

FRIENDS OF CHEMCHAU (FREZCHEM Version 14.2)

Attached is a "beta" version of the FREZCHEM model that includes chloride, perchlorate, sulfate, and bicarbonate-carbonate salts, strong acid chemistry, silicon chemistry, and gas hydrate chemistry. This version includes both temperature (0-100°C) and pressure (1-1000 bars) dependencies. This particular version of FREZCHEM was extended from 25°C to 100°C, which was named as CHEMCHAU (CHEMistry CHAUd, where chaud means "hot" in French). This high temperature version does not contain the solution phases: Fe(II), Fe(III), Al, NO₃, Br, and B(OH)₄⁻, which may be added into CHEMCHAU in the future. The absence of these phases and other solution and atmospheric species are checked off in Table 1 and are simply by-passed when running CHEMCHAU, including solid phases that are a function of these checked species (e.g., all Fe(II) and Fe(III) solid phases). Compared to earlier versions, CHEMCHAU contains higher temperature applications, but with fewer soluble species than previous versions. This folder includes a FORTRAN program listing that you can download directly, three input files (Tables 3,7,8), a list of chemical species in the model (Table 1), instructions for model input (Tables 2,4,5), and three examples of model outputs (Tables 6,9 and Figure 1).

I have not spent 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., FREZCHEM13.3) 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 mineral database, which can be done with the file "Solidphase," see description below. 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).

The validation of this model is discussed in 16 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 Grant (1994) FREZCHEM: A chemical-thermodynamic model for aqueous solutions at subzero temperatures. CRREL Spec. Rept. 94-18. USACRREL, Hanover, NH. (3) 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; (4) 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; (5) Marion (2002) A molal-based model for strong acid chemistry at low temperatures (<200 to 298 K). *Geochim. Cosmochim. Acta*, 66:2499-2516; (6) Marion et al. (2003) Modeling aqueous ferrous iron chemistry at low temperatures with application to Mars. *Geochim. Cosmochim. Acta*, 67:4251-4266; (7) Marion et al. (2005) Effects of pressure on aqueous chemical equilibria at subzero temperatures with applications to Europa. *Geochim. Cosmochim. Acta*, 69:259-274; (8) Marion et al. (2006) Modeling gas hydrate equilibria in electrolyte solutions. *CALPHAD*, 30:248-259; (9) Marion (2007) Adapting molar data (without density) for molal models. *Computers & Geosciences*, 33:829-834. (10) Marion and Kargel (2008) Cold Aqueous Planetary Geochemistry with FREZCHEM: From Modeling to the Search for Life at the Limits. Springer; (11) Marion et al. (2008) Modeling ferrous-ferric iron chemistry with application to Martian surface geochemistry. *Geochim. Cosmochim. Acta*, 72:242-266; (12) Marion et al., (2009) Br/Cl partitioning in chloride minerals in the Burns formation on Mars. *Icarus*, 200:436-445; (13) Marion et al. (2009). Modeling aluminum-silicon chemistries and application to Australian playa lakes as analogues for Mars. *Geochim. Cosmochim. Acta*. 73:3493-3511; (14) Marion et al., (2010). Modeling aqueous perchlorate chemistries with applications to Mars. *Icarus*. 207:675-685; (15) Marion et al. (2010) FREZCHEM: A geochemical model for cold aqueous solutions. *Comput. Geosci.* 36:10-15; and (16) Marion et al. (2011) Modeling hot spring chemistries with applications to Martian silica formation. *Icarus*. 212:629-642.

A fundamental change was made in FREZCHEM 13 and subsequent versions on how to input data into the model. Earlier versions required inputs via the computer screen. Version 13

and later versions require inputs via data files; this approach simplifies and speeds up model inputting. There are four input files that must be built to run FREZCHEM. Table 2 describes the main model inputs; Table 3 presents the main Input.txt file; and Table 4 describes in more detail how to handle gases for these inputs. There are three minor input files that are lumped together in Table 5. Table 2 is just a verbal description of the material that is in the Input.txt file of Table 3. Similarly, Table 4 describes in more detail how gases need to be dealt with in Input.txt (Table 3). In the Input.txt file, note that inputs are all placed to the left of the “,”. Also, do not remove the “,”. That comma separates model input from descriptive words. The three minor files in Table 5 include: (A) SOLIDPHASE.txt, (B) SOLIDMASS.txt, and (C) NUANCES.txt. SOLIDPHASE.txt allows the user to remove all solid phases from equilibrium calculations or some specific minerals. That option allows for a pure solution phase calculation without any minerals precipitating. Or in the Phoenix site case (Table 6), we removed magnesite (MgCO_3) and dolomite [$\text{CaMg}(\text{CO}_3)_2$] from model calculations that eventually led to calcite (CaCO_3) and hydromagnesite [$3\text{Mg}(\text{CO}_3)_2 \cdot \text{MgSO}_4 \cdot 3\text{H}_2\text{O}$] precipitating. Generally model calculations start with aqueous/gas phases, without initial solid phases; but if you want a particular solid phase to control the solution phase chemical composition, then you can specify the solid phase and its mole mass (Table 5); the mole mass is an arbitrary amount that must not completely dissolve in 1.0 kg H_2O . For example, we assumed that Earth seawater would have been saturated with dolomite during Snowball Earth (Marion and Kargel, 2008). Changing the first line of SOLIDMASS.txt from No(0) to YES(1) would allow saturation with dolomite. The NUANCES.txt file allows for temperature, water content, or pressure changes to be adjusted during a specific run. For example, if you want to know the eutectic temperature of a salt assemblage, and you know that this will occur slightly below 259 K, you could change the ΔT term from 5 K between 298 and 263 K (as assigned by Input.txt) to 1 K between 263 and 259 K, and 0.1 K below 259 K (Table 5). This scenario would allow for a more accurate estimate of the eutectic temperature than using either a 5 K or 1 K term for the ΔT decrement. With respect to NUANCES.txt, always retain three steps for temperature, water content, and pressure changes, even if you need to duplicate two steps (e.g., 263.15 0.1, 263.15 0.1).

Table 1. A listing of chemical species in the CHEMCHAU model (FREZCHEM Version 14.2).

