr)	61	CaMg(CO ₃) ₂ (cr)	81	FeSO ₄ •7H ₂ O(cr)	101	α-Fe ₂ O ₃ (cr)
42	Na ₂ SO ₄ (cr)	62	Na ₂ CO ₃ •7H ₂ O(cr)	82	FeSO ₄ •H ₂ O(cr)	102	α-FeO(OH)(cr)
43	MgSO ₄ •6H ₂ O(cr)	63	KHCO ₃ (cr)	83	FeCl ₂ •6H ₂ O(cr)	103	γ-FeO(OH)(cr)
44	MgSO ₄ •7H ₂ O(cr)	64	CaCO ₃ (cr,aragonite)	84	FeCl ₂ •4H ₂ O(cr)	104	FeO(OH) _{0.75} (SO ₄) _{0.125} (cr)
45	K ₂ SO ₄ (cr)	65	CaCO ₃ (cr,vaterite)	85	FeCO ₃ (cr)	105	FeSO ₄ •4H ₂ O(cr)
46	MgSO ₄ •K ₂ SO ₄ •6H ₂ O(cr)	66	HNO ₃ •3H ₂ O(cr)	86	Fe(OH) ₃ (cr)	106	Fe ₂ (SO ₄) ₃ •7H ₂ O(cr)
47	Na ₂ SO ₄ •MgSO ₄ •4H ₂ O(cr)	67	KNO ₃ (cr)	87	CO ₂ •6H ₂ O(cr)	107	Fe(II)Fe(III) ₄ (SO ₄) ₆ (OH) ₂ •20H ₂ O(cr)
48	CaSO ₄ •2H ₂ O(cr)	68	NaNO ₃ (cr)	88	CH ₄ •6H ₂ O(cr)	108	Fe ₅ (SO ₄) ₆ O(OH)•20H ₂ O(cr)
49	CaSO ₄ (cr)	69	HCl•3H ₂ O(cr)	89	FeCl ₃ •10H ₂ O(cr)	109	Fe(II)Fe(III) ₂ (SO ₄) ₄ •22H ₂ O(cr)
50	MgSO ₄ •12H ₂ O(cr)	70	H ₂ SO ₄ •6.5H ₂ O(cr)	90	FeCl ₃ •6H ₂ O(cr)	110	Fe(II)Fe(III) ₂ (SO ₄) ₄ •14H ₂ O(cr)
						111	K ₂ Fe(II) ₅ Fe(III) ₄ (SO ₄) ₁₂ •18H ₂ O(cr)
						112	AlCl ₃ •6H ₂ O(cr)
						113	Al ₂ (SO ₄) ₃ •16H ₂ O(cr)
						114	NaBr
						115	MgBr ₂
						116	Al(OH) ₃ (cr)
						117	SiO ₂ (quartz)(cr)
						118	SiO ₂ (amorphous)
						119	KAl ₃ (SO ₄) ₂ (OH) ₆ (cr)
						120	NaAl ₃ (SO ₄) ₂ (OH) ₆ (cr)
						121	KAl(SO ₄) ₂ •12H ₂ O(cr)
						122	NaAl(SO ₄) ₂ •12H ₂ O(cr)
						123	FeSO ₄ •Al ₂ (SO ₄) ₃ •22H ₂ O(cr)
						124	Al ₂ Si ₂ O ₅ (OH) ₄ (cr)
						125	MgSO ₄ •Al ₂ (SO ₄) ₃ •22H ₂ O(cr)

Table 2. Model Inputs (Version 12.2) (hit return after every entry).

Title: Any alphanumeric character up to 50 characters.

Freeze(1) or Evaporation(2) or Pressure (3) Pathway: Enter 1, 2, or 3 depending on whether you want to simulate a temperature change (1) an evaporation (2), or a pressure change (3).

For evaluating a single point, enter "1".

Equilibrium(1) or Fractional(2) Crystallization: In equilibrium crystallization (1), precipitated solids are allowed to re-equilibrate with the solution phase as environmental conditions change. In fractional crystallization (2), precipitated solids are removed and not allowed to re-equilibrate with the solution phase as environmental conditions change.

Open(1) or Closed(2) Carbon System: If you want the gas partial pressure of CO₂ or CH₄ to be fixed at a given total pressure, enter 1. If you want the total carbon to be fixed, enter 2.

