WPO 38628 (PKG)
WPO 46124

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date: 21 April 1997

to: R. Vann Bynum, Org. 6831, MS 1320

Craig F Novak

from: Craig F. Novak, Org. 6832, MS 1341

subject: Calculation of Actinide Solubilities in WIPP SPC and ERDA6 Brines under MgO Backfill Scenarios containing either Nesquehonite or Hydromagnesite as the Mg-CO_3 Solubility-limiting Phase

Actinide solubility calculations for the WIPP Compliance Certification Application (CCA) were performed assuming that standardized WIPP brines were saturated with halite, anhydrite, brucite, and magnesite (Novak et al., 1996b). Brucite, $Mg(OH)_2$(s), and magnesite, $MgCO_3$(s), were modeled to be present because of brine interactions with the backfill material MgO(s). Ongoing laboratory experiments have suggested that nesquehonite, $MgCO_3 \cdot 3H_2O$(s), or hydromagnesite, $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$(s) or $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$(s) may form instead of magnesite under WIPP-like conditions, at least at early times. This memorandum provides estimated total actinide solubilities by oxidation state when either hydromagnesite or nesquehonite precipitates instead of magnesite.

The calculations in this memorandum repeat the CCA calculations with two exceptions: a revised thermodynamic data base called FMT_970407.CHEMDAT was used, and either hydromagnesite or nesquehonite was precipitated instead of magnesite. In order to have hydromagnesite precipitate, several nonactinide solid phases in the data base were prevented from forming, including dolomite, $CaMg(CO_3)_2$(s), magnesite, calcite and aragonite, both $CaCO_3$(s), pirssonite, $Na_2Ca(CO_3)_2 \cdot 2H_2O$(s), and gaylussite, $CaNa_2(CO_3)_2 \cdot 5H_2O$(s). In order to have nesquehonite precipitate, the solids hydromagnesite and labile salt, $Na_4Ca(SO_4)_3 \cdot 2H_2O$(s), must be prevented from forming, in addition to the solids in the list above. Note that this does not necessarily imply that the equilibrium conditions are supersaturated with respect to these solids, only that the

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mathematical path followed to reach equilibrium conditions could not allow the precipitation of these minerals.

No constraints were placed on the actinide solid phases that could form; equilibrium principles were used to determine the thermodynamically most stable solid phase for each actinide.

Thermodynamic Data Base Files

The primary data base release accompanying this memo is called FMT_970407.CHEMDAT. The CHEMDAT files used for the calculations, based on this file, are called FMT_970407_NESQ.CHEMDAT, FMT_970407_HMAG4323.CHEMDAT, and FMT_970407_HMAG5424.CHEMDAT. These files are contained with these names under SCMS on the WIPP DEC Alpha computers. Changes made to arrive at the FMT_970407.CHEMDAT file are documented below. Information that has not changed since the last major release of the data base file, called FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT (Novak, 1996a), is not discussed here.

The FMT_970407.CHEMDAT file contains an update of several Pitzer parameters for the pairs K^+ with $Th(CO_3)_5^{6-}$, Mg^{2+} with $NpO_2CO_3^-$, $NpO_2(CO_3)_2^{3-}$, and $NpO_2(CO_3)_3^{5-}$, Cl^- with $Th(CO_3)_5^{6-}$, and for the triplets Na^+ with Cl^- and $Th(CO_3)_5^{6-}$, and K^+ with Cl^- and $Th(CO_3)_5^{6-}$.

The revised neptunyl carbonato species parameters are based on the averaged values for K^+ (Novak et al., 1996a) and Na^+, and are supported by a comparison with one Np(V) solubility measurement in a high magnesium brine (Novak et al., 1996c). Further documentation of this comparison is given in a document with the title "Solubility of Np(V) in K-Cl-CO_3 and Na-K-Cl-CO_3 Solutions to High Concentration: Measurements and Thermodynamic Model Predictions," currently undergoing Review and Approval at SNL.

The new ion interaction parameters for Cl^- with $Th(CO_3)_5^{6-}$ and for the triplets Na^+ with Cl^- and $Th(CO_3)_5^{6-}$ are based on the values provided to me in an email message from Andrew R. Felmy of Pacific Northwest National Laboratories. Dr. Felmy and coworkers were performing additional solubility measurements for the Th-Cl-CO_3-HCO_3 system until these were suspended due to WIPP Project exigencies. The email message, reproduced in Table 1, serves as documentation for these parameters. K^+ interaction parameters with $Th(CO_3)_5^{6-}$

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were assigned the same numerical values as those for Na^+, by chemical analogy, to provide reasonable estimates.

Finally, two hydromagnesite solids with the stoichiometries $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O(s)$ and $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O(s)$ were added. For convenience, these solids are called HMAG5424 and HMAG4323, respectively. Both stoichiometries have been proposed but neither appears to be definitive. The analysis in the following section was used to determine dimensionless standard chemical potentials for each of the hydromagnesite stoichiometries; both are used in the FMT simulations discussed in this memo.

The differences between `FMT_970407.CHEMDAT` and `FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT` are given in Table 2 by using the VMS "`DIFFERENCES`" command. The resulting file was shortened by removing the matching lines terminating each different block in the comparison files. Line numbers in the list below refer to the line numbers for file `FMT_970407.CHEMDAT` as given in Table 2. The differences include:

- different title lines 1 and 2;
- total number of species increased from 210 to 212 on line 4;
- two additional solids added, lines 254 and 255;
- new $\beta^{(0)}$ and $\beta^{(1)}$ values for K^+ with $Th(CO_3)_5^{6-}$ in line 339;
- new $\beta^{(0)}$, $\beta^{(1)}$, $\beta^{(2)}$, and $C\phi$ values for K^+ with $NpO_2(CO_3)_3^{5-}$ on lines 439 to 441;
- modification from the previous estimated θ value for Cl^- with $Th(CO_3)_5^{6-}$ from 5.5 to 2.0 in line 2409;
- and addition of the ψ value –0.08 for triplet Na^+ with Cl^- and $Th(CO_3)_5^{6-}$ and the triplet K^+ with Cl^- and $Th(CO_3)_5^{6-}$ in line 3270.

The other `CHEMDAT` files differ from this primary file only by which solids are prevented from forming, as summarized in Table 3.

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Solubility Products for Hydromagnesite and Magnesite

The Harvie et al. (1984) data base was chosen as the primary reference for actinide solubility modeling. The data base contains thermodynamic parameters values at 25°C, including solubility product (Ksp) information in the form of standard chemical potentials. Until now we have added to this data base only those species and parameters necessary to describe actinide solubility and speciation behavior. However, the solid phase hydromagnesite is not included in the Harvie et al. (1984) data base, so we must obtain and add information for this solid.

There are two stoichiometries reported for hydromagnesite, $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O(s)$ and $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O(s)$, which we will also refer to as HMAG4323 and HMAG5424, respectively. The solubility products for these solids can be defined by the reactions

$$Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O(s) \leftrightarrow 4\ Mg^{2+} + 3\ CO_3^{2-} + 2\ OH^- + 3\ H_2O \quad (1)$$

$$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O(s) \leftrightarrow 5\ Mg^{2+} + 4\ CO_3^{2-} + 2\ OH^- + 4\ H_2O \quad (2)$$

It is not clear that either stoichiometry has been settled upon definitively. The solubility product of HMAG4323 was reported as $10^{-30.2}$ in Langmuir (1965). This stoichiometry and Ksp were accepted in Lippmann (1973), although Garrels and Christ (1990) provide the value $10^{-35.5}$ for "natural hydromagnesite" with the same stoichiometry. On the other hand, Robie and Hemingway (1973) prefer the HMAG5424 stoichiometry and the Ksp value $10^{-37.1 \pm 0.4}$ in their data compilation.

Because neither stoichiometry can be considered definitive, we have conducted calculations using both stoichiometries. The HMAG4323 Ksp of Langmuir was selected because it gives a higher solubility and thus would lead to higher solution concentrations than the value of Garrels and Christ (1990).

The corresponding dimensionless standard chemical potentials for the two stoichiometries for hydromagnesite can be calculated using standard thermodynamics, Reactions 1 and 2, and the species dimensionless standard chemical potentials taken from the Harvie et al. (1984) data base. These calculations can be summarized as

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$$\frac{\mu^{\circ}_f}{RT}(\text{HMAG4323})$$

$$= \ln(10^{-30.2}) + 4(-183.468) + 3(-212.944) + 2(-63.435) + 3(-95.6635)$$

$$= -1856.103 \qquad (3)$$

for Reaction 1 and as

$$\frac{\mu^{\circ}_f}{RT}(\text{HMAG5424})$$

$$= \ln(10^{-37.1}) + 5(-183.468) + 4(-212.944) + 2(-63.435) + 4(-95.6635)$$

$$= -2364.066 \qquad (4)$$

for Reaction 2. Because of the use of a different round off scheme in earlier calculations, the dimensionless chemical potentials for HMAG4323 and HMAG5424 were entered into FMT_970407.CHEMDAT as –1856.104 and –2364.06, respectively.

Input and Output Files for FMT v2.2 Simulation Runs

Six different FMT v2.2 runs were performed to calculate actinide solubilities in WIPP brines in equilibrium with brucite+nesquehonite or brucite+hydromagnesite. The files following the naming convention given by the prototype

FMT_<P1>_<P2>_970407_22.<EXT>

were <P1> can assume the values SPC or ERDA6, and <P2> can assume the values NESQ, HMAG4323, or HMAG5424. The <EXT> variable has four values for each run, COM, IN, OUT, and FOR088. The "970407" in the name specifies that a version of the FMT_970407.CHEMDAT data base was used, and the "22" indicates that FMT v2.2 was used. The six different file identifiers thus are:

FMT_ERDA6_NESQ_970407_22.<EXT>
FMT_ERDA6_HMAG4323_970407_22.<EXT>
FMT_ERDA6_HMAG5424_970407_22.<EXT>
FMT_SPC_NESQ_970407_22.<EXT>
FMT_SPC_HMAG4323_970407_22.<EXT>
FMT_SPC_HMAG5424_970407_22.<EXT>

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Each of these unique file identifiers corresponds to SCMS files with the extensions IN, OUT, FOR088, and COM. A "dummy" INGUESS file, the contents of which were ignored, was used for all runs because the flags in the IN files were such that this file was superfluous.

The IN files were constructed using the Element Abundances column called Total Moles from the OUT files of earlier FMT runs (Novak, 1996b). These OUT files, contained under SCMS, are called FMT_ERDA6_BF_960823.OUT and FMT_SPC_BF_960823.OUT. The IN files were created in this way to more clearly demonstrate the continuity of the chemical conditions simulated from one FMT run to the next. One change to the ERDA6 files was required: 0.002 moles of oxygen and 0.001 moles of thorium were added, equivalent to the addition of 0.001 moles of ThO_2(am), was added to ensure enough ThO_2(am) solid to reach the solubility limit.

The FMT source code, executable, build command, and data sets are stored in SCMS. The image information from the executable version 2.2 of FMT used for the runs is:

```
image name: "FMT_FMT2P0_PA96_2"
image file identification: "P PA96_2 2.2"
image file build identification: ""
link date/time: 29-OCT-1996 15:16:12.48
linker identification: "A11-14"
```

Run Results

Partial OUT files, i.e., with the echo printed data base portion removed, are included in this memorandum. Tables 4 to 6 contain the ERDA6 runs NESQ, HMAG4323, and HMAG5424, respectively. Tables 7 to 9 contain the SPC runs NESQ, HMAG4323, and HMAG5424, respectively. In each file, the section following the entry "Elemental Abundance for Flash Problem" lists for each element the total moles in the simulation (an input, extrinsic quantity), the element aqueous molality and Molarity, and the corresponding element concentration in mg/l. Also in each file, the section labeled "Table of Concentrations for Batch Problem" provides concentrations and other chemical information by species.

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References

Garrels, R.M., and C.L. Christ. 1990. *Solutions, Minerals, and Equilibria.* New York: Harper and Row Publications.

Harvie, C.E., N. Møller, and J.H. Weare. 1984. "The Prediction of Mineral Solubilities in Natural Waters: The Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O System to High Ionic Strengths at 25°C," *Geochimica et Cosmochimica Acta.* Vol. 48, no. 4, 723-751.

Langmuir, D., 1965, Stability of Carbonates in the System MgO-CO_2-H_2O. Journal of Geology, v. 73, p. 730-754.

Lippmann, F., 1973, Sedimentary Carbonate Minerals, Springer-Verlag, New York, 228 p.

Novak, C.F. 1996a. "Release of FMT Data Base File HMW_Am3Pu3Th4Np5_960823.CHEMDAT." internal SNL memorandum to R.C. Moore. 23 August 1996. WPO 38628.

Novak, C.F. 1996b. "Predictions of +III, +IV, and +V Actinide Solubilities in WIPP Salado and Castile Brine using the Revised Thermodynamic Data Base File HMW_Am3Pu3Th4Np5_960823.CHEMDAT." internal SNL memorandum to R.V. Bynum. 4 November 1996. WPO 38628.

Novak, C.F., I. Al Mahamid, K.A. Becraft, S.A. Carpenter, N. Hakem, and T. Prussin. 1996a. "Measurement and Thermodynamic Modeling of Np(V) Solubility in Dilute Through Concentrated K_2CO_3 Media." SAND96-1604J. Albuquerque, NM: Sandia National Laboratories.

Novak, C.F., R.C. Moore, and R.V. Bynum. 1996b. "Predictions of Dissolved Actinide Concentrations in Concentrated Electrolyte Solutions: A Conceptual Model and Model Results for the Waste Isolation Pilot Plant (WIPP)." *Proceedings of the 1996 International Conference on Deep Geological Disposal of Radioactive Waste.* 16-19 September 1996. Winnipeg, Manitoba, Canada.

Novak, C.F., H. Nitsche, H.B. Silber, K. Roberts, Ph.C. Torretto, T. Prussin, K. Becraft, S.A. Carpenter, D.E. Hobart, and I. Al Mahamid. 1996c. "Neptunium(V) and Neptunium(VI) Solubilities in Synthetic Brines of Interest to the Waste Isolation Pilot Plant (WIPP)," *Radiochimica Acta.* Vol. 74, 31-36.

Robie, R.A., and Hemingway, B.S., 1973, The Enthalpies of Formation of Nesquehonite, MgCO3.3H2O, and Hydromagnesite, $5MgO{\cdot}4CO_2{\cdot}5H_2O$. Journal of Research of the U.S. Geological Survey, Reston, VA, v. 1, p. 543-547.

Distribution:

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Table 1. Email message from AR Felmy to CF Novak giving new parameter values for Cl^- - $Th(CO_3)_5^{6-}$ and Na^+ - Cl^- - $Th(CO_3)_5^{6-}$ ion interactions.

```
Date: Wed, 26 Mar 1997 07:46:29 -0800
From: ar_felmy@ccmail.pnl.gov (Andrew R Felmy)
Subject: Re: Thermo Parameters for Th++++
To: ar_felmy@pnl.gov, cfnovak@sandia.gov (Craig F. Novak)
Cc: rcmoore@nwer.sandia.gov, rvbynum@nwer.sandia.gov
MIME-version: 1.0

Content-Type: text/plain; charset=US-ASCII
Content-Transfer-Encoding: 7bit
Content-Description: cc:Mail note part

     Craig,

     I have finished my initial analysis of the mixing parameters for
     Th(CO3)5 6- with Cl- and Na+. This analysis is based solely on the
     ThO2(am) solubility data in mixed NaCl-Na2CO3 solutions.  I did not
     analyze the HCO3 data.  There were only a couple of points with solid
     phase present in the HCO3 solutions and I was unsure about
     equilibrium. Unfortunately, we will not be able to do any more work on
     the HCO3 this year. I'm sending along the original data files that I
     used for my analysis.  If you do any fitting you will note a
     redundancy between theta and psi which leads to a numerical precision
     issue involving parameter convergence. As a result it is only possible
     to refine the parameter values for theta to +/- 0.2 units and psi to
     +/- .02 units.  My recommended parameter values are therefore theta =
     2.0 +/- 0.2 and psi = -.08 +/- 0.2.  Never the less, I think you will
     find an ENORMOUS improvement in the predicted Th concentrations.

     Enjoy,

     Andy
```

Note that, because of a typographical error, the error associated with "psi" should read "+/– 0.02" instead of "+/– 0.2", as confirmed by telephone with AR Felmy.

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Table 2. Results of VMS DIFFERENCES comparison command between FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT and FMT_970407.CHEMDAT.

```
**************
File U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2
     1   'FMT_970407_NESQ.chemdat'
     2   'Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy'
     3
     4   27 212 'nNEW T' 'nACTCOEF' 'nECHO' 'nABCD'
******
File U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
     1   'HMW_Am3Pu3Th4Np5.CHEMDAT:  Am(III), Pu(III); Th(IV); Np(V)'
     2   '96.08.23 Memo Release      HMW/FW; Ac-Cit-EDTA-Lac-Ox; MgOAG-CaOAG'
     3
     4   27 210 'nNEW T' 'nACTCOEF' 'nECHO' 'nABCD'
**************
**************
File U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2
   253   'CaMg(CO3)2_DISABLED_____________Dolomite'  0  6 0 0 1 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 999.999 -871.99
   254   'Mg5(CO3)4(OH)2.4H2O_HydroMagne5424' 10 18 0 0 5 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -2364.06     R&H73
   255   'Mg4(CO3)3(OH)2.3H2O_HydroMagne4323'  8 14 0 0 4 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1858.104    Lang65
******
File U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
   253   'CaMg(CO3)2____DISABLED____Dolomite'  0  6 0 0 1 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 999.999 -871.99      HMW84
**************
**************
File U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2
   339     1 1.31     30.        .0      .0       K+ Th(CO3)5===    by analogy with Na+
******
File U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
   337     1  .0        .0        .0      .0       K+ Th(CO3)5===
**************
**************
File U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2
   439     1  .10       .34       .0      .0       Mg++ NpO2CO3-        by analogy with Na+, K+ values
   440     3  .48      4.4        .0      .0       Mg++ NpO2(CO3)2=-    by analogy with Na+, K+ values
   441     3 2.07     22.7      -48.      -.11      Mg++ NpO2(CO3)3=--   average of Na+, K+ values
******
File U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
   437     1  .0        .0        .0      .0       Mg++ NpO2CO3-
   438     3  .0        .0        .0      .0       Mg++ NpO2(CO3)2=-
   439     3  .0        .0        .0      .0       Mg++ NpO2(CO3)3=--
**************
**************
File U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2
  2409   .02 -.006 -.05  .03 -.02 -.065  .12  .074 0 0 .168  0 -.24 -.21 -.26 -.26 .1 0 0  0 0 2.0 0 0 -.09 0 0 0 0 0 0 0 0 0 0 0
******
File U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
  2407   .02 -.006 -.05  .03 -.02 -.065  .12  .074 0 0 .168  0 -.24 -.21 -.26 -.26 .1 0 0  0 0 5.5 0 0 -.09 0 0 0 0 0 0 0 0 0 0 0
**************
**************
File U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2
  3270      -.08  -.08    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Th(CO3)5===: ARF9703
******
File U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
  3268       .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Th(CO3)5===:
**************
**************
File U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2
  5836     ARF970326 == Email from ARFelmy 26Mar97
******
File U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
**************
**************
File U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2
  5853     R&H73  ==  Robie and Hemingway 1973 J.Reas.US.Geol.Surv. v1n5 pp 543-547
  5854     Lang65 ==  Langmuir 1965 J.Geology v73 730-754
******
File U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
**************

Number of difference sections found: 8
Number of difference records found: 16

DIFFERENCES /IGNORE=()/MERGED=1/OUTPUT=U1:[CFNOVAK.FMT.QA_NESQ_HMAG]DB.DIF;1-
    U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407.CHEMDAT;2-
    U1:[CFNOVAK.FMT]FMT_HMW_AM3PU3TH4NP5_960823.CHEMDAT;1
```


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Table 3. Solids that are "DISABLED" (prevented from forming) in variants of the data base file FMT_970407.CHEMDAT.