A. Solution and Atmospheric Species									
#	Species	#	Species	#	Species	#	Species	#	Species
1	Na ⁺ (aq)	11	Cl ⁻ (aq)	21	CO ₂ (aq)	151	O ₂ (g)	166	Si(OH) ₄ ⁰ (aq)
2	K ⁺ (aq)	12	SO ₄ ²⁻ (aq)	22	FeCO ₃ ^o (aq)	152	O ₂ (aq)	167	Si(OH) ₃ ⁻ (aq)
3	Ca ²⁺ (aq)	13	OH ⁻ (aq)	23	HCl(g)	153	H ₂ (g)	168	SrCO ₃ ⁰ (aq)
4	Mg ²⁺ (aq)	14	HCO ₃ ⁻ (aq)	24	CaCO ₃ ^o (aq)	154	CH ₄ (g)	169	B(OH) ₃ ⁰ (aq)
5	H ⁺ (aq)	15	CO ₃ ²⁻ (aq)	25	MgCO ₃ ^o (aq)	155	CH ₄ (aq)	170	F(aq)
6	MgOH ⁺ (aq)	16	HSO ₄ ⁻ (aq)	26	HNO ₃ (g)	156	Fe(OH) ₂ ⁰ (aq)	171	HF ⁰ (aq)
7	Fe ²⁺ (aq)	17	NO ₃ ⁻ (aq)	27	H ₂ SO ₄ (g)	157	Fe(OH) ₃ ⁻ (aq)	172	Sr ²⁺ (aq)
8	FeOH ⁺ (aq)	18	Br ⁻ (aq)	28	H ₂ O(g)	158	FeOH ²⁺ (aq)		
9	Fe ³⁺ (aq)	19	ClO ₄ ⁻ (aq)	29	CO ₂ (g)	159	Fe(OH) ₂ ⁺ (aq)		
10	Al ³⁺ (aq)	20	B(OH) ₄ ⁻ (aq)	30	H ₂ O(l)	160	Fe(OH) ₃ ⁰ (aq)		
						161	Fe(OH) ₄ ⁻ (aq)		
						162	Al(OH) ²⁺ (aq)		
						163	Al(OH) ₂ ⁺ (aq)		
						164	Al(OH) ₃ ⁰ (aq)		
						165	Al(OH) ₄ ⁻ (aq)		
B. Solid Phase Species									
#	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)	111	K ₂ Fe(II) ₅ Fe(III) ₄ (SO ₄) ₁₂ •18H 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)	112	AlCl ₃ •6H ₂ O(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)	113	Al ₂ (SO ₄) ₃ •17H 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)	114	NaBr
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)	115	MgBr ₂
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)	116	Al(OH) ₃ (cr)
37	MgCl ₂ •8H ₂ O(cr)	57	NaHCO ₃ (cr)	77	K ₂ H ₃ (SO ₄) ₄ (cr)	97	Fe ₂ (SO ₄) ₃ •H ₂ SO ₄ •8H ₂ O(cr)	117	SiO ₂ (quartz)(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)	118	SiO ₂ (amorphous)
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)	119	KAl 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)	120	NaAl 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)	121	KAl ₂ (SO ₄) ₂ •12H ₂ O(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)	122	NaAl(SO ₄) ₂ •12H ₂ O(cr)
43	MgSO ₄ •6H ₂ O(cr)	63	KHCO ₃ (cr)	83	FeCl ₂ •6H ₂ O(cr)	103	γ-FeO(OH)(cr)	123	FeSO ₄ •Al ₂ (SO ₄) ₃ •22H ₂ O(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)	124	Al ₂ Si ₂ O ₅ (OH) ₄ (cr)
45	K ₂ SO ₄ (cr)	65	CaCO ₃ (cr,vaterite)	85	FeCO ₃ (cr)	105	FeSO ₄ •4H ₂ O(cr)	125	MgSO ₄ •Al ₂ (SO ₄) ₃ •22H 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)	126	NaClO ₄ •H 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)	127	Mg(ClO ₄) ₂ •8H ₂ O(cr)
48	CaSO ₄ •2H ₂ O(cr)	68	NaNO ₃ (cr)	88	CH ₄ •6H ₂ O(cr)	108	Fe ₃ (SO ₄) ₆ O(OH)•20H ₂ O(cr)	128	Ca(ClO ₄) ₂ •6H ₂ O(cr)
49	CaSO ₄ (cr)	69	HCl•3H ₂ O(cr)	89	HCl•10H ₂ O(cr)	109	Fe(II)Fe(III) ₂ (SO ₄) ₄ •22H ₂ O(cr)	129	KClO ₄ (cr)
50	MgSO ₄ •11H 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)	130	Mg(ClO ₄) ₂ •6H ₂ O(cr)
								131	NaClO ₄ •2H ₂ O(cr)
								132	NaClO(cr) ₄
								133	Na ₂ CO ₃ •H ₂ O(cr)

Table 2. Description of Model Inputs (Version 14.2) (Compare with Table 3).

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.

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.

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

If pH is 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.

Perchlorate (m/kg): Enter perchlorate molality (moles/kg(water)). Otherwise, enter 0.0.

Sulfate (m/kg): Enter sulfate 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.

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).

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 = P_{CO₂}/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.

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 = P_{CH₄}/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).

Initial Temperature(K): Enter the temperature in absolute degrees (K) for start of simulation (e.g., 273.15).

For Temperature Change Pathway(1):

Final Temperature(K): Enter final temperature of simulation (e.g., 263.15).

Temperature Decrement(K): The temperature interval between simulations (e.g. 1). For the above temperature designations, the model would calculate equilibrium starting at

273.15 K and ending at 263.15 K at 1 K intervals. If you want to change the decrement in a run (e.g., to reduce the step size near an equilibrium), see File "NUANCES.txt."

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 Files "NUANCES.txt."

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 File "NUANCES."

Table 3. Input.txt. This is the main input file for applications of CHEMCHAU. In this particular case, the model simulates a perchlorate chemistry at 273.15 K (Table 6).

