

November 18, 2005

**UNITED STATES OF AMERICA
NUCLEAR REGULATORY COMMISSION**

BEFORE THE ATOMIC SAFETY AND LICENSING BOARD

**DOCKETED
USNRC**

November 21, 2005 (7:48am)

**OFFICE OF SECRETARY
RULEMAKINGS AND
ADJUDICATIONS STAFF**

In the Matter of

Docket No. 70-3103

Louisiana Energy Services, L.P.

ASLBP No. 04-826-01-ML

**MOTION FOR PARTIAL SUMMARY DISPOSITION
SUBMITTED ON BEHALF OF INTERVENORS
NUCLEAR INFORMATION AND RESOURCE SERVICE
AND PUBLIC CITIZEN**

Preliminary statement

This motion is submitted on behalf of Intervenor Nuclear Information and Resource Service and Public Citizen ("NIRS/PC") pursuant to the Order of the Atomic Safety and Licensing Board (The "Board") dated November 9, 2005 and 10 CFR 2.710. By this motion NIRS/PC seek a determination by the Board sustaining NIRS/PC Contention EC-4, as remanded by the Commission in its Memorandum and Order dated October 19, 2005, insofar as it concerns the discussion contained in the Draft and Final Environmental Impact Statements¹ concerning possible deep disposal of depleted uranium from the National Enrichment Facility ("NEF"). The contention asserts, in substance, that the EIS discussion fails to comply with the National

¹ The pending contention, remanded by the Commission in its ruling dated October 19, 2005, concerns the Draft Environmental Impact Statement. By motion dated November 11, 2005, NIRS/PC have sought leave to assert a similar contention as to the Final Environmental Impact Statement in order to make the record clear. The Board has already stated its intention to allow the contention to go forward. (Oct. 2005 Tr. 2598). The Board stated also that it would "collapse the process, so that we don't spend time fixing the error, and then having to have another contention that we are going to let the parties deal with that, generally, which is the allegation that this didn't take a sufficiently hard look in this area." (Oct. 2005 T. 2486). Accordingly, this motion addresses the disclosure contained in the Draft and Final Environmental Impact Statements.

Environmental Policy Act, 42 U.S.C.4332 ("NEPA"), because the dose results have no demonstrable basis in data or scientific analysis and because the estimated doses grossly understate the potential impacts of such disposal.

Factual background

In the Draft Environmental Impact Statement for the NEF (September 2004) (NUREG-1790) (NRC Staff Ex. 1, admitted in February 2005)² the Commission Staff published Table 4-19, at page 4-59, purporting to show "Maximum Annual Exposure from Postulated Geologic Disposal Sites." These figures had never before been published. The accompanying text states that an analysis of the impacts of deep disposal of depleted uranium wastes was previously presented in the EIS for the Claiborne Enrichment Center ("CEC") (NIRS/PC Ex. 58; also NRC Staff Ex. 46), and the potential impacts of NEF-generated DU_3O_8 would be proportional to the quantity of material postulated from the CEC. Estimated dose figures at the time of peak dose are stated in Table 4-19 of the NEF Draft EIS. It is suggested, although not expressly stated, that the dose figures are derived from the modeling done in connection with the CEC Final EIS.

The dose figures stated in Table 4-19 are extremely low—so low, in fact, as to be unbelievable on their face. In response to the results shown in the Draft EIS, NIRS/PC did two things:

First, on October 20, 2004, NIRS/PC moved to amend their contentions, stating, among other things, that the Draft EIS fails adequately to support or explain the modeling of disposal of depleted uranium. (NIRS/PC motion to amend and supplement contentions, Oct. 20, 2004, at 13). NIRS/PC stated that the Draft EIS fails adequately to disclose the models used or the

^{2 2} In connection with this motion NIRS/PC have not copied and attached documents previously served upon the parties to this proceeding or marked as exhibits in connection with hearings. Should any party require an additional copy of any such item, NIRS/PC stands ready to provide the document.

parameter values and that the results are unlike those reported in connection with the CEC facility. (id. 16).

Second, on October 21, 2004, NIRS/PC propounded interrogatories to the Commission Staff, requesting disclosure of the models used and the parameter values used in the modeling, together with supporting information about the data underlying the parameter values. (NIRS/PC interrogatories to Commission Staff, Interrogatory No. 10, Oct. 21, 2004).

On November 10, 2004, Commission Staff answered the interrogatories, explaining that the source of the results shown in Table 4-19 is the CEC Final EIS, with an adjustment to reflect the volume of depleted uranium expected from the NEF. (NRC Staff response to NIRS/PC interrogatories and document request, at 6-7, Nov. 10, 2004). Other than pointing to the CEC Final EIS, Staff have furnished essentially no further information on the modeling or the derivation of the parameter values used in producing Table 4-19.

The NEF Final EIS was issued in June 2005 (NRC Staff Ex. 47). The Final EIS likewise contains Table 4-19. Certain errors in transcription of dose results in Table 4-19 that affected the Draft EIS were corrected in the Final EIS. However, the reported results present the same fundamental problems: the results are unexplained and are unbelievably low.

By its ruling dated October 19, 2005, the Commission held that NIRS/PC's contention about deep disposal impacts is timely. The Commission has also suggested that the contention may be amenable to summary disposition. (Memorandum and Order, CLI-05-20, at 24-25 note 48, Oct. 19, 2005). At hearings on October 27, 2005, Commission Staff testified that the transcription errors made in preparing Table 4-19 were corrected in the Final EIS. (Tr. Oct. 2005 at 2850-54). The remanded contention involved the Draft EIS, and the Board has sought to condense the process by allowing the parties to address, in substance, whether the NEPA

documents enable the agency to take a sufficiently "hard look" in this area. (Tr. 2486). By Order dated November 9, 2005, the Board set a schedule for summary disposition motions in connection with these contentions.

The attached affidavits by Dr. Arjun Makhijani and George Rice demonstrate that:

- (a) Scientific results have no credibility if they cannot be reproduced from source data.

(Makhijani Aff. par. 5). Here, the information in the CEC Final EIS does not include all necessary source data, and does not disclose modeling methodology, sufficiently to permit reproduction of the results shown in Table 4-19. The disclosure made in the CEC Final EIS and in the NEF Draft and Final EIS is inadequate to enable other scientists independently to verify the dose results published in the CEC Final EIS. (Makhijani Aff. par. 5). The Commission Staff itself have been unable or unwilling to re-run the models and reproduce the results. Therefore, it is not possible to attribute any credibility to results said to be based upon the CEC Final EIS, such as the results in Table 4-19.

- (b) The NEF Draft EIS says that impacts from disposal of depleted uranium from the NEF will be proportional to the quantity disposed at the CEC facility, and the stated results appear to approximately reflect the ratio between such quantities. However, no discussion of the waste configuration is given in the NEF Final EIS for comparison to that proposed in the CEC Final EIS, nor is a justification offered for concluding that releases or doses will bear such a simple linear relationship to the volume of waste. (Makhijani Aff. par. 4).

- (c) Looking first at the well water scenarios, drinking water doses reported in the CEC Final EIS for the hypothetical granite site are incredibly low, implying a thorium concentration in the range of one atom per liter. In the sandstone/basalt site the U-234 concentration

implied is just one atom per every 200 liters of water, and thorium is present at the ratio of one atom per 1.9 million liters. Such values are so low as to be incredible. (Makhijani Aff. par. 6-9).

- (d) In the river scenarios, at the granite site implied thorium concentrations would be just two atoms per liter. Radium-226 would have a concentration of one atom per 28 liters of water. Again, such values are so low as to be incredible. (Makhijani Aff. par. 10).
- (e) Expert analysis suggests that, although the CEC Final EIS states that depleted U_3O_8 would be the disposal form, the CEC modeling assumed that the dominant solid phase for the depleted uranium would be UO_2 . Assuming the presence of UO_2 , modeling conducted by George Rice using PHREEQC indicates solubility values that are lower by several orders of magnitude than values determined in similar investigations that assumed the presence of DU_3O_8 . (Makhijani Aff. par. 13-15; Rice Aff. par. 5-8). No explanation has been offered for the selection of UO_2 as the solid phase in the CEC Final EIS. (Makhijani Aff. par. 15; Rice Aff. par. 10). The use of inappropriately low solubility values would introduce a non-conservative bias into the analysis, causing erroneous results inconsistent with appropriate environmental modeling. (Makhijani Aff. par. 15).
- (f) The CEC analysis incorporates modeling of flow of groundwater and transport of radionuclides. The specifics of such modeling are not adequately disclosed in the CEC Final EIS, and the results therefore cannot be reproduced. However, the reference to retardation coefficients in the range of 1,200 at page A-13 of the CEC Final EIS suggests that the quantification of retardation was quite high. The use of inappropriately high retardation factors would introduce another non-conservative bias into the analysis,

causing erroneous results inconsistent with appropriate environmental modeling and relevant experience. (Rice Aff. par. 11).

- (g) Without knowing the specific parameter values used at each step of the CEC modeling exercise, the data source for the values, and how the models were used with such values, it is not possible to state what other errors may lie behind the modeling results reported in the CEC Final EIS and said to be used to derive the results reported in Table 4-19 in the NEF draft and Final EIS.

Thus, the dose results stated in Table 4-19, either as originally published or as corrected in the Final EIS, cannot be traced to any scientifically valid analysis and depart by several orders of magnitude from results in similar studies that are appropriately supported in data and modeling.

Argument

A published statement that quantifies the environmental impacts of a proposed action, but which lacks sufficient supporting data and cannot be explained by the issuing agency, fails to meet NEPA requirements. The purpose of impact analysis under NEPA is to require the federal agency to take a “hard look” at the impacts of a proposed action and appropriate alternatives. *Kleppe v. Sierra Club*, 427 U.S. 390, 410 n. 21 (1976). Thus, “Congress wanted each federal agency spearheading a major federal project to put on the table, for the deciding agency’s and for the public’s view, a sufficiently detailed statement of environmental impacts and alternatives so as to permit informed decision making.” *Lands Council v. Powell*, 395 F.3d 1019, 1027 (9th Cir. 2005).

The Commission’s rules specify how such analysis is to be “put on the table.” The regulations call for quantification of relevant factors and disclosure of analytical methods. Under 10 CFR 51.45, “[t]he analysis for environmental reports shall, to the fullest extent practicable,

quantify the various factors considered.” A draft EIS is expressly required to identify its methodology and source data, and the Commission Staff is required to be responsible for the accuracy of the report:

“The draft environmental impact statement . . . will identify any methodologies used and sources relied upon, and will be supported by evidence that the necessary environmental analyses have been made. . . . The NRC Staff will independently evaluate and be responsible for the reliability of all information used in the draft environmental impact statement.”

Further, the draft EIS is required to adhere to the standards of section 51.45, which requires quantification of the factors used in environmental analyses. (10 CFR 51.71(a)).

Thus, to summarize: “We distill from the cases a requirement that, to satisfy NEPA, an agency must go beyond mere assertions. At a minimum, it must provide a detailed, thoughtful analysis drawn from adequate data so that a reviewing court can decide on an objective basis whether the agency fairly assessed other courses of action which might realistically be substituted for the one proposed.” *Boston Edison Co.* (Pilgrim Nuclear Generating Station, Unit 2), 7 NRC 774, 779, ALAB-479 (May 25, 1978). Unless the agency presents a transparent analysis, it is not possible for the public to comment on that analysis or for a reviewing court to determine whether a fair assessment has been made.

An EIS that fails to quantify the factors used in analysis or to identify their sources and the methods of analysis fails NEPA standards. For example, in *Duke Energy Corp.* (Catawba Nuclear Station, Units 1 and 2), 59 NRC 129, LBP-04-4 (March 5, 2004), the applicant had asserted that impacts would be small but had not revealed its analyses. The intervenor asserted that the applicant had failed to quantify its analysis of impacts of the proposed action on severe accident consequences and potential releases. (59 NRC at 149). The Board explained:

“The root of all these contentions is BREDL’s assertion that Duke has failed to account for differences in MOX and LEU fuel behavior (both known differences as well as recent

information on possible differences) and to account for and quantify the impact of such differences on both the DBA analysis for Catawba, and the potential for releases and their consequences, under NEPA.” (id.).

Thus, the intervenor asserted that the applicant “fails to provide quantitative support for its assertion that the consequences of a severe accident involving use of LTA MOX fuel will increase 0.3% at most.” (at 150; see also 153). The Board ruled:

“Regarding the NEPA issues of whether the severe accident consequences associated with MOX LTA use will be significant, and whether Duke has, as required by 10 C.F.R. sec. 51.45(c) and argued in Contention 6, quantified all environmental factors ‘to the fullest extent practicable’ in its ER, we find that BREDL has presented sufficient basis, facts, and expert opinion to demonstrate a genuine dispute on these issues—one factual, one a combined legal/factual issue—which are clearly material to the proposal before us.” (id. 165).

That principle applies here. Here, Commission Staff has violated NEPA requirements in failing to quantify fully the factors and adequately set forth the methodologies, sources, and analyses underlying Staff’s conclusions—viz: that the dose fractions shown in Table 4-19 reflect the performance of appropriate generic sites, properly modeled to reflect realistic conditions.

It is telling that here, where Commission Staff have failed to present transparent analyses, the results strain scientific credulity and depart radically from the conclusions of other analyses. (For a further discussion of this point see Makhijani Aff. par. 6-12). For example, a key element of the analysis of groundwater release is solubility of radionuclides. Here, the analysis by Kozak et al. of Sandia National Laboratory (NIRS/PC Ex. 128)—performed by a Department of Energy laboratory for the Commission Staff in connection with the Claiborne proceeding—considered the behavior of depleted uranium and estimated solubility values in the range of 10^{-6} to 10^{-5} moles per liter for uranium. (NIRS/PC Ex. 128 at 31). Recent work conducted by George Rice modeled depleted uranium in deep disposal and identified solubility values in the same range (approximately 10^{-6} moles per liter for uranium as U_3O_8) (NIRS/PC Ex. 190 at 22). Commission

Staff in the Claiborne Final EIS (NIRS/PC Ex. 58, Table A.6) report the value as approximately 4×10^{-10} moles per liter—and provide no adequate explanation of the derivation of the figure they report and the three-order-of-magnitude difference from the Kozak analysis, which was conducted for the Commission Staff in connection with the same license application.