FMT_970407_NESQ .CHEMDAT	FMT_970407_HMAG4323 .CHEMDAT	FMT_970407_HMAG5424 .CHEMDAT
Aragonite	Aragonite	Aragonite
Calcite	Calcite	Calcite
Dolomite	Dolomite	Dolomite
Gaylussite	Gaylussite	Gaylussite
Labile Salt		
Magnesite	Magnesite	Magnesite
Pirssonite	Pirssonite	Pirssonite
HMAG5424	HMAG5424	
HMAG4323		

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```
INPUT    file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_ERDA6_HMAG4323_970407_22.IN;1
INGUESS  file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]DUMMY.INGUESS;1
OUTPUT   file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_ERDA6_HMAG4323_970407_22.OUT;2
CHEMDAT  file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407_HMAG4323.CHEMDAT;6
Temperature is Hard Coded as 298.15K
Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Hydromagnesite          FMT V2.2
FMT_970407_HMAG4323.chemdat                  HYDROMAGNESITE ADDED
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy

Accuracy of reactions is              1.0000E-06
Minimum elemental abundance is        1.0000E-18
Number of Aqueous Species is           126
```

Table 4

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Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Hydromagnesite FMT V2.2
FMT_970407_HMAG4323.chemdat HYDROMAGNESITE ADDED
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy
Pressure= 1.000 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.13289995E+02	1.11291724E+02	9.78381090E+01	9.86110301E+04	Hydrogen
6.55755271E+01	5.65528407E+01	4.97163923E+01	7.95432447E+05	Oxygen
7.19980915	6.19775745	5.44853516	1.25260570E+05	Sodium
1.10087747E-01	1.11083132E-01	9.76547335E-02	3.81813407E+03	Potassium
2.04429362	4.59065398E-02	4.03570805E-02	9.80878841E+02	Magnesium
1.01344192	1.34387465E-02	1.18141898E-02	4.73512726E+02	Calcium
6.96738842	5.96774208	5.24632543	1.85997976E+05	Chlorine
1.19112712	1.91046897E-01	1.67951997E-01	5.38454101E+03	Sulfur
1.00103149	1.01051302E-03	8.88356111E-04	1.06700452E+01	Carbon
0.0	0.0	0.0	0.0	PosIon:EL
0.0	0.0	0.0	0.0	NegIon:EL
0.0	0.0	0.0	0.0	Oxalate:EL
7.08491570E-02	7.21464334E-02	6.34249376E-02	6.85623575E+02	Boron
1.23704871E-02	1.25969957E-02	1.10741949E-02	8.84872468E+02	Bromine
0.0	0.0	0.0	0.0	Acetate:EL
1.10000068E-02	5.98385449E-08	5.26049008E-08	1.22063412E-02	Th(IV)
1.00041150E-03	1.31196363E-08	1.15336556E-08	2.80267831E-03	Am(III)
0.0	0.0	0.0	0.0	Pu(III)
1.00253377E-03	5.25156921E-07	4.61672786E-07	1.09438703E-01	Np(V)
0.0	0.0	0.0	0.0	ClO4:EL
0.0	0.0	0.0	0.0	Phosphorus
0.0	0.0	0.0	0.0	U(IV)
0.0	0.0	0.0	0.0	Lactate:EL
0.0	0.0	0.0	0.0	EDTA:EL
0.0	0.0	0.0	0.0	Citrate:EL
0.0	0.0	0.0	0.0	Electron:E
7.42184763E-15	7.55774463E-15	6.64411889E-15	0.0	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS	1360.05982636088	grams
H2O MASS	982.018842063433	grams
TDS(g/kg)	384.963065986703	g/kgH2O

Specified Solution Density

DENSITY	1217.54038033208	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	1.11705521092445	liters
TDS	338.426409545678	g/l

Density based on TDS and NaCl solutions 1217.54038033208 g/l
Percent relative error vs NaCl density 0.000000000000000 0 %

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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.14970E-01	7.49304E-01	0.9194	5.45106E+01	4.87985E+01	8.79114E+05	
Na+	Na+	6.19776	6.05945	0.9777	6.08631	5.44854	1.25261E+05	
Cl-	Cl-	5.96774	6.13728	1.028	5.86044	5.24633	1.85998E+05	
CaSO4	Anhydrite	1.01523	1.000	1.000	9.96974E-01	8.92502E-01	1.21503E+05	
Mg(OH)2	Brucite	6.80737E-01	1.000	1.000	6.68497E-01	5.98446E-01	3.49011E+04	
Mg4(CO3)3(OH)2.3H2O	Hydromagne4323	3.38770E-01	1.000	1.000	3.32679E-01	2.97818E-01	1.08795E+05	
SO4=	SO4=	1.91047E-01	3.56983E-03	1.8686E-02	1.87612E-01	1.67952E-01	1.61331E+04	
K+	K+	1.11083E-01	5.43624E-02	0.4894	1.09086E-01	9.76547E-02	3.81813E+03	
B(OH)4-	B(OH)4-	5.39233E-02	5.38049E-03	9.9780E-02	5.29537E-02	4.74047E-02	3.73735E+03	
Mg++	Mg++	3.96372E-02	7.76735E-02	1.960	3.89245E-02	3.48457E-02	8.46924E+02	
Br-	Br-	1.25970E-02	3.54296E-03	0.2813	1.23705E-02	1.10742E-02	8.84872E+02	
ThO2(am)	Hydrous_Thorium_Oxide	1.12014E-02	1.000	1.000	1.09999E-02	9.84727E-03	2.60004E+03	
KNpO2CO3(s)	KNpO2CO3(s)	1.02037E-03	1.000	1.000	1.00202E-03	8.97017E-04	3.30241E+02	
AmOHCO3(c)	AmOHCO3(c)	1.01872E-03	1.000	1.000	1.00040E-03	8.95568E-04	2.86596E+02	
NaCl	Halite	1.12722	1.000	1.000	1.10695	9.90957E-01	5.79142E+04	-6.99E-08
Ca++	Ca++	1.08851E-02	1.21702E-02	1.118	1.06894E-02	9.56923E-03	3.83535E+02	8.15E-08
B(OH)3(aq)	B(OH)3(aq)	7.90331E-03	7.25114E-03	0.9175	7.76120E-03	6.94791E-03	4.29602E+02	1.41E-08
MgB(OH)4+	MgB(OH)4+	5.43293E-03	1.04807E-02	1.929	5.33524E-03	4.77617E-03	4.92634E+02	1.21E-08
Na2Ca(SO4)2	Glauberite	3.33054E-03	1.000	1.000	3.27065E-03	2.92792E-03	8.14474E+02	-1.70E-07
CaB(OH)4+	CaB(OH)4+	2.44581E-03	2.92711E-03	1.197	2.40183E-03	2.15015E-03	2.55694E+02	9.24E-08
MgOH+	MgOH+	4.24254E-04	1.55072E-04	0.3655	4.16625E-04	3.72967E-04	1.54081E+01	-1.22E-07
MgCO3(aq)	MgCO3(aq)	4.12109E-04	4.12109E-04	1.000	4.04699E-04	3.62291E-04	3.05463E+01	-1.70E-08
B4O5(OH)4=	B4O5(OH)4=	3.69277E-04	1.42321E-06	3.8541E-03	3.62637E-04	3.24636E-04	6.20919E+01	1.02E-07
B3O3(OH)4-	B3O3(OH)4-	3.21339E-04	3.45937E-05	0.1077	3.15561E-04	2.82494E-04	4.19383E+01	4.60E-09
CO3=	CO3=	2.57999E-04	6.25593E-06	2.4248E-02	2.53360E-04	2.26810E-04	1.36107E+01	1.07E-07
HCO3-	HCO3-	2.31918E-04	7.95828E-05	0.3432	2.27748E-04	2.03882E-04	1.24403E+01	4.70E-08
CaCO3(aq)	CaCO3(aq)	1.07853E-04	1.07853E-04	1.000	1.05913E-04	9.48148E-05	9.48994	1.14E-07
OH-	OH-	2.37122E-05	1.29634E-05	0.5467	2.32859E-05	2.08458E-05	3.54530E-01	6.72E-08
NpO2CO3-	NpO2CO3-	4.41407E-07	4.92716E-08	0.1116	4.33470E-07	3.88047E-07	1.27689E-01	-6.86E-08
Th(OH)3(CO3)-	Th(OH)3(CO3)-	5.84948E-08	1.64519E-08	0.2813	5.74430E-08	5.14236E-08	1.76418E-02	7.52E-08
NpO2(CO3)2=-	NpO2(CO3)2=-	4.09676E-08	8.49197E-12	2.0729E-04	4.02309E-08	3.60152E-08	1.40122E-02	3.47E-08
CO2(aq)	CO2(aq)	3.86742E-08	1.34550E-07	3.479	3.79788E-08	3.39991E-08	1.49629E-03	4.96E-08
NpO2+	NpO2+	3.72702E-08	7.35032E-08	1.972	3.66000E-08	3.27647E-08	8.81525E-03	-5.74E-08
Am(OH)2+	(after_Cm(III))	9.16129E-09	1.18486E-12	1.2933E-04	8.99656E-09	8.05382E-09	2.23103E-03	-3.63E-07
NpO2OH(aq)	NpO2OH(aq)	4.50727E-09	4.66708E-10	0.1035	4.42622E-09	3.96240E-09	1.13346E-03	-1.49E-07
Am(CO3)3=-	Am(CO3)3=-	3.42928E-09	1.28405E-13	3.7444E-05	3.36761E-09	3.01473E-09	1.27531E-03	1.13E-07
Th(OH)4(aq)	Th(OH)4(aq)	1.28537E-09	1.28537E-09	1.000	1.26225E-09	1.12998E-09	3.39071E-04	3.41E-08
NpO2(CO3)3==-	NpO2(CO3)3==-	9.82269E-10	4.21922E-18	4.2954E-09	9.64607E-10	8.63527E-10	3.87788E-04	1.31E-07
HSO4-	HSO4-	3.59246E-10	1.97958E-10	0.5510	3.52786E-10	3.15818E-10	3.06550E-05	-5.18E-08
AmCO3+	AmCO3+	2.84866E-10	8.14021E-11	0.2858	2.79744E-10	2.50430E-10	7.58825E-05	-7.90E-08
H+	H+	1.29624E-10	5.82477E-10	4.494	1.27293E-10	1.13954E-10	1.14855E-07	4.09E-08
Am(OH)3(aq)	(1e-9m_minimum)	1.21905E-10	1.21905E-10	1.000	1.19713E-10	1.07169E-10	3.15099E-05	1.70E-08
Am(CO3)2-	Am(CO3)2-	9.57666E-11	2.69348E-11	0.2813	9.40446E-11	8.41898E-11	3.05624E-05	4.11E-08
Th(CO3)5===	Th(CO3)5===	5.84114E-11	7.81935E-26	1.3387E-15	5.73611E-11	5.13503E-11	2.73227E-05	2.88E-07
NpO2(OH)2-	NpO2(OH)2-	2.22276E-11	3.56410E-13	1.6035E-02	2.18280E-11	1.95406E-11	5.92201E-06	-1.17E-07

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AmOH++	(after_Cm(III))	1.70150E-11	1.26060E-13	7.4087E-03	1.67091E-11	1.49582E-11	3.88923E-06	-1.85E-08
Am+++	Am+++	9.51551E-12	3.53236E-13	3.7122E-02	9.34441E-12	8.36522E-12	2.03275E-06	-6.72E-08
Th(SO4)3=	Th(SO4)3=	4.32204E-20	7.64809E-22	1.7696E-02	4.24433E-20	3.79957E-20	1.97658E-14	-2.27E-07
Th(SO4)2(aq)	Th(SO4)2(aq)	9.81983E-22	3.12841E-20	31.86	9.64325E-22	8.63275E-22	3.66161E-16	-8.23E-08
Am(OH)3(s)	Am(OH)3(s)	0.0	1.000	1.000	0.0	0.0	0.0	-9.28E-01
Na4Ca(SO4)3.2H2O	Labile_Salt	0.0	1.000	1.000	0.0	0.0	0.0	-7.05E-01
Ca4Cl2(OH)6.13H2O	CaOxychloride_A	0.0	1.000	1.000	0.0	0.0	0.0	-2.18E+01
K2MgCa2(SO4)4.2H2O	Polyhalite	0.0	1.000	1.000	0.0	0.0	0.0	-3.76
Na3H(CO3)2.2H2O	Trona	0.0	1.000	1.000	0.0	0.0	0.0	-6.16
Th++++	Th++++	0.0	0.0	0.4432	0.0	0.0	0.0	-2.62E+01
K2B407.4H2O	K-Tetraborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-6.40
KB508.4H2O	K-Pentaborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-7.02
HCl(aq)	to.titrate.acid.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.49E+02
NaOH(aq)	to.titrate.base.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.95E+02
KNaC03.6H2O	K-Na-Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-6.32
K8H4(CO3)6.3H2O	K-Sequicarbonate	0.0	1.000	1.000	0.0	0.0	0.0	-4.43E+01
K2NaH(CO3)2.2H2O	Potassium_Trona	0.0	1.000	1.000	0.0	0.0	0.0	-1.25E+01
B(OH)3	Borix_Acid_Solid	0.0	1.000	1.000	0.0	0.0	0.0	-2.11
K2C03.3/2H2O	Potassium_Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-1.10E+01
NaAm(CO3)2.6H2O(c)		0.0	1.000	1.000	0.0	0.0	0.0	-1.44
Th(SO4)2.9H2O(s)		0.0	1.000	1.000	0.0	0.0	0.0	-1.92E+01
Th(SO4)2.8H2O(s)		0.0	1.000	1.000	0.0	0.0	0.0	-1.92E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)		0.0	1.000	1.000	0.0	0.0	0.0	-1.51E+01
Th(SO4)2.K2SO4.4H2O(16C,s)		0.0	1.000	1.000	0.0	0.0	0.0	-1.85E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)		0.0	1.000	1.000	0.0	0.0	0.0	-2.01E+01
2[Th(SO4)2.7/2K2SO4(16C,s)]		0.0	1.000	1.000	0.0	0.0	0.0	-4.77E+01
NpO2OH(aged)	NpO2OH(aged)	0.0	1.000	1.000	0.0	0.0	0.0	-2.54
NpO2OH(amor)	NpO2OH(amor)	0.0	1.000	1.000	0.0	0.0	0.0	-3.24
2[NaNpO2C03.7/2H2O(s)]		0.0	1.000	1.000	0.0	0.0	0.0	-1.81
K3NpO2(C03)2(s)	K3NpO2(C03)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-5.40
C02("solid",DISABLED)		0.0	1.000	1.000	0.0	0.0	0.0	-5.09E+02
NaK3(SO4)2	Aphthitalite/Glaserite	0.0	1.000	1.000	0.0	0.0	0.0	-4.10
CaCl2.6H2O	Antarcticite	0.0	1.000	1.000	0.0	0.0	0.0	-5.23
CaC03_DISABLED	A	0.0	1.000	1.000	0.0	0.0	0.0	-6.31E+02
K2SO4	Arcanite	0.0	1.000	1.000	0.0	0.0	0.0	-3.20
MgCl2.6H2O	Bischofite	0.0	1.000	1.000	0.0	0.0	0.0	-4.74
Na2Mg(SO4)2.4H2O	Bloedite	0.0	1.000	1.000	0.0	0.0	0.0	-2.59
Na6C03(SO4)2	Burkeite	0.0	1.000	1.000	0.0	0.0	0.0	-4.63
CaC03_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-6.31E+02
CaCl2.4H2O	CaCl2_Tetrahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-6.56
Ca2Cl2(OH)2.H2O	CaOxychloride_B	0.0	1.000	1.000	0.0	0.0	0.0	-1.07E+01
KMgCl3.6H2O	Carnallite	0.0	1.000	1.000	0.0	0.0	0.0	-5.09
MgSO4.7H2O	Epsomite	0.0	1.000	1.000	0.0	0.0	0.0	-2.55
CaNa2(C03)2.5H2O_DISABLED	Ga	0.0	1.000	1.000	0.0	0.0	0.0	-1.03E+03
CaSO4.2H2O	Gypsum	0.0	1.000	1.000	0.0	0.0	0.0	-3.22E-02
MgSO4.6H2O	Hexahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-2.67
KMgClSO4.3H2O	Kainite	0.0	1.000	1.000	0.0	0.0	0.0	-4.22
KHC03	Kalicinite	0.0	1.000	1.000	0.0	0.0	0.0	-5.65
MgSO4.H2O	Kieserite	0.0	1.000	1.000	0.0	0.0	0.0	-3.56
K2Mg(SO4)2.4H2O	Leonite	0.0	1.000	1.000	0.0	0.0	0.0	-5.06
MgC03_DISABLED	M	0.0	1.000	1.000	0.0	0.0	0.0	-6.13E+02
KHSO4	Mercallite	0.0	1.000	1.000	0.0	0.0	0.0	-1.15E+01

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Na2SO4.10H2O_____Mirabilite	0.0	1.000	1.000	0.0	0.0	0.0	-9.08E-01
K8H6(SO4)7_____Misenite	0.0	1.000	1.000	0.0	0.0	0.0	-7.19E+01
NaHCO3_____Nahcolite	0.0	1.000	1.000	0.0	0.0	0.0	-2.91
Na2CO3.10H2O_____Natron	0.0	1.000	1.000	0.0	0.0	0.0	-4.07
MgCO3.3H2O_____Nesquehonite	0.0	1.000	1.000	0.0	0.0	0.0	-1.52
K2Mg(SO4)2.6H2O_Picromerite/Schoen	0.0	1.000	1.000	0.0	0.0	0.0	-4.96
Na2Ca(CO3)2.2H2O_DISABLED_____Pi	0.0	1.000	1.000	0.0	0.0	0.0	-9.02E+02
K3H(SO4)2__Sesquipotassium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.44E+01
Na3H(SO4)2____Sesquisodium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.10E+01
Na2CO3.7H2O____Na2CO3-Heptahydrate	0.0	1.000	1.000	0.0	0.0	0.0	-4.06
KCl_____Sylvite	0.0	1.000	1.000	0.0	0.0	0.0	-1.38
K2Ca(SO4)2.H2O_____Syngenite	0.0	1.000	1.000	0.0	0.0	0.0	-2.02
Mg2CaCl6.12H2O_____Tachyhydrite	0.0	1.000	1.000	0.0	0.0	0.0	-1.83E+01
Na2SO4_____Thenardite	0.0	1.000	1.000	0.0	0.0	0.0	-5.95E-01
Na2CO3.H2O_____Thermonatrite	0.0	1.000	1.000	0.0	0.0	0.0	-4.25
NaB5O8.5H2O____Sodium_Pentaborate	0.0	1.000	1.000	0.0	0.0	0.0	-6.33
NaBO2.NaCl.2H2O___Teepleite_(20_C)	0.0	1.000	1.000	0.0	0.0	0.0	-1.52
CaMg(CO3)2_DISABLED_____	0.0	1.000	1.000	0.0	0.0	0.0	-8.09E+02
Mg5(CO3)4(OH)2.4H2O_DISABLED_Hydro	0.0	1.000	1.000	0.0	0.0	0.0	-1.46E+03
NaBO2.4H2O_____Sodium_Metaborate	0.0	1.000	1.000	0.0	0.0	0.0	-2.07
Ca(OH)2_____Portlandite	0.0	1.000	1.000	0.0	0.0	0.0	-6.50
Na2B4O7.10H2O_____Borax	0.0	1.000	1.000	0.0	0.0	0.0	-1.61
Mg2Cl(OH)3.4H2O_____MgOxychloride	0.0	1.000	1.000	0.0	0.0	0.0	-6.34E-01
Na3NpO2(CO3)2(s)__Na3NpO2(CO3)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.01

pH (-log[aH+]); pmH(-log[mH+]) 9.2347 9.8873
Osmotic Coefficient= 1.271198
Equilibrium RH (%) = 74.930375
Ionic Strength (m) = 6.660385
Density, kg/m3 = 1217.54
fCO2(g); log[fCO2(g)]= 4.080E-06 -5.39

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -7.84388104E+03

Total Diagonal Inversions 427
Total Stoichiometric Reoptimizations 43

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INPUT    file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_ERDA6_HMAG5424_970407_22.IN;1
INGUESS  file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]DUMMY.INGUESS;1
