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THE PROCHEM SYSTEM FOR MODELING AQUEOUS SYSTEMS
AND ITS APPLICATION TO GEOTHERMAL WELLS

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ABSTRACT

The purpose of this paper is to describe the ProChem Software for modeling and simulation of aqueous based systems and its application to problems involving geothermal wells. The paper describes the system architecture, underlying thermodynamic formulations, mathematical framework and user interface to ProChem. ProChem has been developed over a 16 year period and accurately predicts the chemistry of involved chemical systems of industrial import. Applicability to problems of industrial significance is highlighted with a practical problem concerning modeling of a geothermal well.

INTRODUCTION

The ProChem System is a comprehensive set of computer programs which allow a user to model and simulate aqueous based systems. As such, ProChem is broadly applicable to problems concerning geothermal wells. ProChem is composed of an integrated set of components as follows:

- 1) ElectroChem - Simulation of the phase separation and intraphase speciation for single-stage, steady-state processes. In addition to interphase and intraphase equilibria, ElectroChem can optionally consider reaction kinetics and/or ion exchange phenomena.
- 2) FraChem - Simulation of multistage, steady-state processes involving an aqueous liquid phase.
- 3) TransChem - Simulation of aqueous chemistry over time and space.
- 4) FlowChem - Generalized interface to allow ElectroChem and FraChem to be readily accessible to higher level calling programs. The customary application is to interface with a Flowsheet Simulator.

- 5) DataChem - The ProChem Public Databank, which allows for modeling of a wide range of chemistries, plus utility programs which allow for routine creation of Private Databanks for chemistry not covered by the Public Databank.
- 6) FitChem - Nonlinear regression of ProChem thermodynamic coefficients to fit user provided experimental data.

ProChem simulates aqueous based systems by solving mathematical models which accurately represent these systems. These models are sets of nonlinear algebraic equations containing appropriate thermodynamic parameters. ProChem is thus built upon a thermodynamic framework for aqueous systems. This framework is an amalgam based upon work by Bromley(1), Meissner(2,3), Pitzer(4,5) and Zemaitis(6) among others. Through careful empirical extensions of activity coefficient formulations along with estimation and extrapolation techniques, ProChem is generally applicable over the range 0-300°C, 0-200 atmospheres and 0-30+ ionic strength.

ProChem is applicable to a wide range of problems of industrial interest including, but not limited to:

- 1) Scale prediction in oil wells and geothermal wells
- 2) Study of the chemistry of underground injection wells
- 3) Removal of industrial pollutants from process streams (e.g., incinerator off-gas)
- 4) Gas treating involving sour water and/or amines
- 5) Pollutants in waste water
- 6) Ion exchange chromatography

In order to properly describe ProChem, the material below will address:

- 1) System Overview
- 2) Mathematical Model
- 3) Thermodynamic Framework
- 4) Typical Application
- 5) Conclusions
- 6) References

SYSTEM OVERVIEW

The ProChem System predicts the phase separation and intraphase speciation in chemical systems. ProChem can consider the following chemical phases:

- 1) Aqueous liquid phase
- 2) Vapor phase (optional)
- 3) Organic liquid phase (optional)
- 4) One or more solid phases (optional)
- 5) Solid exchange media phase (optional)

Phenomenologically, ProChem can simultaneously deal with:

- 1) Interphase equilibria
- 2) Intra-aqueous phase equilibria
- 3) Reaction kinetics
- 4) Ion exchange

Architecturally, ProChem is structured as shown in Figure 1. As depicted, the user of ProChem must prepare two simple input files:

- 1) A description of the chemistry to be considered (Model Definition Input File)
- 2) A description of the conditions at which the phase separation and speciation is to be predicted (Case Definition Input File)

ProChem then accesses the ProChem Public Databank and, if applicable, any Private Databank prepared by the user and extracts the thermodynamic information required by the particular chemistry described in the Model Definition Input File. ProChem then writes a single FORTRAN file and a single data file which contain the required model equations and thermodynamic data, respectively. At this point, the user has the generated model, for the particular chemistry described, available for execution of cases whenever desired. The Case Definition Input File provides the specific details on the particular case. Depending upon the options

chosen in the Model Definition Input File, the Case Definition Input File can apply to one of the solvers: ElectroChem, FraChem, or TransChem.