Sodium (m/kg): Enter sodium molality (moles/kg(water)). Otherwise, enter 0.0.

Potassium (m/kg): Enter potassium molality (moles/kg(water)). Otherwise, enter 0.0.

Calcium (m/kg): Enter calcium molality (moles/kg(water)). Otherwise, enter 0.0.

Magnesium (m/kg): Enter magnesium molality (moles/kg(water)). Otherwise, enter 0.0.

Ferrous Iron (m/kg): Enter ferrous iron molality (moles/kg(water)). Otherwise, enter 0.0.

Ferric Iron (m/kg): Enter ferric iron molality (moles/kg(water)). Otherwise, enter 0.0.

Aluminum (m/kg): Enter aluminum molality (moles/kg(water)). Otherwise, enter 0.0.

Silicon (m/kg): Enter silicon molality (moles/kg(water)). Otherwise, enter 0.0.

If Iron, Aluminum, or Silicon are selected, then choose an acidity option:

Acidity ignored, enter 1.

Acidity fixed by pH, enter 2.

Acidity fixed by H⁺ ion concentration, enter 3.

Acidity fixed by alkalinity, enter 4.

Initial pH: Option 1, enter 0; Option 2, enter pH; Options 3 and 4, enter an approximate pH.

Chloride (m/kg): Enter chloride molality (moles/kg(water)). Otherwise, enter 0.0.

Bromide (m/kg): Enter bromide molality (moles/kg(water)). Otherwise, enter 0.0.

Sulfate (m/kg): Enter sulfate molality (moles/kg(water)). Otherwise, enter 0.0.

Nitrate (m/kg): Enter nitrate molality (moles/kg(water)). Otherwise, enter 0.0.

Carbonate Alkalinity: Enter as equivalents/kg(water). If alkalinity = 0.0, then you must enter 0.0. The latter will cause the model to skip all bicarbonate-carbonate, pH chemistries in the model.

Initial pH: If alkalinity > 0.0, then the model will calculate pH, given an initial pH estimate that is specified here. If this estimate is far removed from the true pH, then the model may not converge.

Acidity: Enter as equivalents/kg(water). This is the total hydrogen concentration, if known initially. Generally this is only known for strong acid solutions. For example, for a 1 molal H₂SO₄ solution, enter 2.00. Otherwise, enter 0.0. The equations used to calculate pH for the alkalinity and acidity cases are incompatible. So, a specification of either carbonate alkalinity or acidity requires that the other variable be assigned a value of 0.00. This will channel the calculations to the proper algorithm.

HCl(bars): If the HCl atmospheric concentration is known, then specify here. Otherwise, enter 0.0. If you specify 0.0, then the model will calculate HCl(bars). Note that if you specify HCl(bars) or the other acids below, then these properties override the total acidity specification (see above). That is, the solution is equilibrated with the atmospheric concentration. Note, you can, if desired, specify atmospheric concentrations for some acids (e.g., HCl and HNO₃) and leave other acid partial pressure unspecified (e.g., H₂SO₄ = 0.0).

HNO₃(bars): If the HNO₃ atmospheric concentration is known, then specify here. Otherwise, enter 0.0.

H₂SO₄(bars): If the H₂SO₄ atmospheric concentration is known, then specify here. Otherwise, enter 0.0.

Initial Total Pressure (bars): Enter the initial total pressure of the system.

Initial CO₂(bars): If alkalinity > 0.0 or CO₂ hydrates are simulated, then specify the initial concentration of CO₂(g) in bars.

Mole Fraction of CO₂: Enter the mole fraction of CO₂(g) for the system (mole fraction = CO₂(g)/total pressure). For pure CO₂, enter 1.0. If 0.0, then CO₂(g) is fixed and independent of total pressure.

O₂(bars): If the atmospheric concentration of oxygen is known, then specify here. Otherwise, enter 0.0. If you are interested in ferrous iron chemistry, then you may want to assign O₂ a value of 0.0. Otherwise, it is likely that the insolubility of ferric minerals in the presence of O₂ will cause all the iron to precipitate as a ferric mineral [see discussions in Marion et al., (2003a) iron paper].