Again, in the Claiborne Final EIS Commission Staff relate that they employed retardation coefficients “greater than 1,200” (NIRS/PC Ex. 58 at A-13), without disclosing how much “greater” or whether the same factors were used for all elements. Retardation factors vary from site to site over an extremely wide range—arguing for conservative assumptions in a generic analysis of a hypothetical site—(Rice Aff. par. 11), but Staff offer no explanation of their selection of values for these critical parameters. Neither, for that matter, do Staff disclose the details of the configuration of their model of release, vertical flow, horizontal flow, and dose within which these retardation coefficients operate. Thus, it is not possible for an independent observer to identify the full impact of the parameter selection, even if all of the parameter values had been disclosed.

Notably, the published results of Staff’s undisclosed analysis contrast dramatically with observed values. The U-238 doses from drinking water in the CEC analyses were a hundred thousand to a hundred trillion times lower than typical background doses that are received from uranium that leaches out of ordinary dirt and rocks. (Makhijani Aff. par. 7). Such extreme ratios indicate that the dose estimates published in the CEC Final EIS, and claimed to be the source for those published in NEF Final EIS Table 4-19, are likely to be wrong by several orders of magnitude. The nature of the errors giving rise to these incredible results cannot now be conclusively identified, nor can NIRS/PC effectively propose corrections, because the underlying

data, the modeling methodology, and the full range of parameters used in modeling have not been adequately disclosed, contrary to NEPA and Commission regulations.

Conclusion

NEPA analysis in this instance has been presented in the form of a “black box” whose results and contours are visible but many of whose internal specifics are blocked from investigation. The Commission Staff have published results in the NEF Draft and Final EISs, but no relevant explanation. But the law and the Commission’s rules prohibit NEPA analysis in the form of unexplained assertions. Neither should the Board allow Staff to rely in licensing the NEF upon analyses done in the CEC proceeding that they cannot explain or reproduce.

If the Board allowed Staff to rely upon previous analyses, without taking a sufficiently hard look and no matter how incredible the results, Staff would henceforth refuse to investigate impacts wherever they could refer to old studies without a serious check of their correctness and reliability—contrary to the Commission’s rules calling for transparent and quantified analyses and contrary to the purpose of NEPA.

The Board should grant summary disposition, directing that the discussion of impacts of deep disposal be held inadequate under NEPA and Commission rules and requiring Staff to present a new analysis of such impacts.

Respectfully submitted,



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November 18, 2005

CERTIFICATE OF SERVICE

Pursuant to 10 CFR § 2.305 the undersigned attorney of record certifies that on November 18, 2005, the foregoing Motion for Partial Summary Disposition submitted on behalf of Intervenor Nuclear Information and Resource Service and Public Citizen and the accompanying declarations by Arjun Makhijani and George Rice were served by electronic mail and first class mail upon the following:

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**UNITED STATES OF AMERICA
NUCLEAR REGULATORY COMMISSION**

BEFORE THE ATOMIC SAFETY AND LICENSING BOARD

In the Matter of

Docket No. 70-3103

Louisiana Energy Services, L.P.
National Enrichment Facility

ASLBP No. 04-826-01-ML

DECLARATION OF ARJUN MAKHIJANI

State of Maryland)

:

County of Montgomery)

I, Dr. Arjun Makhijani, hereby state and declare that,

- 1) I have been retained on behalf of Nuclear Information and Resource Service and Public Citizen (NIRS/PC) to investigate and present testimony about certain issues in the National Enrichment Facility case. I have previously been certified as an expert witness in the present case.

- 2) The conclusions reached and described herein relate to the treatment of mine disposal as presented in the National Enrichment Facility Final Environmental Impact Statement

(NEF FEIS) and the reasonableness of NRC Staff's reliance on the results presented in the Claiborne Enrichment Center Final Environmental Impact Statement (CEC FEIS). These conclusions are my carefully considered scientific opinions. In preparing this affidavit, I have relied on my own work, as well as the work of George Rice, a professional hydrologist, who has previously been certified as an expert witness for NIRS/PC in the present case. I have also relied on the work of Dr. Brice Smith, a Senior Scientist at the Institute for Energy and Environmental Research. Dr. Smith is a co-author of the November 24, 2004, and July 5, 2005, reports on the costs and risks of management and disposal of depleted uranium from the proposed National Enrichment Facility which have been filed with the Board.

- 3) The analysis presented in the CEC FEIS for mine disposal considers a total inventory of 91,000 metric tons of DU_3O_8 . The total inventory considered in the NEF FEIS is 157,000 metric tons of DU_3O_8 , approximately 1.72 times the Claiborne waste inventory. The bulk density for the DU_3O_8 assumed in the CEC FEIS is 3.0 grams per cubic centimeter which results in a total waste volume of approximately 30,300 cubic meters. Assuming the same bulk density of 3.0 grams per cubic centimeter, the DU_3O_8 from the proposed NEF would occupy a volume of approximately 52,300 cubic meters. (CEC FEIS 1994 p. A-7 and NEF FEIS 2005 p. 4-60)
- 4) The peak dose estimates presented in Table 4-19 of the NEF FEIS claim to be based on the results of the analysis presented in the CEC FEIS. The values in the NEF FEIS are not, however, broken down by radionuclide and only a total annual effective dose equivalent is reported. The NRC Staff claim that "[t]he potential impacts from the disposal of the proposed NEF-generated U_3O_8 for similar geologic disposal sites would be proportional to the quantity of material postulated from the Claiborne Enrichment Center enrichment facility." (NEF FEIS 2005 p. 4-63 to 4-64) Comparing the values in the two EISs, I find that that total doses reported in the NEF FEIS are on average 1.76 times the total doses reported in the CEC FEIS for well and river scenarios. This is

consistent with the ratio of DU that would be generated by the proposed NEF compared to that which would have been generated by the proposed CEC. However, no justification is offered for the NRC Staff's claim that the impacts from mine disposal would simply scale linearly with the amount of waste. No information is given as to how the configuration of the DU_3O_8 from the NEF would compare to the approximately 100 x 100 x 3 meter configuration of the CEC DU_3O_8 . Increasing the depth of the waste, increasing its cross sectional area, or some combination of both, could impact either the amount of time required to transport the material to the aquifer or the amount of material that would eventually reach the well. In addition, in the model proposed by the NRC Staff in the CEC FEIS, the point at which the well was located (200 meters down gradient from the mine) was supposedly chosen so as to maximize the resulting dose in that case. However, no information on the variation of dose with distance from the mine is provided. No discussion is offered in the NEF FEIS of any of these potential issues, and the doses reported in Table 4-19 appear to have simply been scaled by a constant factor. To verify that this approach is correct and that increasing the volume of the waste simply increases the peak dose proportionally, the NRC Staff would have to redo the calculation for at least one of the generic sites (i.e., either granite or sandstone/basalt mines) for both the well and river scenarios. However, because the underlying analysis supporting the CEC FEIS is apparently no longer available even to the NRC Staff, such a verification of the claim underlying the Staff's environmental analysis presented in the NEF FEIS is not now possible.

- 5) Turning to a consideration of the dose estimates presented in the CEC FEIS, I have concluded that the doses for the well water pathways presented in the CEC FEIS for deep disposal are incredibly low (literally). These results are not scientifically credible on their face and cannot therefore be accepted in their present form as legitimate estimates of the environmental impacts from disposal of depleted uranium. Any suitably hard look at the results presented in the CEC FEIS would raise serious doubts regarding their validity and would not support their use as the basis for an impacts analysis in the NEF FEIS, even if the issue of scaling the results discussed above could be resolved.

In addition, a central tenet of valid scientific inquiry is that the results must be reproducible by independent third parties. In this case the NRC Staff has relied on scientifically incredible results, which cannot be reproduced by the experts for NIRS/PC from the information provided in the CEC FEIS. The apparent inability of the NRC Staff to reproduce these dose estimates themselves, particularly in light of the serious questions raised by NIRS/PC as far back as November 2004 about their reasonableness (see Makhijani and Smith 2004 pp. 21 to 23 and 25 to 29), should disqualify this analysis from any further consideration in the present case since it is scientifically unacceptable.

- 6) Table A.7 of the CEC FEIS lists the following for the projected doses from the well water scenarios for disposal of 91,000 metric tons of DU_3O_8 in generic granite and sandstone/basalt sites:

	Granite Site (mrem per year)		Sandstone/Basalt Site (mrem per year)	
	Drinking Water	Agricultural	Drinking Water	Agricultural
U-238	5.0×10^{-9}	2.3×10^{-10}	2.3×10^{-15}	1.0×10^{-16}
U-234	5.3×10^{-9}	1.6×10^{-10}	2.5×10^{-15}	7.5×10^{-17}
Th-230	3.1×10^{-12}	1.8×10^{-11}	1.6×10^{-18}	9.0×10^{-18}
Ra-226	4.9×10^{-3}	1.3×10^{-1}	4.0×10^{-6}	1.0×10^{-4}

(CEC FEIS 1994 p. A-14)

The reported drinking water doses are unbelievably low (again in the literal sense). For disposal in a granite site, the drinking water doses reported in the CEC FEIS imply a concentration for thorium-230 in the well water that would be equal to approximately one atom of thorium per liter of water. For the sandstone/basalt site the results are even more incredible. The drinking water doses reported imply a concentration of U-234 equal to just one atom in every 200 liters of well water and a concentration for thorium-230 of just one atom in every 1.9 million liters of water. No comment on these remarkably low concentrations is made in either the CEF or NEF final EIS.

- 7) Another way to consider the reasonableness of the dose estimates in the CEC FEIS is compare them to typical doses received from natural background uranium. Assuming a daily consumption of two liters as was done in the CEC FEIS, the annual background dose to an adult due to drinking water containing uranium that has leached out of ordinary dirt and rocks is summarized in the following table:

	Population averaged background uranium concentration in domestic water supplies (pCi/L)*	Annual Effective Dose Equivalent (mrem per year)
Eastern States	0.01	1.9×10^{-3}
Midwestern States	0.35	6.5×10^{-2}
Western States	3.50	6.5×10^{-1}

*(Eisenbud and Gesell 1997 p. 141-142)

The peak doses received from drinking well water contaminated with both U-238 and U-234 (excluding the other decay products) as reported in the CEC FEIS for the generic sandstone/basalt and granite sites were 4.8×10^{-15} and 1.03×10^{-8} mrem per year respectively. (CEC FEIS 1994 p. A-14) Comparing the CEC FEIS estimates to the typical background doses from naturally occurring uranium, we find that the drinking water doses estimated by the NRC Staff from a well drilled into an aquifer located in a geologic stratum above a disposal site with 91,000 metric tons of pure DU_3O_8 powder were more than a hundred thousand to a hundred trillion times lower than typical background levels received from uranium that dissolves out of ordinary rocks and dirt. No comment on this incredible assertion is found in either the CEC or NEF final environmental impact statements. The NEF FEIS is especially deficient since IEER had already pointed out the above problems in the November 2004 report.

- 8) A third way to consider the reasonableness of the CEC FEIS dose estimates is to consider the amount of energy deposited in the human body implied by these incredibly low doses. For a 70 kilogram adult, the highest well water dose for uranium-238 estimated by the NRC Staff in the CEC FEIS (5×10^{-9} mrem per year) is less than the dose that would be received from the disintegration of just 23 uranium-238 atoms in the entire body over an

entire year. The lowest drinking water dose for U-238 reported in the CEC FEIS (2.3×10^{-15} mrem per year) would imply that less than one atom of uranium-238 would disintegrate in the person's body over their entire lifetime. In fact, the decay of just a single uranium-238 atom in a 70 kilogram adult in one year would result in an absorbed dose nearly five orders of magnitude larger than the drinking water dose reported in the CEC FEIS for the generic sandstone/basalt disposal scenario.¹

- 9) Finally, the doses presented for the sandstone/basalt mine are also incredible from the point of view of the radionuclide solubilities reported in the CEC. As noted in paragraph 6, the implied concentration of the radionuclides in the well water from the reported peak doses is remarkably low. Using the solubilities given in Table A.6 of the CEC FEIS (see paragraphs 13 to 15 for a further discussion of these solubility estimates), I find that if even just one part in a million of the DU waste dissolved into the water in the sandstone/basalt mine was mixed into the aquifer from which the drinking water is withdrawn, then the total volume required to dilute this amount of waste to the levels implied by the dose estimates in Table A.7 of the CEC FEIS would be nearly 23.5 billion cubic meters of water.² For a sense of scale, this amount of water would fill a cube more than 7.8 kilometers on a side. (CEC FEIS 1994 p. A-13 to A-14) The use of higher uranium solubilities as discussed in paragraphs 13 to 15 would make the required dilution even less believable. (Makhijani and Smith 2004 p. 22)

- 10) Turning to the river scenarios, Table A.8 of the CEC FEIS presents the following projected doses for disposal in generic granite and sandstone/basalt sites:

¹ In the November 2004 report, a similar calculation resulted in values that were about a factor of four lower than the ones in this paragraph. The prior calculations ignored uranium biokinetics for simplicity. The present calculations in this paragraph take them into account. This makes no material difference to my conclusions since all the numbers are very small.

² This calculation assumes a 30 percent porosity of the waste in the mine. The amount of contaminated water from the mine assumed to be mixed uniformly into the aquifer is therefore approximately 9.1 liters.