OUTPUT   file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_ERDA6_HMAG5424_970407_22.OUT;3
CHEMDAT  file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407_HMAG5424.CHEMDAT;4
Temperature is Hard Coded as 298.15K
Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Hydromagnesite          FMT V2.2
FMT_970407_HMAG5424.chemdat                  HYDROMAGNESITE ADDED
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy

Accuracy of reactions is              1.0000E-06
Minimum elemental abundance is        1.0000E-18
Number of Aqueous Species is           126
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Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Hydromagnesite FMT V2.2
FMT_970407_HMAG5424.chemdat HYDROMAGNESITE ADDED
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy
Pressure= 1.000 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.13289995E+02	1.11291684E+02	9.78385649E+01	9.86114896E+04	Hydrogen
6.55755271E+01	5.65521148E+01	4.97160035E+01	7.95426226E+05	Oxygen
7.19980915	6.19785660	5.44864965	1.25263202E+05	Sodium
1.10087747E-01	1.11083500E-01	9.76555468E-02	3.81816587E+03	Potassium
2.04429362	4.57038304E-02	4.01790773E-02	9.76552474E+02	Magnesium
1.01344192	1.34147538E-02	1.17931566E-02	4.72669718E+02	Calcium
6.96738842	5.96781223	5.24641341	1.86001095E+05	Chlorine
1.19112712	1.91037611E-01	1.67944675E-01	5.38430628E+03	Sulfur
1.00103149	7.77233695E-04	6.83280425E-04	8.20688119	Carbon
0.0	0.0	0.0	0.0	PosIon:EL
0.0	0.0	0.0	0.0	NegIon:EL
0.0	0.0	0.0	0.0	Oxalate:EL
7.08491570E-02	7.21466708E-02	6.34254643E-02	6.85629269E+02	Boron
1.23704871E-02	1.25970371E-02	1.10742869E-02	8.84879817E+02	Bromine
0.0	0.0	0.0	0.0	Acetate:EL
1.10000068E-02	4.62894405E-08	4.06938979E-08	9.44253475E-03	Th(IV)
1.00041150E-03	1.44943642E-08	1.27422619E-08	3.09636965E-03	Am(III)
0.0	0.0	0.0	0.0	Pu(III)
1.00253377E-03	5.27808841E-07	4.64006452E-07	1.09991894E-01	Np(V)
0.0	0.0	0.0	0.0	ClO4:EL
0.0	0.0	0.0	0.0	Phosphorus
0.0	0.0	0.0	0.0	U(IV)
0.0	0.0	0.0	0.0	Lactate:EL
0.0	0.0	0.0	0.0	EDTA:EL
0.0	0.0	0.0	0.0	Citrate:EL
0.0	0.0	0.0	0.0	Electron:E
-1.51527455E-14	-1.54302491E-14	-1.35650155E-14	0.0	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS	1360.03977930042	grams
H2O MASS	982.015610558398	grams
TDS(g/kg)	384.947209267957	g/kgH2O

Specified Solution Density

DENSITY	1217.53254524176	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	1.11704593410303	liters
TDS	338.414166509250	g/l

Density based on TDS and NaCl solutions 1217.53254524176 g/l
Percent relative error vs NaCl density 0.000000000000000 0 %

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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.14972E-01	7.49308E-01	0.9194	5.45104E+01	4.87987E+01	8.79118E+05	
Na+	Na+	6.19786	6.05965	0.9777	6.08639	5.44865	1.25263E+05	
Cl-	Cl-	5.96781	6.13707	1.028	5.86048	5.24641	1.86001E+05	
CaSO4	Anhydrite	1.01527	1.000	1.000	9.97012E-01	8.92543E-01	1.21509E+05	
Mg(OH)2	Brucite	7.65344E-01	1.000	1.000	7.51579E-01	6.72828E-01	3.92390E+04	
Mg5(CO3)4(OH)2.4H2O	HydroMagne5424	2.54137E-01	1.000	1.000	2.49566E-01	2.23416E-01	1.04478E+05	
SO4=	SO4=	1.91038E-01	3.56959E-03	1.8685E-02	1.87602E-01	1.67945E-01	1.61324E+04	
K+	K+	1.11084E-01	5.43636E-02	0.4894	1.09086E-01	9.76555E-02	3.81817E+03	
B(OH)4-	B(OH)4-	5.39422E-02	5.38237E-03	9.9780E-02	5.29721E-02	4.74216E-02	3.73868E+03	
Mg++	Mg++	3.95413E-02	7.74957E-02	1.960	3.88302E-02	3.47615E-02	8.44879E+02	
Br-	Br-	1.25970E-02	3.54304E-03	0.2813	1.23705E-02	1.10743E-02	8.84880E+02	
ThO2(am)	Hydrous_Thorium_Oxide	1.12014E-02	1.000	1.000	1.10000E-02	9.84737E-03	2.60007E+03	
KNpO2CO3(s)	KNpO2CO3(s)	1.02037E-03	1.000	1.000	1.00202E-03	8.97023E-04	3.30243E+02	
AmOHCO3(c)	AmOHCO3(c)	1.01872E-03	1.000	1.000	1.00040E-03	8.95574E-04	2.86598E+02	
NaCl	Halite	1.12718	1.000	1.000	1.10690	9.90920E-01	5.79121E+04	-6.93E-08
Ca++	Ca++	1.08850E-02	1.21711E-02	1.118	1.06892E-02	9.56917E-03	3.83532E+02	8.08E-08
B(OH)3(aq)	B(OH)3(aq)	7.89708E-03	7.24536E-03	0.9175	7.75506E-03	6.94247E-03	4.29266E+02	1.41E-08
MgB(OH)4+	MgB(OH)4+	5.42215E-03	1.04604E-02	1.929	5.32463E-03	4.76671E-03	4.91658E+02	1.23E-08
Na2Ca(SO4)2	Glauberite	3.31643E-03	1.000	1.000	3.25678E-03	2.91553E-03	8.11027E+02	-1.69E-07
CaB(OH)4+	CaB(OH)4+	2.44674E-03	2.92833E-03	1.197	2.40273E-03	2.15097E-03	2.55792E+02	9.14E-08
MgOH+	MgOH+	4.23741E-04	1.54894E-04	0.3655	4.16121E-04	3.72519E-04	1.53896E+01	-1.21E-07
B4O5(OH)4=	B4O5(OH)4=	3.68923E-04	1.42190E-06	3.8542E-03	3.62288E-04	3.24327E-04	6.20328E+01	1.01E-07
B3O3(OH)4-	B3O3(OH)4-	3.20945E-04	3.45501E-05	0.1077	3.15173E-04	2.82148E-04	4.18870E+01	4.57E-09
MgCO3(aq)	MgCO3(aq)	3.16593E-04	3.16593E-04	1.000	3.10899E-04	2.78322E-04	2.34665E+01	-1.69E-08
CO3=	CO3=	1.98633E-04	4.81699E-06	2.4251E-02	1.95061E-04	1.74622E-04	1.04789E+01	1.06E-07
HCO3-	HCO3-	1.78369E-04	6.12080E-05	0.3432	1.75162E-04	1.56808E-04	9.56796	4.65E-08
CaCO3(aq)	CaCO3(aq)	8.30509E-05	8.30509E-05	1.000	8.15573E-05	7.30116E-05	7.30767	1.13E-07
OH-	OH-	2.37387E-05	1.29783E-05	0.5467	2.33118E-05	2.08691E-05	3.54928E-01	6.66E-08
NpO2CO3-	NpO2CO3-	4.41397E-07	4.92705E-08	0.1116	4.33458E-07	3.88040E-07	1.27687E-01	-6.81E-08
NpO2+	NpO2+	4.83999E-08	9.54581E-08	1.972	4.75294E-08	4.25492E-08	1.14477E-02	-5.66E-08
Th(OH)3(CO3)-	Th(OH)3(CO3)-	4.49883E-08	1.26534E-08	0.2813	4.41793E-08	3.95501E-08	1.35684E-02	7.45E-08
NpO2(CO3)2=-	NpO2(CO3)2=-	3.15409E-08	6.53857E-12	2.0730E-04	3.09737E-08	2.77282E-08	1.07881E-02	3.41E-08
CO2(aq)	CO2(aq)	2.97112E-08	1.03365E-07	3.479	2.91769E-08	2.61197E-08	1.14952E-03	4.92E-08
Am(OH)2+	(after_Cm(III))	1.19128E-08	1.54056E-12	1.2932E-04	1.16985E-08	1.04727E-08	2.90110E-03	-3.60E-07
NpO2OH(aq)	NpO2OH(aq)	5.86043E-09	6.06806E-10	0.1035	5.75503E-09	5.15201E-09	1.47375E-03	-1.48E-07
Am(CO3)3=-	Am(CO3)3=-	2.03029E-09	7.60420E-14	3.7454E-05	1.99378E-09	1.78487E-09	7.55048E-04	1.12E-07
Th(OH)4(aq)	Th(OH)4(aq)	1.28538E-09	1.28538E-09	1.000	1.26227E-09	1.13000E-09	3.39077E-04	3.38E-08
NpO2(CO3)3==-	NpO2(CO3)3==-	5.81997E-10	2.50144E-18	4.2980E-09	5.71530E-10	5.11644E-10	2.29766E-04	1.30E-07
HSO4-	HSO4-	3.58838E-10	1.97719E-10	0.5510	3.52385E-10	3.15461E-10	3.06204E-05	-5.11E-08
AmCO3+	AmCO3+	2.84533E-10	8.13088E-11	0.2858	2.79416E-10	2.50139E-10	7.57943E-05	-7.83E-08
Am(OH)3(aq)	(1e-9m_minimum)	1.58684E-10	1.58684E-10	1.000	1.55830E-10	1.39502E-10	4.10167E-05	1.69E-08
H+	H+	1.29470E-10	5.81813E-10	4.494	1.27142E-10	1.13820E-10	1.14719E-07	4.07E-08
Am(CO3)2-	Am(CO3)2-	7.36533E-11	2.07157E-11	0.2813	7.23287E-11	6.47500E-11	2.35054E-05	4.07E-08
NpO2(OH)2-	NpO2(OH)2-	2.89335E-11	4.63929E-13	1.6034E-02	2.84132E-11	2.54360E-11	7.70868E-06	-1.16E-07
AmOH++	(after_Cm(III))	2.20969E-11	1.63717E-13	7.4091E-03	2.16995E-11	1.94257E-11	5.05084E-06	-1.81E-08

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Th(CO3)5===	Th(CO3)5===	1.57103E-11	2.10671E-26	1.3410E-15	1.54277E-11	1.38112E-11	7.34872E-06	2.86E-07
Am+++	Am+++	1.23407E-11	4.58230E-13	3.7132E-02	1.21188E-11	1.08489E-11	2.63629E-06	-6.64E-08
Th(SO4)3=	Th(SO4)3=	4.30122E-20	7.61165E-22	1.7697E-02	4.22386E-20	3.78128E-20	1.96706E-14	-2.25E-07
Th(SO4)2(aq)	Th(SO4)2(aq)	9.77330E-22	3.11371E-20	31.86	9.59754E-22	8.59189E-22	3.64428E-16	-8.08E-08
Na3NpO2(CO3)2(s)	Na3NpO2(CO3)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.13
Mg2Cl(OH)3.4H2O	Mgoxychloride	0.0	1.000	1.000	0.0	0.0	0.0	-6.35E-01
Na2B4O7.10H2O	Borax	0.0	1.000	1.000	0.0	0.0	0.0	-1.62
Ca(OH)2	Portlandite	0.0	1.000	1.000	0.0	0.0	0.0	-6.50
NaBO2.4H2O	Sodium_Metaborate	0.0	1.000	1.000	0.0	0.0	0.0	-2.07
CaMg(CO3)2_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-8.10E+02
NaBO2.NaCl.2H2O	Teepleite_(20_C)	0.0	1.000	1.000	0.0	0.0	0.0	-1.52
NaB5O8.5H2O	Sodium_Pentaborate	0.0	1.000	1.000	0.0	0.0	0.0	-6.33
Na2CO3.H2O	Thermonatrite	0.0	1.000	1.000	0.0	0.0	0.0	-4.36
Na2SO4	Thenardite	0.0	1.000	1.000	0.0	0.0	0.0	-5.95E-01
Mg2CaCl6.12H2O	Tachyhydrite	0.0	1.000	1.000	0.0	0.0	0.0	-1.83E+01
K2Ca(SO4)2.H2O	Syngenite	0.0	1.000	1.000	0.0	0.0	0.0	-2.02
KCl	Sylvite	0.0	1.000	1.000	0.0	0.0	0.0	-1.38
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.0	1.000	1.000	0.0	0.0	0.0	-4.17
Na3H(SO4)2	Sesquisodium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.10E+01
K3H(SO4)2	Sesquipotassium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.44E+01
Na2Ca(CO3)2.2H2O_DISABLED	Pi	0.0	1.000	1.000	0.0	0.0	0.0	-9.02E+02
K2Mg(SO4)2.6H2O_Picromerite/Schoen		0.0	1.000	1.000	0.0	0.0	0.0	-4.96
MgCO3.3H2O	Nesquehonite	0.0	1.000	1.000	0.0	0.0	0.0	-1.64
Na2CO3.10H2O	Natron	0.0	1.000	1.000	0.0	0.0	0.0	-4.18
NaHCO3	Nahcolite	0.0	1.000	1.000	0.0	0.0	0.0	-3.03
K8H6(SO4)7	Misenite	0.0	1.000	1.000	0.0	0.0	0.0	-7.19E+01
Na2SO4.10H2O	Mirabillite	0.0	1.000	1.000	0.0	0.0	0.0	-9.08E-01
KHSO4	Mercallite	0.0	1.000	1.000	0.0	0.0	0.0	-1.15E+01
MgCO3_DISABLED	M	0.0	1.000	1.000	0.0	0.0	0.0	-6.13E+02
K2Mg(SO4)2.4H2O	Leonite	0.0	1.000	1.000	0.0	0.0	0.0	-5.06
MgSO4.H2O	Kieserite	0.0	1.000	1.000	0.0	0.0	0.0	-3.56
KHCO3	Kalicinite	0.0	1.000	1.000	0.0	0.0	0.0	-5.76
KMgClSO4.3H2O	Kainite	0.0	1.000	1.000	0.0	0.0	0.0	-4.22
MgSO4.6H2O	Hexahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-2.68
CaSO4.2H2O	Gypsum	0.0	1.000	1.000	0.0	0.0	0.0	-3.22E-02
CaNa2(CO3)2.5H2O_DISABLED	Ca	0.0	1.000	1.000	0.0	0.0	0.0	-1.03E+03
MgSO4.7H2O	Epsomite	0.0	1.000	1.000	0.0	0.0	0.0	-2.55
KMgCl3.6H2O	Carnallite	0.0	1.000	1.000	0.0	0.0	0.0	-5.09
Ca2Cl2(OH)2.H2O	CaOxychloride_B	0.0	1.000	1.000	0.0	0.0	0.0	-1.07E+01
Mg4(CO3)3(OH)2.3H2O_HydroMagne4323		0.0	1.000	1.000	0.0	0.0	0.0	-3.44E-01
CaCl2.4H2O	CaCl2_Tetrahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-6.56
CaCO3_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-6.31E+02
Na6CO3(SO4)2	Burkeite	0.0	1.000	1.000	0.0	0.0	0.0	-4.75
Na2Mg(SO4)2.4H2O	Bloedite	0.0	1.000	1.000	0.0	0.0	0.0	-2.60
MgCl2.6H2O	Bischofite	0.0	1.000	1.000	0.0	0.0	0.0	-4.74
K2SO4	Arcanite	0.0	1.000	1.000	0.0	0.0	0.0	-3.20
CaCO3_DISABLED	A	0.0	1.000	1.000	0.0	0.0	0.0	-6.31E+02
CaCl2.6H2O	Antarcticite	0.0	1.000	1.000	0.0	0.0	0.0	-5.23
NaK3(SO4)2	Aphthitalite/Glaserite	0.0	1.000	1.000	0.0	0.0	0.0	-4.10
CO2("solid",DISABLED)		0.0	1.000	1.000	0.0	0.0	0.0	-5.09E+02
K3NpO2(CO3)2(s)	K3NpO2(CO3)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-5.52
2[NaNpO2CO3.7/2H2O(s)]		0.0	1.000	1.000	0.0	0.0	0.0	-1.81

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Np02OH(amor)_____Np02OH(amor)	0.0	1.000	1.000	0.0	0.0	0.0	-3.13
Np02OH(aged)_____Np02OH(aged)	0.0	1.000	1.000	0.0	0.0	0.0	-2.43
2[Th(S04)2.7/2K2S04(16C,s)]_____	0.0	1.000	1.000	0.0	0.0	0.0	-4.77E+01
Th(S04)2.2K2S04.2H20(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-2.01E+01
Th(S04)2.K2S04.4H20(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.85E+01
Th(S04)2.Na2S04.6H20(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.51E+01
Th(S04)2.8H20(s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.92E+01
Th(S04)2.9H20(s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.92E+01
NaAm(C03)2.6H20(c)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.55
K2C03.3/2H20___Potassium_Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-1.11E+01
B(OH)3_____Borix_Acid_Solid	0.0	1.000	1.000	0.0	0.0	0.0	-2.11
K2NaH(C03)2.2H20___Potassium_Trona	0.0	1.000	1.000	0.0	0.0	0.0	-1.28E+01
K8H4(C03)6.3H20___K-Sequicarbonate	0.0	1.000	1.000	0.0	0.0	0.0	-4.50E+01
KNaC03.6H20_____K-Na-Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-6.44
NaOH(aq) to.titrate.base.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.95E+02
HCl(aq) to.titrate.acid.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.49E+02
K8B508.4H20____K-Pentaborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-7.02
K2B407.4H20___K-Tetraborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-6.40
Th++++ Th++++	0.0	0.0	0.4434	0.0	0.0	0.0	-2.62E+01
Na3H(C03)2.2H20_____Trona	0.0	1.000	1.000	0.0	0.0	0.0	-6.39
K2MgCa2(S04)4.2H20_____Polyhalite	0.0	1.000	1.000	0.0	0.0	0.0	-3.77
Ca4C12(OH)6.13H20__CaOxychloride_A	0.0	1.000	1.000	0.0	0.0	0.0	-2.18E+01
Na4Ca(S04)3.2H20_____Labile_Salt	0.0	1.000	1.000	0.0	0.0	0.0	-7.05E-01
Am(OH)3(s)_____Am(OH)3(s)	0.0	1.000	1.000	0.0	0.0	0.0	-8.13E-01

pH (-log[aH+]); pmH(-log[mH+])	9.2352	9.8878
Osmotic Coefficient=	1.271189	
Equilibrium RH (%) =	74.930812	
Ionic Strength (m) =	6.660117	
Density, kg/m3 =	1217.53	
fC02(g); log[fC02(g)]=	3.135E-06	-5.50

NOTES: - Water "molality" is mole fraction H20 in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -7.84414422E+03

Total Diagonal Inversions 589
Total Stoichiometric Reoptimizations 56

Oh/ac

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INPUT    file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_ERDA6_NESQ_970407_22.IN;1
INGUESS  file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]DUMMY.INGUESS;1
OUTPUT   file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_ERDA6_NESQ_970407_22.OUT;6
CHEMDAT  file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407_NESQ.CHEMDAT;8
Temperature is Hard Coded as 298.15K
Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Nesquehonite          FMT V2.2
FMT_970407_NESQ.chemdat
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy

Accuracy of reactions is              1.0000E-06
Minimum elemental abundance is        1.0000E-18
Number of Aqueous Species is           126
```