Inasmuch as the aforementioned ProChem simulation blocks: ElectroChem, TransChem and FraChem, are based upon the solution of a set of nonlinear algebraic equations the user is given the option of:

- 1) Solving many alternative kinds of problems by "switching the roles of variables". Specifically:
 - a) ElectroChem performs, as its standard, an isothermal calculation wherein temperature, pressure and inflows are fixed by the user. However, the user can readily "free" one or more of these normally fixed variables given and "fix" a corresponding number of normally calculated variables. An example would be fixing pH and freeing a particular inflow component to which the pH is sensitive.
 - b) FraChem performs, as its standard, a calculation wherein all feed conditions, sidedraw rates and exchanger duties are fixed by the user, while all product and internal streams are calculated. As an alternative, however, the user can fix specific aspects of any product stream or internal stream (e.g., ppm of a particular component) and free one of the normally fixed variables (e.g., reboiler duty).
- 2) Producing a gain matrix. In such cases, ElectroChem provides the sensitivity of the calculated variables to incremental changes in any user provided fixed variable. These "process sensitivities" can be very useful in making decisions on process adjustments and/or optimization.

MATHEMATICAL MODEL

The mathematical model employed in ProChem is a deterministic set of nonlinear algebraic equations.

The equation set is composed of:

- 1) Equilibrium K-equations

For each vapor-liquid, solid-liquid and liquid intraphase equilibrium there is an equation of the form:

$$K = \frac{\pi_{iP} (\gamma_{iP})^{n_{iP}} (m_{iP})^{n_{iP}}}{\pi_{iR} (\gamma_{iR})^{n_{iR}} (m_{iP})^{n_{iR}}} \quad (1)$$

where,

K = The thermodynamic equilibrium constant; a function of temperature and pressure

γ_{iP}, γ_{iR} = activity coefficient or, for vapors, fugacity coefficient of the i^{th} product and reactant, respectively; a function of temperature, pressure and composition.

n_{iP}, n_{iR} = stoichiometric coefficient of the i^{th} product and reactant, respectively.

m_{iP}, m_{iR} = molality or, for vapors, partial pressure of i^{th} product and reactant respectively

2) An electroneutrality equation

$$\sum_{i=1}^{NC} |z_i| m_i = \sum_{i=1}^{NA} |z_i| m_i \quad (2)$$

where,

z_i = species charge

NC, NA = number of cations and anions respectively

3) Equations for solutions involving a second liquid phase, (liquid-liquid equilibrium):

$$a_i^A = a_i^O \quad i=1, NM \quad (3)$$

where,

a_i = activity of species

A, O = represent aqueous and organic phases respectively

NM = number of molecular species distributing between phases

4) The required number of material balances, NB, to complete the model and to assure that the number of equations and number of unknowns are equal. Normally these balances include an overall, a vapor phase, an organic phase and several component balances.

Thus, assuming NK equilibrium equations, the model has NK+NB+NM+1 equations. The customary unknowns are:

- 1) The liquid phase H₂O rate plus all ionic and molecular species molalities
- 2) The vapor phase composition; species mole fractions plus overall vapor rate
- 3) The organic phase composition; species mole fractions plus overall organic phase rate

As noted above, the number of NB equations required is that number which assures that the number of equations equals the overall number of unknowns. This is a natural consequence of the phase rule.

To better understand this modeling concept, consider the aqueous based system represented by H₂O-CO₂-NaCl. The reactions considered will be:



Based upon the general model described earlier, this leads to:

1) Equilibrium K-equations

$$KH_2OVAP = \frac{a_{H_2O AQ}}{f_{H_2OVAP} P_{H_2OVAP}} \quad (10)$$

$$KCO_2VAP = \frac{\gamma_{CO_2 AQ} m_{CO_2 AQ}}{f_{CO_2VAP} P_{CO_2VAP}} \quad (11)$$

$$KH_2O AQ = \frac{\gamma_{H^+ ION} m_{H^+ ION} \gamma_{OH^- ION} m_{OH^- ION}}{a_{H_2O AQ}} \quad (12)$$

$$KCO_2 AQ = \frac{\gamma_{H^+ ION} m_{H^+ ION} \gamma_{HCO_3^- ION} m_{HCO_3^- ION}}{CO_2 AQ m_{CO_2 AQ} a_{H_2O AQ}} \quad (13)$$

$$KHCO_3^- ION = \frac{\gamma_{H^+ ION} m_{H^+ ION} \gamma_{CO_3^{2-} ION} m_{CO_3^{2-} ION}}{HCO_3^- ION m_{HCO_3^- ION}} \quad (14)$$

$$KNaCl PPT = \gamma_{Na^+ ION} m_{Na^+ ION} \gamma_{Cl^- ION} m_{Cl^- ION} \quad (15)$$

It is worth noting that all solid phase activities are assumed to be one and that the solvent, water, must be represented by its activity not by activity coefficient times molality.

2) Electroneutrality equation

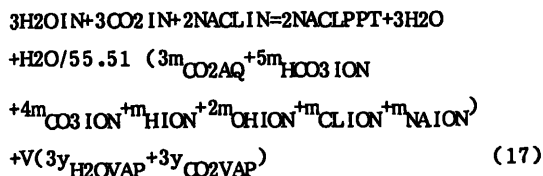
$$H^+ ION + Na^+ ION = HCO_3^- ION + 2CO_3^{2-} ION + OH^- ION + Cl^- ION \quad (16)$$

3) Liquid-liquid equilibrium equations

There are none in this example.

4) Material balance equations

a) Overall material balance:



b) Vapor balance:

$$y_{\text{H}_2\text{OVAP}} + y_{\text{CO}_2\text{VAP}} = 1 \quad (18)$$

c) Sodium balance

$$\text{NaClIN} = \text{H}_2\text{O}/55.51 (m_{\text{NAION}}) + \text{NaClPPT} \quad (19)$$

d) Chlorine balance

$$\text{NaClIN} = \text{H}_2\text{O}/55.51 (m_{\text{CLION}}) + \text{NaClPPT} \quad (20)$$

e) Carbon balance

$$\begin{aligned}
 \text{CO}_2\text{IN} = \text{H}_2\text{O}/55.51 (m_{\text{CO}_3\text{ION}} + m_{\text{HCO}_3\text{ION}} + m_{\text{CO}_2\text{AQ}}) \\
 + V(y_{\text{CO}_2\text{VAP}}) & \quad (21)
 \end{aligned}$$

Equations (10)-(21) are the required 12 equations. Assuming temperature and pressure are known and further assuming that deterministic formulations are available for the K-values, activity and fugacity coefficients, the corresponding 12 unknowns (calculated variables) are:

$$\begin{aligned}
 V, y_{\text{H}_2\text{OVAP}}, y_{\text{CO}_2\text{VAP}}, \text{H}_2\text{O}, m_{\text{HION}}, m_{\text{OHION}}, m_{\text{CO}_3\text{ION}}, \\
 m_{\text{HCO}_3\text{ION}}, m_{\text{NAION}}, m_{\text{CLION}}, m_{\text{CO}_2\text{AQ}}, \text{NaClPPT}
 \end{aligned}$$

THERMODYNAMIC FRAMEWORK

The mathematical model described above utilizes several thermodynamic quantities. Specifically, these are:

- 1) K-values - Normally strong functions of temperature and weaker functions of pressure
- 2) Liquid phase activity coefficients - Normally strong functions of temperature and composition and a weaker function of pressure
- 3) Vapor phase fugacity coefficients - Normally significant functions of temperature, pressure and composition particularly at elevated pressures.

ProChem provides formulations for each of these as follows.

K-values

By considering basic thermodynamic relationships and assuming a constant heat capacity of reaction, the general equation:

$$\ln K(T) = - \frac{\Delta G_{\text{RXN}}^{\circ}}{RT^{\circ}} - \frac{\Delta H_{\text{RXN}}^{\circ}}{R} \left(\frac{1}{T} - \frac{1}{T^{\circ}} \right) - \frac{\Delta C_{p,\text{RXN}}^{\circ}}{R} \left[\ln \frac{T^{\circ}}{T} - \frac{T^{\circ}}{T} + 1 \right] \quad (22)$$

can be derived, where,

T = temperature in Kelvins

T[°] = temperature of the standard state; normally 298.15

$\Delta G_{\text{RXN}}^{\circ}$ = free energy of reaction at the standard state. This is formed by taking the difference of the contributions of the free energies of the products and the reactants.