Initial CH₄(bars): If CH₄ hydrates are simulated, then specify the initial concentration of CH₄(g) in bars.

Mole Fraction of CH₄: Enter the mole fraction of CH₄(g) for the system (mole fraction = CH₄(g)/total pressure). For pure CH₄, enter 1.0. If 0.0, then CH₄(g) is fixed and independent of total pressure.

Mixed CH₄-CO₂ Gas Hydrate?: If both CH₄(g) and CO₂(g) are specified as inputs, then you can use this data to estimate the stability of a mixed CH₄-CO₂ gas hydrate (YES = 1) or treat the two gases as independent gas hydrates (NO = 0).

Molar to Molal Conversion?: If you want to convert molar data into molal concentrations, then enter (YES = 1) or (NO = 0). If yes, then:

Salinity/liter: You must enter the total aqueous salinity (g salt/liter), which can be calculated from molar data [g salt/liter = $\sum(\text{moles/liter}) \times (\text{g salt/mole})$]. In the case depicted in Table 4, the SL value is 316.57 g salt/liter (5.417 x 58.44).

Initial Temperature(K): Enter the temperature in absolute degrees (K) for start of simulation (e.g., 298.15).

For Temperature Change Pathway(1):

Final Temperature(K): Enter final temperature of simulation (e.g., 273.15).

Temperature Decrement(K): The temperature interval between simulations (e.g. 5). For the above temperature designations, the model would calculate equilibrium starting at 298.15 K and ending at 273.15 K at 5 K intervals. If you want to change the decrement in a run (e.g., to reduce the step size near an equilibrium), see the comments near the end of the main program.

For Evaporation Pathway(2):

Initial Water (g): Normally enter "1000" at this point. The standard weight basis of the model is 1000 g water plus associated salts. In you enter 100, instead of 1000, the initial ion concentrations, specified above, will be multiplied by 10.0 (1000/100) as the starting compositions for calculations. This feature of the model is useful in precisely locating where minerals start to precipitate during the evaporation process without having to calculate every small change between 1000 g and 1 g.

Final Water (g): Enter the final amount of water that you want to remain in the system (e.g., 100).

Water Decrement (g): Enter the water decrement for simulations (e.g., 50 g). Specifying initial = 1000, final = 100, and decrement = 50 would result in calculations at 1000g,

950g,100g. If you want to change the decrement in a run (e.g., to reduce the step size near an equilibrium), see the comments near the end of the main program.

For Pressure Pathway(3):

Final Pressure(bars): Enter the final pressure of the simulation [e.g., 101.01325 bars (100 atm)].

Pressure Increment(bars): Enter the pressure increment. For example, if initial pressure is 1.01 bars, final pressure is 101.01 bars, and pressure increment is 1.0 bars, then the simulation would calculate at 1.01, 2.01, 3.01,101.01325 bars. If you want to change the increment in a run, see the comments near the end of the main program.

Inputting Gases into the Model

SYSTEM INPUTS	NO GASES	FIXED GAS CONCS.	VARIABLE GAS CONCS.
1. OPEN CARBON SYSTEM	1	1	1
2. INITIAL TOTAL PRESSURE	USER SPECIFICATION	USER SPECIFICATION	USER SPECIFICATION
3. INITIAL CO ₂	0	USER SPECIFICATION	USER SPECIFICATION
4. MOLE FRACTION OF CO ₂	0	0	USER SPECIFICATION
5. INITIAL O ₂	0	USER SPECIFICATION	0
6. INITIAL CH ₄	0	USER SPECIFICATION	USER SPECIFICATION
7. MOLE FRACTION OF CH ₄	0	0	USER SPECIFICATION
8. MIXED CH ₄ -CO ₂ GAS HYDRATE	----	2	1
CLOSED CARBON			
1. OPEN CARBON SYSTEM	2		
2. INITIAL TOTAL PRESSURE	USER SPECIFICATION		
3. INITIAL CO ₂	USER SPECIFICATION		
4. MOLE FRACTION OF CO ₂	USER SPECIFICATION		
5. INITIAL O ₂	0		
6. INITIAL CH ₄	USER SPECIFICATION		
7. MOLE FRACTION OF CH ₄	USER SPECIFICATION		
8. MIXED CH ₄ -CO ₂ GAS HYDRATE	1		

NO GASES means that you do not want any gases considered in these chemical equilibrium calculations.