	Granite Site (mrem per year)		Sandstone/Basalt Site (mrem per year)	
	Drinking Water	Fish Ingestion	Drinking Water	Fish Ingestion
U-238	2.6×10^{-12}	3.7×10^{-12}	7.9×10^{-11}	1.1×10^{-10}
U-234	2.9×10^{-12}	4.1×10^{-12}	8.8×10^{-11}	1.2×10^{-10}
Th-230	5.6×10^{-12}	1.6×10^{-11}	1.7×10^{-10}	4.7×10^{-10}
Ra-226	1.3×10^{-11}	2.6×10^{-11}	4.0×10^{-10}	7.8×10^{-10}

(CEC FEIS 1994 p. A-15)

The drinking water doses reported in the CEC FEIS assume that the daughters of uranium-238 are in secular equilibrium at the river due to the decay of the radium initially in the mine water during the time required to travel the five kilometers assumed to be the distance between the mine and the river outcropping. The drinking water doses reported for U-234, Th-230, and Ra-226 are then consistent with simply scaling the U-238 dose by the relevant dose conversion factors for the other radionuclides. However, these reported doses are again incredibly low and unbelievable. For disposal in a granite site, the drinking water doses imply a concentration for thorium-230 in the water that would be equivalent to less than two atoms per liter of water. For radium-226, the doses in the CEC FEIS imply a concentration of just one atom of radium-226 in every 28 liters of water.

- 11) As paragraphs 6 to 10 above demonstrate, even a minimal effort spent in reviewing the reasonableness of the results presented in the CEC FEIS would be sufficient to cast grave doubts upon their validity. In addition, I have also found, on a closer examination, that the dose estimates for the well scenarios appear to be internally inconsistent. In Table A.6 the CEC FEIS, the following information is given regarding the solubility of uranium, thorium, and radium in the deep ground water:

Nuclide	Solubility in CEC FEIS (mg/L)	Dominant Solid Phase in CEC FEIS	Dominant Aqueous Phase in CEC FEIS
Uranium	1×10^{-4}	UO ₂	U(OH) ₄
Thorium	5×10^{-13}	ThO ₂	Th(OH) ₃ ⁺¹
Radium	1×10^{-2}	RaSO ₄	Ra ⁺²

(CEC FEIS 1994 p. A-13)

For the given values for the solubility, the masses of U-238, U-234, Th-230, and Ra-226 at secular equilibrium in the CEC depleted uranium are more than sufficient to saturate the volume of water that would be contained in the pore space of the waste. If a well was drilled directly into the mine, the annual dose from drinking this water would be dominated by the radium component and would amount to several thousand rem per year (see the table below).³

	U-238	U-234	Th-230	Ra-226
Activity in mine water at solubility limit (pCi/L)	3.30E-02	3.30E-02	1.00E-05	1.00E+07
Annual drinking water dose (mrem per year)	6.83E-03	6.13E-03	4.00E-06	9.67E+06

- 12) The CEC FEIS, however, does not consider a well sunk into the waste itself, but instead considers a well sunk into an aquifer above the waste emplacement zone and 200 meters down gradient from the mine. (CEC FEIS 1994 p. A-10, A-11 and A-14) Comparing the doses reported in Table A.7 for the sandstone/basalt mine, I find that the dose from each individual radionuclide listed is an average of 2.6 trillion times less than that which would be estimated from drinking the mine water directly. Significantly, the dose reported for each of the four individual radionuclides is reduced by approximately the same amount.

Comparing the above results for the sandstone/basalt site to those for the granite site, on the other hand, I find that the doses for U-238, U-234, and Th-230 reported in Table A.7 are all reduced by approximately 1.3 million times from the doses that would be received from drinking the mine water directly. While the reduction in the dose from each of these three radionuclides are all approximately equal, the radium-226 dose reported in Table A.7 is nearly 2 billion times less than that which would be received from drinking

³ This calculation assumes the consumption of two liters per day.

the mine water directly. No discussion of this difference between the uranium and thorium behavior on the one hand and the radium behavior on the other is offered anywhere in the CEC or NEF FEIS.

Given the far shorter half-life of radium compared to the uranium and thorium isotopes (1,600 years for Ra-226 versus 77,000 years for Th-230, 248,000 years for U-234, and 4.5 billion years for U-238), it is possible that the lower radium dose reported for the granite site could result from radioactive decay during transport if it took on the order of 17,000 years for the radioactive material to migrate from the mine to the well. However, the transport path assumed for the sandstone/basalt site appears to be significantly longer than that assumed for the granite site and in the case of the sandstone/basalt mine the radium dose was not reduced relative to the uranium and thorium doses as would be expected if significant radioactive decay was occurring during transport. (CEC FEIS 1994 p. A-11) Thus, the results reported for the granite and sandstone/basalt sites appear to be inconsistent with respect to their treatment of radium.

This is a potentially significant inconsistency with respect to the radiological impacts of mine disposal as presented in the CEC FEIS. If the radium drinking water dose for the generic granite site was consistent with the uranium and thorium doses reported in Table A.7, then the bone surface dose under these assumptions would exceed the 25 millirem per year organ specific dose limit in 10 CFR 61.41 (2005).⁴ A final resolution of this matter is not now possible since the underlying calculations supporting the CEC analysis are apparently no longer available even to the NRC Staff and the NRC Staff has forwarded no re-runs of the model to show the plausibility of their claimed results.

- 13) Turning away from the reported doses, a further issue arises with respect to the reported solubilities for uranium, thorium, and radium. The CEC FEIS states that the solubilities

⁴ This calculation assumes that the radium dose from drinking the well water would be 1.3 million times less than dose received from drinking the mine water directly, in agreement with the uranium and thorium doses reported in the CEC FEIS. This would then result in an annual effective dose equivalent of 7.6 millirem per year for radium-226. The bone surface dose is approximately 19 times the effective dose equivalent.

for these elements were calculated using the PHREEQE code, but does not specify all of the parameters used in performing these calculations. To check these solubility calculations, George Rice conducted runs of the PHREEQC program for a variety of different solid phases using the information that was provided in the CEC FEIS as well as reasonable values for inputs that were not provided (see declaration of George Rice, November 18, 2005 (Rice 2005)). His results of interest to the present discussion are summarized in the following table:

Nuclide	Solubility from George Rice (mg/L)	Dominant Solid Phase from George Rice	Dominant Aqueous Phase from George Rice
Uranium	7.0×10^{-1}	U ₃ O ₈ (with CO ₂)	UO ₂ (CO ₃) ₃ ⁻⁴
	1.8×10^{-1}	U ₃ O ₈ (without CO ₂)	UO ₂ (CO ₃) ₂ ⁻²
	2.1×10^{-4}	UO ₂ (with CO ₂)	U(OH) ₅ ⁻¹
	2.5×10^{-5}	UO ₂ (without CO ₂)	U(OH) ₅ ⁻¹
Thorium	n.a.	ThO ₂ *	n.a.
Radium	1.2×10^{-2}	RaSO ₄	Ra ⁺²

* According to information supplied by George Rice, the data required to calculate the solubility for ThO₂ was unavailable and so this calculation could not be done in the time allowed.

- 14) The solubility and dominant aqueous phase for radium found in the work of Mr. Rice is consistent with the results presented in the CEC FEIS (see paragraph 11). For uranium in the form of UO₂, the solubility reported in the CEC FEIS (1×10^{-4} milligrams per liter) is on the same order of magnitude as the results from Mr. Rice (2.5×10^{-5} to 2.1×10^{-4} milligrams per liter), however, the dominant aqueous phase predicted by Mr. Rice's calculation is not the same as that reported in the CEC FEIS. Due to the lack of all relevant input data, this conflict cannot now be resolved. Finally, as noted above, the thorium calculation in the CEC FEIS could not be reproduced due to the lack of relevant data on ThO₂ for use in the PHREEQC database. It is necessary to address this detail since the results for uranium are likely to be in error.

15) One of the most important questions raised by the work of George Rice is why the dominant solid phase for uranium in the CEC FEIS was taken to be UO_2 when the depleted uranium was to be disposed of in the form of DU_3O_8 . The importance of this distinction is clear from the table in paragraph 13. The solubility of U_3O_8 under the assumed conditions with or without the presence of CO_2 (i.e. air) is more than three orders of magnitude greater than the corresponding solubility of UO_2 . There is no discussion of why UO_2 was chosen as the dominant phase in the CEC FEIS and no mention is made of the fact that this choice is likely to underestimate the impacts from disposal of U_3O_8 which is significantly more soluble under the assumed conditions. Further, the NEF FEIS did not adjust its CEC dose estimates upward in view of the fact that UO_2 has been ruled out as the final form of DU for disposal by the NRC Staff.

The higher solubility of U_3O_8 found by Mr. Rice compared to the uranium solubility of UO_2 reported in the CEC FEIS is supported by the work of Kozak *et al.* carried out at Sandia National Laboratory. In this work, which was conducted to support the Claiborne Enrichment Center environmental impact analysis, the authors noted that

One important point to make is that U_3O_8 does not exist in solution, but rather speciates to other oxide, hydroxide, and complex forms, all of which are soluble to some extent. In addition, U_3O_8 is thermodynamically unstable in ground water. U_3O_8 is therefore expected to convert to other oxide forms; the favored form under oxidizing conditions is schoepite, but other complexes may be favored depending on site-specific conditions. (Kozak et al. 1992 p. 30-31)

Kozak *et al.* went on to note that due to the significance of site specific chemistries on the behavior of uranium, "on a generic basis, we cannot specify a solubility limit for U_3O_8 with much confidence." (Kozak et al. 1992 p. 31) Considering the general behavior of schoepite, the authors of the Sandia study concluded that the minimum solubility for uranium in this form would be approximately 10^{-6} moles/liter with or without the presence of CO_2 . Over a wider range of pH values, $4 < \text{pH} < 9$, the authors concluded that "we can have confidence that the solubility limit is less than 10^{-5} moles/liter." (Kozak et al. 1992 p. 31) Thus, from Kozak *et al.*, the solubility of uranium would be expected to fall within the range of 0.24 and 2.4 milligrams per liter. This range is

consistent with George Rice's calculations for U_3O_8 in the presence of CO_2 (i.e. 0.70 milligrams per liter). However, even the smallest value reported by either Kozak *et al.* or Mr. Rice for U_3O_8 is still more than three orders of magnitude greater than the uranium solubility used in the CEC FEIS.

The one "extremely important" qualification that Kozak *et al.* put on their conclusions regarding the solubility of uranium is that

... the solubility of uranium compounds can be much less than the schoepite in water values, since uranium can form very insoluble complexes with minerals. The potential for these lower solubilities can only be evaluated for specific geochemical conditions. (Kozak et al. 1992 p. 34)

I share this conclusion regarding the need for site specific evaluations as part of providing a credible and scientifically reasonable estimate of the impacts from depleted uranium disposal (see Makhijani and Smith 2004 p. 21 to 23 and 25 to 28). In conducting generic screening calculations, however, it is necessary to make use of the higher solubility estimates given the fact that they will correspond to the chemical form actually proposed for disposal and they do not require the use of information regarding the presence of other minerals which would necessitate site specific considerations.

- 16) Assuming that a well was drilled directly into the mine and using the higher uranium solubility calculated by Mr. Rice (i.e., the solubility for U_3O_8 in the presence of CO_2), the water would exceed the EPA drinking water limit for uranium of 30 micrograms per liter by more than 20 times. (40 CFR 141.66 (2005)) In addition, assuming an adult would drink two liters of this water per day, the uranium-238 alone would result in a bone surface dose in excess of the 25 millirem dose limit to the critical organ. While such estimates are conservative in that they do not take into account any dilution of the mine water, they are reasonable as screening calculations which can provide further information with which to judge the incredibility of the dose estimates presented by the NRC Staff in the CEC FEIS and reiterated in the NEF FEIS. Even a dilution of this

waste with any reasonable volume of water, would not produce doses as low as those reported in the NEF FEIS.

17) Another concern regarding the NRC Staff's use of the results from the analysis in the CEC case is that more than a decade has gone by since the analysis underlying the CEC FEIS was completed. In that time a significant amount of work has been done on radionuclide transport and bioaccumulation and plant transfer factors. In order to have confidence that the results presented in the NEF FEIS are consistent with today's scientific understanding and the current norms of environmental pathway analyses, a critical review of the relevant inputs and default assumptions in the CEC analysis would be required. However, there is no evidence in the FEIS that the NRC Staff conducted such a review.

18) A final concern is that the NRC Staff responsible for the environmental impact assessment appear unable to discern incorrect results even when they are completely unphysical and impossible. At the October 2005 licensing board hearing, NRC Staff witnesses testified that they reviewed the performance assessment used to support the original licensing of the Envirocare site and concluded the results presented in it were "scientifically reasonable" and that the analysis "was done with a model that was considered acceptable." (ASLB Hearing Oct. 2005 p. 2885 to 2887) However, some of the results in this performance assessment are literally impossible, including one in which the allowable U-238 concentration per gram of soil would far exceed the weight of the Earth. (Baird et al. 1990 p. 5-13)

19) I conclude, therefore, that the NEF FEIS mine disposal doses are almost certainly incorrect. They were included in the final EIS in a manner that does not indicate the slightest respect for the scientific method in that the NRC Staff cannot provide some of the essential details of how the calculations were done and has, to all evidence, not tried

or has been unable to reproduce the results. Further, evidence of the incredible, unscientific and unsupportable nature of these results are provided by calculations in IEER's November 2004 report, the calculations reported here, and the 1992 report from Sandia commissioned by the NRC in connection with the proposed Claiborne Enrichment Center. The NEF FEIS contains no legitimate or scientifically valid calculations of mine disposal dose.