$\Delta H_{\text{RXN}}^{\circ}$ = corresponding heat of reaction at the standard state

$\Delta C_{p,\text{RXN}}^{\circ}$ = corresponding heat capacity of reaction at the standard state

R = Gas Constant

The derivation of this relationship can be found in the Handbook of Aqueous Electrolyte Thermodynamics (7). Values for constituent G[°], H[°] and Cp[°] are usually available in the excellent compilations of the NBS (8) or the Russian Academy of Sciences (9).

Liquid Phase Activities and Activity Coefficients

The key to successful simulation of aqueous systems is to accurately predict:

- 1) Activity coefficients of ions in solution
- 2) Activity coefficients of molecules in solution
- 3) Activity of water

In ProChem, these quantities can be represented in terms of a number of alternative as well as complementary formulations. The common element of all these formulations is that they involve the interaction of pairs of species in solution. A general assumption is made that:

- 1) Interactions between like charged ions are not significant.
- 2) Higher level interactions (involving more than two species) are not significant

Ions: For ions the formulation used is:

$$\log_{10} \gamma_i = \text{DH}_i + \text{BZ}_i + \text{P}_i \quad (23)$$

where,

DH_i = The Debye-Huckel term defined as

$$DH_i = \frac{-A |z_i|^2 I^{1/2}}{1 + I^{1/2}} \quad (24)$$

where,

A = The Debye-Huckel constant; a known function of T , the temperature

$$I = \text{Ionic Strength} = 1/2 \sum_i z_i^2 m_i$$

The Debye-Huckel term predicts the long-range or electrostatic effects. For dilute solutions of ionic strength less than 0.1 this term is all that is needed.

BZ_i = The Bromley-Zemaitis term for ion-ion interactions defined as:

$$BZ_i = \sum_{j=1}^{NO} \left(\frac{|z_i| + |z_j|}{2} \right)^2 \beta_{ij} m_j \quad (25)$$

$$\beta_{ij} = \frac{(0.06 + 0.6 B_{ij}) |z_i z_j|}{(1 + 1.5 |z_i z_j| I)^2} + B_{ij} + C_{ij} I + D_{ij} I^2 \quad (26)$$

where,

NO = The number of ions with charge opposite to that of the ion being represented

B_{ij} , C_{ij} , D_{ij} - The three interaction coefficients, for each cation:anion interaction. These are each made 3 parameter functions of temperature. Thus, for each cation:anion interaction there are 9 coefficients that must be established.

P_i = The Pitzer term for ion-molecule interactions, defined as:

$$P_i = \sum_{j=1}^{NM} BP_{ij} m_j + \frac{z_i^2}{4I^2} BPS_j \quad (27)$$

$$BP_{ij} = \beta_{ij}^{(0)} + \beta_{ij}^{(1)} (1+2I^{1/2}) \frac{(1-\exp(-2I^{1/2}))}{2I} \quad (28)$$

$$BPS_j = 0.86859 m_j \sum_{k=1}^{NS} BPP_{jk} m_k \quad (29)$$

$$BPP_{jk} = \beta_{jk}^{(1)} [1 - (1+2I^{1/2} + 2I) \exp(-2I^{1/2})] \quad (30)$$

where,

NM = The number of molecular species in solution

NS = The number of species in solution

$\beta_{ij}^{(0)}$, $\beta_{ij}^{(1)}$ = The two interaction coefficients, for each ion:molecule and molecule:molecule interaction. Each of these is made a 3 parameter function of temperature. Thus, for each interaction there are 6 coefficients that must be established.