Table 6

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Information Only

Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Nesquehonite FMT V2.2
FMT_970407_NESQ.chemdat
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy
Pressure= 1.000 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.13289995E+02	1.11305737E+02	9.77567721E+01	9.85290506E+04	Hydrogen
6.55755271E+01	5.66727172E+01	4.97740910E+01	7.96355592E+05	Oxygen
7.19980915	6.17815175	5.42610101	1.24744814E+05	Sodium
1.10087747E-01	1.16165322E-01	1.02024812E-01	3.98899672E+03	Potassium
2.04429362	7.74238037E-02	6.79992004E-02	1.65272057E+03	Magnesium
1.01344192	1.60879610E-02	1.41296143E-02	5.66314940E+02	Calcium
6.96738842	5.95806841	5.23280785	1.85518737E+05	Chlorine
1.19112712	1.93110373E-01	1.69603537E-01	5.43748939E+03	Sulfur
1.00103149	3.54438887E-02	3.11293940E-02	3.73895152E+02	Carbon
0.0	0.0	0.0	0.0	PosIon:EL
0.0	0.0	0.0	0.0	NegIon:EL
0.0	0.0	0.0	0.0	Oxalate:EL
7.08491570E-02	7.47605014E-02	6.56600951E-02	7.09785628E+02	Boron
1.23704871E-02	1.30534202E-02	1.14644605E-02	9.16056249E+02	Bromine
0.0	0.0	0.0	0.0	Acetate:EL
1.10000068E-02	1.18682054E-03	1.04235188E-03	2.41865351E+02	Th(IV)
1.00041150E-03	2.44034482E-06	2.14328783E-06	5.20818943E-01	Am(III)
0.0	0.0	0.0	0.0	Pu(III)
1.00253377E-03	8.91914272E-07	7.83343809E-07	1.85690240E-01	Np(V)
0.0	0.0	0.0	0.0	Cl04:EL
0.0	0.0	0.0	0.0	Phosphorus
0.0	0.0	0.0	0.0	U(IV)
0.0	0.0	0.0	0.0	Lactate:EL
0.0	0.0	0.0	0.0	EDTA:EL
0.0	0.0	0.0	0.0	Citrate:EL
0.0	0.0	0.0	0.0	Electron:E
1.53072073E-14	1.61522669E-14	1.41860924E-14	0.0	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS	1315.37541171348	grams
H2O MASS	947.681672924009	grams
TDS(g/kg)	387.992877033248	g/kgH2O

Specified Solution Density

DENSITY	1219.03602412117	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	1.07902915556721	liters
TDS	340.763488078488	g/l

Density based on TDS and NaCl solutions 1219.03602412117 g/l
Percent relative error vs NaCl density 0.000000000000000 0 %

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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.14652E-01	7.48604E-01	0.9189	5.26046E+01	4.87518E+01	8.78273E+05	
Na+	Na+	6.17815	6.05934	0.9808	5.85492	5.42610	1.24745E+05	
Cl-	Cl-	5.95807	6.13739	1.030	5.64635	5.23281	1.85519E+05	
Mg(OH)2	Brucite	1.06310	1.000	1.000	1.00748	9.33689E-01	5.44524E+04	
CaSO4	Anhydrite	1.04283	1.000	1.000	9.88271E-01	9.15889E-01	1.24687E+05	
MgCO3.3H2O	Nesquehonite	1.01663	1.000	1.000	9.63442E-01	8.92879E-01	1.23539E+05	
SO4=	SO4=	1.93110E-01	3.56996E-03	1.8487E-02	1.83007E-01	1.69604E-01	1.62917E+04	
K+	K+	1.16165E-01	5.69985E-02	0.4907	1.10088E-01	1.02025E-01	3.98900E+03	
Mg++	Mg++	5.58333E-02	1.06894E-01	1.915	5.29122E-02	4.90368E-02	1.19184E+03	
B(OH)4-	B(OH)4-	5.29445E-02	5.23525E-03	9.8882E-02	5.01745E-02	4.64997E-02	3.66600E+03	
Br-	Br-	1.30534E-02	3.62498E-03	0.2777	1.23705E-02	1.14645E-02	9.16056E+02	
ThO2(am)	Hydrous_Thorium_Oxide	1.04205E-02	1.000	1.000	9.87528E-03	9.15200E-03	2.41647E+03	
Na3NpO2(CO3)2(s)	Na3NpO2(CO3)2(s)	1.05699E-03	1.000	1.000	1.00169E-03	9.28324E-04	4.25205E+02	
NaAm(CO3)2.6H2O(c)		1.05320E-03	1.000	1.000	9.98099E-04	9.24997E-04	4.57040E+02	
NaCl	Halite	1.39397	1.000	1.000	1.32104	1.22428	7.15504E+04	4.90E-08
MgCO3(aq)	MgCO3(aq)	1.37617E-02	1.37617E-02	1.000	1.30417E-02	1.20865E-02	1.01907E+03	3.63E-08
Ca++	Ca++	1.10770E-02	1.21698E-02	1.099	1.04975E-02	9.72866E-03	3.89925E+02	-6.24E-08
Na2Ca(SO4)2	Glauberite	1.04722E-02	1.000	1.000	9.92430E-03	9.19744E-03	2.55850E+03	1.14E-07
B(OH)3(aq)	B(OH)3(aq)	9.01155E-03	8.27681E-03	0.9185	8.54008E-03	7.91460E-03	4.89375E+02	8.25E-08
MgB(OH)4+	MgB(OH)4+	7.32427E-03	1.40342E-02	1.916	6.94108E-03	6.43271E-03	6.63496E+02	3.17E-09
HCO3-	HCO3-	6.66303E-03	2.26325E-03	0.3397	6.31443E-03	5.85196E-03	3.57069E+02	-3.35E-08
CO3=	CO3=	6.46438E-03	1.51800E-04	2.3482E-02	6.12618E-03	5.67749E-03	3.40702E+02	-1.02E-07
CaCO3(aq)	CaCO3(aq)	2.61694E-03	2.61694E-03	1.000	2.48003E-03	2.29839E-03	2.30044E+02	-7.63E-08
CaB(OH)4+	CaB(OH)4+	2.39398E-03	2.84800E-03	1.190	2.26873E-03	2.10257E-03	2.50035E+02	-6.90E-09
Th(CO3)5===	Th(CO3)5===	1.18514E-03	1.24342E-18	1.0492E-15	1.12313E-03	1.04087E-03	5.53832E+02	-2.74E-07
MgOH+	MgOH+	5.04543E-04	1.81917E-04	0.3606	4.78146E-04	4.43126E-04	1.83066E+01	1.06E-07
B4O5(OH)4=	B4O5(OH)4=	4.64666E-04	1.76378E-06	3.7958E-03	4.40356E-04	4.08104E-04	7.80565E+01	2.15E-07
B3O3(OH)4-	B3O3(OH)4-	4.09188E-04	4.39789E-05	0.1075	3.87780E-04	3.59379E-04	5.33524E+01	2.15E-07
OH-	OH-	2.05179E-05	1.10504E-05	0.5386	1.94445E-05	1.80203E-05	3.06477E-01	-7.54E-08
Am(CO3)3=-	Am(CO3)3=-	2.43703E-06	8.59478E-11	3.5267E-05	2.30953E-06	2.14038E-06	9.05439E-01	-5.14E-08
Th(OH)3(CO3)-	Th(OH)3(CO3)-	1.68323E-06	4.67439E-07	0.2777	1.59517E-06	1.47833E-06	5.07171E-01	-5.53E-08
CO2(aq)	CO2(aq)	1.28627E-06	4.48887E-06	3.490	1.21898E-06	1.12970E-06	4.97178E-02	-1.07E-08
NpO2(CO3)2=-	NpO2(CO3)2=-	4.34636E-07	8.76385E-11	2.0164E-04	4.11897E-07	3.81729E-07	1.48518E-01	-1.03E-07
NpO2(CO3)3==-	NpO2(CO3)3==-	2.66756E-07	1.05657E-15	3.9608E-09	2.52799E-07	2.34284E-07	1.05211E-01	-2.17E-07
NpO2CO3-	NpO2CO3-	1.89796E-07	2.09558E-08	0.1104	1.79866E-07	1.66693E-07	5.48512E-02	-1.62E-09
Am(CO3)2-	Am(CO3)2-	2.67550E-09	7.42995E-10	0.2777	2.53552E-09	2.34982E-09	8.53026E-04	2.56E-08
Th(OH)4(aq)	Th(OH)4(aq)	1.28297E-09	1.28297E-09	1.000	1.21585E-09	1.12680E-09	3.38115E-04	-2.43E-08
NpO2+	NpO2+	6.59088E-10	1.28835E-09	1.955	6.24606E-10	5.78859E-10	1.55740E-04	1.37E-08
HSO4-	HSO4-	4.20334E-10	2.32019E-10	0.5520	3.98343E-10	3.69168E-10	3.58335E-05	4.47E-08
AmCO3+	AmCO3+	3.25030E-10	9.25398E-11	0.2847	3.08025E-10	2.85465E-10	8.64984E-05	1.36E-07
Am(OH)2+	(after_Cm(III))	3.07084E-10	4.03367E-14	1.3135E-04	2.91018E-10	2.69704E-10	7.47119E-05	3.18E-07
H+	H+	1.53080E-10	6.82675E-10	4.460	1.45071E-10	1.34446E-10	1.35508E-07	-7.03E-09
NpO2OH(aq)	NpO2OH(aq)	6.70973E-11	6.97322E-12	0.1039	6.35868E-11	5.89297E-11	1.68571E-05	5.87E-08
Am(OH)3(aq)	(1e-9m_minimum)	3.53765E-12	3.53765E-12	1.000	3.35257E-12	3.10702E-12	9.13532E-07	2.04E-08
AmOH++	(after_Cm(III))	6.86043E-13	5.03444E-15	7.3384E-03	6.50150E-13	6.02532E-13	1.56663E-07	8.83E-08

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Am+++	Am+++	4.65117E-13	1.65493E-14	3.5581E-02	4.40783E-13	4.08500E-13	9.92654E-08	1.54E-07
Np02(OH)2-	Np02(OH)2-	2.85392E-13	4.53938E-15	1.5906E-02	2.70461E-13	2.50652E-13	7.59630E-08	9.82E-09
Th(SO4)3=	Th(SO4)3=	8.27354E-20	1.44594E-21	1.7477E-02	7.84069E-20	7.26643E-20	3.78007E-14	2.19E-07
Th(SO4)2(aq)	Th(SO4)2(aq)	1.86691E-21	5.91433E-20	31.68	1.76923E-21	1.63965E-21	6.95465E-16	1.28E-07
Mg2Cl(OH)3.4H20	MgOxychloride	0.0	1.000	1.000	0.0	0.0	0.0	-5.67E-01
Na2B407.10H20	Borax	0.0	1.000	1.000	0.0	0.0	0.0	-1.52
Ca(OH)2	Portlandite	0.0	1.000	1.000	0.0	0.0	0.0	-6.64
NaB02.4H20	Sodium_Metaborate	0.0	1.000	1.000	0.0	0.0	0.0	-2.08
Mg5(C03)4(OH)2.4H20_DISABLED	Hydro	0.0	1.000	1.000	0.0	0.0	0.0	-1.45E+03
CaMg(C03)2_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-8.06E+02
NaB02.NaCl.2H20	Teepleite_(20_C)	0.0	1.000	1.000	0.0	0.0	0.0	-1.53
NaB508.5H20	Sodium_Pentaborate	0.0	1.000	1.000	0.0	0.0	0.0	-6.11
Na2C03.H20	Thermonatrite	0.0	1.000	1.000	0.0	0.0	0.0	-2.86
Na2S04	Thenardite	0.0	1.000	1.000	0.0	0.0	0.0	-5.95E-01
Mg2CaCl6.12H20	Tachyhydrite	0.0	1.000	1.000	0.0	0.0	0.0	-1.80E+01
K2Ca(S04)2.H20	Syngenite	0.0	1.000	1.000	0.0	0.0	0.0	-1.98
KCl	Sylvite	0.0	1.000	1.000	0.0	0.0	0.0	-1.36
Na2C03.7H20	Na2C03-Heptahydrate	0.0	1.000	1.000	0.0	0.0	0.0	-2.67
Na3H(S04)2	Sesquisodium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.09E+01
K3H(S04)2	Sesquipotassium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.43E+01
Na2Ca(C03)2.2H20_DISABLED	Pi	0.0	1.000	1.000	0.0	0.0	0.0	-8.99E+02
K2Mg(S04)2.6H20	Picromerite/Schoen	0.0	1.000	1.000	0.0	0.0	0.0	-4.78
Na2C03.10H20	Natron	0.0	1.000	1.000	0.0	0.0	0.0	-2.69
NaHC03	Nahcolite	0.0	1.000	1.000	0.0	0.0	0.0	-1.46
K8H6(S04)7	Misenite	0.0	1.000	1.000	0.0	0.0	0.0	-7.13E+01
Na2S04.10H20	Mirabilite	0.0	1.000	1.000	0.0	0.0	0.0	-9.12E-01
KHS04	Mercallite	0.0	1.000	1.000	0.0	0.0	0.0	-1.15E+01
MgC03_DISABLED	M	0.0	1.000	1.000	0.0	0.0	0.0	-6.11E+02
Na4Ca(S04)3.2H20_DISABLED	Lab	0.0	1.000	1.000	0.0	0.0	0.0	-1.20E+03
K2Mg(S04)2.4H20	Leonite	0.0	1.000	1.000	0.0	0.0	0.0	-4.88
MgS04.H20	Kieserite	0.0	1.000	1.000	0.0	0.0	0.0	-3.42
KHC03	Kalicinite	0.0	1.000	1.000	0.0	0.0	0.0	-4.17
KMgClS04.3H20	Kainite	0.0	1.000	1.000	0.0	0.0	0.0	-4.06
MgS04.6H20	Hexahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-2.54
CaS04.2H20	Gypsum	0.0	1.000	1.000	0.0	0.0	0.0	-3.30E-02
CaNa2(C03)2.5H20_DISABLED	Ca	0.0	1.000	1.000	0.0	0.0	0.0	-1.02E+03
MgS04.7H20	Epsomite	0.0	1.000	1.000	0.0	0.0	0.0	-2.42
KMgCl3.6H20	Carnallite	0.0	1.000	1.000	0.0	0.0	0.0	-4.94
Ca2Cl2(OH)2.H20	CaOxychloride_B	0.0	1.000	1.000	0.0	0.0	0.0	-1.08E+01
Mg4(C03)3(OH)2.3H20_DISABLED	Hydro	0.0	1.000	1.000	0.0	0.0	0.0	-1.24E+03
CaCl2.4H20	CaCl2_Tetrahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-6.56
CaC03_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-6.29E+02
Na6C03(S04)2	Burkeite	0.0	1.000	1.000	0.0	0.0	0.0	-3.25
Na2Mg(S04)2.4H20	Bloedite	0.0	1.000	1.000	0.0	0.0	0.0	-2.46
MgCl2.6H20	Bischofite	0.0	1.000	1.000	0.0	0.0	0.0	-4.60
K2S04	Arcanite	0.0	1.000	1.000	0.0	0.0	0.0	-3.16
CaC03_DISABLED	A	0.0	1.000	1.000	0.0	0.0	0.0	-6.29E+02
CaCl2.6H20	Antarcticite	0.0	1.000	1.000	0.0	0.0	0.0	-5.24
NaK3(S04)2	Aphthitalite/Glaserite	0.0	1.000	1.000	0.0	0.0	0.0	-4.04
C02("solid",DISABLED)		0.0	1.000	1.000	0.0	0.0	0.0	-5.07E+02
K3Np02(C03)2(s)	K3Np02(C03)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-4.33
KNp02C03(s)	KNp02C03(s)	0.0	1.000	1.000	0.0	0.0	0.0	-3.51E-01