FIXED GAS CONCS. means that you want the user specified gas concentrations to remain fixed as T, P, and H₂O content change. For example, atm. CO₂ is equal to 3.80e-4 bars.

VARIABLE GAS CONCS. were specifically designed for CO₂ and CH₄ gas hydrate equilibrium which allows gas pressures to increase as total pressure increases.

CLOSED CARBON was specifically designed for CO₂ and CH₄ gas hydrate equilibrium in small volumes (e.g, ice pockets). The aqueous component contains 1.0 kg of water. The air component contains 0.1 liter. To change the aqueous/air ratio, change the 0.1 liter multiplier in FC12.2 lines 254 and 270.

Model Output.

"Ion.Str." is the ionic strength of the equilibrium solution (see Table 3). "RHO" is the density of the solution. "Phi" is the osmotic coefficient of the equilibrium solution. "H2O(g)" is the amount of water remaining as liquid. "Ice" is the amount of water that is present as ice. The mass basis for calculation in the model is 1.0 kg of water (except for evaporation); therefore, the water in liquid water + ice + hydrated salts should always sum to 1.0 kg. The data under "Initial Conc." are the input concentrations. "Final Conc." are the equilibrium concentrations. Act. coef. (activity coefficient) and activity are self-explanatory. Moles are the # of moles in the solution or solid phase. For the major constituents, the "Mass Balance" column should generally agree with the input column ("Initial Conc."); this is the best check on the internal consistency of the calculations. The "Accum Moles" in the solids section are the net # of moles of that solid that have precipitated. For equilibrium crystallization, accum. moles = moles(solid). For fractional crystallization accum. moles = moles (solids); in this case, moles represent the solids that have precipitated in the last interval (e.g., between 15 and 10 °C), while accum. moles represent the total precipitate (e.g., between 25 and 10 °C).

Table 3 is a case where we examined evaporation of an Australian acidic saline playa lake. What began with 1000 g of water, evaporated down to 1.2 g at a fixed pH = 3.0 and a fixed temperature of 15°C. During this process, ten solid phases precipitated. What began as a predominately NaCl solution ended up as a predominately MgCl₂ solution. This simulation was done using fractional crystallization, which accounts for the early CaSO₄•2H₂O (gypsum) precipitation when the ionic strength

initial density = 1.00 g/cm³), we were able to calculate density and convert molar to molal concentrations. In turn, molal concentrations could be directly imported into FREZCHEM to explore geochemical processes. Note that all the potential solid phases were assigned high solubility products to prevent their precipitation (Table 4). FORTRAN statements to accomplish this negation of solid phases are at the end of the “Parameter” subroutine and must be implemented by the user. See the previously cited 2007 paper for a fuller discussion of the techniques used in this algorithm.

Table 3. Australian playa lake evaporation.