Molecules other than Water: For molecules other than water, the preferred formulation is the Pitzer. The formulation is

$$\log_e \gamma_i = 2 \sum_{j=1}^{NS} BP_{ij} m_j \quad (31)$$

Water activity: The water activity for multicomponent systems is an integrated form of the Gibbs-Duhem equation with a mixing rule suggested by Meissner and Kusik. The formulation can be represented as:

$$\log_e a_{H_2O} = \frac{1}{\sum_{i=1}^{NC} z_i^2 m_i + \sum_{i=1}^{NA} z_i^2 m_i} \left[\sum_{i=1}^{NC} z_i^2 m_i \sum_{j=1}^{NM} |z_i z_j| \beta_{ij} m_i m_j - 0.01801 \sum_{i=1}^{NM} [m_i + 2 \sum_{j=1}^{NS} BPW_{ij} m_i m_j] \right]$$

$$BPW_{ij} = \beta_{ij}^{(0)} + \beta_{ij}^{(1)} \exp(-2I^{1/2})$$

The above formulations are, in cases where the requisite interaction coefficients have been fit to cover the conditions being simulated, quite adequate for predicting systems in which water is the principal solvent. In cases involving additional, organic, solvents, an NRTL formulation can be included to cover organic molecule:aqueous species interactions.

Vapor phase fugacity coefficients

Three alternative methods are provided:

- 1) Ideal, all fugacity coefficients are assumed to be 1.0
- 2) Nothnagel (10) method, generally valid up to 20 atmospheres
- 3) Nakamura (11) method, generally valid up to 200 atmospheres

TYPICAL APPLICATION

ProChem delivers to the user an extremely simple interface for problem solving. Specifically, the user presents to ProChem two input files:

- 1) Model Definition Input File - A simple description of the chemistry to be considered
- 2) Case Definition Input File - A simple specification of the case to be executed

As a practical illustration consider a common problem in modeling geothermal wells. EDTA is being used as an agent for preventing scale formation. In the example shown the chemistry is initially being studied to determine the likely scales.

Figure 2 illustrates the Model Definition File in which the user describes the molecular inflows, the product species names and the equilibrium equations. Figure 3 illustrates the case being simulated.

ProChem, behind the scenes, creates the required FORTRAN and Thermo Data files to solve the highly nonlinear model described earlier. The user need not be involved in this. Figure 4 illustrates the output report. For the case shown we see a summary of the solids formed, scaling tendencies and a full detailed speciation summary.

From results like this reasonable decisions can be made concerning the economics of using caustic to resolve this problem.

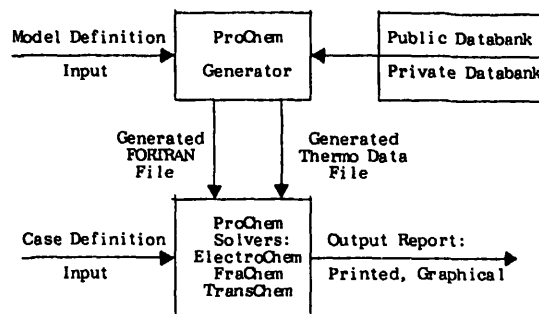
CONCLUSIONS

The OLI ProChem System is a broad based simulation system applicable to a wide spectrum of problems involving aqueous chemistry including modeling of geothermal wells. A Public Databank which can be supplemented by user provided Private Databanks covers a range of conditions which allows application of ProChem to most problems of industrial importance. A sophisticated program generator allows highly involved problems to be addressed based upon a simple user statement of the problem.

ProChem is applicable to systems involving several phenomena; namely equilibrium, ion exchange and reaction kinetics. ProChem's utility is particularly enhanced by its applicability to single-stage steady state and multistage steady state, as well as time/space varying systems. An additional flexibility is the ease with which the single and multistage steady-state components can interface with higher level calling programs.