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2[NaNpO2CO3.7/2H2O(s)]	0.0	1.000	1.000	0.0	0.0	0.0	-2.55
NpO2OH(amor) NpO2OH(amor)	0.0	1.000	1.000	0.0	0.0	0.0	-5.07
NpO2OH(aged) NpO2OH(aged)	0.0	1.000	1.000	0.0	0.0	0.0	-4.37
2[Th(SO4)2.7/2K2SO4(16C,s)]	0.0	1.000	1.000	0.0	0.0	0.0	-4.69E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.97E+01
Th(SO4)2.K2SO4.4H2O(16C,s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.82E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.48E+01
Th(SO4)2.8H2O(s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.89E+01
Th(SO4)2.9H2O(s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.90E+01
Am(OH)3(s) Am(OH)3(s)	0.0	1.000	1.000	0.0	0.0	0.0	-2.47
AmOHCO3(c) AmOHCO3(c)	0.0	1.000	1.000	0.0	0.0	0.0	-1.36E-02
K2CO3.3/2H2O Potassium_Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-9.53
B(OH)3 Borix_Acid_Solid	0.0	1.000	1.000	0.0	0.0	0.0	-2.05
K2NaH(CO3)2.2H2O Potassium_Trona	0.0	1.000	1.000	0.0	0.0	0.0	-9.66
K8H4(CO3)6.3H2O K-Sequicarbonate	0.0	1.000	1.000	0.0	0.0	0.0	-3.56E+01
KNaCO3.6H2O K-Na-Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-4.92
NaOH(aq) to.titrate.base.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.95E+02
HCl(aq) to.titrate.acid.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.49E+02
KB5O8.4H2O K-Pentaborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-6.78
K2B4O7.4H2O K-Tetraborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-6.27
Na3H(CO3)2.2H2O Trona	0.0	1.000	1.000	0.0	0.0	0.0	-3.32
Ca4Cl2(OH)6.13H2O CaOxychloride_A	0.0	1.000	1.000	0.0	0.0	0.0	-2.22E+01
K2MgCa2(SO4)4.2H2O Polyhalite	0.0	1.000	1.000	0.0	0.0	0.0	-3.59
Th++++ Th++++	0.0	0.0	0.4076	0.0	0.0	0.0	-2.59E+01

pH (-log[aH+]); pmH(-log[mH+]) 9.1658 9.8151
Osmotic Coefficient= 1.272623
Equilibrium RH (%) = 74.860425
Ionic Strength (m) = 6.723099
Density, kg/m3 = 1219.04
fCO2(g); log[fCO2(g)]= 1.361E-04 -3.87

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -7.84040976E+03

Total Diagonal Inversions 539
Total Stoichiometric Reoptimizations 52

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INPUT file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_SPC_HMAG4323_970407_22.IN;1
INGUESS file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]DUMMY.INGUESS;1
OUTPUT file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_SPC_HMAG4323_970407_22.OUT;2
CHEMDAT file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407_HMAG4323.CHEMDAT;6
Temperature is Hard Coded as 298.15K
Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Hydromagnesite4232 FMT V2.2
FMT_970407_HMAG4323.chemdat HYDROMAGNESITE ADDED
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy

Accuracy of reactions is	1.0000E-06
Minimum elemental abundance is	1.0000E-18
Number of Aqueous Species is	126

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Table 7

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Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Hydromagnesite4232 FMT V2.2
FMT_970407_HMAG4323.chemdat HYDROMAGNESITE ADDED
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy
Pressure= 1.000 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.36767180E+02	1.11125029E+02	9.69571705E+01	9.77231321E+04	Hydrogen
7.99098636E+01	5.58605885E+01	4.87386562E+01	7.79789256E+05	Oxygen
5.69295395	4.68470928	4.08743340	9.39691537E+04	Sodium
1.04775026	1.06745730	9.31362090E-01	3.64146744E+04	Potassium
6.80724482	5.09375430E-01	4.44432732E-01	1.08019376E+04	Magnesium
1.03305403	3.29234186E-02	2.87258553E-02	1.15133228E+03	Calcium
9.81438839	6.67598166	5.82482899	2.06507662E+05	Chlorine
1.06024227	6.06495690E-02	5.29170668E-02	1.69652116E+03	Sulfur
1.00104081	5.37821567E-04	4.69252136E-04	5.63618741	Carbon
0.0	0.0	0.0	0.0	PosIon:EL
0.0	0.0	0.0	0.0	NegIon:EL
0.0	0.0	0.0	0.0	Oxalate:EL
2.71882500E-02	2.77261605E-02	2.41912204E-02	2.61507092E+02	Boron
1.35941250E-02	1.38630803E-02	1.20956102E-02	9.66487636E+02	Bromine
0.0	0.0	0.0	0.0	Acetate:EL
1.00497956E-03	1.74893178E-08	1.52595214E-08	3.54079036E-03	Th(IV)
1.00438590E-03	8.31128677E-08	7.25164126E-08	1.76214883E-02	Am(III)
0.0	0.0	0.0	0.0	Pu(III)
1.00263669E-03	1.23214086E-07	1.07504936E-07	2.54838515E-02	Np(V)
0.0	0.0	0.0	0.0	ClO4:EL
0.0	0.0	0.0	0.0	Phosphorus
0.0	0.0	0.0	0.0	U(IV)
0.0	0.0	0.0	0.0	Lactate:EL
0.0	0.0	0.0	0.0	EDTA:EL
0.0	0.0	0.0	0.0	Citrate:EL
0.0	0.0	0.0	0.0	Electron:E
-8.80070450E-15	-8.97482352E-15	-7.83058056E-15	0.0	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS	1381.58270717752	grams
H2O MASS	980.599170279779	grams
TDS(g/kg)	408.916863332991	g/kgH2O

Specified Solution Density

DENSITY	1229.28734709803	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	1.12388914637331	liters
TDS	356.782106306194	g/l

Density based on TDS and NaCl solutions 1229.28734709803 g/l
Percent relative error vs NaCl density 0.000000000000000 0 %

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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.09536E-01	7.29339E-01	0.9009	5.44318E+01	4.84316E+01	8.72505E+05	
Cl-	Cl-	6.67598	8.18249	1.226	6.54646	5.82483	2.06508E+05	
Na+	Na+	4.68471	4.54489	0.9702	4.59382	4.08743	9.39692E+04	
Mg2Cl(OH)3.4H2O	MgOxychloride	2.21170	1.000	1.000	2.16879	1.92972	3.99734E+05	
K+	K+	1.06746	4.84416E-01	0.4538	1.04675	9.31362E-01	3.64147E+04	
CaSO4	Anhydrite	1.02057	1.000	1.000	1.00077	8.90452E-01	1.21224E+05	
Mg(OH)2	Brucite	6.51460E-01	1.000	1.000	6.38821E-01	5.68402E-01	3.31490E+04	
Mg4(CO3)3(OH)2.3H2O	Hydromagne4323	3.39421E-01	1.000	1.000	3.32836E-01	2.96146E-01	1.08185E+05	
SO4=	SO4=	6.06496E-02	1.20548E-03	1.9876E-02	5.94729E-02	5.29171E-02	5.08309E+03	
Br-	Br-	1.38631E-02	3.79232E-03	0.2736	1.35941E-02	1.20956E-02	9.66488E+02	
MgB(OH)4+	MgB(OH)4+	1.16306E-02	2.56341E-02	2.204	1.14049E-02	1.01477E-02	1.04668E+03	
ThO2(am)	Hydrous_Thorium_Oxide	1.02485E-03	1.000	1.000	1.00496E-03	8.94183E-04	2.36097E+02	
AmOHCO3(c)	AmOHCO3(c)	1.02417E-03	1.000	1.000	1.00430E-03	8.93597E-04	2.85966E+02	
KNpO2CO3(s)	KNpO2CO3(s)	1.02235E-03	1.000	1.000	1.00252E-03	8.92006E-04	3.28396E+02	
NaCl	Halite	1.12088	1.000	1.000	1.09913	9.77972E-01	5.71554E+04	-3.12E-09
Mg++	Mg++	4.95582E-01	1.00696	2.032	4.85967E-01	4.32398E-01	1.05094E+04	3.61E-09
Ca++	Ca++	3.16324E-02	3.60402E-02	1.139	3.10187E-02	2.75994E-02	1.10618E+03	-5.30E-09
B(OH)4-	B(OH)4-	9.93060E-03	1.01510E-03	0.1022	9.73794E-03	8.66450E-03	6.83102E+02	-2.91E-07
B(OH)3(aq)	B(OH)3(aq)	4.81580E-03	4.92564E-03	1.023	4.72237E-03	4.20181E-03	2.59806E+02	2.42E-07
MgOH+	MgOH+	1.73931E-03	5.58347E-04	0.3210	1.70556E-03	1.51755E-03	6.26936E+01	-2.14E-09
CaB(OH)4+	CaB(OH)4+	1.26574E-03	1.63536E-03	1.292	1.24118E-03	1.10436E-03	1.31330E+02	3.01E-08
MgCO3(aq)	MgCO3(aq)	4.23390E-04	4.23390E-04	1.000	4.15176E-04	3.69410E-04	3.11465E+01	-1.04E-09
HCO3-	HCO3-	6.07667E-05	2.21029E-05	0.3637	5.95878E-05	5.30192E-05	3.23508	-1.82E-09
CO3=	CO3=	2.82196E-05	4.95768E-07	1.7568E-02	2.76721E-05	2.46217E-05	1.47753	-6.64E-09
CaCO3(aq)	CaCO3(aq)	2.53109E-05	2.53109E-05	1.000	2.48198E-05	2.20839E-05	2.21036	-4.07E-09
B3O3(OH)4-	B3O3(OH)4-	1.96779E-05	3.26574E-06	0.1660	1.92961E-05	1.71690E-05	2.54887	-5.61E-09
OH-	OH-	7.71536E-06	3.60038E-06	0.4667	7.56567E-06	6.73169E-06	1.14488E-01	-2.70E-09
B4O5(OH)4=	B4O5(OH)4=	6.10041E-06	2.67545E-08	4.3857E-03	5.98206E-06	5.32264E-06	1.01804	-1.89E-08
Am(OH)2+	(after_Cm(III))	8.10022E-08	4.15249E-12	5.1264E-05	7.94306E-08	7.06748E-08	1.95780E-02	-8.03E-09
NpO2CO3-	NpO2CO3-	7.23831E-08	5.52938E-09	7.6391E-02	7.09788E-08	6.31546E-08	2.07814E-02	-3.70E-09
NpO2+	NpO2+	4.72672E-08	1.04088E-07	2.202	4.63502E-08	4.12409E-08	1.10957E-02	2.44E-09
CO2(aq)	CO2(aq)	4.11878E-08	1.34550E-07	3.267	4.03888E-08	3.59366E-08	1.58156E-03	1.57E-09
Th(OH)3(CO3)-	Th(OH)3(CO3)-	1.62582E-08	4.44752E-09	0.2736	1.59428E-08	1.41854E-08	4.86657E-03	-1.15E-09
NpO2OH(aq)	NpO2OH(aq)	2.32016E-09	1.83556E-10	7.9113E-02	2.27515E-09	2.02435E-09	5.79075E-04	-2.45E-09
NpO2(CO3)2=-	NpO2(CO3)2=-	1.21969E-09	7.55224E-14	6.1920E-05	1.19602E-09	1.06418E-09	4.14037E-04	-1.06E-08
Th(OH)4(aq)	Th(OH)4(aq)	1.21778E-09	1.21778E-09	1.000	1.19416E-09	1.06252E-09	3.18828E-04	7.94E-10
AmCO3+	AmCO3+	1.12610E-09	2.93093E-10	0.2603	1.10426E-09	9.82532E-10	2.97716E-04	-4.05E-10
H+	H+	4.30229E-10	2.04137E-09	4.745	4.21882E-10	3.75377E-10	3.78343E-07	3.40E-09
Am+++	Am+++	3.68946E-10	1.60490E-11	4.3500E-02	3.61788E-10	3.21908E-10	7.82235E-05	2.41E-09
HSO4-	HSO4-	3.07434E-10	2.34275E-10	0.7620	3.01470E-10	2.68238E-10	2.60367E-05	6.23E-09
Am(CO3)3=-	Am(CO3)3=-	2.82206E-10	2.90354E-15	1.0289E-05	2.76731E-10	2.46226E-10	1.04161E-04	-1.18E-08
AmOH++	(after_Cm(III))	1.86704E-10	1.59071E-12	8.5200E-03	1.83082E-10	1.62900E-10	4.23552E-05	6.54E-09
Am(OH)3(aq)	(1e-9m_minimum)	1.18657E-10	1.18657E-10	1.000	1.16355E-10	1.03529E-10	3.04398E-05	1.83E-10
Am(CO3)2-	Am(CO3)2-	2.80949E-11	7.68549E-12	0.2736	2.75498E-11	2.45129E-11	8.89864E-06	-2.37E-09
NpO2(CO3)3==-	NpO2(CO3)3==-	2.04378E-11	2.97363E-21	1.4550E-10	2.00413E-11	1.78321E-11	8.00794E-06	-2.59E-08

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Th(CO3)5===	Th(CO3)5===	1.33218E-11	3.89163E-29	2.9212E-18	1.30634E-11	1.16234E-11	6.18461E-06	-6.42E-08
NpO2(OH)2-	NpO2(OH)2-	3.50704E-12	3.89315E-14	1.1101E-02	3.43900E-12	3.05991E-12	9.27341E-07	-4.54E-09
Th(SO4)3=	Th(SO4)3=	8.31974E-20	4.68935E-21	5.6364E-02	8.15833E-20	7.25902E-20	3.77622E-14	5.26E-09
Th(SO4)2(aq)	Th(SO4)2(aq)	1.18237E-20	5.68030E-19	48.04	1.15943E-20	1.03162E-20	4.37566E-15	1.13E-08
Th++++	Th++++	0.0	0.0	0.3873	0.0	0.0	0.0	-2.40E+01
K2MgCa2(SO4)4.2H2O	Polyhalite	0.0	1.000	1.000	0.0	0.0	0.0	-1.72
Ca(OH)2	Portlandite	0.0	1.000	1.000	0.0	0.0	0.0	-7.14
K2NaH(CO3)2.2H2O	Potassium_Trona	0.0	1.000	1.000	0.0	0.0	0.0	-1.24E+01
K8H4(CO3)6.3H2O	K-Sequicarbonate	0.0	1.000	1.000	0.0	0.0	0.0	-4.12E+01
NaB5O8.5H2O	Sodium_Pentaborate	0.0	1.000	1.000	0.0	0.0	0.0	-7.81
Na2CO3.H2O	Thermonatrite	0.0	1.000	1.000	0.0	0.0	0.0	-5.61
Na2SO4	Thenardite	0.0	1.000	1.000	0.0	0.0	0.0	-1.32
Mg2CaCl6.12H2O	Tachyhydrite	0.0	1.000	1.000	0.0	0.0	0.0	-1.50E+01
K2Ca(SO4)2.H2O	Syngenite	0.0	1.000	1.000	0.0	0.0	0.0	-5.99E-01
KCl	Sylvite	0.0	1.000	1.000	0.0	0.0	0.0	-3.02E-01
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.0	1.000	1.000	0.0	0.0	0.0	-5.49
Na3H(SO4)2	Sesquisodium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.17E+01
K3H(SO4)2	Sesquipotassium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.19E+01
Mg5(CO3)4(OH)2.4H2O_DISABLED	Hydro	0.0	1.000	1.000	0.0	0.0	0.0	-1.46E+03
CaMg(CO3)2_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-8.10E+02
Na2Ca(CO3)2.2H2O_DISABLED	Pi	0.0	1.000	1.000	0.0	0.0	0.0	-9.04E+02
K2Mg(SO4)2.6H2O	Picromerite/Schoen	0.0	1.000	1.000	0.0	0.0	0.0	-2.96
MgCO3.3H2O	Nesquehonite	0.0	1.000	1.000	0.0	0.0	0.0	-1.55
Na2CO3.10H2O	Natron	0.0	1.000	1.000	0.0	0.0	0.0	-5.54
NaHCO3	Nahcolite	0.0	1.000	1.000	0.0	0.0	0.0	-3.60
K8H6(SO4)7	Misenite	0.0	1.000	1.000	0.0	0.0	0.0	-6.43E+01
Na2SO4.10H2O	Mirabilite	0.0	1.000	1.000	0.0	0.0	0.0	-1.75
KHSO4	Mercallite	0.0	1.000	1.000	0.0	0.0	0.0	-1.05E+01
MgCO3_DISABLED	M	0.0	1.000	1.000	0.0	0.0	0.0	-6.13E+02
Na4Ca(SO4)3.2H2O	Labile_Salt	0.0	1.000	1.000	0.0	0.0	0.0	-2.17
K2Mg(SO4)2.4H2O	Leonite	0.0	1.000	1.000	0.0	0.0	0.0	-3.03
MgSO4.H2O	Kieserite	0.0	1.000	1.000	0.0	0.0	0.0	-2.93
KHCO3	Kalicinite	0.0	1.000	1.000	0.0	0.0	0.0	-5.25
KMgClSO4.3H2O	Kainite	0.0	1.000	1.000	0.0	0.0	0.0	-2.54
MgSO4.6H2O	Hexahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-2.10
CaSO4.2H2O	Gypsum	0.0	1.000	1.000	0.0	0.0	0.0	-5.57E-02
Na2Ca(SO4)2	Glauberite	0.0	1.000	1.000	0.0	0.0	0.0	-7.21E-01
CaNa2(CO3)2.5H2O_DISABLED	Ca	0.0	1.000	1.000	0.0	0.0	0.0	-1.03E+03
MgSO4.7H2O	Epsomite	0.0	1.000	1.000	0.0	0.0	0.0	-1.99
KMgCl3.6H2O	Carnallite	0.0	1.000	1.000	0.0	0.0	0.0	-2.73
Ca2Cl2(OH)2.H2O	CaOxychloride_B	0.0	1.000	1.000	0.0	0.0	0.0	-1.06E+01
NaBO2.NaCl.2H2O	Teepleite_(20_C)	0.0	1.000	1.000	0.0	0.0	0.0	-2.37
CaCl2.4H2O	CaCl2_Tetrahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-5.88
CaCO3_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-6.32E+02
Na6CO3(SO4)2	Burkeite	0.0	1.000	1.000	0.0	0.0	0.0	-7.43
Na2Mg(SO4)2.4H2O	Bloedite	0.0	1.000	1.000	0.0	0.0	0.0	-2.72
MgCl2.6H2O	Bischofite	0.0	1.000	1.000	0.0	0.0	0.0	-3.45
K2SO4	Arcanite	0.0	1.000	1.000	0.0	0.0	0.0	-1.77
CaCO3_DISABLED	A	0.0	1.000	1.000	0.0	0.0	0.0	-6.32E+02
CaCl2.6H2O	Antarcticite	0.0	1.000	1.000	0.0	0.0	0.0	-4.58
NaK3(SO4)2	Aphthitalite/Glaserite	0.0	1.000	1.000	0.0	0.0	0.0	-2.32
CO2("solid",DISABLED)		0.0	1.000	1.000	0.0	0.0	0.0	-5.09E+02