TITLE: This is a Mars Phoenix test case.
1, FREEZE(1) OR EVAPORATION(2) OR PRESSURE(3) SCENARIO ? CALLED PATH BELOW.
2, EQUILIBRIUM(1) OR FRACTIONAL(2) CRYSTALLIZATION?
1.5E-3, SODIUM(M/KG).
0.3E-3, POTASSIUM(M/KG).
0.4E-3, CALCIUM(M/KG).
2.5E-3, MAGNESIUM(M/KG).
0.00, SILICA (M/KG).

FOR FE,AL,SI, AND ALKALINE CHEMISTRIES,DO YOU WANT ACIDITY IGNORED(1),OR FIXED BY PH(2), OR ACIDITY(3), OR ALKALINITY(4)? IF YES, THEN ENTER NUM. NOTE THAT OPTIONS 3 AND 4 REQUIRE A FURTHER SPECIFICATION BELOW. OPTIONS 2-4 WILL ADJUST SOLUTION-PHASE CHARGE BALANCE AS AL, FE, OR SI REACTIONS PRODUCE ACIDITY BY ASSUMING H+ REACTS WITH ROCKS TO RELEASE NA,K,CA,MG,OR FE(II) IONS. SOME OF THE LATTER IONS MUST BE PRESENT AS INPUT TO SERVE AS AN ION SINK/SOURCE.

4, SPECIFY ABOVE ACIDITY OPTION.
7.70, SPECIFY INITIAL PH.
0.45E-3, CHLORIDE(M/KG).
3.0E-3, PERCHLORATE(M/KG).
0.8E-3, SULFATE(M/KG).
2.55E-3, ALKALINITY(EQUIVALENTS/KG).
0.00, ACIDITY(EQUIVALENTS/KG).
0.00, IF YOU WANT TO SPECIFY HCL(BARS), ENTER VALUE HERE.
0.00, IF YOU WANT TO SPECIFY H2SO4(BARS), ENTER VALUE HERE.
1.01325, INITIAL TOTAL PRESSURE(BARS).
3.0E-3, INITIAL CO2(BARS).
0.0, ENTER MOLE FRACTION OF CO2, 0=FIXED CO2, 1=PURE CO2.
0.00, INITIAL O2(BARS).
0.0, INITIAL CH4(BARS).
0.0, ENTER MOLE FRACTION OF CH4, 0=FIXED CHR, 1=PURE CH4.
0, CONSIDER A MIXED CO2-CH4 GAS HYDRATE(YES=1, NO=0)?
273.15, INITIAL TEMPERATURE(K).
273.15, FINAL TEMPERATURE(K), IF PATH =1, OTHERWISE, SET = 0.
0.00, TEMPERATURE DECREMENT(K), IF PATH = 1, OTHERWISE, SET = 0.
1000, INITIAL WATER(G), IF PATH = 2, OTHERWISE, SET = 1000.
0.00, FINAL WATER (G), IF PATH = 2, OTHERWISE, SET = 0.
0, WATER DECREMENT(K), IF PATH = 2, OTHERWISE, SET = 0.
0, FINAL PRESSURE(BARS), IF PATH = 3, OTHERWISE, SET = 0.
0, PRESSURE INCREMENT(BARS), IF PATH = 3, OTHERWISE, SET = 0.

Table 4. Inputting Gases into the Model

SYSTEM INPUTS	NO GASES	FIXED GAS CONCS.	VARIABLE GAS CONCS.
1. INITIAL TOTAL PRESSURE	USER SPECIFICATION	USER SPECIFICATION	USER SPECIFICATION
2. INITIAL CO2	0	USER SPECIFICATION	USER SPECIFICATION
3. MOLE FRACTION OF CO2	0	0	USER SPECIFICATION
4. INITIAL O2	0	USER SPECIFICATION	0
5. INITIAL CH4	0	USER SPECIFICATION	USER SPECIFICATION
6. MOLE FRACTION OF CH4	0	0	USER SPECIFICATION
7. MIXED CH4-CO2 GAS HYDRATE	0	0	1

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

FIXED GAS CONCS. mean 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 3.90×10^{-4} bars.

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

Table 5. Minor input files for FREZCHEM 14.2

(A). SOLIDPHASE.txt

0, WANT ALL SOLID PHASES TO BE REMOVED, YES=1, NO=0.
2, WANT SPECIFIC SOLID PHASES REMOVED, SPECIFY # OF CASES.
53, SPECIFY SAMPLE # TO BE REMOVED.
61, SPECIFY SAMPLE # TO BE REMOVED.

(B). SOLIDMASS.txt

0, WANT STARTING MINERALS TO CONTAIN MASS, YES=1, NO=0.
1, SPECIFY NUMBER OF MINERALS TO HAVE INITIAL MASS.
61 10.000, SPECIFY MINERAL NUMBER AND MASS(MOLES).

(C). NUANCES.txt

0, WANT TO REDUCE TEMPERATURE DECREMENT AT LOWER T? YES=1, NO=0.
263.15 1.0, TEMPERATURE AND ΔT , WHERE CHANGE SHOULD BE MADE.
259.15 0.1, TEMPERATURE AND ΔT , WHERE CHANGE SHOULD BE MADE.
0, WANT TO REDUCE WATER DECREMENT AT LOWER WATER? YES=1,NO=0.
100 1, WATER CONTENT AND ΔH_2O , WHERE CHANGE SHOULD BE MADE.
10 0.1, WATER CONTENT AND ΔH_2O , WHERE CHANGE SHOULD BE MADE.
0, WANT TO INCREASE(OR DECREASE) PRESSURE INCREMENT AT HIGHER P? YES = 1, N=0.
17 1, PRESSURE AND ΔP , WHERE CHANGE SHOULD BE MADE.
50 10, PRESSURE AND ΔP , WHERE CHANGE SHOULD BE MADE.

Model Outputs.

We will illustrate three model outputs. The first case (Table 6) will largely present definitions of outputs. Tables 7 and 8 will deal with high temperature outputs. "Ion.Str." is the ionic strength of the equilibrium solution (see Table 6). "RHO" is the density of the solution. "Phi" is the osmotic coefficient of the equilibrium solution. "H2O(g)" is the amount of water present as liquid. "Ice" is the amount of water that forms 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 at 273 K. "Final Conc." are the equilibrium concentrations at 273 K. Act. coef. (activity coefficient) and activity are self-explanatory. Moles are the # of moles in the solution 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 \geq moles (solids); in this case, moles represent the solids that have precipitated in the last interval (e.g., between 274 K and 273 K), while accum. moles represent the total precipitate (e.g., between 283 K and 273 K). This calculation for CHEMCHAU is limited to a lower temperature limit of 273 K (0°C). In FREZCHEM 13, allowing the temperature to drop to 263 K, formed ice, gypsum, calcite, hydromagnesite, meridianite, and KClO_4 to precipitate (see 2011 paper cited above).