Temp(K)	Ion.Str.	RHO	Phi	H2O(g)	Ice(g)	Press.(bars)
288.15	17.238	1.33492	3.6273	1.2322	0.00000	1.0132
Solution SPECIES	Initial Conc.	Final Conc.	Act.Coeff.	Activity	Moles	Mass Balance
NA	0.65900	0.56713E-01	1.6037	0.90948E-01	0.69883E-04	0.66447
K	0.46000E-02	0.13379E-01	0.56113E-01	0.75073E-03	0.16486E-04	0.46704E-02
CA	0.38000E-02	0.11681E-02	5.1220	0.59830E-02	0.14394E-05	0.38066E-02
MG	0.52000E-01	5.6987	48.149	274.38	0.70221E-02	0.52471E-01
H	0.13206E-02	0.40637E-04	24.608	0.10000E-02	0.50074E-07	
FE(III)	0.85000E-04	0.63162E-05	0.22684E-02	0.14328E-07	0.77831E-08	0.85000E-04
AL	0.31000E-02	0.15522E-02	5.0837	0.78911E-02	0.19127E-05	0.31000E-02
CL	0.74580	11.356	34.385	390.49	0.13994E-01	0.74580
SO4	0.19500E-01	0.59026E-01	0.19342	0.11417E-01	0.72734E-04	0.19500E-01
OH	0.00000	0.19394E-10	0.76622E-01	0.14860E-11	0.23898E-13	
HSO4	0.00000	0.76464E-05	105.48	0.80653E-03	0.94222E-08	
FEIII(OH)	0.00000	0.85658E-09	14.159	0.12129E-07	0.10555E-11	
FEIII(OH)2	0.00000	0.23825E-07	0.49886E-01	0.11885E-08	0.29358E-10	
FEIII(OH)3	0.00000	0.28869E-13	1.0000	0.28869E-13	0.35573E-16	
FEIII(OH)4	0.00000	0.12543E-18	0.49886E-01	0.62574E-20	0.15457E-21	
AL(OH)	0.00000	0.92410E-06	14.159	0.13085E-04	0.11387E-08	
AL(OH)2	0.00000	0.27316E-06	0.49886E-01	0.13627E-07	0.33660E-09	
AL(OH)3	0.00000	0.41438E-12	1.0000	0.41438E-12	0.51061E-15	
AL(OH)4	0.00000	0.22329E-14	0.49886E-01	0.11139E-15	0.27515E-17	
SI(OH)4	0.13000E-02	0.78523E-05	1.0000	0.78523E-05	0.96759E-08	0.13000E-02
SIO(OH)3	0.00000	0.17009E-10	0.49886E-01	0.84848E-12	0.20959E-13	
H2O(BAR)	0.16647E-01			.55492E-02		
H2O(L)	55.508			.32526	0.68400E-01	0.34415

Solid SPECIES	Moles	Equil. Constant	Accum. Moles
ICE	0.00000	1.1526	0.00000
NACL.2H2O	0.00000	27.382	0.00000
NACL	0.14564E-04	35.526	0.66440
KCL	0.00000	6.0723	0.00000
CACL2.6H2O	0.00000	3701.3	0.00000
MGCL2.6H2O	0.14484E-02	49505.	0.28271E-01
MGCL2.8H2O	0.00000	11380.	0.00000
MGCL2.12H2O	0.00000	7548.7	0.00000
KMGCL3.6H2O	0.33103E-05	14510.	0.36213E-02
CACL2.2MGCL2.12H2O	0.00000	0.34440E+18	0.00000
NA2SO4.10H2O	0.00000	0.18719E-01	0.00000
NA2SO4	0.00000	0.50537	0.00000
MGSO4.6H2O	0.00000	0.22071E-01	0.00000
MGSO4.7H2O	0.00000	0.98588E-02	0.94960E-02
K2SO4	0.00000	0.11595E-01	0.00000
MGSO4.K2SO4.6H2O	0.00000	0.25506E-04	0.00000
NA2SO4.MGSO4.4H2O	0.00000	0.39130E-02	0.00000
CASO4.2H2O	0.00000	0.24833E-04	0.37725E-02
CASO4	0.30048E-06	0.68254E-04	0.32583E-04
MGSO4.12H2O	0.00000	0.16978E-01	0.00000
NA2SO4.3K2SO4	0.00000	0.14070E-07	0.00000
CACO3(CALCITE)	0.00000	0.52102E-07	0.00000
MGCO3	0.00000	0.13390E-07	0.00000
MGCO3.3H2O	0.00000	0.55426E-05	0.00000
MGCO3.5H2O	0.00000	0.70324E-05	0.00000
CACO3.6H2O	0.00000	0.15152E-06	0.00000
NAHCO3	0.00000	0.30108	0.00000
NA2CO3.10H2O	0.00000	0.60306E-01	0.00000
NAHCO3.NA2CO3.2H2O	0.00000	0.74329E-01	0.00000
3MGCO3.MG(OH)2.3H2O	0.00000	0.75962E-36	0.00000
CAMG(CO3)2	0.00000	0.14365E-16	0.00000
NA2CO3.7H2O	0.00000	0.20601	0.00000
KHCO3	0.00000	1.1129	0.00000
CACO3(ARAGONITE)	0.00000	0.52599E-08	0.00000
CACO3(VATERITE)	0.00000	0.14575E-07	0.00000
HNO3.3H2O	0.00000	2026.8	0.00000