References:

- | | |
|-----------------------------|--|
| 10 CFR 61.41,
2005 | United States. Nuclear Regulatory Commission. <i>Code of Federal Regulations. Title 10 Energy. Part 61: Licensing requirements for land disposal of radioactive waste. Section 41: Protection of the general population from releases of radioactivity.</i> (1-1-05 Edition). |
| 40 CFR 141.66,
2005 | United States. Environmental Protection Agency. <i>Code of Federal Regulations. Title 40: Protection of Environment. Part 141: National primary drinking water regulations. Section 66: Maximum contaminant levels for radionuclides.</i> (7-1-05 Edition). |
| ASLB Hearing
Oct. 2005 | U.S. Nuclear Regulatory Commission Atomic Safety and Licensing Board, "Closed Hearing in the Matter of Louisiana Energy Services, L.P. (National Enrichment Facility)", Docket No. 70-3103-ML, ASLBP No. 04-826-01-ML, October 27, 2005. |
| Baird et al. 1990 | R.D. Baird, M.K. Bollenbacher, E.S. Murphy, R. Shuman, and P.B. Klein, "Evaluation of the Potential Public Health Impacts Associated with Radioactive Waste Disposal at a Site Near Clive, Utah", Rogers and Associates Engineering Corporation, June 1990 (RAE-9004/2-1). |
| CEC FEIS 1994 | U.S. Nuclear Regulatory Commission. "Final Environmental Impact Statement for the Construction and Operation of Claiborne Enrichment Center, Homer, Louisiana", August 1994 (NUREG-1484, Vol. 1). |
| Eisenbud and
Gesell 1997 | Merril Eisenbud and Thomas Gesell, <i>Environmental Radioactivity: From Natural, Industrial, and Military Sources</i> , 4th ed. New York: Academic Press, 1997. |
| Kozak et al. 1992 | Matthew W. Kozak, Thomas A. Feeney, Christi D. Leigh, Harlan W. Stockman. <i>Performance assessment of the proposed disposal of depleted uranium as Class A Low-level Waste.</i> FIN A1764 Final Letter Report submitted December 16, 1992 to F.W. Ross (Low-Level Waste Management Branch, Office of Nuclear Material Safety and Safeguards, Nuclear Regulatory Commission). Albuquerque, NM: Sandia National Laboratories, 1992. |

Makhijani and Smith 2004	Arjun Makhijani and Brice Smith, "Costs and Risks of Management and Disposal of Depleted Uranium from the National Enrichment Facility Proposed to be Built in Lea County New Mexico by LES", November 24, 2004.
NEF FEIS 2005	U.S. Nuclear Regulatory Commission, "Environmental Impact Statement for the Proposed National Enrichment Facility in Lea County, New Mexico: Final Report", Chapters 1 through 10 and Appendices A through G, June 2005 (NUREG-1790, Vol. 1).
Rice 2005	U.S. Nuclear Regulatory Commission, Atomic Safety and Licensing Board, In the Matter of Louisiana Energy Services, L.P. (National Enrichment Facility), "Declaration of George Rice," Docket No. 70-3103-ML, ASLBP No. 04-826-01-ML, November 18, 2005.

I declare under penalty of perjury that the foregoing are my true and correct professional opinions and conclusions. Executed at Takoma Park, Maryland this 18th day of November, 2005.



Arjun Makhijani, Ph.D.

**UNITED STATES OF AMERICA
NUCLEAR REGULATORY COMMISSION**

BEFORE THE ATOMIC SAFETY AND LICENSING BOARD

In the Matter of

Docket No. 70-3103

Louisiana Energy Services, L.P.
National Enrichment Facility

ASLBP No. 04-826-01-ML

DECLARATION OF GEORGE RICE

State of Texas)
 :
County of Bexar)

George Rice, under penalty of perjury, states as follows:

1. I am a professional hydrologist and have been retained on behalf of Nuclear Information and Resource Service and Public Citizen (NIRS/PC) to investigate and present testimony about certain issues in this case.

2. I used the geochemical code PHREEQC to estimate equilibrium concentrations of uranium, radium, and thorium in water.

3. PHREEQC is a public domain code available from the United States Geological Survey.

A fact sheet on PHREEQC can be found at the following address:

<ftp://brrcrftp.cr.usgs.gov/geochem/pc/phreeqc/PhreeqcI.FactSheet.pdf>

4. I performed three sets of simulations. All three sets used the solution chemistry provided in the Claiborne FEIS¹ (table A.5)². In the first set of simulations I also used a solution chemistry from Los Alamos National Laboratory.

¹ NRC, 1994.

5. In the first set of simulations (runs one through eight) I equilibrated the solution described in the FEIS with U_3O_8 and UO_2 . In some of the runs I fixed the partial pressure of CO_2 to simulate contact with the atmosphere. These runs assumed that an unlimited supply of uranium minerals was available to dissolve into the solution. The results of these simulations are summarized in Attachment 1, a letter from me to Arjun Makhijani (November 15th, 2004).
6. In the second set of simulations (runs nine through 14) I equilibrated the solution described in the FEIS with radium and thorium minerals³. These runs assumed that an unlimited supply of radium and thorium minerals was available to dissolve into the solution. The results of these simulations are summarized in Attachment 2, a letter from me to Brice Smith (November 12th, 2005).
7. In the third set of simulations (runs 15 through 20) I equilibrated the solution described in the FEIS with radium and thorium minerals. However, in these runs I assumed the supply of radium and thorium minerals was limited. The results of these simulations are summarized in Attachment 3, a letter from me to Arjun Makhijani and Brice Smith (November 15th, 2005).
8. The outputs for the first, second, and third sets of simulations are provided as attachments 4, 5, and 6, respectively.
9. The following comments concern the Claiborne FEIS:
10. A list of dominant solid phases is presented in Table A.6. However, there is no explanation of how they were chosen. The choice of UO_2 as the dominant uranium phase

² Note – the solution chemistry in the FEIS was incomplete. I added appropriate amounts of calcium and sodium to achieve cation/anion balance. In addition, no temperature was provided so I assumed a temperature of 25 C.

³ I was unable to simulate the dissolution of one thorium mineral (ThO_2) because I could not find the data required (solubility product for the dissolution reaction) to add it to the database.

is particularly surprising as the discussions of both the near surface and deep disposal options indicate that uranium will be disposed in the form of U_3O_8 , not UO_2 ⁴.

11. Retardation coefficients greater than 1200 are assumed for uranium, radium, and thorium⁵. This would result in very low groundwater transport rates. However, according to the PHREEQC runs the dominant aqueous uranium species would be anionic complexes (e.g., $UO_2(CO_3)_2^{2-}$, $U(OH)_5^-$). These uranium complexes are likely to be mobile. That is, these uranium complexes would be readily transported by groundwater. My experience with uranium mill wastes on the UMTRA⁶ Project is that uranium is often mobile. In addition, dissolved species being transported through fractures tend to be more mobile than those transported through granular media. An analyses of radionuclide transport through fractured tuff suggested that the radionuclides would migrate at the same rate as the water⁷. Finally, it should be noted that retardation coefficients are highly site specific. In the absence of site specific data, estimates of retardation coefficients are questionable.

References

Krier, D., P. Longmire, R.H. Gilkeson, and H.J. Turin, 1997, *Geologic, Geohydrologic, and Geochemical Data Summary of Material Disposal Area G, Technical Area 54, Los Alamos National Laboratory*, February 1997, LAUR-95-2696.

NRC, 1994, *Final Environmental Impact Statement for the Construction and Operation of Claiborne Enrichment Center, Homer, Louisiana*, NUREG-1484, August 1994.

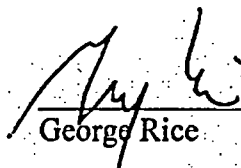
⁴ NRC, 1994, sections A.2.2 and A.2.3.

⁵ NRC, 1994, page A-13.

⁶ UMTRA = uranium mill tailings remedial action.

⁷ Krier et al., 1997, page 49.

Signed:

 Nov. 18, 2008
George Rice (date)

Attachment 1

November 15, 2004

Hello Arjun,

Here are the results of the six PHREEQC runs we discussed, and three others. The complete output for each run is attached to the email. These runs are preliminary.

Runs one through 6 use the solution chemistry provided by LES in the Claiborne EIS (pg A-12). Note – Ca and Na were added to the solution for cation/anion balance. Assumed temperature = 25 C.

Runs seven through nine use the water chemistry from LANL well R-15⁸. Depth of sample = 1018 feet.

Where a solution is equilibrated with CO₂, the partial pressure of CO₂ is equal to the atmospheric partial pressure 10^{-3.5} atm.

Results

Run 1: Equilibration with U3O8

Total U concentration (molality)⁹ = 7.529e-07 ~ 1.79 x 10⁻⁴ g/L = 179 µg/L
Dominant U species in solution = UO₂(CO₃)₂-2

Run 2: Equilibration with UO2

Total U concentration (molality) = 1.065e-10 ~ 2.53 x 10⁻⁸ g/L = 0.0253 µg/L
Dominant U species in solution = U(OH)₅-

Run 3: Equilibration with U3O8 and UO2

Total U concentration (molality) = 2.282e-05 ~ 5.43 x 10⁻³ g/L = 5430 µg/L
Dominant U species in solution = UO₂(CO₃)₂-2

Run 4: Equilibration with U3O8 and CO2

Total U concentration (molality) = 2.937e-06 ~ 6.99 x 10⁻⁴ g/L = 699 µg/L
Dominant U species in solution = UO₂(CO₃)₃-4

⁸ Longmire, P., 2002, *Characterization Well R-15 Geochemistry Report*, LA-13896-MS, March 2002.

⁹ Conversions from molality to g/L assume atomic weight of U = 238.

Run 5: Equilibration with UO₂ and CO₂

Total U concentration (molality) = $9.008 \times 10^{-10} \sim 2.14 \times 10^{-7}$ g/L = 0.214 µg/L

Dominant U species in solution = U(OH)₅⁻

Run 6: Equilibration with U₃O₈, UO₂, and CO₂

Total U concentration (molality) = $5.446 \times 10^{-5} \sim 1.30 \times 10^{-2}$ g/L = 12,960 µg/L

Dominant U species in solution = UO₂(CO₃)₃⁻⁴

Run 7: LANL well R-15, Equilibration with U₃O₈

Total U concentration (molality) = $1.372 \times 10^{-6} \sim 3.27 \times 10^{-4}$ g/L = 327 µg/L

Dominant U species in solution = UO₂(CO₃)₂⁻²

Run 8: LANL well R-15, Equilibration with U₃O₈ and CO₂

Total U concentration (molality) = $1.273 \times 10^{-6} \sim 3.03 \times 10^{-4}$ g/L = 303 µg/L

Dominant U species in solution = UO₂(CO₃)₂⁻²

Run 8: LANL well R-15, Equilibration with UO₂

Total U concentration (molality) = $5.065 \times 10^{-7} \sim 1.21 \times 10^{-4}$ g/L = 121 µg/L

Dominant U species in solution = UO₂(CO₃)₂⁻²

Attachment 2

November 12, 2005

Hello Brice,

Here are the results of six PHREEQC runs. Runs nine through 11 are for radium species. Runs 12 through 14 are for thorium species. (Runs one through eight are for uranium species and were provided in November 2004.)

All of the runs use the solution chemistry provided by LES in the Claiborne EIS (pg A-12). Note – Ca and Na were added to the solution for cation/anion balance. Assumed temperature = 25 C.

The runs used the database compiled by Lawrence Livermore National Laboratory. This is the only PHREEQC database that contains data for Ra or Th. However, it does not contain data for ThO₂. I could not find a reference that contains the data required to add ThO₂ to the database (solubility product for dissolution reaction).

Let me know if you want the output for any of the runs or if you need anything else.

George

Radium Species

Run 9: Equilibration with RaSO₄

Total Ra concentration (molality)¹⁰ = 5.229e-08 ~ 1.18 x 10⁻⁵ g/L = 11.8 µg/L
Dominant (only) Ra species in solution = Ra+2

Run 10: Equilibration with Ra(NO₃)₂

Total Ra concentration (molality) = 2.668e-01 ~ 60.3 g/L = 6.03 x 10⁷ µg/L
Dominant (only) Ra species in solution = Ra+2

Run 11: Equilibration with RaCl₂·2H₂O

Total Ra concentration (molality) = 9.125e-01 ~ 206 g/L = 2.06 x 10⁸ µg/L
Dominant (only) Ra species in solution = Ra+2

Thorium Species

Run 12¹¹: Equilibration with Th(NO₃)₄·5H₂O

¹⁰ Conversions from molality to g/L assume atomic weight of Ra = 226.

¹¹ Program produced a convergence warning.

Total Th concentration (molality)¹² = $1.356 \times 10^0 \sim 315 \text{ g/L} = 3.15 \times 10^8 \text{ } \mu\text{g/L}$
Dominant Th species in solution = Th⁴⁺

Run 13: Equilibration with Th(OH)₄

Total Th concentration (molality) = $4.473 \times 10^{-7} \sim 1.04 \times 10^{-4} \text{ g/L} = 1.04 \times 10^2 \text{ } \mu\text{g/L}$
Dominant Th species in solution = Th(OH)₄

Run 14: Equilibration with Th(SO₄)₂

Total Th concentration (molality) = $\sim 2.250 \times 10^{-4} = 5.22 \times 10^{-2} \text{ g/L} = 5.22 \times 10^4 \text{ } \mu\text{g/L}$
Dominant Th species in solution = Th(OH)₄

¹² Conversions from molality to g/L assume atomic weight of Th = 232.

Attachment 3

November 15, 2005

Hello Arjun and Brice,

The results of the revised PHREEQC runs are given below.

As with the previous runs, all of these runs use the solution chemistry provided by LES in the Claiborne EIS (pg A-12). Note – Ca and Na were added to the solution for cation/anion balance. Assumed temperature = 25 C.

These runs also used the database compiled by Lawrence Livermore National Laboratory. This is the only PHREEQC database that contains data for Ra or Th.

These runs make sense in that the highly soluble species are limited by the amount of mass available (e.g., $\text{Ra}(\text{NO}_3)_2$, $\text{Th}(\text{NO}_3)_4 \cdot 5\text{H}_2\text{O}$) while the results for the less soluble species (e.g., RaSO_4 , $\text{Th}(\text{OH})_4$) remain unchanged.

Let me know if you want the output for any of the runs or if you need anything else.

George

In these runs I limited the amounts of Ra and Th available for dissolution. I calculated the amounts as follows:

Amount of water in which minerals may dissolve = 1.0 L.

Total amount of waste = 133,000 metric tons = $1.33 \text{ E}+8 \text{ Kg}$

Total amount of Ra = 44 Kg

Ratio Ra to waste = $3.31 \text{ E}-7$

Total amount Th = 2000 Kg

Ratio Th to waste = $1.50 \text{ E}-5$

Ra and Th are assumed to be evenly distributed throughout waste.

Bulk density of waste = 3 g/cc = 3 Kg/L

Porosity of waste = 0.3.