We chose evaporation of the Crystal Creek case to represent formation of solid phases at high temperatures and low pH using CHEMCHAU. Table 7 is the Crystal Creek input file for CHEMCHAU. Crystal Creek is a predominantly NaCl system (Fig. 1). Silica began precipitating immediately at the initial 1000 g of water indicating that the solution was slightly supersaturated. Other salts that precipitated included matteuccite ($\text{NaHSO}_4 \cdot \text{H}_2\text{O}$), halite (NaCl), and anhydrite (CaSO_4). Matteuccite typically forms in volcanic craters (<http://webmineral.com>), which is where Crystal Creek exists in Yellowstone hot springs.

Table 6. TITLE: This is a Mars Phoenix test case.

Temp(K)	Ion.Str.	RHO	Phi	H2O(g)	Ice(g)	Press.(bars)
273.15	0.11295E-01	1.000382	0.93902	1000.0	0.00000	1.0132
Solution SPECIES	Initial Conc.	Final Conc.	Act.Coeff.	Activity	Moles	Mass Balance
NA	0.15000E-02	0.15000E-02	0.89325	0.13399E-02	0.15000E-02	0.15000E-02
K	0.30000E-03	0.30000E-03	0.88979	0.26694E-03	0.30000E-03	0.30000E-03
CA	0.40000E-03	0.39941E-03	0.63549	0.25382E-03	0.39941E-03	0.40000E-03
MG	0.25000E-02	0.24980E-02	0.66603	0.16637E-02	0.24980E-02	0.25000E-02
H	0.00000	0.29683E-07	0.89298	0.26507E-07	0.29683E-07	
MGOH	0.00000	0.10098E-07	0.89076	0.89953E-08	0.10098E-07	
CL	0.45000E-03	0.45000E-03	0.90232	0.40604E-03	0.45000E-03	0.45000E-03
SO4	0.80000E-03	0.80000E-03	0.65085	0.52068E-03	0.80000E-03	0.80000E-03
OH	0.00000	0.49129E-07	0.89306	0.43875E-07	0.49129E-07	
HCO3	0.25500E-02	0.25384E-02	0.89826	0.22801E-02	0.25384E-02	0.25500E-02
CO3	0.00000	0.31800E-05	0.63623	0.20232E-05	0.31800E-05	
HSO4	0.00000	0.72371E-09	0.90041	0.65164E-09	0.72371E-09	
CLO4	0.30000E-02	0.30000E-02	0.91490	0.27447E-02	0.30000E-02	0.30000E-02
CO2	0.00000	0.22865E-03	1.0018	0.22906E-03	0.22865E-03	
CACO3	0.00000	0.59174E-06	1.0000	0.59174E-06	0.59174E-06	
MGCO3	0.00000	0.20270E-05	1.0000	0.20270E-05	0.20270E-05	
CO2 (BAR)	0.00000	0.30000E-02	0.99301	0.29790E-02	0.00000	
H2O (BAR)	0.00000			.61150E-02		
H2O (L)	0.00000			.99980	55.508	55.508
Solid SPECIES	Moles	Equil. Constant	Accum. Moles			
ICE	0.00000	0.99993	0.00000			
NACL.2H2O	0.00000	17.960	0.00000			
NACL	0.00000	31.336	0.00000			
KCL	0.00000	3.7732	0.00000			
CACL2.6H2O	0.00000	1859.3	0.00000			
MGCL2.6H2O	0.00000	55958.	0.00000			
MGCL2.8H2O	0.00000	7080.1	0.00000			
MGCL2.12H2O	0.00000	706.24	0.00000			
KMGCL3.6H2O	0.00000	7819.3	0.00000			
CACL2.2MGCL2.12H2O	0.00000	0.27626E+19	0.00000			
NA2SO4.10H2O	0.00000	0.30861E-02	0.00000			
NA2SO4	0.00000	0.49095	0.00000			
MGSO4.6H2O	0.00000	0.19915E-01	0.00000			
MGSO4.7H2O	0.00000	0.61561E-02	0.00000			
K2SO4	0.00000	0.63529E-02	0.00000			
MGSO4.K2SO4.6H2O	0.00000	0.92572E-05	0.00000			
NA2SO4.MGSO4.4H2O	0.00000	0.34591E-02	0.00000			
CASO4.2H2O	0.00000	0.21911E-04	0.00000			
CASO4	0.00000	0.86711E-04	0.00000			
MGSO4.11H2O	0.00000	0.47447E-02	0.00000			
NA2SO4.3K2SO4	0.00000	0.14241E-08	0.00000			
CACO3 (CALCITE)	0.00000	0.41547E-08	0.00000			
MGCO3	0.00000	0.10000E+21	0.00000			
MGCO3.3H2O	0.00000	0.90460E-05	0.00000			
MGCO3.5H2O	0.00000	0.64327E-05	0.00000			
CACO3.6H2O	0.00000	0.62689E-07	0.00000			
NAHCO3	0.00000	0.19053	0.00000			
NA2CO3.10H2O	0.00000	0.15830E-01	0.00000			
NAHCO3.NA2CO3.2H2O	0.00000	0.50599E-01	0.00000			
3MGCO3.MG(OH)2.3H2O	0.00000	0.88117E-35	0.00000			
CAMG(CO3)2	0.00000	0.10000E+21	0.00000			
NA2CO3.7H2O	0.00000	0.87302E-01	0.00000			
KHCO3	0.00000	0.68522	0.00000			
CACO3 (ARAGONITE)	0.00000	0.60523E-08	0.00000			
CACO3 (VATERITE)	0.00000	0.18081E-07	0.00000			
HNO3.3H2O	0.00000	703.94	0.00000			
KNO3	0.00000	0.16734	0.00000			
NANO3	0.00000	2.4768	0.00000			
HCL.3H2O	0.00000	14693.	0.00000			
H2SO4.6.5H2O	0.00000	13.391	0.00000			
H2SO4.4H2O	0.00000	999.90	0.00000			
HCL.6H2O	0.00000	1000.0	0.00000			
NANO3.NA2SO4.2H2O	0.00000	0.12949	0.00000			
NA3H(SO4)2	0.00000	0.15009	0.00000			