References

- (1) L.A. Bromley, "Thermodynamic properties of strong electrolytes in aqueous solutions", *AIChE J*, 19:313-320 (1973)
- (2) H.P. Meissner, C.L. Kusik, "Aqueous solutions of two or more strong electrolytes - vapor pressures and solubilities", *IEC Proc. Des. Dev.*, 12:205-208 (1973)
- (3) H.P. Meissner, N.A. Peppas, "Activity coefficients - aqueous solutions of polybasic acids and their salts", *AIChE J*, 19:806-809 (1973)
- (4) K.S. Pitzer, "Theory: ion interaction approach", Activity Coefficients in Electrolyte Solutions, 1:157-208, R.M. Pytkowicz, ed., CRC Press, Boca Raton, FL (1979)
- (5) K.S. Pitzer; "Thermodynamics of aqueous electrolytes at various temperatures, pressures and compositions", Thermodynamics of Aqueous Systems with Industrial Applications, 451-466, S.A. Newman, ed., ACS Symposium Series 133 (1980)
- (6) J.F. Zemaitis, Jr., "Predicting vapor-liquid-solid equilibria in multicomponent aqueous solutions of electrolytes", Thermodynamics of Aqueous Systems with Industrial Applications, 227-246, S.A. Newman, ed., ACS Symposium Series 133 (1980)
- (7) J.F. Zemaitis, Jr., D.M. Clark, M. Rafal, N.C. Scrivner, Handbook of Aqueous Electrolyte Thermodynamics, *AIChE* (1986)
- (8) D.D. Wagman et. al., "Selected values of chemical thermodynamic properties", NBS Tech Note 270-3 to 8, (1968-1973)
- (9) V.P. Glushko, editor, "Thermal constants of compounds", Russian Academy of Sciences, vols. I-X (1965-1981)
- (10) K.H. Nothnagel, D.S. Abrams, J.M. Prausnitz, "Generalized correlation of fugacity coefficients in mixtures at moderate pressures", *IEC Process Des. Dev.*, 12:25-35 (1973)
- (11) R. Nakamura, G.J.F. Breedveld, J.M. Prausnitz, "Thermodynamic properties of gas mixtures containing polar and nonpolar components", *IEC Process Des. Dev.*, 15:557-564 (1976)

Figure 1
ProChem StructureFigure 2
Chemistry Model Definition Input File

```

ECES DISK TERM
COM *** INFLOWS ***
INPUT
H2OIN
CO2IN
NH3IN
H2SIN
BACL2IN