KNO3	0.00000	0.44289	0.00000
NANO3	0.00000	4.9358	0.00000
HCL.3H2O	0.00000	18764.	0.00000
H2SO4.6.5H2O	0.00000	3.5355	0.00000
H2SO4.4H2O	0.00000	999.90	0.00000
HCL.6H2O	0.00000	1000.0	0.00000
NANO3.NA2SO4.2H2O	0.00000	0.55856	0.00000
NA3H(SO4)2	0.00000	0.12125	0.00000
NAHSO4.H2O	0.00000	52.099	0.00000
K3H(SO4)2	0.00000	0.12991E-03	0.00000
K5H3(SO4)4	0.00000	0.93217E-07	0.00000
K8H6(SO4)7.H2O	0.00000	0.17749E-11	0.00000
KHSO4	0.00000	2.5607	0.00000
MGSO4.H2O	0.14620E-04	1.0178	0.40608E-02
FESO4.7H2O	0.00000	0.35395E-02	0.00000
FESO4.H2O	0.00000	0.17918	0.00000
FECL2.6H2O	0.00000	2305.8	0.00000
FECL2.4H2O	0.00000	5754.6	0.00000
FECO3	0.00000	0.10071E-10	0.00000
FE(OH)3	0.00000	8014.6	0.00000
CO2.6H2O	0.00000	44.468	0.00000
CH4.6H2O	0.00000	103.58	0.00000
FECL3.10H2O	0.00000	3.6853	0.00000
FECL3.6H2O	0.00000	31.794	0.00000
FECL3.2KCL.H2O	0.00000	2183.5	0.00000
FE2(SO4)3	0.00000	1.1642	0.00000
FE2(SO4)3.2K2SO4.14H	0.00000	0.14132E-13	0.00000
K2SO4.FESO4.6H2O	0.00000	0.25106E-04	0.00000
NA2SO4.FESO4.4H2O	0.00000	0.12041E-02	0.00000
FE2(SO4)3.9H2O	0.00000	0.18627E-01	0.00000
FE2(SO4)3.H2SO4.8H2O	0.00000	2.0667	0.00000
KFE3(SO4)2(OH)6	0.00000	0.94255E-11	0.00000
NAFE3(SO4)2(OH)6	0.00000	0.64126E-05	0.00000
H3OFE3(SO4)2(OH)6	0.00000	0.21772E-04	0.00000
a-FE2O3	0.81528E-09	7.0637	0.42496E-04
a-FEO(OH)	0.00000	3.7117	0.00000
g-FEO(OH)	0.00000	214.02	0.00000
FEO(OH)3/4(SO4)1/8	0.00000	40.346	0.00000
FESO4.4H2O	0.00000	0.26077E-01	0.00000
FE2(SO4)3.7H2O	0.00000	0.45199E-01	0.00000
FE(II)FE(III)4(SO4)6	0.00000	0.63352E-22	0.00000
FE(III)5(SO4)6(OH).	0.00000	0.46784E-22	0.00000
FE(II)FE(III)2(SO4)4	0.00000	0.26902E-16	0.00000
FE(II)FE(III)2(SO4)4	0.00000	0.67753E-11	0.00000
K2FE(II)5FE(III)4(SO	0.00000	0.23590E-36	0.00000
ALCL3.6H2O	0.00000	0.19085E+07	0.00000
AL2(SO4)3.17H2O	0.00000	0.91746E-06	0.00000
NABR	0.00000	0.00000	0.00000
MGBR2	0.00000	0.00000	0.00000
AL(OH)3	0.00000	0.38140E+09	0.00000
SIO2(QUARTZ)	0.20177E-08	0.74234E-04	0.13000E-02
SIO2(AMORPHOUS)	0.00000	0.15828E-02	0.00000
KAL3(SO4)2(OH)6	0.13320E-06	56.778	0.10327E-02
NAAL3(SO4)2(OH)6	0.00000	49890.	0.00000
KAL(SO4)2.12H2O	0.00000	0.36704E-06	0.00000
NAAL(SO4)2.12H2O	0.00000	0.43872E-04	0.00000
FESO4.AL2(SO4)3.22H2	0.00000	0.27653E-08	0.00000
AL2SI2O5(OH)4	0.00000	0.70144E+07	0.00000
MGSO4.AL2(SO4).22H2O	0.00000	0.96704E-08	0.00000