NAHSO4.H2O	0.00000	32.663	0.00000
K3H(SO4)2	0.00000	0.67048E-04	0.00000
K5H3(SO4)4	0.00000	0.34065E-07	0.00000
K8H6(SO4)7.H2O	0.00000	0.56476E-12	0.00000
KHSO4	0.00000	1.4339	0.00000
MGSO4.H2O	0.00000	3.5255	0.00000
FESO4.7H2O	0.00000	0.18773E-02	0.00000
FESO4.H2O	0.00000	0.27235	0.00000
FECL2.6H2O	0.00000	2387.6	0.00000
FECL2.4H2O	0.00000	11921.	0.00000
FECO3	0.00000	0.12776E-10	0.00000
FE(OH)3	0.00000	50377.	0.00000
CO2.6H2O	0.00000	10.251	0.00000
CH4.6H2O	0.00000	24.965	0.00000
FECL3.10H2O	0.00000	0.84910E-01	0.00000
FECL3.6H2O	0.00000	0.64059	0.00000
FECL3.2KCL.H2O	0.00000	11.463	0.00000
FE2(SO4)3	0.00000	302.00	0.00000
FE2(SO4)3.2K2SO4.14H	0.00000	0.14132E-13	0.00000
K2SO4.FESO4.6H2O	0.00000	0.65369E-05	0.00000
NA2SO4.FESO4.4H2O	0.00000	0.12041E-02	0.00000
FE2(SO4)3.9H2O	0.00000	0.21248	0.00000
FE2(SO4)3.H2SO4.8H2O	0.00000	79.073	0.00000
KFE3(SO4)2(OH)6	0.00000	0.10605E-09	0.00000
NAFE3(SO4)2(OH)6	0.00000	0.15873E-03	0.00000
H3OFE3(SO4)2(OH)6	0.00000	0.39862E-02	0.00000
a-FE2O3	0.00000	142.26	0.00000
a-FEO(OH)	0.00000	15.373	0.00000
g-FEO(OH)	0.00000	1117.3	0.00000
FEO(OH)3/4(SO4)1/8	0.00000	216.07	0.00000
FESO4.4H2O	0.00000	0.22553E-01	0.00000
FE2(SO4)3.7H2O	0.00000	1.0231	0.00000
FE(II)FE(III)4(SO4)6	0.00000	0.78198E-20	0.00000
FE(III)5(SO4)6O(OH).	0.00000	0.82950E-20	0.00000
FE(II)FE(III)2(SO4)4	0.00000	0.23825E-16	0.00000
FE(II)FE(III)2(SO4)4	0.00000	0.65980E-10	0.00000
K2FE(II)5FE(III)4(SO	0.00000	0.81200E-33	0.00000
ALCL3.6H2O	0.00000	0.10884E+06	0.00000
AL2(SO4)3.17H2O	0.00000	0.10529E-05	0.00000
NABR	0.00000	0.00000	0.00000
MGBR2	0.00000	0.00000	0.00000
AL(OH)3	0.00000	0.42578E+10	0.00000
SIO2(QUARTZ)	0.00000	0.41759E-04	0.00000
SIO2(AMORPHOUS)	0.00000	0.11483E-02	0.00000
KAL3(SO4)2(OH)6	0.00000	11289.	0.00000
NAAL3(SO4)2(OH)6	0.00000	0.18014E+08	0.00000
KAL(SO4)2.12H2O	0.00000	0.99627E-07	0.00000
NAAL(SO4)2.12H2O	0.00000	0.29724E-04	0.00000
FESO4.AL2(SO4)3.22H2	0.00000	0.27653E-08	0.00000
AL2SI2O5(OH)4	0.00000	0.29822E+09	0.00000
MGSO4.AL2(SO4).22H2O	0.00000	0.96704E-08	0.00000
NACLO4.H2O	0.00000	86.917	0.00000
MG(CLO4)2.8H2O	0.00000	0.17149E+06	0.00000
CA(CLO4)2.6H2O	0.00000	0.93572E+06	0.00000
KCLO4	0.00000	0.17504E-02	0.00000
MG(CLO4)2.6H2O	0.00000	0.91236E+06	0.00000
NACLO4.2H2O	0.00000	58.954	0.00000
NACLO4	0.00000	1384.3	0.00000
NA2CO3.H2O	0.00000	0.99120	0.00000

pH= 7.57665 pHF= 7.52749 pHT= 7.51703 pH(SWS)= 7.51703
pHMacinnis = 7.52053 Temp. = 273.150

CONVERGENCE CRITERION = 0.100000 %
Iterations = 4

Table 7. TITLE: This is the Crystal Creek case.

2, FREEZE(1) OR EVAPORATION(2) OR PRESSURE(3) SCENARIO ? CALLED PATH BELOW.
1, EQUILIBRIUM(1) OR FRACTIONAL(2) CRYSTALLIZATION?
1.9420e-2, SODIUM(M/KG).
7.80e-4, POTASSIUM(M/KG).
1.52e-4, CALCIUM(M/KG).
0.00, MAGNESIUM(M/KG).
6.41e-3, SILICA (M/KG).

FOR FE,AL,SI, AND ALKALINE CHEMISTRIES,DO YOU WANT ACIDITY
IGNORED(1),OR FIXED BY PH(2), OR ACIDITY(3), OR
ALKALINITY(4)? IF YES, THEN ENTER NUM. NOTE THAT OPTIONS 3
AND 4 REQUIRE A FURTHER SPECIFICATION BELOW. OPTIONS 2-4
WILL ADJUST SOLUTION-PHASE CHARGE BALANCE AS AL, FE, OR SI
REACTIONS PRODUCE ACIDITY BY ASSUMING H+ REACTS WITH ROCKS
TO RELEASE NA,K,CA,MG,OR FE(II) IONS. SOME OF THE LATTER
IONS MUST BE PRESENT AS INPUT TO SERVE AS AN ION SINK/SOURCE.