CACL2IN
CUCL2IN
FEIICL2IN
FEIICL3IN
KCLIN
LICLIN
MGCL2IN
MNCL2IN
NACLIN
NA2SIN
NA2SO3IN
NA2SO4IN
PBCL2IN
SIO2IN
SRCL2IN
ZNCL2IN
NA4EDTAIN
CA2EDTAIN
CASIO3IN
CA2SIO4IN
BOH3IN
COM **** SPECIES ****
SPECIES
COM VAPOR (VAPS)
H2OVAP
CO2VAP
NH3VAP
H2SVAP
COM AQUEOUS MOLECULES (AQS)
CO2AQ
NH3AQ
H2SAQ
CASO4AQ
H4SIO4AQ
NA4EDTAAQ
CA2EDTAAQ
BOH3AQ
COM CATIONS
HION
NH4ION
BAION
BAOHION
CAION
CARCO3ION
CAOHION
CUION
FEIION
FEIHC03ION
FEIIOHION
FEIIOHION
KION
LIION
MGION
MGCLION
MGHC03ION
MNION
MNHCO3ION
MNOHION
NAION
PBION
SRION
ZNION
ZNHCO3ION
COM ANIONS
OHION
HCO3ION
CO3ION
NH2CO2ION
HSION
SION
CLION
NASO4ION
H3SIO4ION
HSO3ION
SO3ION
HSO4ION
SO4ION
EDTAION
BOH3OHION
COM PRECIPITATES AND HYDRATES
BACO3PPT
BASO4PPT
CACO3PPT
CASO3PPT
CASO4.2H2O
CUPES2PPT
FEIISIO3PPT
FE3O4PPT
MGCO3PPT
NH42SO4PPT
NH42SO3PPT
SIO2PPT
SRCO3PPT
SRSO4PPT
CASIO3PPT
CA2SIO4PPT
COM *** EQUILIBRIUM EQUATIONS ***
EQUILIBRIUM
COM
H2OVAP=H2O
CO2VAP=CO2AQ
NH3VAP=NH3AQ
H2SVAP=H2SAQ
COM
H2O=HION+OHION
CO2AQ+H2O=HION+HCO3ION
NH3AQ+H2O=NH4ION+OHION
H2SAQ=HION+HSION
CASO4AQ=CAION+SO4ION
H4SIO4AQ=HION+H3SIO4ION
NA4EDTAAQ=4NAION+EDTAION
CA2EDTAAQ=2CAION+EDTAION
BOH3AQ+H2O=BOH3OHION+HION
COM
HCO3ION=HION+CO3ION
NH2CO2ION+H2O=NH3AQ+HCO3ION
HSION=HION+SION
BAOHION=BAION+OHION
CAHCO3ION=CAION+HCO3ION
CAOHION=CAION+OHION
FEIHC03ION=FEIION+HCO3ION
FEIIOHION=FEIION+OHION
HSO3ION=HION+SO3ION
HSO4ION=HION+SO4ION
MGCLION=MGION+CLION
MGHC03ION=MGION+HCO3ION
MNHCO3ION=MNION+HCO3ION
MNOHION=MNION+OHION
NASO4ION=NAION+SO4ION
ZNHCO3ION=ZNION+HCO3ION
COM
BACO3PPT=BAION+CO3ION
BASO4PPT=BAION+SO4ION
CACO3PPT=CAION+CO3ION
CASO3PPT=CAION+SO3ION
CASO4.2H2O=CAION+SO4ION+2H2O
CUPES2PPT=CUION+FEIION+2SION
OX FEIISIO3PPT+H2O+HION=FEIION+H3SIO4ION
OX FE3O4PPT+8HION=FEIION+2FEIIOHION+4H2O
MGCO3PPT=MGION+CO3ION
NH42SO3PPT=2NH4ION+SO3ION
NH42SO4PPT=2NH4ION+SO4ION
OX SIO2PPT+2H2O=H4SIO4AQ
SRCO3PPT=SRION+CO3ION
SRSO4PPT=SRION+SO4ION
OX CASIO3PPT+H2O+HION=CAION+H3SIO4ION
OX CA2SIO4PPT+2H2O=SIO2PPT+2CAION+4OHION
END
  