Therefore 1 L of waste = 0.3 L of water and 3.33 L of waste = 1.0 L of water

3.33 L of waste = 10 kg of waste

Amount of Ra in 10 kg = $10 (3.31\text{E-}7) \text{ kg} = 3.31 \text{ E-}6 \text{ Kg}$.

Amount of Th in 10 kg = $10 (1.50 \text{ E-}4) \text{ kg} = 1.50 \text{ E-}4 \text{ Kg}$.

One mole Ra = 226 g.

Moles Ra available for dissolution into 1.0 L water = $3.31 \text{ E-}6 \text{ Kg} / 0.226 \text{ Kg}$
= $1.46 \text{ E-}5$ moles Ra (3.3 mg).

One mole Th = 232 g.

Moles Th available for dissolution into 1.0 L water = $1.50 \text{ E-}4 \text{ Kg} / 0.232 \text{ Kg}$
= $6.47 \text{ E-}4$ moles Th (150 mg)

Radium Species

(assume $1.46 \text{ E-}5$ moles Ra available for dissolution).

Run 15: Equilibration with RaSO_4

Total Ra concentration (molality)¹³ = $5.229\text{e-}08 \sim 1.18\text{E-}5 \text{ g/L} = 11.8 \text{ }\mu\text{g/L}$
Dominant (only) Ra species in solution = Ra^{+2}

Run 16: Equilibration with $\text{Ra}(\text{NO}_3)_2$

Total Ra concentration (molality) = $1.460\text{e-}05 \sim 3.3\text{E-}3 \text{ g/L} = 3300 \text{ }\mu\text{g/L}$
Dominant (only) Ra species in solution = Ra^{+2}

Run 17: Equilibration with $\text{RaCl}_2 \cdot 2\text{H}_2\text{O}$

Total Ra concentration (molality) = $1.460\text{e-}05 \sim 3.3\text{E-}3 \text{ g/L} = 3300 \text{ }\mu\text{g/L}$
Dominant (only) Ra species in solution = Ra^{+2}

Thorium Species

(assume $6.47 \text{ E-}4$ moles Th available for dissolution)

Run 18: Equilibration with $\text{Th}(\text{NO}_3)_4 \cdot 5\text{H}_2\text{O}$

Total Th concentration (molality)¹⁴ = $6.470\text{e-}04 \sim 0.15 \text{ g/L} = 1.50 \text{ E+}5 \text{ }\mu\text{g/L}$
Dominant Th species in solution = $\text{Th}(\text{OH})_4$

Run 19: Equilibration with $\text{Th}(\text{OH})_4$

Total Th concentration (molality) = $4.473\text{e-}07 \sim 1.04 \text{ E-}4 \text{ g/L} = 104 \text{ }\mu\text{g/L}$

¹³ Conversions from molality to g/L assume atomic weight of Ra = 226.

¹⁴ Conversions from molality to g/L assume atomic weight of Th = 232.

Dominant Th species in solution = $\text{Th}(\text{OH})_4$

Run 20: Equilibration with $\text{Th}(\text{SO}_4)_2$

Total Th concentration (molality) = $2.250\text{e-}04 \sim 5.22 \text{ E-}2 \text{ g/L} = 5.22 \text{ E+}4 \text{ } \mu\text{g/L}$

Dominant Th species in solution = $\text{Th}(\text{OH})_4$

Attachment 4

Run 1

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

TITLE Run-1 - Equil with U3O8 only
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.
pH 7.8
temp 25.0
pe -1.69 $\# = -100$ mV, $pe = eh/0.059$ (Stumm & Morgan, pg 422)
units ppm
Alkalinity 205.7 as HCO₃
Ca 141.9
Cl 4.4
Na 2.85
S 178.2
EQUILIBRIUM_PHASES 1
U3O8(C) 0.0 10.0
END

TITLE

Run-1 - Equil with U3O8 only

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.373e-03	3.373e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04

S

1.856e-03 1.856e-03

-----Description of solution-----

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.083e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.438e-03
 Total CO2 (mol/kg) = 3.438e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -4.968e-07
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = -0.00
 Iterations = 7
 Total H = 1.110159e+02
 Total O = 5.552395e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	7.068e-07	6.338e-07	-6.151	-6.198	-0.047
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.438e-03				
HCO3-	3.228e-03	2.912e-03	-2.491	-2.536	-0.045
H2CO3	1.034e-04	1.036e-04	-3.986	-3.984	0.001
CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
CO3-2	1.299e-05	8.600e-06	-4.887	-5.065	-0.179
NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
Ca	3.542e-03				
Ca+2	3.054e-03	2.045e-03	-2.515	-2.689	-0.174
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
CaOH+	3.603e-08	3.256e-08	-7.443	-7.487	-0.044
Cl	1.242e-04				
Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
H(0)	8.510e-16				
H2	4.255e-16	4.266e-16	-15.371	-15.370	0.001
Na	1.240e-04				
Na+	1.232e-04	1.109e-04	-3.909	-3.955	-0.046
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
O(0)	0.000e+00				
O2	0.000e+00	0.000e+00	-61.641	-61.640	0.001
S(-2)	1.370e-26				
HS-	1.012e-26	9.076e-27	-25.995	-26.042	-0.047
H2S	1.255e-27	1.258e-27	-26.902	-26.900	0.001
S5-2	2.230e-28	1.455e-28	-27.652	-27.837	-0.185

S4-2	1.301e-28	8.489e-29	-27.886	-28.071	-0.185
S6-2	1.154e-28	7.532e-29	-27.938	-28.123	-0.185
S-2	1.049e-31	6.916e-32	-30.979	-31.160	-0.181
S3-2	4.584e-32	2.991e-32	-31.339	-31.524	-0.185
S2-2	2.602e-33	1.698e-33	-32.585	-32.770	-0.185
S(6)	1.856e-03				
SO4-2	1.461e-03	9.498e-04	-2.835	-3.022	-0.187
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
HSO4-	1.624e-09	1.461e-09	-8.789	-8.835	-0.046

-----Saturation indices-----
--

Phase	SI	log IAP	log KT	
Anhydrite	-1.07	-5.71	-4.64	CaSO4
Aragonite	0.58	-7.75	-8.34	CaCO3
Calcite	0.72	-7.75	-8.47	CaCO3
CH4(g)	-29.45	-69.55	-40.10	CH4
CO2(g)	-2.51	-20.67	-18.16	CO2
Gypsum	-0.86	-5.71	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.89	12.91	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-11.67	-12.98	-1.31	Na2CO3:10H2O
O2(g)	-58.68	24.44	83.12	O2
Portlandite	-9.76	12.91	22.68	Ca(OH)2
SULFUR	-19.51	-21.62	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-13.10	-12.98	0.12	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----
--

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
U3O8(C)	0.00	-6.54	-6.54	1.000e+01	1.000e+01	-2.510e-07

-----Solution composition-----
--

Elements	Molality	Moles
C	3.438e-03	3.438e-03
Ca	3.542e-03	3.542e-03

Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
U	7.529e-07	7.529e-07

-----Description of solution-----
--

	pH =	7.799	Charge balance
	pe =	-1.527	Adjusted to redox
equilibrium	Activity of water =	1.000	
	Ionic strength =	1.083e-02	
	Mass of water (kg) =	1.000e+00	
	Total alkalinity (eq/kg) =	3.375e-03	
	Total CO2 (mol/kg) =	3.438e-03	
	Temperature (deg C) =	25.000	
	Electrical balance (eq) =	-4.968e-07	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.00	
	Iterations =	12	
	Total H =	1.110159e+02	
	Total O =	5.552396e+01	

-----Distribution of species-----
--

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	7.043e-07	6.316e-07	-6.152	-6.200	-0.047
	H+	1.746e-08	1.590e-08	-7.758	-7.799	-0.041
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.438e-03					
	HCO3-	3.226e-03	2.911e-03	-2.491	-2.536	-0.045
	H2CO3	1.037e-04	1.039e-04	-3.984	-3.983	0.001
	CaHCO3+	6.826e-05	6.168e-05	-4.166	-4.210	-0.044
	CaCO3	2.483e-05	2.490e-05	-4.605	-4.604	0.001
	CO3-2	1.294e-05	8.567e-06	-4.888	-5.067	-0.179
	UO2 (CO3) 2-2	2.863e-07	1.868e-07	-6.543	-6.729	-0.185
	UO2 (CO3) 3-4	2.126e-07	3.854e-08	-6.672	-7.414	-0.742
	NaHCO3	1.812e-07	1.817e-07	-6.742	-6.741	0.001
	NaCO3-	1.952e-08	1.761e-08	-7.709	-7.754	-0.045
	UO2CO3	2.723e-09	2.730e-09	-8.565	-8.564	0.001
Ca	3.542e-03					
	Ca+2	3.054e-03	2.045e-03	-2.515	-2.689	-0.174
	CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
	CaHCO3+	6.826e-05	6.168e-05	-4.166	-4.210	-0.044
	CaCO3	2.483e-05	2.490e-05	-4.605	-4.604	0.001
	CaOH+	3.591e-08	3.245e-08	-7.445	-7.489	-0.044
Cl	1.242e-04					
	Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
	UO2Cl+	5.199e-18	4.673e-18	-17.284	-17.330	-0.046
	UCl+3	1.912e-35	7.318e-36	-34.718	-35.136	-0.417
H(0)	4.052e-16					
	H2	2.026e-16	2.031e-16	-15.693	-15.692	0.001
Na	1.240e-04					
	Na+	1.232e-04	1.109e-04	-3.909	-3.955	-0.046

	NaSO4-	5.852e-07	5.279e-07	-6.233	-6.277	-0.045
	NaHCO3	1.812e-07	1.817e-07	-6.742	-6.741	0.001
	NaCO3-	1.952e-08	1.761e-08	-7.709	-7.754	-0.045
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-60.997	-60.996	0.001
S(-2)		7.063e-28				
	HS-	5.218e-28	4.679e-28	-27.283	-27.330	-0.047
	H2S	6.490e-29	6.506e-29	-28.188	-28.187	0.001
	S5-2	1.146e-29	7.476e-30	-28.941	-29.126	-0.185
	S4-2	6.684e-30	4.362e-30	-29.175	-29.360	-0.185
	S6-2	5.930e-30	3.869e-30	-29.227	-29.412	-0.185
	S-2	5.392e-33	3.553e-33	-32.268	-32.449	-0.181
	S3-2	2.355e-33	1.537e-33	-32.628	-32.813	-0.185
	S2-2	1.337e-34	8.723e-35	-33.874	-34.059	-0.185
S(6)		1.856e-03				
	SO4-2	1.461e-03	9.498e-04	-2.835	-3.022	-0.187
	CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
	NaSO4-	5.852e-07	5.279e-07	-6.233	-6.277	-0.045
	HSO4-	1.629e-09	1.466e-09	-8.788	-8.834	-0.046
	UO2SO4	1.227e-14	1.230e-14	-13.911	-13.910	0.001
	UO2(SO4)2-2	5.335e-16	3.481e-16	-15.273	-15.458	-0.185
	U(SO4)2	1.526e-29	1.529e-29	-28.817	-28.815	0.001
	USO4+2	1.271e-30	8.296e-31	-29.896	-30.081	-0.185
U(3)		4.254e-40				
	U+3	4.254e-40	1.628e-40	-39.371	-39.788	-0.417
U(4)		2.507e-07				
	U(OH)5-	2.505e-07	2.252e-07	-6.601	-6.648	-0.046
	U(OH)4	1.496e-10	1.500e-10	-9.825	-9.824	0.001
	U(OH)3+	9.704e-15	8.722e-15	-14.013	-14.059	-0.046
	U(OH)2+2	9.830e-20	6.414e-20	-19.007	-19.193	-0.185
	UOH+3	1.079e-25	4.130e-26	-24.967	-25.384	-0.417
	U(SO4)2	1.526e-29	1.529e-29	-28.817	-28.815	0.001
	USO4+2	1.271e-30	8.296e-31	-29.896	-30.081	-0.185
	U+4	1.667e-32	3.022e-33	-31.778	-32.520	-0.742
	UCl+3	1.912e-35	7.318e-36	-34.718	-35.136	-0.417
	U6(OH)15+9	0.000e+00	0.000e+00	-91.616	-95.371	-3.755
U(5)		5.783e-10				
	UO2+	5.783e-10	5.198e-10	-9.238	-9.284	-0.046
U(6)		5.016e-07				
	UO2(CO3)2-2	2.863e-07	1.868e-07	-6.543	-6.729	-0.185
	UO2(CO3)3-4	2.126e-07	3.854e-08	-6.672	-7.414	-0.742
	UO2CO3	2.723e-09	2.730e-09	-8.565	-8.564	0.001
	UO2OH+	1.440e-11	1.294e-11	-10.842	-10.888	-0.046
	UO2+2	3.880e-14	2.532e-14	-13.411	-13.597	-0.185
	UO2SO4	1.227e-14	1.230e-14	-13.911	-13.910	0.001
	UO2(SO4)2-2	5.335e-16	3.481e-16	-15.273	-15.458	-0.185
	(UO2)2(OH)2+2	8.795e-18	5.739e-18	-17.056	-17.241	-0.185
	UO2Cl+	5.199e-18	4.673e-18	-17.284	-17.330	-0.046
	(UO2)3(OH)5+	4.529e-18	4.070e-18	-17.344	-17.390	-0.046

-----Saturation indices-----
--

Phase	SI	log IAP	log KT	
Anhydrite	-1.07	-5.71	-4.64	CaSO4
Aragonite	0.58	-7.76	-8.34	CaCO3