3, SPECIFY ABOVE ACIDITY OPTION.
3.5, SPECIFY INITIAL PH.
2.038e-2, CHLORIDE(M/KG).
0.00, PERCHLORATE(M/KG).
5.48e-4, SULFATE(M/KG).
0.00, ALKALINITY(EQUIVALENTS/KG).
9.76e-4, ACIDITY(EQUIVALENTS/KG).
0.00, IF YOU WANT TO SPECIFY HCL(BARS), ENTER VALUE HERE.
0.00, IF YOU WANT TO SPECIFY H2SO4(BARS), ENTER VALUE HERE.
1.01325, INITIAL TOTAL PRESSURE(BARS).
0.00, INITIAL CO2(BARS).
0.00, ENTER MOLE FRACTION OF CO2, 0=FIXED CO2, 1=PURE CO2.
0.00, INITIAL O2(BARS).
0.0, INITIAL CH4(BARS).
0.0, ENTER MOLE FRACTION OF CH4, 0=FIXED CH4, 1=PURE CH4.
353.45, INITIAL TEMPERATURE(K).
0.00, FINAL TEMPERATURE(K), IF PATH =1, OTHERWISE, SET = 0.
0.00, TEMPERATURE DECREMENT(K), IF PATH = 1, OTHERWISE, SET = 0.
1000.0, INITIAL WATER(G), IF PATH = 2, OTHERWISE, SET = 1000.
1.00, FINAL WATER (G), IF PATH = 2, OTHERWISE, SET = 0.
10.00, WATER DECREMENT(K), IF PATH = 2, OTHERWISE, SET = 0.
0.00, FINAL PRESSURE(BARS), IF PATH = 3, OTHERWISE, SET = 0.
0.00, PRESSURE INCREMENT(BARS), IF PATH = 3, OTHERWISE, SET = 0.

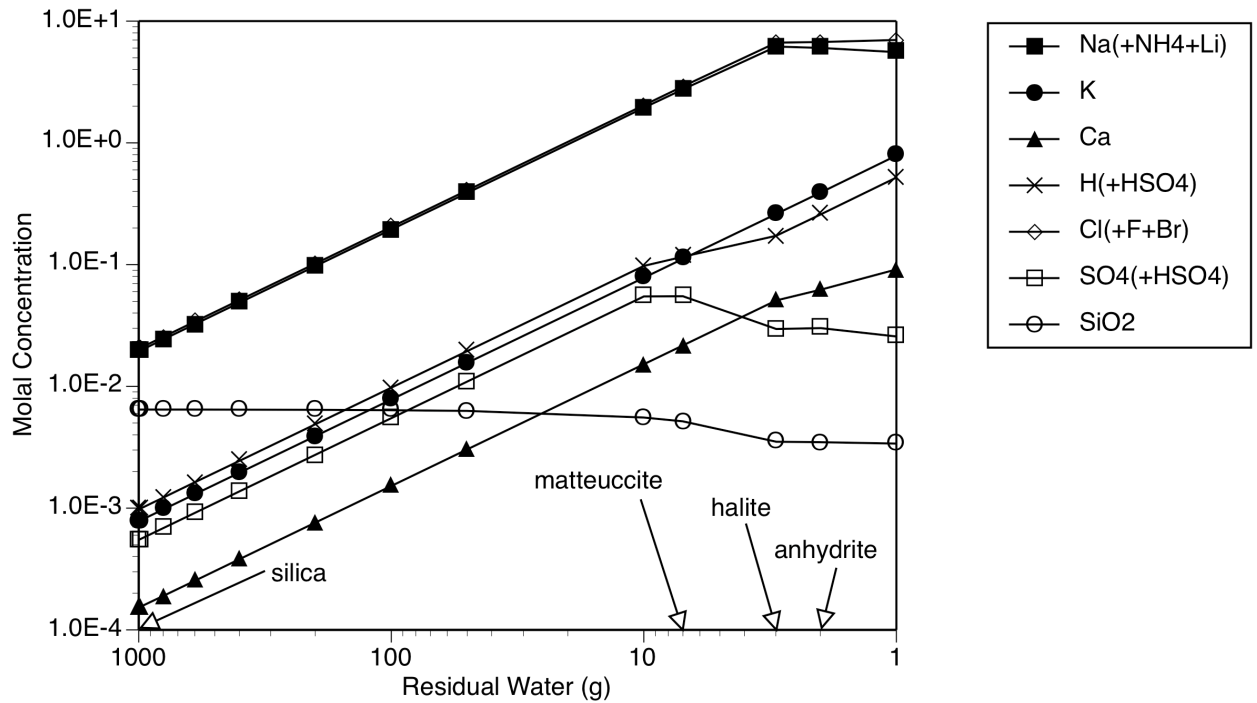


Figure 1. Evaporation of a low pH (3.67-3.77) and high temperature (353.45 K) solution from Crystal Creek (Table 7)

Silica can precipitate at high pH values and at high temperatures (355 K), which is why we chose the Sodi Springs case (Table 8) from Iceland for a simulation that was done with the CHEMCHAU model. Because we could not control pH through unmeasured bicarbonate/carbonate chemistry at these high pH values, this simulation was run at a fixed pH = 8.45 (Table 8).

This case is a predominantly NaCl system, similar to the Crystal Spring case (Fig. 1). Silica began precipitating shortly after evaporation began. The only other solid phases that precipitated were anhydrite (CaSO_4) and thenardite (Na_2SO_4). Had this simulation been done at lower temperatures (e.g., 25°C), then hydrated forms of these salts would have precipitated [gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), mirabilite ($\text{Na}_2\text{SO}_4 \cdot 10\text{H}_2\text{O}$)]. Anhydrous salts were also prevalent at the high temperature in the Crystal Creek case (Fig. 1, halite and anhydrite). Table 9 is the output of this simulation after evaporation had dropped from 1000 g of water to 1.0 g.

Table 8. TITLE: This is the Sodi Spring case.