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K3NpO2(CO3)2(s)____K3NpO2(CO3)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-4.61
Na3NpO2(CO3)2(s)__Na3NpO2(CO3)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-3.44
NpO2OH(amor)_____NpO2OH(amor)	0.0	1.000	1.000	0.0	0.0	0.0	-3.65
NpO2OH(aged)_____NpO2OH(aged)	0.0	1.000	1.000	0.0	0.0	0.0	-2.95
2[Th(SO4)2.7/2K2SO4(16C,s)]_____	0.0	1.000	1.000	0.0	0.0	0.0	-3.52E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.60E+01
Th(SO4)2.K2SO4.4H2O(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.59E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.46E+01
Th(SO4)2.8H2O(s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.80E+01
Th(SO4)2.9H2O(s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.81E+01
NaAm(CO3)2.6H2O(c)_____	0.0	1.000	1.000	0.0	0.0	0.0	-2.18
Am(OH)3(s)_____Am(OH)3(s)	0.0	1.000	1.000	0.0	0.0	0.0	-9.40E-01
B(OH)3_____Borix_Acid_Solid	0.0	1.000	1.000	0.0	0.0	0.0	-2.28
KB5O8.4H2O____K-Pentaborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-7.42
K2B4O7.4H2O___K-Tetraborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-6.25
Na2B4O7.10H2O_____Borax	0.0	1.000	1.000	0.0	0.0	0.0	-3.68
NaOH(aq) to.titrate.base.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.95E+02
HCl(aq) to.titrate.acid.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.48E+02
Na3H(CO3)2.2H2O_____Trona	0.0	1.000	1.000	0.0	0.0	0.0	-8.22
NaBO2.4H2O_____Sodium_Metaborate	0.0	1.000	1.000	0.0	0.0	0.0	-2.94
K2CO3.3/2H2O___Potassium_Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-1.02E+01
Ca4Cl2(OH)6.13H2O__CaOxychloride_A	0.0	1.000	1.000	0.0	0.0	0.0	-2.31E+01
KNaCO3.6H2O_____K-Na-Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-6.67
2[NaNpO2CO3.7/2H2O(s)]_____	0.0	1.000	1.000	0.0	0.0	0.0	-4.04

pH (-log[aH+]); pmH(-log[mH+]) 8.6901 9.3663
Osmotic Coefficient= 1.341477
Equilibrium RH (%) = 72.933903
Ionic Strength (m) = 7.409130
Density, kg/m3 = 1229.29
fCO2(g); log[fCO2(g)]= 4.080E-06 -5.39

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -1.00705329E+04

Total Diagonal Inversions 630
Total Stoichiometric Reoptimizations 60

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INPUT    file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_SPC_HMAG5424_970407_22.IN;2
INGUESS  file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]DUMMY.INGUESS;1
OUTPUT   file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_SPC_HMAG5424_970407_22.OUT;3
CHEMDAT  file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407_HMAG5424.CHEMDAT;4
Temperature is Hard Coded as 298.15K
Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Hydromagnesite5424        FMT V2.2
FMT_970407_HMAG5424.chemdat                  HYDROMAGNESITE ADDED
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy

Accuracy of reactions is              1.0000E-06
Minimum elemental abundance is        1.0000E-18
Number of Aqueous Species is           126
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Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Hydromagnesite5424 FMT V2.2
FMT_970407_HMAG5424.chemdat HYDROMAGNESITE ADDED
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy
Pressure= 1.000 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.36767180E+02	1.11125015E+02	9.69574659E+01	9.77234299E+04	Hydrogen
7.99098636E+01	5.58601996E+01	4.87384715E+01	7.79786301E+05	Oxygen
5.69295395	4.68471257	4.08744924	9.39695179E+04	Sodium
1.04775026	1.06745883	9.31366380E-01	3.64148421E+04	Potassium
6.80724482	5.09262502E-01	4.44335611E-01	1.07995770E+04	Magnesium
1.03305403	3.29195802E-02	2.87225974E-02	1.15120170E+03	Calcium
9.81438839	6.67599572	5.82485973	2.06508752E+05	Chlorine
1.06024227	6.06457699E-02	5.29139199E-02	1.69642027E+03	Sulfur
1.00104081	4.13187987E-04	3.60509828E-04	4.33008354	Carbon
0.0	0.0	0.0	0.0	PosIon:EL
0.0	0.0	0.0	0.0	NegIon:EL
0.0	0.0	0.0	0.0	Oxalate:EL
2.71882500E-02	2.77261999E-02	2.41913315E-02	2.61508293E+02	Boron
1.35941250E-02	1.38631000E-02	1.20956657E-02	9.66492075E+02	Bromine
0.0	0.0	0.0	0.0	Acetate:EL
1.00497956E-03	1.37114670E-08	1.19633648E-08	2.77595643E-03	Th(IV)
1.00438590E-03	1.07633709E-07	9.39112728E-08	2.28204393E-02	Am(III)
0.0	0.0	0.0	0.0	Pu(III)
1.00263669E-03	1.37882922E-07	1.20303954E-07	2.85178358E-02	Np(V)
0.0	0.0	0.0	0.0	ClO4:EL
0.0	0.0	0.0	0.0	Phosphorus
0.0	0.0	0.0	0.0	U(IV)
0.0	0.0	0.0	0.0	Lactate:EL
0.0	0.0	0.0	0.0	EDTA:EL
0.0	0.0	0.0	0.0	Citrate:EL
0.0	0.0	0.0	0.0	Electron:E
5.75362954E-15	5.86747153E-15	5.11941590E-15	0.0	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS	1381.57083223157	grams
H2O MASS	980.597777461594	grams
TDS(g/kg)	408.906754620580	g/kgH2O

Specified Solution Density

DENSITY	1229.28242702612	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	1.12388398455664	liters
TDS	356.774418249366	g/l

Density based on TDS and NaCl solutions 1229.28242702612 g/l
Percent relative error vs NaCl density 0.000000000000000 0 %

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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.09537E-01	7.29341E-01	0.9009	5.44317E+01	4.84318E+01	8.72508E+05	
Cl-	Cl-	6.67600	8.18246	1.226	6.54647	5.82486	2.06509E+05	
Na+	Na+	4.68471	4.54491	0.9702	4.59382	4.08745	9.39695E+04	
Mg2Cl(OH)3.4H2O	Mgoxychloride	2.21170	1.000	1.000	2.16879	1.92972	3.99734E+05	
K+	K+	1.06746	4.84418E-01	0.4538	1.04675	9.31366E-01	3.64148E+04	
CaSO4	Anhydrite	1.02057	1.000	1.000	1.00077	8.90459E-01	1.21225E+05	
Mg(OH)2	Brucite	7.36289E-01	1.000	1.000	7.22004E-01	6.42418E-01	3.74656E+04	
Mg5(CO3)4(OH)2.4H2O	HydroMagne5424	2.54597E-01	1.000	1.000	2.49657E-01	2.22138E-01	1.03880E+05	
SO4=	SO4=	6.06458E-02	1.20540E-03	1.9876E-02	5.94691E-02	5.29139E-02	5.08278E+03	
Br-	Br-	1.38631E-02	3.79233E-03	0.2736	1.35941E-02	1.20957E-02	9.66492E+02	
MgB(OH)4+	MgB(OH)4+	1.16305E-02	2.56340E-02	2.204	1.14048E-02	1.01477E-02	1.04667E+03	
ThO2(am)	Hydrous_Thorium_Oxide	1.02485E-03	1.000	1.000	1.00497E-03	8.94190E-04	2.36099E+02	
AmOHCO3(c)	AmOHCO3(c)	1.02415E-03	1.000	1.000	1.00428E-03	8.93580E-04	2.85960E+02	
KNpO2CO3(s)	KNpO2CO3(s)	1.02234E-03	1.000	1.000	1.00250E-03	8.91997E-04	3.28393E+02	
NaCl	Halite	1.12088	1.000	1.000	1.09914	9.77979E-01	5.71558E+04	8.62E-12
Mg++	Mg++	4.95568E-01	1.00695	2.032	4.85952E-01	4.32387E-01	1.05092E+04	2.80E-10
Ca++	Ca++	3.16343E-02	3.60426E-02	1.139	3.10205E-02	2.76012E-02	1.10626E+03	1.70E-09
B(OH)4-	B(OH)4-	9.93069E-03	1.01510E-03	0.1022	9.73801E-03	8.66460E-03	6.83110E+02	4.49E-08
B(OH)3(aq)	B(OH)3(aq)	4.81580E-03	4.92564E-03	1.023	4.72236E-03	4.20182E-03	2.59807E+02	-1.86E-08
MgOH+	MgOH+	1.73928E-03	5.58344E-04	0.3210	1.70554E-03	1.51754E-03	6.26929E+01	2.18E-11
CaB(OH)4+	CaB(OH)4+	1.26582E-03	1.63548E-03	1.292	1.24126E-03	1.10444E-03	1.31339E+02	1.09E-08
MgCO3(aq)	MgCO3(aq)	3.25260E-04	3.25260E-04	1.000	3.18949E-04	2.83792E-04	2.39277E+01	1.44E-11
HCO3-	HCO3-	4.66829E-05	1.69802E-05	0.3637	4.57771E-05	4.07312E-05	2.48530	-4.31E-11
CO3=	CO3=	2.16791E-05	3.80867E-07	1.7568E-02	2.12584E-05	1.89152E-05	1.13508	3.03E-10
B3O3(OH)4-	B3O3(OH)4-	1.96779E-05	3.26575E-06	0.1660	1.92961E-05	1.71691E-05	2.54888	5.04E-08
CaCO3(aq)	CaCO3(aq)	1.94460E-05	1.94460E-05	1.000	1.90687E-05	1.69668E-05	1.69819	1.18E-09
OH-	OH-	7.71540E-06	3.60040E-06	0.4667	7.56570E-06	6.73175E-06	1.14489E-01	1.42E-10
B4O5(OH)4=	B4O5(OH)4=	6.10040E-06	2.67546E-08	4.3857E-03	5.98204E-06	5.32265E-06	1.01804	6.95E-08
Am(OH)2+	(after_Cm(III))	1.05442E-07	5.40525E-12	5.1263E-05	1.03396E-07	9.19988E-08	2.54850E-02	-3.15E-10
NpO2CO3-	NpO2CO3-	7.23830E-08	5.52936E-09	7.6390E-02	7.09787E-08	6.31548E-08	2.07815E-02	-2.60E-11
NpO2+	NpO2+	6.15261E-08	1.35488E-07	2.202	6.03324E-08	5.36820E-08	1.44430E-02	7.24E-11
CO2(aq)	CO2(aq)	3.16419E-08	1.03365E-07	3.267	3.10280E-08	2.76078E-08	1.21501E-03	9.09E-11
Th(OH)3(CO3)-	Th(OH)3(CO3)-	1.24901E-08	3.41674E-09	0.2736	1.22478E-08	1.08977E-08	3.73867E-03	5.68E-11
NpO2OH(aq)	NpO2OH(aq)	3.02013E-09	2.38932E-10	7.9113E-02	2.96153E-09	2.63509E-09	7.53779E-04	-1.30E-10
Th(OH)4(aq)	Th(OH)4(aq)	1.21779E-09	1.21779E-09	1.000	1.19416E-09	1.06253E-09	3.18831E-04	5.83E-11
AmCO3+	AmCO3+	1.12610E-09	2.93092E-10	0.2603	1.10425E-09	9.82527E-10	2.97715E-04	3.42E-11
NpO2(CO3)2=-	NpO2(CO3)2=-	9.37009E-10	5.80189E-14	6.1919E-05	9.18829E-10	8.17548E-10	3.18080E-04	5.00E-10
Am+++	Am+++	4.80231E-10	2.08906E-11	4.3501E-02	4.70914E-10	4.19005E-10	1.01818E-04	5.86E-10
H+	H+	4.30225E-10	2.04136E-09	4.745	4.21878E-10	3.75375E-10	3.78341E-07	1.35E-10
HSO4-	HSO4-	3.07416E-10	2.34259E-10	0.7620	3.01452E-10	2.68223E-10	2.60352E-05	-1.32E-09
AmOH++	(after_Cm(III))	2.43029E-10	2.07059E-12	8.5200E-03	2.38314E-10	2.12045E-10	5.51331E-05	1.00E-10
Am(CO3)3=-	Am(CO3)3=-	1.66549E-10	1.71363E-15	1.0289E-05	1.63318E-10	1.45316E-10	6.14725E-05	5.29E-10
Am(OH)3(aq)	(1e-9m_minimum)	1.54456E-10	1.54456E-10	1.000	1.51459E-10	1.34764E-10	3.96235E-05	4.37E-11
Am(CO3)2-	Am(CO3)2-	2.15833E-11	5.90424E-12	0.2736	2.11646E-11	1.88316E-11	6.83623E-06	2.76E-11
NpO2(CO3)3==-	NpO2(CO3)3==-	1.20619E-11	1.75499E-21	1.4550E-10	1.18278E-11	1.05241E-11	4.72610E-06	2.24E-09

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Np02(OH)2-	Np02(OH)2-	4.56510E-12	5.06768E-14	1.1101E-02	4.47653E-12	3.98309E-12	1.20712E-06	-1.45E-10
Th(C03)5===	Th(C03)5===	3.56405E-12	1.04136E-29	2.9218E-18	3.49490E-12	3.10966E-12	1.65460E-06	4.58E-09
Th(S04)3=	Th(S04)3=	8.31790E-20	4.68834E-21	5.6365E-02	8.15651E-20	7.25743E-20	3.77540E-14	-3.19E-09
Th(S04)2(aq)	Th(S04)2(aq)	1.18218E-20	5.67945E-19	48.04	1.15925E-20	1.03146E-20	4.37499E-15	-2.11E-09
Th++++	Th++++	0.0	0.0	0.3873	0.0	0.0	0.0	-2.40E+01
Ca(OH)2	Portlandite	0.0	1.000	1.000	0.0	0.0	0.0	-7.14
K2NaH(C03)2.2H20	Potassium_Trona	0.0	1.000	1.000	0.0	0.0	0.0	-1.27E+01
K8H4(C03)6.3H20	K-Sequicarbonate	0.0	1.000	1.000	0.0	0.0	0.0	-4.19E+01
NaB508.5H20	Sodium_Pentaborate	0.0	1.000	1.000	0.0	0.0	0.0	-7.81
Na2C03.H20	Thermonatrite	0.0	1.000	1.000	0.0	0.0	0.0	-5.72
Na2S04	Thenardite	0.0	1.000	1.000	0.0	0.0	0.0	-1.32
Mg2CaCl6.12H20	Tachyhydrite	0.0	1.000	1.000	0.0	0.0	0.0	-1.50E+01
K2Ca(S04)2.H20	Syngenite	0.0	1.000	1.000	0.0	0.0	0.0	-5.99E-01
KCl	Sylvite	0.0	1.000	1.000	0.0	0.0	0.0	-3.02E-01
Na2C03.7H20	Na2C03-Heptahydrate	0.0	1.000	1.000	0.0	0.0	0.0	-5.60
Na3H(S04)2	Sesquisodium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.17E+01
K3H(S04)2	Sesquipotassium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.19E+01
Mg4(C03)3(OH)2.3H20	HydroMagne4323	0.0	1.000	1.000	0.0	0.0	0.0	-3.44E-01
CaMg(C03)2	DISABLED	0.0	1.000	1.000	0.0	0.0	0.0	-8.10E+02
Na2Ca(C03)2.2H20	DISABLED_Pi	0.0	1.000	1.000	0.0	0.0	0.0	-9.04E+02
K2Mg(S04)2.6H20	Picromerite/Schoen	0.0	1.000	1.000	0.0	0.0	0.0	-2.96
MgC03.3H20	Nesquehonite	0.0	1.000	1.000	0.0	0.0	0.0	-1.66
Na2C03.10H20	Natron	0.0	1.000	1.000	0.0	0.0	0.0	-5.65
NaHC03	Nahcolite	0.0	1.000	1.000	0.0	0.0	0.0	-3.71
K8H6(S04)7	Misenite	0.0	1.000	1.000	0.0	0.0	0.0	-6.43E+01
Na2S04.10H20	Mirabilite	0.0	1.000	1.000	0.0	0.0	0.0	-1.75
KHS04	Mercallite	0.0	1.000	1.000	0.0	0.0	0.0	-1.05E+01
MgC03_DISABLED	M	0.0	1.000	1.000	0.0	0.0	0.0	-6.13E+02
Na4Ca(S04)3.2H20	Labile_Salt	0.0	1.000	1.000	0.0	0.0	0.0	-2.17
K2Mg(S04)2.4H20	Leonite	0.0	1.000	1.000	0.0	0.0	0.0	-3.03
MgS04.H20	Kieserite	0.0	1.000	1.000	0.0	0.0	0.0	-2.93
KHC03	Kalicinite	0.0	1.000	1.000	0.0	0.0	0.0	-5.37
KMgClS04.3H20	Kainite	0.0	1.000	1.000	0.0	0.0	0.0	-2.54
MgS04.6H20	Hexahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-2.10
CaS04.2H20	Gypsum	0.0	1.000	1.000	0.0	0.0	0.0	-5.57E-02
Na2Ca(S04)2	Glauberite	0.0	1.000	1.000	0.0	0.0	0.0	-7.21E-01
CaNa2(C03)2.5H20	DISABLED_Ga	0.0	1.000	1.000	0.0	0.0	0.0	-1.03E+03
MgS04.7H20	Epsomite	0.0	1.000	1.000	0.0	0.0	0.0	-1.99
KMgCl3.6H20	Carnallite	0.0	1.000	1.000	0.0	0.0	0.0	-2.73
Ca2Cl2(OH)2.H20	CaOxychloride_B	0.0	1.000	1.000	0.0	0.0	0.0	-1.06E+01
NaB02.NaCl.2H20	Teepleite_(20_C)	0.0	1.000	1.000	0.0	0.0	0.0	-2.37
CaCl2.4H20	CaCl2_Tetrahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-5.88
CaC03_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-6.32E+02
Na6C03(S04)2	Burkeite	0.0	1.000	1.000	0.0	0.0	0.0	-7.54
Na2Mg(S04)2.4H20	Bloedite	0.0	1.000	1.000	0.0	0.0	0.0	-2.72
MgCl2.6H20	Bischofite	0.0	1.000	1.000	0.0	0.0	0.0	-3.45
K2S04	Arcanite	0.0	1.000	1.000	0.0	0.0	0.0	-1.77
CaC03_DISABLED	A	0.0	1.000	1.000	0.0	0.0	0.0	-6.32E+02
CaCl2.6H20	Antarcticite	0.0	1.000	1.000	0.0	0.0	0.0	-4.58
NaK3(S04)2	Aphthitalite/Glaserite	0.0	1.000	1.000	0.0	0.0	0.0	-2.32
C02("solid",DISABLED)		0.0	1.000	1.000	0.0	0.0	0.0	-5.09E+02
K3Np02(C03)2(s)	K3Np02(C03)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-4.72