Iterations = 14

Table 4. Conversion of a molar NaCl solution into a molal concentration.

rho	SA	CF				
1.17800	268.735	1.16086				
1.20181	263.411	1.12964				
1.19726	264.411	1.13547				
1.19812	264.223	1.13437				
1.19796	264.259	1.13458				
1.19799	264.252	1.13454				
1.19798	264.253	1.13455				
1.19798	264.253	1.13454				
1.19798	264.253	1.13455				
Temp(K)	Ion.Str.	RHO	Phi	H2O(g)	Ice(g)	Press.(bars)
298.15	6.1458	1.19798	1.2846	1000.0	0.00000	1.0132
Solution	Initial	Final				Mass
SPECIES	Conc.	Conc.	Act.Coeff.	Activity	Moles	Balance
NA	5.4170	6.1458	1.0109	6.2128	6.1458	6.1458
CL	5.4170	6.1458	1.0109	6.2128	6.1458	6.1458
H2O(BAR)	0.24948E-01			.23840E-01		
H2O(L)	55.508			.75242	55.508	55.508
Solid			Equil.	Accum.		
SPECIES	Moles		Constant	Moles		
ICE	0.00000		0.10000E+31	0.00000		
NACL.2H2O	0.00000		0.10000E+31	0.00000		
NACL	0.00000		0.10000E+31	0.00000		
KCL	0.00000		0.10000E+31	0.00000		
CACL2.6H2O	0.00000		0.10000E+31	0.00000		
MGCL2.6H2O	0.00000		0.10000E+31	0.00000		
MGCL2.8H2O	0.00000		0.10000E+31	0.00000		
MGCL2.12H2O	0.00000		0.10000E+31	0.00000		
KMGCL3.6H2O	0.00000		0.10000E+31	0.00000		
CACL2.2MGCL2.12H2O	0.00000		0.10000E+31	0.00000		
NA2SO4.10H2O	0.00000		0.10000E+31	0.00000		
NA2SO4	0.00000		0.10000E+31	0.00000		
MGSO4.6H2O	0.00000		0.10000E+31	0.00000		
MGSO4.7H2O	0.00000		0.10000E+31	0.00000		
K2SO4	0.00000		0.10000E+31	0.00000		
MGSO4.K2SO4.6H2O	0.00000		0.10000E+31	0.00000		
NA2SO4.MGSO4.4H2O	0.00000		0.10000E+31	0.00000		
CASO4.2H2O	0.00000		0.10000E+31	0.00000		
CASO4	0.00000		0.10000E+31	0.00000		
MGSO4.12H2O	0.00000		0.10000E+31	0.00000		
NA2SO4.3K2SO4	0.00000		0.10000E+31	0.00000		
CACO3(CALCITE)	0.00000		0.10000E+31	0.00000		
MGCO3	0.00000		0.10000E+31	0.00000		
MGCO3.3H2O	0.00000		0.10000E+31	0.00000		
MGCO3.5H2O	0.00000		0.10000E+31	0.00000		
CACO3.6H2O	0.00000		0.10000E+31	0.00000		
NAHCO3	0.00000		0.10000E+31	0.00000		
NA2CO3.10H2O	0.00000		0.10000E+31	0.00000		
NAHCO3.NA2CO3.2H2O	0.00000		0.10000E+31	0.00000		
3MGCO3.MG(OH)2.3H2O	0.00000		0.10000E+31	0.00000		
CAMG(CO3)2	0.00000		0.10000E+31	0.00000		
NA2CO3.7H2O	0.00000		0.10000E+31	0.00000		
KHCO3	0.00000		0.10000E+31	0.00000		
CACO3(ARAGONITE)	0.00000		0.10000E+31	0.00000		
CACO3(VATERITE)	0.00000		0.10000E+31	0.00000		
HNO3.3H2O	0.00000		0.10000E+31	0.00000		
KNO3	0.00000		0.10000E+31	0.00000		
NANO3	0.00000		0.10000E+31	0.00000		
HCL.3H2O	0.00000		0.10000E+31	0.00000		
H2SO4.6.5H2O	0.00000		0.10000E+31	0.00000		
H2SO4.4H2O	0.00000		0.10000E+31	0.00000		
HCL.6H2O	0.00000		0.10000E+31	0.00000		
NANO3.NA2SO4.2H2O	0.00000		0.10000E+31	0.00000		
NA3H(SO4)2	0.00000		0.10000E+31	0.00000		
NAHSO4.H2O	0.00000		0.10000E+31	0.00000		
K3H(SO4)2	0.00000		0.10000E+31	0.00000		