2, FREEZE(1) OR EVAPORATION(2) OR PRESSURE(3) SCENARIO ? CALLED PATH BELOW.
1, EQUILIBRIUM(1) OR FRACTIONAL(2) CRYSTALLIZATION?
7.283-3, SODIUM(M/KG).
2.30e-4, POTASSIUM(M/KG).
2.80e-5, CALCIUM(M/KG).
0.00, MAGNESIUM(M/KG).
6.19e-3, SILICA (M/KG).

FOR FE,AL,SI, AND ALKALINE CHEMISTRIES,DO YOU WANT ACIDITY IGNORED(1),OR FIXED BY PH(2), OR ACIDITY(3), OR ALKALINITY(4)? IF YES, THEN ENTER NUM. NOTE THAT OPTIONS 3 AND 4 REQUIRE A FURTHER SPECIFICATION BELOW. OPTIONS 2-4 WILL ADJUST SOLUTION-PHASE CHARGE BALANCE AS AL, FE, OR SI REACTIONS PRODUCE ACIDITY BY ASSUMING H+ REACTS WITH ROCKS TO RELEASE NA,K,CA,MG,OR FE(II) IONS. SOME OF THE LATTER IONS MUST BE PRESENT AS INPUT TO SERVE AS AN ION SINK/SOURCE.

2, SPECIFY ABOVE ACIDITY OPTION.
8.45, SPECIFY INITIAL PH.
4.089e-3, CHLORIDE(M/KG).
0.00, PERCHLORATE(M/KG).
1.114e-3, SULFATE(M/KG).
0.00, ALKALINITY(EQUIVALENTS/KG).
0.00, ACIDITY(EQUIVALENTS/KG).
0.00, IF YOU WANT TO SPECIFY HCL(BARS), ENTER VALUE HERE.
0.00, IF YOU WANT TO SPECIFY H2SO4(BARS), ENTER VALUE HERE.
1.01325, INITIAL TOTAL PRESSURE(BARS).
0.00, INITIAL CO2(BARS).
0.00, ENTER MOLE FRACTION OF CO2, 0=FIXED CO2, 1=PURE CO2.
0.00, INITIAL O2(BARS).
0.0, INITIAL CH4(BARS).
0.0, ENTER MOLE FRACTION OF CH4, 0=FIXED CH4, 1=PURE CH4.
355.15, INITIAL TEMPERATURE(K).
0.00, FINAL TEMPERATURE(K), IF PATH =1, OTHERWISE, SET = 0.
0.00, TEMPERATURE DECREMENT(K), IF PATH = 1, OTHERWISE, SET = 0.
1000.0, INITIAL WATER(G), IF PATH = 2, OTHERWISE, SET = 1000.
1.00, FINAL WATER (G), IF PATH = 2, OTHERWISE, SET = 0.
10.00, WATER DECREMENT(K), IF PATH = 2, OTHERWISE, SET = 0.
0.00, FINAL PRESSURE(BARS), IF PATH = 3, OTHERWISE, SET = 0.
0.00, PRESSURE INCREMENT(BARS), IF PATH = 3, OTHERWISE, SET = 0.

Table 9. TITLE: This is the Sodi Spring case.

Temp(K)	Ion.Str.	RHO	Phi	H2O(g)	Ice(g)	Press.(bars)
355.15	7.2400	1.200835	1.0697	1.0000	0.00000	1.0132
Solution SPECIES	Initial Conc.	Final Conc.	Act.Coeff.	Activity	Moles	Mass Balance
NA	0.72830E-02	6.7867	0.67895	4.6078	0.67867E-02	0.72830E-02
K	0.23000E-03	0.23000	0.45056	0.10363	0.23000E-03	0.23000E-03
CA	0.28000E-04	0.23502E-02	0.31289	0.73535E-03	0.23502E-05	0.28000E-04
H	0.00000	0.74417E-08	0.47679	0.35481E-08	0.74417E-11	
CL	0.40890E-02	4.0890	0.91618	3.7463	0.40890E-02	0.40890E-02
SO4	0.11140E-02	0.84022	0.14336E-01	0.12045E-01	0.84022E-03	0.11140E-02
HSO4	0.00000	0.17819E-09	511.50	0.91145E-07	0.17819E-12	
SI(OH)4	0.61900E-02	0.41272E-02	1.0000	0.41272E-02	0.41272E-05	0.61898E-02
SIO(OH)3	0.00000	0.39725E-02	0.23749	0.94344E-03	0.39725E-05	
H2O(BAR)	0.00000			.40719		
H2O(L)	0.00000			.79420	0.55508E-01	0.55508E-01
Solid SPECIES	Moles	Equil. Constant	Accum. Moles			
ICE	0.00000	2.0250	0.00000			
NACL.2H2O	0.00000	35.032	0.00000			
NACL	0.00000	40.063	0.00000			
KCL	0.00000	19.273	0.00000			
CACL2.6H2O	0.00000	0.91263E+06	0.00000			
MGCL2.6H2O	0.00000	9318.0	0.00000			
MGCL2.8H2O	0.00000	58095.	0.00000			
MGCL2.12H2O	0.00000	0.16406E+09	0.00000			
KMGCL3.6H2O	0.00000	22199.	0.00000			
CACL2.2MGCL2.12H2O	0.00000	0.31485E+14	0.00000			
NA2SO4.10H2O	0.00000	5.0955	0.00000			
NA2SO4	0.24813E-03	0.25574	0.24813E-03			
MGSO4.6H2O	0.00000	0.17197E-01	0.00000			
MGSO4.7H2O	0.00000	0.22045E-01	0.00000			
K2SO4	0.00000	0.40118E-01	0.00000			
MGSO4.K2SO4.6H2O	0.00000	0.45489E-04	0.00000			
NA2SO4.MGSO4.4H2O	0.00000	0.67874E-02	0.00000			
CASO4.2H2O	0.00000	0.22555E-04	0.00000			
CASO4	0.25650E-04	0.88573E-05	0.25650E-04			
MGSO4.11H2O	0.00000	10.152	0.00000			
NA2SO4.3K2SO4	0.00000	0.39042E-03	0.00000			
CACO3(CALCITE)	0.00000	0.96752E-09	0.00000			
MGCO3	0.00000	0.17543E-08	0.00000			
MGCO3.3H2O	0.00000	0.16517E-05	0.00000			
MGCO3.5H2O	0.00000	0.15775E-02	0.00000			
CACO3.6H2O	0.00000	0.31415E-05	0.00000			
NAHCO3	0.00000	1.2397	0.00000			
NA2CO3.10H2O	0.00000	75.798	0.00000			
NAHCO3.NA2CO3.2H2O	0.00000	0.45884	0.00000			
3MGCO3.MG(OH)2.3H2O	0.00000	0.16741E-39	0.00000			
CAMG(CO3)2	0.00000	0.64143E-18	0.00000			
NA2CO3.7H2O	0.00000	26.544	0.00000			
KHCO3	0.00000	23.493	0.00000			
CACO3(ARAGONITE)	0.00000	0.12444E-08	0.00000			
CACO3(VATERITE)	0.00000	0.26631E-08	0.00000			
HNO3.3H2O	0.00000	0.22817E+06	0.00000			
KNO3	0.00000	5.1946	0.00000			
NANO3	0.00000	0.30453E+09	0.00000			
HCL.3H2O	0.00000	55932.	0.00000			
H2SO4.6.5H2O	0.00000	0.27471E-05	0.00000			
H2SO4.4H2O	0.00000	999.90	0.00000			
HCL.6H2O	0.00000	1000.0	0.00000			
NANO3.NA2SO4.2H2O	0.00000	0.57040E+08	0.00000			
NA3H(SO4)2	0.00000	0.34621E+19	0.00000			
NAHSO4.H2O	0.00000	0.54901E-01	0.00000			
K3H(SO4)2	0.00000	0.27296	0.00000			
K5H3(SO4)4	0.00000	0.83614E-05	0.00000			
K8H6(SO4)7.H2O	0.00000	0.73339E-05	0.00000			
KHSO4	0.00000	34.130	0.00000			
MGSO4.H2O	0.00000	0.27513E-01	0.00000			
FESO4.7H2O	0.00000	0.90152	0.00000			
FESO4.H2O	0.00000	0.27607E-01	0.00000			