B ₂ O ₃ (OH) ₂	-3.54	2.00	5.54	UO ₂ (OH) ₂
Calcite	0.72	-7.76	-8.47	CaCO ₃
CH ₄ (g)	-30.73	-70.83	-40.10	CH ₄
CO ₂ (g)	-2.50	-20.66	-18.16	CO ₂
Gummite	-8.40	2.00	10.40	UO ₃
Gypsum	-0.86	-5.71	-4.85	CaSO ₄ ·2H ₂ O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.89	12.91	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na ₂ SO ₄ ·10H ₂ O
Natron	-11.67	-12.98	-1.31	Na ₂ CO ₃ ·10H ₂ O
O ₂ (g)	-58.04	25.08	83.12	O ₂
Portlandite	-9.77	12.91	22.68	Ca(OH) ₂
Rutherfordine	-4.20	-18.66	-14.46	UO ₂ CO ₃
Schoepite	-3.40	2.00	5.40	UO ₂ (OH) ₂ ·H ₂ O
SULFUR	-20.48	-22.59	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na ₂ SO ₄
Thermonatrite	-13.10	-12.98	0.12	Na ₂ CO ₃ ·H ₂ O
U ₃ O ₈ (C)	-0.00	21.11	21.11	U ₃ O ₈
U ₄ O ₉ (C)	10.62	7.24	-3.38	U ₄ O ₉
UO ₂ (am)	-2.26	-1.33	0.93	UO ₂
UO ₃ (C)	-5.72	2.00	7.72	UO ₃
Uraninite	3.37	-1.33	-4.70	UO ₂

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 2

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

TITLE Run-2 Equil with UO2 only
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.
pH 7.8
temp 25.0
pe -1.69 $\# = -100$ mV, $pe = eh/0.059$ (Stumm & Morgan, pg 422)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2
EQUILIBRIUM_PHASES 1
Uraninite 0.0 10.0
END

TITLE

Run-2 Equil with UO2 only

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.373e-03	3.373e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----
--

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.083e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.438e-03
 Total CO2 (mol/kg) = 3.438e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -4.968e-07
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
 Iterations = 7
 Total H = 1.110159e+02
 Total O = 5.552395e+01

-----Distribution of species-----

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	7.068e-07	6.338e-07	-6.151	-6.198	-0.047
	H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)		3.438e-03				
	HCO3-	3.228e-03	2.912e-03	-2.491	-2.536	-0.045
	H2CO3	1.034e-04	1.036e-04	-3.986	-3.984	0.001
	CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
	CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
	CO3-2	1.299e-05	8.600e-06	-4.887	-5.065	-0.179
	NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
	NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
Ca		3.542e-03				
	Ca+2	3.054e-03	2.045e-03	-2.515	-2.689	-0.174
	CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
	CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
	CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
	CaOH+	3.603e-08	3.256e-08	-7.443	-7.487	-0.044
Cl		1.242e-04				
	Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
H(0)		8.510e-16				
	H2	4.255e-16	4.266e-16	-15.371	-15.370	0.001
Na		1.240e-04				
	Na+	1.232e-04	1.109e-04	-3.909	-3.955	-0.046
	NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
	NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
	NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-61.641	-61.640	0.001
S(-2)		1.370e-26				
	HS-	1.012e-26	9.076e-27	-25.995	-26.042	-0.047
	H2S	1.255e-27	1.258e-27	-26.902	-26.900	0.001
	S5-2	2.230e-28	1.455e-28	-27.652	-27.837	-0.185
	S4-2	1.301e-28	8.489e-29	-27.886	-28.071	-0.185
	S6-2	1.154e-28	7.532e-29	-27.938	-28.123	-0.185
	S-2	1.049e-31	6.916e-32	-30.979	-31.160	-0.181
	S3-2	4.584e-32	2.991e-32	-31.339	-31.524	-0.185

S(6)	S2-2	2.602e-33	1.698e-33	-32.585	-32.770	-0.185
		1.856e-03				
	SO4-2	1.461e-03	9.498e-04	-2.835	-3.022	-0.187
	CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
	NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
	HSO4-	1.624e-09	1.461e-09	-8.789	-8.835	-0.046

-----Saturation indices-----

--

Phase	SI	log IAP	log KT	
Anhydrite	-1.07	-5.71	-4.64	CaSO4
Aragonite	0.58	-7.75	-8.34	CaCO3
Calcite	0.72	-7.75	-8.47	CaCO3
CH4(g)	-29.45	-69.55	-40.10	CH4
CO2(g)	-2.51	-20.67	-18.16	CO2
Gypsum	-0.86	-5.71	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.89	12.91	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-11.67	-12.98	-1.31	Na2CO3:10H2O
O2(g)	-58.68	24.44	83.12	O2
Portlandite	-9.76	12.91	22.68	Ca(OH)2
SULFUR	-19.51	-21.62	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-13.10	-12.98	0.12	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

--

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
Uraninite	0.00	-13.92	-13.92	1.000e+01	1.000e+01	-1.065e-10

-----Solution composition-----

--

Elements	Molality	Moles
C	3.438e-03	3.438e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
U	1.065e-10	1.065e-10

-----Description of solution-----

```

--
                                pH = 7.800      Charge balance
                                pe = -3.034     Adjusted to redox
equilibrium
                                Activity of water = 1.000
                                Ionic strength = 1.083e-02
                                Mass of water (kg) = 1.000e+00
                                Total alkalinity (eq/kg) = 3.373e-03
                                Total CO2 (mol/kg) = 3.438e-03
                                Temperature (deg C) = 25.000
                                Electrical balance (eq) = -4.968e-07
                                Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
                                Iterations = 8
                                Total H = 1.110159e+02
                                Total O = 5.552395e+01