```


Figure 3
Case Execution Input File

```

ECES DISK TERM
UNITIN FAHR PSIA LBS BTUS HOURS
UNITOUT FAHR PSIA LBS BTUS HOURS
COM
COM HIGH PRESSURE, SUBSURFACE EQUILIBRIUM TO DETERMINE ENTHALPY
COM
PHGUESS 6.0
TEMPERATURE 550
PRESSURE 1400
COM
COM INFLOWS IN POUNDS/HR
COM
H2OIN 2201500
CO2IN 5700
NH3IN 1400
H2SIN 60
NA2SO3IN 170
SIO2IN 1170
BACL2IN 900
CUCL2IN 250
FEIICL2IN 6500
LICLIN 3500
HNCL2IN 6500
PBCL2IN 300
SRCL2IN 2000
ZNCL2IN 2400
CACL2IN 173000
KCLIN 64000
NACLIN 380000
NA2SO4IN 400
NA2SIN 250
FEIICL3IN 0
MGCL2IN 0
NA4EDTAIN 0
CA2EDTAIN 0
BOH3IN 0
CASIO3IN 1
CA2SIO4IN 1
END
    
```

OLI ELECTROCHEM.....VERSION 5.0 (1 FEB 1987)

ELECTROCHEM SUMMARY OF RESULTS

SPECIES NAME	INFLOWS POUNDS/HR	VAPOR POUNDS/HR	LIQUID POUNDS/HR	MOLALITY	SOLID POUNDS/HR
H2O	2.2015E+06		2.2006E+06		
BOH3					
CA2EDTA					
CO2	5.7000E+03		4.7515E+03	4.9061E-02	
H2S	6.0000E+01		4.2407E+01	5.6546E-04	
NA4EDTA					
NH3	1.4000E+03		2.8929E+01	7.7187E-04	
BACL2	9.0000E+02				
CA2SIO4	1.0000E+00				
CACL2	1.7300E+05				
CASIO3	1.0000E+00				
CUCL2	2.5000E+02				
FEIICL2	6.5000E+03				
FEIICL3					
KCL	6.4000E+04				
LICL	3.5000E+03				
MGCL2					
HNCL2	6.5000E+03				
NA2S	2.5000E+02				
NA2SO3	1.7000E+02				
NA2SO4	4.0000E+02				
NACL	3.8000E+05				
PBCL2	3.0000E+02				
SIO2	1.1700E+03				
SRCL2	2.0000E+03				
ZNCL2	2.4000E+03				
H4SIO4			2.9299E-01	1.3852E-06	
CASO4			4.8432E+01	1.6166E-04	
BACO3PPT					
BASO4PPT					4.3531E-02
CACO3PPT					1.2237E-03
CASO3PPT					1.5953E-02
CUFES2PPT					3.4128E-02
FE3O4PPT					
FEIISIO3PPT					2.5705E+03
HCCO3PPT					
NH42SO3PPT					
NH42SO4PPT					
SRCO3PPT					
SRSO4PPT					
CASO4.2H2O					
BAION			3.3739E+02	1.1163E-03	
BAOHION			8.1239E-03	2.3918E-08	
BOH3OHION					
CAHCO3ION			6.5702E+02	2.9532E-03	
CAION			6.1655E+04	6.9904E-01	
CAOHION			4.2574E-01	3.3890E-06	
CLION			3.8436E+05	4.9265E-00	
CO3ION			3.9514E-09	2.9922E-14	
CUION			2.4260E-14	1.7350E-19	
EDTAION					
FEIHC3ION			2.8452E+02	1.1064E-03	
FEIION			1.1330E+03	9.2190E-03	
FEIIOHION			5.2578E+02	3.2795E-03	
H3SIO4ION			2.2199E-04	1.0607E-09	
HCO3ION			9.5249E-01	7.0936E-06	
HION			8.7656E-02	3.9517E-05	
HSION			2.2173E-02	3.0467E-07	
HSO3ION			1.6946E+00	9.4988E-06	
HSO4ION			3.7379E+01	1.7498E-04	
KION			3.3566E+04	3.9009E-01	
LIION			5.7304E+02	3.7516E-02	
MGCLION					
MGHC3ION					
MGION					
MNHCO3ION			2.9956E+01	1.1739E-04	
MNION			2.8216E+03	2.3339E-02	
MNOHION			2.5392E+00	1.6038E-05	
NAION			1.4982E+05	2.9613E-00	
NASO4ION			1.8616E+01	7.1059E-05	
NH2CO2ION			1.6513E-04	1.2500E-09	
NH4ION			1.4522E+03	3.6583E-02	
OHION			5.0432E-03	1.3475E-07	
PBION			2.2351E+02	4.9021E-04	
SION			6.2074E-06	8.7973E-11	
SO3ION			1.6411E-07	9.3144E-13	
SO4ION			5.1701E+00	2.4457E-05	
SRION			1.1054E+03	5.7329E-03	
ZNHCO3ION			1.6768E+01	5.3894E-05	
ZNION			1.1435E+03	7.9488E-03	
TOTALS	2.8500E+06	0.0000E+00	2.8453E+06		4.7304E+03

Figure 4
Case Execution Output File

PRECIPITATE INCLUSION ANALYSIS

SCALE TEND = TENDENCY FOR PRECIPITATE TO FORM
(SCALE TEND > 1 FOR DRIVING FORCE TO PRECIPITATE)

SPECIES	VALUE	SCALE TEND	STATUS
BACO3PPT		4.01203E-03	EXCLUDED
BASO4PPT	845.99		INCLUDED
CACO3PPT	5545.7		INCLUDED
CASO3PPT	602.31		INCLUDED
CASO4.2H2O		2.96465E-02	EXCLUDED
CUFES2PPT	843.42		INCLUDED
FEIISIO3PPT	8837.6		INCLUDED
FE3O4PPT		0.00000E+00	EXCLUDED
HCCO3PPT		0.00000E+00	EXCLUDED
NH42SO3PPT		1.36320E-18	EXCLUDED
NH42SO4PPT		3.44574E-22	EXCLUDED
SIO2PPT		6.23871E-04	EXCLUDED
SRCO3PPT		6.48450E-04	EXCLUDED
SRSO4PPT		1.32489E-02	EXCLUDED
CASIO3PPT		5.75649E-04	EXCLUDED
CA2SIO4PPT		7.22636E-06	EXCLUDED