OH/K

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Na3NpO2(CO3)2(s)__Na3NpO2(CO3)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-3.55
2[NaNpO2CO3.7/2H2O(s)]_____	0.0	1.000	1.000	0.0	0.0	0.0	-4.04
NpO2OH(amor)_____NpO2OH(amor)	0.0	1.000	1.000	0.0	0.0	0.0	-3.53
NpO2OH(aged)_____NpO2OH(aged)	0.0	1.000	1.000	0.0	0.0	0.0	-2.83
2[Th(SO4)2.7/2K2SO4(16C,s)]_____	0.0	1.000	1.000	0.0	0.0	0.0	-3.52E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.60E+01
Th(SO4)2.K2SO4.4H2O(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.59E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.46E+01
Th(SO4)2.8H2O(s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.80E+01
Th(SO4)2.9H2O(s)_____	0.0	1.000	1.000	0.0	0.0	0.0	-1.81E+01
NaAm(CO3)2.6H2O(c)_____	0.0	1.000	1.000	0.0	0.0	0.0	-2.29
Am(OH)3(s)_____Am(OH)3(s)	0.0	1.000	1.000	0.0	0.0	0.0	-8.25E-01
B(OH)3_____Borix_Acid_Solid	0.0	1.000	1.000	0.0	0.0	0.0	-2.28
KB5O8.4H2O____K-Pentaborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-7.42
K2B4O7.4H2O____K-Tetraborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-6.25
Na2B4O7.10H2O_____Borax	0.0	1.000	1.000	0.0	0.0	0.0	-3.68
NaOH(aq) to.titrate.base.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.95E+02
HCl(aq) to.titrate.acid.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.48E+02
Na3H(CO3)2.2H2O_____Trona	0.0	1.000	1.000	0.0	0.0	0.0	-8.45
NaBO2.4H2O_____Sodium_Metaborate	0.0	1.000	1.000	0.0	0.0	0.0	-2.94
K2CO3.3/2H2O___Potassium_Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-1.03E+01
Ca4Cl2(OH)6.13H2O__CaOxychloride_A	0.0	1.000	1.000	0.0	0.0	0.0	-2.31E+01
KNaCO3.6H2O_____K-Na-Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-6.78
K2MgCa2(SO4)4.2H2O_____Polyhalite	0.0	1.000	1.000	0.0	0.0	0.0	-1.72

pH (-log[aH+]); pmH(-log[mH+]) 8.6901 9.3663
Osmotic Coefficient= 1.341479
Equilibrium RH (%) = 72.934080
Ionic Strength (m) = 7.409086
Density, kg/m3 = 1229.28
fCO2(g); log[fCO2(g)]= 3.135E-06 -5.50

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -1.00707962E+04

Total Diagonal Inversions 1098
Total Stoichiometric Reoptimizations 98

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INPUT file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_SPC_NESQ_970407_22.IN;1
INGUESS file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]DUMMY.INGUESS;1
OUTPUT file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_SPC_NESQ_970407_22.OUT;6
CHEMDAT file name is U1:[CFNOVAK.FMT.QA_NESQ_HMAG]FMT_970407_NESQ.CHEMDAT;8
Temperature is Hard Coded as 298.15K
Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Nesquehonite FMT V2.2
FMT_970407_NESQ.chemdat
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy

Accuracy of reactions is	1.0000E-06
Minimum elemental abundance is	1.0000E-18
Number of Aqueous Species is	126

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Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Nesquehonite FMT V2.2
FMT_970407_NESQ.chemdat
Added Th(CO3)5-Cl(-Na) Parms, assigned K+-Th(CO3)5=== by analogy
Pressure= 1.000 [=] ATM Temperature= 2.98E+02 [=] Kelvin

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter	
Using NaCl Density Correlation				
1.36767180E+02	1.11131305E+02	9.68401618E+01	9.76051991E+04	Hydrogen
7.99098636E+01	5.59371744E+01	4.87438263E+01	7.79871975E+05	Oxygen
5.69295395	4.66062408	4.06128220	9.33679437E+04	Sodium
1.04775026	1.10984588	9.67123126E-01	3.78128701E+04	Potassium
6.80724482	5.30417100E-01	4.62207097E-01	1.12339435E+04	Magnesium
1.03305403	3.33990592E-02	2.91040432E-02	1.16649805E+03	Calcium
9.81438839	6.69363414	5.83285344	2.06792153E+05	Chlorine
1.06024227	6.22262109E-02	5.42241121E-02	1.73842503E+03	Sulfur
1.00104081	2.25651760E-02	1.96633640E-02	2.36176665E+02	Carbon
0.0	0.0	0.0	0.0	PosIon:EL
0.0	0.0	0.0	0.0	NegIon:EL
0.0	0.0	0.0	0.0	Oxalate:EL
2.71882500E-02	2.88271623E-02	2.51200782E-02	2.71548045E+02	Boron
1.35941250E-02	1.44135812E-02	1.25600391E-02	1.00359736E+03	Bromine
0.0	0.0	0.0	0.0	Acetate:EL
1.00497956E-03	7.22041910E-04	6.29189547E-04	1.45995947E+02	Th(IV)
1.00438590E-03	3.63740149E-07	3.16964287E-07	7.70223218E-02	Am(III)
0.0	0.0	0.0	0.0	Pu(III)
1.00263669E-03	1.36328963E-07	1.18797479E-07	2.81607285E-02	Np(V)
0.0	0.0	0.0	0.0	ClO4:EL
0.0	0.0	0.0	0.0	Phosphorus
0.0	0.0	0.0	0.0	U(IV)
0.0	0.0	0.0	0.0	Lactate:EL
0.0	0.0	0.0	0.0	EDTA:EL
0.0	0.0	0.0	0.0	Citrate:EL
0.0	0.0	0.0	0.0	Electron:E
-1.22725890E-14	-1.30123828E-14	-1.13390305E-14	0.0	Charge:EL

Solution Parameters, Calculated

SOLUTION MASS	1332.61669529897	grams
H2O MASS	943.146941901166	grams
TDS(g/kg)	412.947056386272	g/kgH2O

Specified Solution Density

DENSITY	1231.24642240165	kg/m^3 = g/l

Solution Parameters Based on Specified Density

SOLUTION VOL	1.08233142533693	liters
TDS	359.843338445578	g/l

Density based on TDS and NaCl solutions 1231.24642240165 g/l
Percent relative error vs NaCl density 0.000000000000000 0 %

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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.08781E-01	7.28367E-01	0.9006	5.23528E+01	4.83704E+01	8.71403E+05	
Cl-	Cl-	6.69363	8.19070	1.224	6.31308	5.83285	2.06792E+05	
Na+	Na+	4.66062	4.54033	0.9742	4.39565	4.06128	9.33679E+04	
Mg2Cl(OH)3.4H2O	MgOxychloride	2.33687	1.000	1.000	2.20401	2.03635	4.21821E+05	
K+	K+	1.10985	5.05594E-01	0.4556	1.04675	9.67123E-01	3.78129E+04	
CaSO4	Anhydrite	1.06193	1.000	1.000	1.00155	9.25367E-01	1.25977E+05	
MgCO3.3H2O	Nesquehonite	1.03669	1.000	1.000	9.77752E-01	9.03376E-01	1.24991E+05	
Mg(OH)2	Brucite	9.76748E-01	1.000	1.000	9.21217E-01	8.51141E-01	4.96382E+04	
SO4=	SO4=	6.22262E-02	1.22438E-03	1.9676E-02	5.86885E-02	5.42241E-02	5.20864E+03	
Br-	Br-	1.44136E-02	3.91477E-03	0.2716	1.35941E-02	1.25600E-02	1.00360E+03	
MgB(OH)4+	MgB(OH)4+	1.20960E-02	2.67696E-02	2.213	1.14083E-02	1.05405E-02	1.08719E+03	
AmOHCO3(c)	AmOHCO3(c)	1.06457E-03	1.000	1.000	1.00404E-03	9.27667E-04	2.96869E+02	
KNpO2CO3(s)	KNpO2CO3(s)	1.06294E-03	1.000	1.000	1.00251E-03	9.26249E-04	3.41003E+02	
Th(CO3)5===	Th(CO3)5===	7.21467E-04	2.06954E-21	2.8685E-18	6.80449E-04	6.28688E-04	3.34515E+02	
NaCl	Halite	1.37550	1.000	1.000	1.29730	1.19862	7.00505E+04	-2.87E-10
Mg++	Mg++	5.01618E-01	1.01573	2.025	4.73099E-01	4.37111E-01	1.06240E+04	-2.73E-10
Ca++	Ca++	3.12405E-02	3.54838E-02	1.136	2.94644E-02	2.72231E-02	1.09110E+03	-3.27E-10
MgCO3(aq)	MgCO3(aq)	1.49410E-02	1.49410E-02	1.000	1.40915E-02	1.30196E-02	1.09774E+03	-1.85E-10
B(OH)4-	B(OH)4-	1.03236E-02	1.05092E-03	0.1018	9.73669E-03	8.99603E-03	7.09240E+02	-1.89E-08
B(OH)3(aq)	B(OH)3(aq)	5.02573E-03	5.12159E-03	1.019	4.74000E-03	4.37943E-03	2.70789E+02	5.82E-08
HCO3-	HCO3-	2.15044E-03	7.75578E-04	0.3607	2.02818E-03	1.87390E-03	1.14340E+02	-3.26E-10
MgOH+	MgOH+	1.76232E-03	5.60771E-04	0.3182	1.66213E-03	1.53569E-03	6.34431E+01	-4.16E-10
CaB(OH)4+	CaB(OH)4+	1.28670E-03	1.66693E-03	1.296	1.21354E-03	1.12123E-03	1.33336E+02	3.77E-08
CO3=	CO3=	9.91290E-04	1.73442E-05	1.7497E-02	9.34932E-04	8.63813E-04	5.18367E+01	-1.57E-09
CaCO3(aq)	CaCO3(aq)	8.71815E-04	8.71815E-04	1.000	8.22250E-04	7.59703E-04	7.60380E+01	1.88E-09
ThO2(am)	Hydrous_Thorium_Oxide	3.43518E-04	1.000	1.000	3.23988E-04	2.99343E-04	7.90375E+01	1.26E-08
B3O3(OH)4-	B3O3(OH)4-	2.21857E-05	3.66999E-06	0.1654	2.09244E-05	1.93327E-05	2.87008	1.11E-07
OH-	OH-	7.70090E-06	3.58482E-06	0.4655	7.26308E-06	6.71059E-06	1.14129E-01	-7.46E-10
B4O5(OH)4=	B4O5(OH)4=	7.15108E-06	3.12104E-08	4.3644E-03	6.74452E-06	6.23147E-06	1.19187	1.48E-07
CO2(aq)	CO2(aq)	1.44907E-06	4.74178E-06	3.272	1.36668E-06	1.26272E-06	5.55722E-02	1.64E-10
Th(OH)3(CO3)-	Th(OH)3(CO3)-	5.73827E-07	1.55853E-07	0.2716	5.41203E-07	5.00034E-07	1.71546E-01	-1.76E-08
Am(CO3)3=-	Am(CO3)3=-	3.59244E-07	3.56911E-12	9.9351E-06	3.38820E-07	3.13046E-07	1.32427E-01	-2.63E-09
NpO2CO3-	NpO2CO3-	7.00723E-08	5.29778E-09	7.5604E-02	6.60885E-08	6.10612E-08	2.00926E-02	-5.43E-10
NpO2(CO3)2=-	NpO2(CO3)2=-	4.12118E-08	2.53144E-12	6.1425E-05	3.88688E-08	3.59121E-08	1.39722E-02	-1.68E-09
NpO2(CO3)3==-	NpO2(CO3)3==-	2.36899E-08	3.48702E-18	1.4719E-10	2.23431E-08	2.06435E-08	9.27046E-03	-3.61E-09
Am(OH)2+	(after_Cm(III))	2.35014E-09	1.18182E-13	5.0287E-05	2.21653E-09	2.04792E-09	5.67304E-04	2.34E-10
NpO2+	NpO2+	1.29115E-09	2.85063E-09	2.208	1.21775E-09	1.12511E-09	3.02709E-04	-1.05E-10
Th(OH)4(aq)	Th(OH)4(aq)	1.21454E-09	1.21454E-09	1.000	1.14549E-09	1.05835E-09	3.17577E-04	-1.70E-08
AmCO3+	AmCO3+	1.13274E-09	2.94366E-10	0.2599	1.06834E-09	9.87069E-10	2.99091E-04	-1.09E-10
Am(CO3)2-	Am(CO3)2-	9.94246E-10	2.70040E-10	0.2716	9.37720E-10	8.66389E-10	3.14515E-04	-5.79E-10
H+	H+	4.30789E-10	2.04750E-09	4.753	4.06298E-10	3.75391E-10	3.78357E-07	5.97E-11
HSO4-	HSO4-	3.14896E-10	2.38663E-10	0.7579	2.96993E-10	2.74401E-10	2.66349E-05	-1.43E-09
NpO2OH(aq)	NpO2OH(aq)	6.36930E-11	5.00528E-12	7.8584E-02	6.00719E-11	5.55023E-11	1.58767E-05	-2.96E-12
Am+++	Am+++	1.06161E-11	4.60739E-13	4.3400E-02	1.00125E-11	9.25086E-12	2.24796E-06	-1.28E-10
AmOH++	(after_Cm(III))	5.27987E-12	4.54690E-14	8.6118E-03	4.97969E-12	4.60089E-12	1.19627E-06	4.06E-10