```

-----Distribution of species-----

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--
Species      Molality      Activity      Log      Log      Log
              Molality      Activity      Molality  Activity  Gamma
OH-           7.068e-07      6.338e-07      -6.151    -6.198    -0.047
H+            1.740e-08      1.585e-08      -7.759    -7.800    -0.041
H2O           5.551e+01      9.999e-01      1.744     -0.000     0.000
C(4)          3.438e-03
HCO3-         3.228e-03      2.912e-03      -2.491    -2.536    -0.045
H2CO3         1.034e-04      1.036e-04      -3.986    -3.984     0.001
CaHCO3+       6.828e-05      6.171e-05      -4.166    -4.210    -0.044
CaCO3         2.493e-05      2.499e-05      -4.603    -4.602     0.001
CO3-2         1.299e-05      8.600e-06      -4.887    -5.065    -0.179
NaHCO3        1.813e-07      1.818e-07      -6.742    -6.741     0.001
NaCO3-        1.960e-08      1.768e-08      -7.708    -7.753    -0.045
UO2 (CO3) 2-2 1.184e-13      7.728e-14      -12.927   -13.112   -0.185
UO2 (CO3) 3-4 8.829e-14      1.601e-14      -13.054   -13.796   -0.742
UO2CO3        1.122e-15      1.125e-15      -14.950   -14.949     0.001
Ca            3.542e-03
Ca+2          3.054e-03      2.045e-03      -2.515    -2.689    -0.174
CaSO4         3.947e-04      3.957e-04      -3.404    -3.403     0.001
CaHCO3+       6.828e-05      6.171e-05      -4.166    -4.210    -0.044
CaCO3         2.493e-05      2.499e-05      -4.603    -4.602     0.001
CaOH+         3.603e-08      3.256e-08      -7.443    -7.487    -0.044
Cl            1.242e-04
Cl-           1.242e-04      1.112e-04      -3.906    -3.954    -0.048
UO2Cl+        2.134e-24      1.918e-24      -23.671   -23.717   -0.046
UCl+3         7.969e-39      3.050e-39      -38.099   -38.516   -0.417
H(0)          4.141e-13
H2            2.071e-13      2.076e-13      -12.684   -12.683     0.001
Na            1.240e-04
Na+           1.232e-04      1.109e-04      -3.909    -3.955    -0.046
NaSO4-        5.852e-07      5.280e-07      -6.233    -6.277    -0.045
NaHCO3        1.813e-07      1.818e-07      -6.742    -6.741     0.001
NaCO3-        1.960e-08      1.768e-08      -7.708    -7.753    -0.045
O(0)          0.000e+00

```

S(-2)	O2	0.000e+00	0.000e+00	-67.016	-67.014	0.001
		7.684e-16				
	HS-	5.675e-16	5.089e-16	-15.246	-15.293	-0.047
	H2S	7.034e-17	7.052e-17	-16.153	-16.152	0.001
	S5-2	1.250e-17	8.159e-18	-16.903	-17.088	-0.185
	S4-2	7.295e-18	4.760e-18	-17.137	-17.322	-0.185
	S6-2	6.472e-18	4.223e-18	-17.189	-17.374	-0.185
	S-2	5.884e-21	3.878e-21	-20.230	-20.411	-0.181
	S3-2	2.570e-21	1.677e-21	-20.590	-20.775	-0.185
	S2-2	1.459e-22	9.520e-23	-21.836	-22.021	-0.185
S(6)		1.856e-03				
	SO4-2	1.461e-03	9.498e-04	-2.835	-3.022	-0.187
	CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
	NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
	HSO4-	1.624e-09	1.461e-09	-8.789	-8.835	-0.046
	UO2SO4	5.039e-21	5.052e-21	-20.298	-20.297	0.001
	UO2(SO4) 2-2	2.190e-22	1.429e-22	-21.660	-21.845	-0.185
	U(SO4) 2	6.358e-33	6.374e-33	-32.197	-32.196	0.001
	USO4+2	5.298e-34	3.457e-34	-33.276	-33.461	-0.185
U(3)		0.000e+00				
	U+3	0.000e+00	0.000e+00	-41.245	-41.662	-0.417
U(4)		1.063e-10				
	U(OH) 5-	1.062e-10	9.546e-11	-9.974	-10.020	-0.046
	U(OH) 4	6.321e-14	6.337e-14	-13.199	-13.198	0.001
	U(OH) 3+	4.086e-18	3.672e-18	-17.389	-17.435	-0.046
	U(OH) 2+2	4.125e-23	2.692e-23	-22.385	-22.570	-0.185
	UOH+3	4.513e-29	1.727e-29	-28.346	-28.763	-0.417
	U(SO4) 2	6.358e-33	6.374e-33	-32.197	-32.196	0.001
	USO4+2	5.298e-34	3.457e-34	-33.276	-33.461	-0.185
	U+4	6.945e-36	1.259e-36	-35.158	-35.900	-0.742
	UCl+3	7.969e-39	3.050e-39	-38.099	-38.516	-0.417
	U6(OH) 15+9	0.000e+00	0.000e+00	-111.875	-115.629	-3.754
U(5)		7.617e-15				
	UO2+	7.617e-15	6.846e-15	-14.118	-14.165	-0.046
U(6)		2.079e-13				
	UO2(CO3) 2-2	1.184e-13	7.728e-14	-12.927	-13.112	-0.185
	UO2(CO3) 3-4	8.829e-14	1.601e-14	-13.054	-13.796	-0.742
	UO2CO3	1.122e-15	1.125e-15	-14.950	-14.949	0.001
	UO2OH+	5.931e-18	5.330e-18	-17.227	-17.273	-0.046
	UO2+2	1.593e-20	1.039e-20	-19.798	-19.983	-0.185
	UO2SO4	5.039e-21	5.052e-21	-20.298	-20.297	0.001
	UO2(SO4) 2-2	2.190e-22	1.429e-22	-21.660	-21.845	-0.185
	UO2Cl+	2.134e-24	1.918e-24	-23.671	-23.717	-0.046
	(UO2) 2(OH) 2+2	1.492e-30	9.739e-31	-29.826	-30.011	-0.185
	(UO2) 3(OH) 5+	3.188e-37	2.865e-37	-36.497	-36.543	-0.046

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.07	-5.71	-4.64	CaSO4
Aragonite	0.58	-7.75	-8.34	CaCO3
B_UO2(OH) 2	-9.93	-4.38	5.54	UO2(OH) 2
Calcite	0.72	-7.75	-8.47	CaCO3
CH4(g)	-18.70	-58.80	-40.10	CH4
CO2(g)	-2.51	-20.67	-18.16	CO2

Gummite	-14.79	-4.38	10.40	UO3
Gypsum	-0.86	-5.71	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.89	12.91	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-11.67	-12.98	-1.31	Na2CO3:10H2O
O2(g)	-64.05	19.07	83.12	O2
Portlandite	-9.76	12.91	22.68	Ca(OH)2
Rutherfordine	-10.59	-25.05	-14.46	UO2CO3
Schoepite	-9.79	-4.38	5.40	UO2(OH)2:H2O
SULFUR	-11.45	-13.56	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-13.10	-12.98	0.12	Na2CO3:H2O
U3O8(C)	-16.14	4.97	21.11	U3O8
U4O9(C)	-5.88	-9.27	-3.38	U4O9
UO2(am)	-5.63	-4.70	0.93	UO2
UO3(C)	-12.10	-4.38	7.72	UO3
Uraninite	0.00	-4.70	-4.70	UO2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 3

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

TITLE Run-3 - Equil with U3O8 and UO2
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.
pH 7.8
temp 25.0
pe -1.69 $\# = -100$ mV, $pe = eh/0.059$ (Stumm & Morgan, pg 422)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2
EQUILIBRIUM_PHASES 1
U3O8(C) 0.0 10.0
Uraninite 0.0 10.0
END

TITLE

Run-3 - Equil with U3O8 and UO2

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.373e-03	3.373e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

--

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.083e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.438e-03
 Total CO2 (mol/kg) = 3.438e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -4.968e-07
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
 Iterations = 7
 Total H = 1.110159e+02
 Total O = 5.552395e+01

-----Distribution of species-----

--

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	7.068e-07	6.338e-07	-6.151	-6.198	-0.047
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.438e-03				
HCO3-	3.228e-03	2.912e-03	-2.491	-2.536	-0.045
H2CO3	1.034e-04	1.036e-04	-3.986	-3.984	0.001
CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
CO3-2	1.299e-05	8.600e-06	-4.887	-5.065	-0.179
NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
Ca	3.542e-03				
Ca+2	3.054e-03	2.045e-03	-2.515	-2.689	-0.174
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
CaOH+	3.603e-08	3.256e-08	-7.443	-7.487	-0.044
Cl	1.242e-04				
Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
H(0)	8.510e-16				
H2	4.255e-16	4.266e-16	-15.371	-15.370	0.001
Na	1.240e-04				
Na+	1.232e-04	1.109e-04	-3.909	-3.955	-0.046
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
O(0)	0.000e+00				
O2	0.000e+00	0.000e+00	-61.641	-61.640	0.001
S(-2)	1.370e-26				
HS-	1.012e-26	9.076e-27	-25.995	-26.042	-0.047
H2S	1.255e-27	1.258e-27	-26.902	-26.900	0.001
S5-2	2.230e-28	1.455e-28	-27.652	-27.837	-0.185
S4-2	1.301e-28	8.489e-29	-27.886	-28.071	-0.185
S6-2	1.154e-28	7.532e-29	-27.938	-28.123	-0.185

S-2	1.049e-31	6.916e-32	-30.979	-31.160	-0.181
S3-2	4.584e-32	2.991e-32	-31.339	-31.524	-0.185
S2-2	2.602e-33	1.698e-33	-32.585	-32.770	-0.185
S(6)	1.856e-03				
SO4-2	1.461e-03	9.498e-04	-2.835	-3.022	-0.187
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
HSO4-	1.624e-09	1.461e-09	-8.789	-8.835	-0.046

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.07	-5.71	-4.64	CaSO4
Aragonite	0.58	-7.75	-8.34	CaCO3
Calcite	0.72	-7.75	-8.47	CaCO3
CH4(g)	-29.45	-69.55	-40.10	CH4
CO2(g)	-2.51	-20.67	-18.16	CO2
Gypsum	-0.86	-5.71	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.89	12.91	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-11.67	-12.98	-1.31	Na2CO3:10H2O
O2(g)	-58.68	24.44	83.12	O2
Portlandite	-9.76	12.91	22.68	Ca(OH)2
SULFUR	-19.51	-21.62	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-13.10	-12.98	0.12	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
U3O8(C)	0.00	-6.54	-6.54	1.000e+01	1.000e+01	-1.141e-05
Uraninite	0.00	-13.92	-13.92	1.000e+01	1.000e+01	1.141e-05

-----Solution composition-----

Elements	Molality	Moles
C	3.438e-03	3.438e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04

Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
U	2.282e-05	2.282e-05

-----Description of solution-----

--

	pH =	7.769	Charge balance
	pe =	1.033	Adjusted to redox
equilibrium	Activity of water =	1.000	
	Ionic strength =	1.091e-02	
	Mass of water (kg) =	1.000e+00	
	Total alkalinity (eq/kg) =	3.419e-03	
	Total CO2 (mol/kg) =	3.438e-03	
	Temperature (deg C) =	25.000	
	Electrical balance (eq) =	-4.968e-07	
	Percent error, 100*(Cat- An)/(Cat+ An) =	-0.00	
	Iterations =	10	
	Total H =	1.110159e+02	
	Total O =	5.552402e+01	

-----Distribution of species-----

--

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	6.578e-07	5.897e-07	-6.182	-6.229	-0.047
	H+	1.871e-08	1.703e-08	-7.728	-7.769	-0.041
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)		3.438e-03				
	HCO3-	3.172e-03	2.860e-03	-2.499	-2.544	-0.045
	H2CO3	1.091e-04	1.094e-04	-3.962	-3.961	0.001
	CaHCO3+	6.710e-05	6.062e-05	-4.173	-4.217	-0.044
	CaCO3	2.278e-05	2.284e-05	-4.642	-4.641	0.001
	UO2 (CO3) 2-2	1.347e-05	8.777e-06	-4.871	-5.057	-0.186
	CO3-2	1.188e-05	7.860e-06	-4.925	-5.105	-0.180
	UO2 (CO3) 3-4	9.213e-06	1.662e-06	-5.036	-5.779	-0.744
	NaHCO3	1.780e-07	1.785e-07	-6.749	-6.748	0.001
	UO2CO3	1.395e-07	1.398e-07	-6.856	-6.854	0.001
	NaCO3-	1.791e-08	1.615e-08	-7.747	-7.792	-0.045
Ca		3.542e-03				
	Ca+2	3.058e-03	2.045e-03	-2.515	-2.689	-0.175
	CaSO4	3.943e-04	3.953e-04	-3.404	-3.403	0.001
	CaHCO3+	6.710e-05	6.062e-05	-4.173	-4.217	-0.044
	CaCO3	2.278e-05	2.284e-05	-4.642	-4.641	0.001
	CaOH+	3.354e-08	3.030e-08	-7.475	-7.519	-0.044
Cl		1.242e-04				
	Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
	UO2Cl+	2.902e-16	2.607e-16	-15.537	-15.584	-0.046
	UC1+3	1.066e-38	4.069e-39	-37.972	-38.391	-0.418
H(0)		3.519e-21				
	H2	1.759e-21	1.764e-21	-20.755	-20.754	0.001
Na		1.240e-04				
	Na+	1.233e-04	1.109e-04	-3.909	-3.955	-0.046
	NaSO4-	5.846e-07	5.272e-07	-6.233	-6.278	-0.045

	NaHCO3	1.780e-07	1.785e-07	-6.749	-6.748	0.001
	NaCO3-	1.791e-08	1.615e-08	-7.747	-7.792	-0.045
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-50.874	-50.873	0.001
S(-2)		0.000e+00				
	HS-	0.000e+00	0.000e+00	-47.498	-47.546	-0.047
	H2S	0.000e+00	0.000e+00	-48.374	-48.372	0.001
	S5-2	0.000e+00	0.000e+00	-49.186	-49.372	-0.186
	S4-2	0.000e+00	0.000e+00	-49.420	-49.606	-0.186
	S6-2	0.000e+00	0.000e+00	-49.472	-49.658	-0.186
	S-2	0.000e+00	0.000e+00	-52.513	-52.695	-0.182
	S3-2	0.000e+00	0.000e+00	-52.873	-53.059	-0.186
	S2-2	0.000e+00	0.000e+00	-54.119	-54.305	-0.186
S(6)		1.856e-03				
	SO4-2	1.461e-03	9.488e-04	-2.835	-3.023	-0.188
	CaSO4	3.943e-04	3.953e-04	-3.404	-3.403	0.001
	NaSO4-	5.846e-07	5.272e-07	-6.233	-6.278	-0.045
	HSO4-	1.744e-09	1.568e-09	-8.758	-8.805	-0.046
	UO2SO4	6.844e-13	6.861e-13	-12.165	-12.164	0.001
	UO2(SO4)2-2	2.975e-14	1.939e-14	-13.526	-13.712	-0.186
	U(SO4)2	8.467e-33	8.488e-33	-32.072	-32.071	0.001
	USO4+2	7.073e-34	4.609e-34	-33.150	-33.336	-0.186
U(3)		0.000e+00				
	U+3	0.000e+00	0.000e+00	-45.185	-45.604	-0.418
U(4)		9.891e-11				
	U(OH)5-	9.885e-11	8.881e-11	-10.005	-10.052	-0.046
	U(OH)4	6.321e-14	6.337e-14	-13.199	-13.198	0.001
	U(OH)3+	4.393e-18	3.947e-18	-17.357	-17.404	-0.046
	U(OH)2+2	4.772e-23	3.109e-23	-22.321	-22.507	-0.186
	UOH+3	5.621e-29	2.145e-29	-28.250	-28.669	-0.418
	U(SO4)2	8.467e-33	8.488e-33	-32.072	-32.071	0.001
	USO4+2	7.073e-34	4.609e-34	-33.150	-33.336	-0.186
	U+4	9.319e-36	1.681e-36	-35.031	-35.775	-0.744
	UC1+3	1.066e-38	4.069e-39	-37.972	-38.391	-0.418
	U6(OH)15+9	0.000e+00	0.000e+00	-111.581	-115.347	-3.766
U(5)		8.884e-11				
	UO2+	8.884e-11	7.982e-11	-10.051	-10.098	-0.046
U(6)		2.282e-05				
	UO2(CO3)2-2	1.347e-05	8.777e-06	-4.871	-5.057	-0.186
	UO2(CO3)3-4	9.213e-06	1.662e-06	-5.036	-5.779	-0.744
	UO2CO3	1.395e-07	1.398e-07	-6.856	-6.854	0.001
	UO2OH+	7.505e-10	6.743e-10	-9.125	-9.171	-0.046
	UO2+2	2.169e-12	1.413e-12	-11.664	-11.850	-0.186
	UO2SO4	6.844e-13	6.861e-13	-12.165	-12.164	0.001
	(UO2)3(OH)5+	5.587e-13	5.020e-13	-12.253	-12.299	-0.046
	UO2(SO4)2-2	2.975e-14	1.939e-14	-13.526	-13.712	-0.186
	(UO2)2(OH)2+2	2.391e-14	1.558e-14	-13.621	-13.807	-0.186
	UO2Cl+	2.902e-16	2.607e-16	-15.537	-15.584	-0.046

-----Saturation indices-----
--

Phase	SI	log IAP	log KT	
Anhydrite	-1.08	-5.71	-4.64	CaSO4
Aragonite	0.54	-7.79	-8.34	CaCO3
B_UO2(OH)2	-1.86	3.69	5.54	UO2(OH)2

Calcite	0.68	-7.79	-8.47	CaCO3
CH4(g)	-50.96	-91.06	-40.10	CH4
CO2(g)	-2.48	-20.64	-18.16	CO2
Gummite	-6.72	3.69	10.40	UO3
Gypsum	-0.86	-5.71	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.95	12.85	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-11.70	-13.02	-1.31	Na2CO3:10H2O
O2(g)	-47.91	35.21	83.12	O2
Portlandite	-9.83	12.85	22.68	Ca(OH)2
Rutherfordine	-2.49	-16.95	-14.46	UO2CO3
Schoepite	-1.72	3.69	5.40	UO2(OH)2:H2O
SULFUR	-35.60	-37.71	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-13.14	-13.01	0.12	Na2CO3:H2O
U3O8(C)	-0.00	21.11	21.11	U3O8
U4O9(C)	2.19	-1.20	-3.38	U4O9
UO2(am)	-5.63	-4.70	0.93	UO2
UO3(C)	-4.03	3.69	7.72	UO3
Uraninite	-0.00	-4.70	-4.70	UO2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 4

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

TITLE Run-4 - Equil with U3O8 and CO2
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 $\# = -100$ mV, $pe = eh/0.059$ (Stumm & Morgan, pg 422)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1

U3O8(C) 0.0 10.0
CO2(g) -3.5

END

TITLE

Run-4 - Equil with U3O8 and CO2

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.373e-03	3.373e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

--

pH	=	7.800
pe	=	-1.690
Activity of water	=	1.000
Ionic strength	=	1.083e-02
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	3.438e-03
Total CO2 (mol/kg)	=	3.438e-03
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-4.968e-07
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.00
Iterations	=	7
Total H	=	1.110159e+02
Total O	=	5.552395e+01

-----Distribution of species-----

--

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	7.068e-07	6.338e-07	-6.151	-6.198	-0.047
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.438e-03				
HCO3-	3.228e-03	2.912e-03	-2.491	-2.536	-0.045
H2CO3	1.034e-04	1.036e-04	-3.986	-3.984	0.001
CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
CO3-2	1.299e-05	8.600e-06	-4.887	-5.065	-0.179
NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
Ca	3.542e-03				
Ca+2	3.054e-03	2.045e-03	-2.515	-2.689	-0.174
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
CaOH+	3.603e-08	3.256e-08	-7.443	-7.487	-0.044
Cl	1.242e-04				
Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
H(0)	8.510e-16				
H2	4.255e-16	4.266e-16	-15.371	-15.370	0.001
Na	1.240e-04				
Na+	1.232e-04	1.109e-04	-3.909	-3.955	-0.046
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
O(0)	0.000e+00				
O2	0.000e+00	0.000e+00	-61.641	-61.640	0.001
S(-2)	1.370e-26				
HS-	1.012e-26	9.076e-27	-25.995	-26.042	-0.047
H2S	1.255e-27	1.258e-27	-26.902	-26.900	0.001
S5-2	2.230e-28	1.455e-28	-27.652	-27.837	-0.185
S4-2	1.301e-28	8.489e-29	-27.886	-28.071	-0.185
S6-2	1.154e-28	7.532e-29	-27.938	-28.123	-0.185

S-2	1.049e-31	6.916e-32	-30.979	-31.160	-0.181
S3-2	4.584e-32	2.991e-32	-31.339	-31.524	-0.185
S2-2	2.602e-33	1.698e-33	-32.585	-32.770	-0.185
S(6)	1.856e-03				
SO4-2	1.461e-03	9.498e-04	-2.835	-3.022	-0.187
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
HSO4-	1.624e-09	1.461e-09	-8.789	-8.835	-0.046

-----Saturation indices-----

--

Phase	SI	log IAP	log KT	
Anhydrite	-1.07	-5.71	-4.64	CaSO4
Aragonite	0.58	-7.75	-8.34	CaCO3
Calcite	0.72	-7.75	-8.47	CaCO3
CH4(g)	-29.45	-69.55	-40.10	CH4
CO2(g)	-2.51	-20.67	-18.16	CO2
Gypsum	-0.86	-5.71	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.89	12.91	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-11.67	-12.98	-1.31	Na2CO3:10H2O
O2(g)	-58.68	24.44	83.12	O2
Portlandite	-9.76	12.91	22.68	Ca(OH)2
SULFUR	-19.51	-21.62	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-13.10	-12.98	0.12	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

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Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
CO2(g)	-3.50	-21.66	-18.16	1.000e+01	1.000e+01	3.315e-04
U3O8(C)	-0.00	-6.54	-6.54	1.000e+01	1.000e+01	-9.791e-07

-----Solution composition-----

--

Elements	Molality	Moles
C	3.106e-03	3.106e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04

Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
U	2.937e-06	2.937e-06

-----Description of solution-----