FECL2.6H2O	0.00000	0.31684E+14	0.00000
FECL2.4H2O	0.00000	33.212	0.00000
FECO3	0.00000	0.44473E-11	0.00000
FE(OH)3	0.00000	14.496	0.00000
CO2.6H2O	0.00000	26467.	0.00000
CH4.6H2O	0.00000	0.26990E+10	0.00000
FECL3.10H2O	0.00000	0.49839E+08	0.00000
FECL3.6H2O	0.00000	0.15525E+15	0.00000
FECL3.2KCL.H2O	0.00000	0.33308E+14	0.00000
FE2(SO4)3	0.00000	0.59318E-08	0.00000
FE2(SO4)3.2K2SO4.14H	0.00000	0.14132E-13	0.00000
K2SO4.FESO4.6H2O	0.00000	0.10235E-01	0.00000
NA2SO4.FESO4.4H2O	0.00000	0.12041E-02	0.00000
FE2(SO4)3.9H2O	0.00000	0.43489E-05	0.00000
FE2(SO4)3.H2SO4.8H2O	0.00000	0.75491E-05	0.00000
KFE3(SO4)2(OH)6	0.00000	0.23071E-14	0.00000
NAFE3(SO4)2(OH)6	0.00000	0.10457E-09	0.00000
H3OFE3(SO4)2(OH)6	0.00000	0.36714E-12	0.00000
a-FE2O3	0.00000	0.23398E-03	0.00000
a-FEO(OH)	0.00000	0.28142E-01	0.00000
g-FEO(OH)	0.00000	0.73251	0.00000
FEO(OH)3/4(SO4)1/8	0.00000	0.12651	0.00000
FESO4.4H2O	0.00000	0.49879E-01	0.00000
FE2(SO4)3.7H2O	0.00000	0.10020E-05	0.00000
FE(II)FE(III)4(SO4)6	0.00000	0.41390E-29	0.00000
FE(III)5(SO4)6O(OH).	0.00000	0.88087E-30	0.00000
FE(II)FE(III)2(SO4)4	0.00000	0.40833E-16	0.00000
FE(II)FE(III)2(SO4)4	0.00000	0.27235E-14	0.00000
K2FE(II)5FE(III)4(SO	0.00000	0.00000	0.00000
ALCL3.6H2O	0.00000	0.60068E+10	0.00000
AL2(SO4)3.17H2O	0.00000	0.26102E-07	0.00000
NABR	0.00000	0.00000	0.00000
MGBR2	0.00000	0.00000	0.00000
AL(OH)3	0.00000	95889.	0.00000
SIO2(QUARTZ)	0.00000	0.10000E+21	0.00000
SIO2(AMORPHOUS)	0.61817E-02	0.65436E-02	0.61817E-02
KAL3(SO4)2(OH)6	0.00000	0.72115E-06	0.00000
NAAL3(SO4)2(OH)6	0.00000	0.81601E-04	0.00000
KAL(SO4)2.12H2O	0.00000	0.12427E-03	0.00000
NAAL(SO4)2.12H2O	0.00000	0.24969E-03	0.00000
FESO4.AL2(SO4)3.22H2	0.00000	0.27653E-08	0.00000
AL2SI2O5(OH)4	0.00000	17.837	0.00000
MGSO4.AL2(SO4).22H2O	0.00000	0.96704E-08	0.00000
NACLO4.H2O	0.00000	389.08	0.00000
MG(CLO4)2.8H2O	0.00000	9971.6	0.00000
CA(CLO4)2.6H2O	0.00000	0.10397E+06	0.00000
KCLO4	0.00000	0.28528	0.00000
MG(CLO4)2.6H2O	0.00000	0.11977E+07	0.00000
NACLO4.2H2O	0.00000	3416.2	0.00000
NACLO4	0.00000	1284.0	0.00000
NA2CO3.H2O	0.00000	1.5238	0.00000

pH= 8.45000 pHF= 8.12833 pHT= 8.11805 pH(SWS)= 8.11805
pHMacinnis = 9.45481 Temp. = 355.150

CONVERGENCE CRITERION = 0.100000 %
Iterations = 4