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Am(OH)3(aq)	(1e-9m_minimum)	3.36245E-12	3.36245E-12	1.000	3.17128E-12	2.93005E-12	8.61498E-07	5.20E-11
NpO2(OH)2-	NpO2(OH)2-	9.67185E-14	1.05701E-15	1.0929E-02	9.12198E-14	8.42808E-14	2.55423E-08	-4.01E-10
Th(SO4)3=	Th(SO4)3=	8.34029E-20	4.98600E-21	5.9782E-02	7.86612E-20	7.26776E-20	3.78077E-14	-2.43E-08
Th(SO4)2(aq)	Th(SO4)2(aq)	1.22515E-20	5.94639E-19	48.54	1.15550E-20	1.06760E-20	4.52825E-15	-2.12E-08
Th++++	Th++++	0.0	0.0	0.3707	0.0	0.0	0.0	-2.40E+01
K2NaH(CO3)2.2H2O	Potassium_Trona	0.0	1.000	1.000	0.0	0.0	0.0	-9.32
K8H4(CO3)6.3H2O	K-Sequicarbonate	0.0	1.000	1.000	0.0	0.0	0.0	-3.18E+01
NaB5O8.5H2O	Sodium_Pentaborate	0.0	1.000	1.000	0.0	0.0	0.0	-7.73
Na2CO3.H2O	Thermonatrite	0.0	1.000	1.000	0.0	0.0	0.0	-4.07
Na2SO4	Thenardite	0.0	1.000	1.000	0.0	0.0	0.0	-1.31
Mg2CaCl6.12H2O	Tachyhydrite	0.0	1.000	1.000	0.0	0.0	0.0	-1.50E+01
K2Ca(SO4)2.H2O	Syngenite	0.0	1.000	1.000	0.0	0.0	0.0	-5.56E-01
KCl	Sylvite	0.0	1.000	1.000	0.0	0.0	0.0	-2.83E-01
Na2CO3.7H2O	Na2CO3-Heptahydrate	0.0	1.000	1.000	0.0	0.0	0.0	-3.95
Na3H(SO4)2	Sesquisodium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.17E+01
K3H(SO4)2	Sesquipotassium_Sulfate	0.0	1.000	1.000	0.0	0.0	0.0	-1.19E+01
Mg4(CO3)3(OH)2.3H2O_DISABLED_Hydro		0.0	1.000	1.000	0.0	0.0	0.0	-1.24E+03
Mg5(CO3)4(OH)2.4H2O_DISABLED_Hydro		0.0	1.000	1.000	0.0	0.0	0.0	-1.45E+03
CaMg(CO3)2_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-8.07E+02
Na2Ca(CO3)2.2H2O_DISABLED	Pi	0.0	1.000	1.000	0.0	0.0	0.0	-9.01E+02
K2Mg(SO4)2.6H2O_Picromerite/Schoen		0.0	1.000	1.000	0.0	0.0	0.0	-2.91
Na2CO3.10H2O	Natron	0.0	1.000	1.000	0.0	0.0	0.0	-4.00
NaHCO3	Nahcolite	0.0	1.000	1.000	0.0	0.0	0.0	-2.05
K8H6(SO4)7	Misenite	0.0	1.000	1.000	0.0	0.0	0.0	-6.41E+01
Na2SO4.10H2O	Mirabilite	0.0	1.000	1.000	0.0	0.0	0.0	-1.75
KHSO4	Mercallite	0.0	1.000	1.000	0.0	0.0	0.0	-1.05E+01
MgCO3_DISABLED	M	0.0	1.000	1.000	0.0	0.0	0.0	-6.11E+02
Na4Ca(SO4)3.2H2O_DISABLED	Lab	0.0	1.000	1.000	0.0	0.0	0.0	-1.20E+03
K2Mg(SO4)2.4H2O	Leonite	0.0	1.000	1.000	0.0	0.0	0.0	-2.98
MgSO4.H2O	Kieserite	0.0	1.000	1.000	0.0	0.0	0.0	-2.92
KHCO3	Kalicinite	0.0	1.000	1.000	0.0	0.0	0.0	-3.69
KMgClSO4.3H2O	Kainite	0.0	1.000	1.000	0.0	0.0	0.0	-2.51
MgSO4.6H2O	Hexahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-2.10
CaSO4.2H2O	Gypsum	0.0	1.000	1.000	0.0	0.0	0.0	-5.68E-02
Na2Ca(SO4)2	Glauberite	0.0	1.000	1.000	0.0	0.0	0.0	-7.15E-01
CaNa2(CO3)2.5H2O_DISABLED	Ga	0.0	1.000	1.000	0.0	0.0	0.0	-1.03E+03
MgSO4.7H2O	Epsomite	0.0	1.000	1.000	0.0	0.0	0.0	-1.99
KMgCl3.6H2O	Carnallite	0.0	1.000	1.000	0.0	0.0	0.0	-2.71
Ca2Cl2(OH)2.H2O	CaOxychloride_B	0.0	1.000	1.000	0.0	0.0	0.0	-1.06E+01
NaBO2.NaCl.2H2O	Teepleite_(20_C)	0.0	1.000	1.000	0.0	0.0	0.0	-2.35
CaCl2.4H2O	CaCl2_Tetrahydrite	0.0	1.000	1.000	0.0	0.0	0.0	-5.89
CaCO3_DISABLED		0.0	1.000	1.000	0.0	0.0	0.0	-6.30E+02
Na6CO3(SO4)2	Burkeite	0.0	1.000	1.000	0.0	0.0	0.0	-5.87
Na2Mg(SO4)2.4H2O	Bloedite	0.0	1.000	1.000	0.0	0.0	0.0	-2.71
MgCl2.6H2O	Bischofite	0.0	1.000	1.000	0.0	0.0	0.0	-3.45
K2SO4	Arcanite	0.0	1.000	1.000	0.0	0.0	0.0	-1.73
CaCO3_DISABLED	A	0.0	1.000	1.000	0.0	0.0	0.0	-6.30E+02
CaCl2.6H2O	Antarcticite	0.0	1.000	1.000	0.0	0.0	0.0	-4.59
NaK3(SO4)2	Aphthitalite/Glaserite	0.0	1.000	1.000	0.0	0.0	0.0	-2.25
CO2("solid",DISABLED)		0.0	1.000	1.000	0.0	0.0	0.0	-5.07E+02
K3NpO2(CO3)2(s)	K3NpO2(CO3)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-3.02
Na3NpO2(CO3)2(s)	Na3NpO2(CO3)2(s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.92

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2[NaNpO2CO3.7/2H2O(s)]	0.0	1.000	1.000	0.0	0.0	0.0	-4.08
NpO2OH(amor) NpO2OH(amor)	0.0	1.000	1.000	0.0	0.0	0.0	-5.21
NpO2OH(aged) NpO2OH(aged)	0.0	1.000	1.000	0.0	0.0	0.0	-4.51
2[Th(SO4)2.7/2K2SO4(16C,s)]	0.0	1.000	1.000	0.0	0.0	0.0	-3.48E+01
Th(SO4)2.2K2SO4.2H2O(16C,s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.59E+01
Th(SO4)2.K2SO4.4H2O(16C,s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.58E+01
Th(SO4)2.Na2SO4.6H2O(16C,s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.46E+01
Th(SO4)2.8H2O(s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.80E+01
Th(SO4)2.9H2O(s)	0.0	1.000	1.000	0.0	0.0	0.0	-1.81E+01
NaAm(CO3)2.6H2O(c)	0.0	1.000	1.000	0.0	0.0	0.0	-6.36E-01
Am(OH)3(s) Am(OH)3(s)	0.0	1.000	1.000	0.0	0.0	0.0	-2.49
B(OH)3 Borix_Acid_Solid	0.0	1.000	1.000	0.0	0.0	0.0	-2.26
KB5O8.4H2O K-Pentaborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-7.32
K2B4O7.4H2O K-Tetraborate_(30_C)	0.0	1.000	1.000	0.0	0.0	0.0	-6.15
Na2B4O7.10H2O Borax	0.0	1.000	1.000	0.0	0.0	0.0	-3.62
NaOH(aq) to.titrate.base.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.95E+02
HCl(aq) to.titrate.acid.only	0.0	0.0	1.000	0.0	0.0	0.0	-2.48E+02
Na3H(CO3)2.2H2O Trona	0.0	1.000	1.000	0.0	0.0	0.0	-5.13
NaBO2.4H2O Sodium_Metaborate	0.0	1.000	1.000	0.0	0.0	0.0	-2.93
K2CO3.3/2H2O Potassium_Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-8.59
Ca4Cl2(OH)6.13H2O CaOxychloride_A	0.0	1.000	1.000	0.0	0.0	0.0	-2.32E+01
KNaCO3.6H2O K-Na-Carbonate	0.0	1.000	1.000	0.0	0.0	0.0	-5.11
Ca(OH)2 Portlandite	0.0	1.000	1.000	0.0	0.0	0.0	-7.15
K2MgCa2(SO4)4.2H2O Polyhalite	0.0	1.000	1.000	0.0	0.0	0.0	-1.67

pH (-log[aH+]); pmH(-log[mH+]) 8.6888 9.3657
Osmotic Coefficient= 1.340579
Equilibrium RH (%) = 72.836675
Ionic Strength (m) = 7.458238
Density, kg/m3 = 1231.25
fCO2(g); log[fCO2(g)]= 1.438E-04 -3.84

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
- Gas "molality" and "activity" are gas partial pressures
- "Descriptor" means:
*dG/RT/ln10 for species with nonzero concs. (convergence criterion)
*Saturation Index for minerals, SI=log10(IAP/Ksp)
*log10(activity) for aqueous species with very small concentrations
*log10(partial pressure) for gases

Total G/RT= -1.00669938E+04

Total Diagonal Inversions 375
Total Stoichiometric Reoptimizations 40

ah/oh

Information Only

Actinide and selected ion solubilities calculated using the FMT code for different solid phases.

SPC brine

Conditions	Database and code version	+3 actinides molar	+4 actinides molar	+5 actinides molar	+6 actinides[2] molar	log f_{CO2}	Ca^{2+} molal	Mg^{2+} molal	HCO_3^- molal	CO_3^{2-} molal	pcH	pmH
CCA calculations	FMT_HMW_960501FANG FMT 2.0	5.82E-07	4.40E-06	2.30E-06	8.70E-06	-6.9	3.18E-02	0.496	1.78E-06	8.34E-07	9.42	9.37
No backfill	TBD	4.00E-03	5.00E-04	2.00E-04	8.00E-05	0.5 to 2.2	-	-	-	-	-	4.0 - 6.0
Nesquehonite solid	FMT_970407 FMT 2.2	3.17E-07	6.28E-04	1.19E-07	8.70E-06	-3.8	3.12E-02	0.496	2.15E-03	9.91E-04	9.42	9.36
Hydromagnesite ($Ksp=10^{-37.1}$)	FMT_970407 FMT 2.2	9.40E-08	1.20E-08	1.20E-07	8.70E-06	-5.5	3.20E-02	0.5	4.70E-05	2.20E-05	9.42	9.37
Hydromagnesite ($Ksp=10^{-30.2}$)	FMT _970407 FMT 2.2	7.20E-08	1.50E-08	1.10E-07	8.70E-06	-5.39	3.20E-02	0.5	6.10E-05	2.80E-05	9.42	9.37

ERDA6 brine

Conditions	Database and code version	+3 actinides molar	+4 actinides molar	+5 actinides molar	+6 actinides[2] molar	log f_{CO2}	Ca^{2+} molal	Mg^{2+} molal	HCO_3^- molal	CO_3^{2-} molal	pcH	pmH
CCA calculations	FMT_HMW_960501FANG FMT 2.0	6.52E-08	6.00E-09	2.20E-06	8.70E-06	-6.9	1.09E-02	3.86E-02	7.08E-06	7.97E-06	9.94	9.9
No backfill	TBD	2.00E-03	7.00E-05	6.00E-04	8.00E-05	0 to 2	-	-	-	-	-	4.5 - 6.0
Nesquehonite solid	FMT_970407 FMT 2.2	2.14E-06	1.04E-03	7.83E-07	8.70E-06	-3.8	1.10E-02	5.58E-02	6.66E-03	6.46E-03	9.87	9.82
Hydromagnesite ($Ksp=10^{-37.1}$)	FMT_970407 FMT 2.2	1.30E-06	4.10E-08	4.60E-07	8.70E-07	-5.5	1.10E-02	4.00E-02	1.80E-04	2.00E-04	9.94	9.89
Hydromagnesite ($Ksp=10^{-30.2}$)	FMT _970407 FMT 2.2	1.20E-08	5.30E-08	4.60E-07	1.10E-02	-5.39	1.10E-02	4.00E-02	2.30E-04	2.80E-04	9.94	9.89

Information Only

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History of CMS Library WP$NONPA_CMSROOT:[FMT]

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 21-APR-1997 15:08:36 CFNOVAK CREATE ELEMENT FMT_ERDA6_HMAG5424_970407_22.IN "APRIL 97 MGO RUNS"
 21-APR-1997 15:08:37 CFNOVAK CREATE ELEMENT FMT_ERDA6_NESQ_970407_22.IN "APRIL 97 MGO RUNS"
 21-APR-1997 15:08:38 CFNOVAK CREATE ELEMENT FMT_SPC_HMAG4323_970407_22.IN "APRIL 97 MGO RUNS"
 21-APR-1997 15:08:39 CFNOVAK CREATE ELEMENT FMT_SPC_HMAG5424_970407_22.IN "APRIL 97 MGO RUNS"
 21-APR-1997 15:08:40 CFNOVAK CREATE ELEMENT FMT_SPC_NESQ_970407_22.IN "APRIL 97 MGO RUNS"
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%CMS-W-NOHIS, no history records found
$ cfe *_22.in
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%CMS-I-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_SPC_NESQ_970407_22.IN fetched
%CMS-I-FETCHES, 6 elements fetched
$ dir

Directory UI:[CCCRAFT.NANCY]

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Total of 6 files.
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Information Only

File=FMT_SPC_HMAG5424_970407.IN

'Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Hydromagnesite5424'
'CHEMFILE'
'BATCH' 'EXPLICIT'

'nMOLES' 'nEXACT'
1.36767180E+02 Hydrogen
7.99098638E+01 Oxygen
5.69295395E+00 Sodium
1.04775026E+00 Potassium
6.80724482E+00 Magnesium
1.03305403E+00 Calcium
9.81438839E+00 Chlorine
1.06024227E+00 Sulfur
1.00104081E+00 Carbon
0.00000000E+00 PosIon:EL
0.00000000E+00 NegIon:EL
0.00000000E+00 Oxalate:EL
2.71882500E-02 Boron
1.35941250E-02 Bromine
0.00000000E+00 Acetate:EL
1.00497956E-03 Th(IV)
1.00438590E-03 Am(III)
0.00000000E+00 Pu(III)
1.00263669E-03 Np(V)
0.00000000E+00 ClO4:EL
0.00000000E+00 Phosphorus
0.00000000E+00 U(IV)
0.00000000E+00 Lactate:EL
0.00000000E+00 EDTA:EL
0.00000000E+00 Citrate:EL
0.00000000E+00 Electron:E
0.0 Charge:EL

Information Only

File=FMT_SPC_NESQ_970407.IN

'Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Nesquehonite'
'CHEMFILE'
'BATCH' 'EXPLICIT'

'nMOLES' 'nEXACT'
1.36767180E+02 Hydrogen
7.99098638E+01 Oxygen
5.69295395E+00 Sodium
1.04775026E+00 Potassium
6.80724482E+00 Magnesium
1.03305403E+00 Calcium
9.81438839E+00 Chlorine
1.06024227E+00 Sulfur
1.00104081E+00 Carbon
0.00000000E+00 PosIon:EL
0.00000000E+00 NegIon:EL
0.00000000E+00 Oxalate:EL
2.71882500E-02 Boron
1.35941250E-02 Bromine
0.00000000E+00 Acetate:EL
1.00497956E-03 Th(IV)
1.00438590E-03 Am(III)
0.00000000E+00 Pu(III)
1.00263669E-03 Np(V)
0.00000000E+00 ClO4:EL
0.00000000E+00 Phosphorus
0.00000000E+00 U(IV)
0.00000000E+00 Lactate:EL
0.00000000E+00 EDTA:EL
0.00000000E+00 Citrate:EL
0.00000000E+00 Electron:E
0.0 Charge:EL

Information Only

File=FMT_ERDA6_HMAG4323_970407.IN

'Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Hydromagnesite'
'CHEMFILE'
'BATCH' 'EXPLICIT'

'nMOLES' 'nEXACT'
1.13289995E+02 Hydrogen
6.57555273E+01 Oxygen
7.19980915E+00 Sodium
1.10087747E-01 Potassium
2.04429362E+00 Magnesium
1.01344192E+00 Calcium
6.96738842E+00 Chlorine
1.19112712E+00 Sulfur
1.00103149E+00 Carbon
0.00000000E+00 PosIon:EL
0.00000000E+00 NegIon:EL
0.00000000E+00 Oxalate:EL
7.08491570E-02 Boron
1.23704871E-02 Bromine
0.00000000E+00 Acetate:EL
11.00000678E-03 Th(IV)
1.00041150E-03 Am(III)
0.00000000E+00 Pu(III)
1.00253377E-03 Np(V)
0.00000000E+00 ClO4:EL
0.00000000E+00 Phosphorus
0.00000000E+00 U(IV)
0.00000000E+00 Lactate:EL
0.00000000E+00 EDTA:EL
0.00000000E+00 Citrate:EL
0.00000000E+00 Electron:E
0.0 Charge

Information Only

File=FMT_ERDA6_HMAG5424_970407.IN

'CHEMFILE'
'BATCH' 'EXPLICIT'

'nMOLES' 'nEXACT'
1.13289995E+02 Hydrogen
6.57555273E+01 Oxygen
7.19980915E+00 Sodium
1.10087747E-01 Potassium
2.04429362E+00 Magnesium
1.01344192E+00 Calcium
6.96738842E+00 Chlorine
1.19112712E+00 Sulfur
1.00103149E+00 Carbon
0.00000000E+00 PosIon:EL
0.00000000E+00 NegIon:EL
0.00000000E+00 Oxalate:EL
7.08491570E-02 Boron
1.23704871E-02 Bromine
0.00000000E+00 Acetate:EL
11.00000678E-03 Th(IV)
1.00041150E-03 Am(III)
0.00000000E+00 Pu(III)
1.00253377E-03 Np(V)
0.00000000E+00 ClO4:EL
0.00000000E+00 Phosphorus
0.00000000E+00 U(IV)
0.00000000E+00 Lactate:EL
0.00000000E+00 EDTA:EL
0.00000000E+00 Citrate:EL
0.00000000E+00 Electron:E
0.0 Charge

Information Only

File=FMT_ERDA6_NESQ_970407.IN

'Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Nesquehonite'
'CHEMFILE'
'BATCH' 'EXPLICIT'

'nMOLES' 'nEXACT'
1.13289995E+02 Hydrogen
6.57555273E+01 Oxygen
7.19980915E+00 Sodium
1.10087747E-01 Potassium
2.04429362E+00 Magnesium
1.01344192E+00 Calcium
6.96738842E+00 Chlorine
1.19112712E+00 Sulfur
1.00103149E+00 Carbon
0.00000000E+00 PosIon:EL
0.00000000E+00 NegIon:EL
0.00000000E+00 Oxalate:EL
7.08491570E-02 Boron
1.23704871E-02 Bromine
0.00000000E+00 Acetate:EL
I I.00000678E-03 Th(IV)
1.00041150E-03 Am(III)
0.00000000E+00 Pu(III)
1.00253377E-03 Np(V)
0.00000000E+00 ClO4:EL
0.00000000E+00 Phosphorus
0.00000000E+00 U(IV)
0.00000000E+00 Lactate:EL
0.00000000E+00 EDTA:EL
0.00000000E+00 Citrate:EL
0.00000000E+00 Electron:E
0.0 Charge

Information Only

File=FMT_SPC_HMAG4323_970407.IN

'Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Hydromagnesite4232'
'CHEMFILE'
'BATCH' 'EXPLICIT'

'nMOLES' 'nEXACT'
1.36767180E+02 Hydrogen
7.99098638E+01 Oxygen
5.69295395E+00 Sodium
1.04775026E+00 Potassium
6.80724482E+00 Magnesium
1.03305403E+00 Calcium
9.81438839E+00 Chlorine
1.06024227E+00 Sulfur
1.00104081E+00 Carbon
0.00000000E+00 PosIon:EL
0.00000000E+00 NegIon:EL
0.00000000E+00 Oxalate:EL
2.71882500E-02 Boron
1.35941250E-02 Bromine
0.00000000E+00 Acetate:EL
1.00497956E-03 Th(IV)
1.00438590E-03 Am(III)
0.00000000E+00 Pu(III)
1.00263669E-03 Np(V)
0.00000000E+00 ClO4:EL
0.00000000E+00 Phosphorus
0.00000000E+00 U(IV)
0.00000000E+00 Lactate:EL
0.00000000E+00 EDTA:EL
0.00000000E+00 Citrate:EL
0.00000000E+00 Electron:E
0.0 Charge:EL

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