K5H3(SO4)4	0.00000	0.10000E+31	0.00000
K8H6(SO4)7.H2O	0.00000	0.10000E+31	0.00000
KHSO4	0.00000	0.10000E+31	0.00000
MGSO4.H2O	0.00000	0.10000E+31	0.00000
FESO4.7H2O	0.00000	0.10000E+31	0.00000
FESO4.H2O	0.00000	0.10000E+31	0.00000
FECL2.6H2O	0.00000	0.10000E+31	0.00000
FECL2.4H2O	0.00000	0.10000E+31	0.00000
FECO3	0.00000	0.10000E+31	0.00000
FE(OH)3	0.00000	0.10000E+31	0.00000
CO2.6H2O	0.00000	0.10000E+31	0.00000
CH4.6H2O	0.00000	0.10000E+31	0.00000
FECL3.10H2O	0.00000	0.10000E+31	0.00000
FECL3.6H2O	0.00000	0.10000E+31	0.00000
FECL3.2KCL.H2O	0.00000	0.10000E+31	0.00000
FE2(SO4)3	0.00000	0.10000E+31	0.00000
FE2(SO4)3.2K2SO4.14H	0.00000	0.10000E+31	0.00000
K2SO4.FESO4.6H2O	0.00000	0.10000E+31	0.00000
NA2SO4.FESO4.4H2O	0.00000	0.10000E+31	0.00000
FE2(SO4)3.9H2O	0.00000	0.10000E+31	0.00000
FE2(SO4)3.H2SO4.8H2O	0.00000	0.10000E+31	0.00000
KFE3(SO4)2(OH)6	0.00000	0.10000E+31	0.00000
NAFE3(SO4)2(OH)6	0.00000	0.10000E+31	0.00000
H3OFE3(SO4)2(OH)6	0.00000	0.10000E+31	0.00000
a-Fe2O3	0.00000	0.10000E+31	0.00000
a-FeO(OH)	0.00000	0.10000E+31	0.00000
g-FeO(OH)	0.00000	0.10000E+31	0.00000
FeO(OH)3/4(SO4)1/8	0.00000	0.10000E+31	0.00000
FESO4.4H2O	0.00000	0.10000E+31	0.00000
FE2(SO4)3.7H2O	0.00000	0.10000E+31	0.00000
FE(II)FE(III)4(SO4)6	0.00000	0.10000E+31	0.00000
FE(III)5(SO4)6O(OH).	0.00000	0.10000E+31	0.00000
FE(II)FE(III)2(SO4)4	0.00000	0.10000E+31	0.00000
FE(II)FE(III)2(SO4)4	0.00000	0.10000E+31	0.00000
K2FE(II)5FE(III)4(SO	0.00000	0.10000E+31	0.00000
ALCL3.6H2O	0.00000	0.10000E+31	0.00000
AL2(SO4)3.17H2O	0.00000	0.10000E+31	0.00000
NABR	0.00000	0.10000E+31	0.00000
MGBR2	0.00000	0.10000E+31	0.00000
AL(OH)3	0.00000	0.10000E+31	0.00000
SIO2(QUARTZ)	0.00000	0.10000E+31	0.00000
SIO2(AMORPHOUS)	0.00000	0.10000E+31	0.00000
KAL3(SO4)2(OH)6	0.00000	0.10000E+31	0.00000
NAAL3(SO4)2(OH)6	0.00000	0.10000E+31	0.00000
KAL(SO4)2.12H2O	0.00000	0.10000E+31	0.00000
NAAL(SO4)2.12H2O	0.00000	0.10000E+31	0.00000
FESO4.AL2(SO4)3.22H2	0.00000	0.10000E+31	0.00000
AL2SI2O5(OH)4	0.00000	0.10000E+31	0.00000
MGSO4.AL2(SO4).22H2O	0.00000	0.10000E+31	0.00000

Iterations = 9