```

equilibrium
pH = 8.728
pe = -2.204
Charge balance
Adjusted to redox

Activity of water = 1.000
Ionic strength = 1.054e-02
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 3.381e-03
Total CO2 (mol/kg) = 3.106e-03
Temperature (deg C) = 25.000
Electrical balance (eq) = -4.968e-07
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 11
Total H = 1.110159e+02
Total O = 5.552330e+01

```

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.979e-06	5.368e-06	-5.223	-5.270	-0.047
H+	2.052e-09	1.871e-09	-8.688	-8.728	-0.040
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.106e-03				
HCO3-	2.765e-03	2.497e-03	-2.558	-2.603	-0.044
CaCO3	1.743e-04	1.748e-04	-3.759	-3.758	0.001
CO3-2	9.390e-05	6.248e-05	-4.027	-4.204	-0.177
CaHCO3+	5.631e-05	5.094e-05	-4.249	-4.293	-0.043
H2CO3	1.047e-05	1.049e-05	-4.980	-4.979	0.001
UO2 (CO3) 3-4	1.649e-06	3.050e-07	-5.783	-6.516	-0.733
UO2 (CO3) 2-2	3.091e-07	2.027e-07	-6.510	-6.693	-0.183
NaHCO3	1.556e-07	1.559e-07	-6.808	-6.807	0.001
NaCO3-	1.423e-07	1.285e-07	-6.847	-6.891	-0.044
UO2CO3	4.052e-10	4.062e-10	-9.392	-9.391	0.001
Ca	3.542e-03				
Ca+2	2.927e-03	1.969e-03	-2.534	-2.706	-0.172
CaSO4	3.846e-04	3.855e-04	-3.415	-3.414	0.001
CaCO3	1.743e-04	1.748e-04	-3.759	-3.758	0.001
CaHCO3+	5.631e-05	5.094e-05	-4.249	-4.293	-0.043
CaOH+	2.934e-07	2.655e-07	-6.532	-6.576	-0.043
Cl	1.242e-04				
Cl-	1.242e-04	1.114e-04	-3.906	-3.953	-0.047
UO2Cl+	1.061e-19	9.546e-20	-18.974	-19.020	-0.046
UC1+3	1.670e-39	6.464e-40	-38.777	-39.190	-0.412
H(0)	1.266e-16				
H2	6.328e-17	6.344e-17	-16.199	-16.198	0.001
Na	1.240e-04				
Na+	1.231e-04	1.110e-04	-3.910	-3.955	-0.045
NaSO4-	5.919e-07	5.346e-07	-6.228	-6.272	-0.044

	NaHCO3	1.556e-07	1.559e-07	-6.808	-6.807	0.001
	NaCO3-	1.423e-07	1.285e-07	-6.847	-6.891	-0.044
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-59.986	-59.985	0.001
S(-2)		1.746e-30				
	HS-	5.907e-31	5.304e-31	-30.229	-30.275	-0.047
	S5-2	1.098e-31	7.203e-32	-30.959	-31.143	-0.183
	S4-2	6.408e-32	4.202e-32	-31.193	-31.377	-0.183
	S6-2	5.684e-32	3.728e-32	-31.245	-31.429	-0.183
	H2S	8.656e-33	8.677e-33	-32.063	-32.062	0.001
	S-2	5.169e-35	3.424e-35	-34.287	-34.466	-0.179
	S3-2	2.258e-35	1.481e-35	-34.646	-34.830	-0.183
	S2-2	1.281e-36	8.404e-37	-35.892	-36.076	-0.183
S(6)		1.856e-03				
	SO4-2	1.471e-03	9.613e-04	-2.832	-3.017	-0.185
	CaSO4	3.846e-04	3.855e-04	-3.415	-3.414	0.001
	NaSO4-	5.919e-07	5.346e-07	-6.228	-6.272	-0.044
	HSO4-	1.938e-10	1.745e-10	-9.713	-9.758	-0.045
	UO2SO4	2.535e-16	2.541e-16	-15.596	-15.595	0.001
	UO2(SO4)2-2	1.109e-17	7.276e-18	-16.955	-17.138	-0.183
	U(SO4)2	1.379e-33	1.382e-33	-32.861	-32.859	0.001
	USO4+2	1.129e-34	7.407e-35	-33.947	-34.130	-0.183
U(3)		0.000e+00				
	U+3	0.000e+00	0.000e+00	-42.754	-43.166	-0.412
U(4)		9.791e-07				
	U(OH)5-	9.790e-07	8.810e-07	-6.009	-6.055	-0.046
	U(OH)4	6.888e-11	6.905e-11	-10.162	-10.161	0.001
	U(OH)3+	5.249e-16	4.724e-16	-15.280	-15.326	-0.046
	U(OH)2+2	6.232e-22	4.088e-22	-21.205	-21.389	-0.183
	UOH+3	8.000e-29	3.097e-29	-28.097	-28.509	-0.412
	U(SO4)2	1.379e-33	1.382e-33	-32.861	-32.859	0.001
	USO4+2	1.129e-34	7.407e-35	-33.947	-34.130	-0.183
	U+4	1.441e-36	2.665e-37	-35.841	-36.574	-0.733
	UCl+3	1.670e-39	6.464e-40	-38.777	-39.190	-0.412
	U6(OH)15+9	0.000e+00	0.000e+00	-102.047	-105.757	-3.710
U(5)		5.597e-11				
	UO2+	5.597e-11	5.037e-11	-10.252	-10.298	-0.046
U(6)		1.958e-06				
	UO2(CO3)3-4	1.649e-06	3.050e-07	-5.783	-6.516	-0.733
	UO2(CO3)2-2	3.091e-07	2.027e-07	-6.510	-6.693	-0.183
	UO2CO3	4.052e-10	4.062e-10	-9.392	-9.391	0.001
	UO2OH+	2.493e-12	2.244e-12	-11.603	-11.649	-0.046
	UO2+2	7.876e-16	5.166e-16	-15.104	-15.287	-0.183
	UO2SO4	2.535e-16	2.541e-16	-15.596	-15.595	0.001
	UO2(SO4)2-2	1.109e-17	7.276e-18	-16.955	-17.138	-0.183
	(UO2)3(OH)5+	1.704e-18	1.533e-18	-17.769	-17.814	-0.046
	(UO2)2(OH)2+2	2.631e-19	1.726e-19	-18.580	-18.763	-0.183
	UO2Cl+	1.061e-19	9.546e-20	-18.974	-19.020	-0.046

-----Saturation indices-----
 --

Phase	SI	log IAP	log KT	
Anhydrite	-1.09	-5.72	-4.64	CaSO4
Aragonite	1.43	-6.91	-8.34	CaCO3
B_UO2(OH)2	-3.38	2.17	5.54	UO2(OH)2

Calcite	1.56	-6.91	-8.47	CaCO3
CH4(g)	-33.75	-73.85	-40.10	CH4
CO2(g)	-3.50	-21.66	-18.16	CO2
Gummite	-8.23	2.17	10.40	UO3
Gypsum	-0.88	-5.72	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-18.05	14.75	32.80	CaO
Mirabilite	-9.81	-10.93	-1.11	Na2SO4:10H2O
Natron	-10.80	-12.11	-1.31	Na2CO3:10H2O
O2(g)	-57.02	26.10	83.12	O2
Portlandite	-7.93	14.75	22.68	Ca(OH)2
Rutherfordine	-5.03	-19.49	-14.46	UO2CO3
Schoepite	-3.24	2.17	5.40	UO2(OH)2:H2O
SULFUR	-23.85	-25.96	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-12.24	-12.11	0.12	Na2CO3:H2O
U3O8(C)	-0.00	21.11	21.11	U3O8
U4O9(C)	9.78	6.40	-3.38	U4O9
UO2(am)	-2.60	-1.66	0.93	UO2
UO3(C)	-5.55	2.17	7.72	UO3
Uraninite	3.04	-1.66	-4.70	UO2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 5

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

TITLE Run-5 - Equil with UO2 and CO2
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.
pH 7.8
temp 25.0
pe -1.69 $\# = -100$ mV, $pe = eh/0.059$ (Stumm & Morgan, pg 422)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2
EQUILIBRIUM PHASES 1
CO2(g) -3.5
Uraninite 0.0 10.0
END

TITLE

Run-5 - Equil with UO2 and CO2

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.373e-03	3.373e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

--

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.083e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.438e-03
 Total CO2 (mol/kg) = 3.438e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -4.968e-07
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
 Iterations = 7
 Total H = 1.110159e+02
 Total O = 5.552395e+01

-----Distribution of species-----

--

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	7.068e-07	6.338e-07	-6.151	-6.198	-0.047
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.438e-03				
HCO3-	3.228e-03	2.912e-03	-2.491	-2.536	-0.045
H2CO3	1.034e-04	1.036e-04	-3.986	-3.984	0.001
CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
CO3-2	1.299e-05	8.600e-06	-4.887	-5.065	-0.179
NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
Ca	3.542e-03				
Ca+2	3.054e-03	2.045e-03	-2.515	-2.689	-0.174
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
CaOH+	3.603e-08	3.256e-08	-7.443	-7.487	-0.044
Cl	1.242e-04				
Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
H(0)	8.510e-16				
H2	4.255e-16	4.266e-16	-15.371	-15.370	0.001
Na	1.240e-04				
Na+	1.232e-04	1.109e-04	-3.909	-3.955	-0.046
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
O(0)	0.000e+00				
O2	0.000e+00	0.000e+00	-61.641	-61.640	0.001
S(-2)	1.370e-26				
HS-	1.012e-26	9.076e-27	-25.995	-26.042	-0.047
H2S	1.255e-27	1.258e-27	-26.902	-26.900	0.001
S5-2	2.230e-28	1.455e-28	-27.652	-27.837	-0.185
S4-2	1.301e-28	8.489e-29	-27.886	-28.071	-0.185
S6-2	1.154e-28	7.532e-29	-27.938	-28.123	-0.185

S-2	1.049e-31	6.916e-32	-30.979	-31.160	-0.181
S3-2	4.584e-32	2.991e-32	-31.339	-31.524	-0.185
S2-2	2.602e-33	1.698e-33	-32.585	-32.770	-0.185
S(6)	1.856e-03				
SO4-2	1.461e-03	9.498e-04	-2.835	-3.022	-0.187
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
HSO4-	1.624e-09	1.461e-09	-8.789	-8.835	-0.046

-----Saturation indices-----

--

Phase	SI	log IAP	log KT	
Anhydrite	-1.07	-5.71	-4.64	CaSO4
Aragonite	0.58	-7.75	-8.34	CaCO3
Calcite	0.72	-7.75	-8.47	CaCO3
CH4(g)	-29.45	-69.55	-40.10	CH4
CO2(g)	-2.51	-20.67	-18.16	CO2
Gypsum	-0.86	-5.71	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.89	12.91	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-11.67	-12.98	-1.31	Na2CO3:10H2O
O2(g)	-58.68	24.44	83.12	O2
Portlandite	-9.76	12.91	22.68	Ca(OH)2
SULFUR	-19.51	-21.62	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-13.10	-12.98	0.12	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

--

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
CO2(g)	-3.50	-21.66	-18.16	1.000e+01	1.000e+01	3.300e-04
Uraninite	0.00	-13.92	-13.92	1.000e+01	1.000e+01	-9.008e-10

-----Solution composition-----

--

Elements	Molality	Moles
C	3.108e-03	3.108e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04

Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
U	9.008e-10	9.008e-10

-----Description of solution-----

```

equilibrium
              pH = 8.729      Charge balance
              pe = -4.067     Adjusted to redox

              Activity of water = 1.000
              Ionic strength = 1.052e-02
              Mass of water (kg) = 1.000e+00
              Total alkalinity (eq/kg) = 3.373e-03
              Total CO2 (mol/kg) = 3.108e-03
              Temperature (deg C) = 25.000
              Electrical balance (eq) = -4.968e-07
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
              Iterations = 10
              Total H = 1.110159e+02
              Total O = 5.552329e+01
  
```

-----Distribution of species-----

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	5.991e-06	5.380e-06	-5.222	-5.269	-0.047
	H+	2.048e-09	1.867e-09	-8.689	-8.729	-0.040
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C (4)		3.108e-03				
	HCO3-	2.771e-03	2.503e-03	-2.557	-2.602	-0.044
	CaCO3	1.751e-04	1.755e-04	-3.757	-3.756	0.001
	CO3-2	9.428e-05	6.275e-05	-4.026	-4.202	-0.177
	CaHCO3+	5.642e-05	5.105e-05	-4.249	-4.292	-0.043
	H2CO3	1.047e-05	1.049e-05	-4.980	-4.979	0.001
	NaHCO3	1.559e-07	1.563e-07	-6.807	-6.806	0.001
	NaCO3-	1.429e-07	1.291e-07	-6.845	-6.889	-0.044
	UO2 (CO3) 3-4	2.877e-13	5.327e-14	-12.541	-13.273	-0.732
	UO2 (CO3) 2-2	5.373e-14	3.525e-14	-13.270	-13.453	-0.183
	UO2CO3	7.017e-17	7.034e-17	-16.154	-16.153	0.001
Ca		3.542e-03				
	Ca+2	2.926e-03	1.969e-03	-2.534	-2.706	-0.172
	CaSO4	3.846e-04	3.856e-04	-3.415	-3.414	0.001
	CaCO3	1.751e-04	1.755e-04	-3.757	-3.756	0.001
	CaHCO3+	5.642e-05	5.105e-05	-4.249	-4.292	-0.043
	CaOH+	2.940e-07	2.660e-07	-6.532	-6.575	-0.043
Cl		1.242e-04				
	Cl-	1.242e-04	1.114e-04	-3.906	-3.953	-0.047
	UO2Cl+	1.829e-26	1.646e-26	-25.738	-25.784	-0.046
	UCl+3	0.000e+00	0.000e+00	-41.819	-42.230	-0.412
H (0)		6.709e-13				
	H2	3.354e-13	3.362e-13	-12.474	-12.473	0.001
Na		1.240e-04				
	Na+	1.231e-04	1.110e-04	-3.910	-3.955	-0.045
	NaSO4-	5.920e-07	5.347e-07	-6.228	-6.272	-0.044

	NaHCO3	1.559e-07	1.563e-07	-6.807	-6.806	0.001
	NaCO3-	1.429e-07	1.291e-07	-6.845	-6.889	-0.044
O(0)	0.000e+00					
	O2	0.000e+00	0.000e+00	-67.434	-67.433	0.001
S(-2)	1.377e-15					
	HS-	4.653e-16	4.178e-16	-15.332	-15.379	-0.047
	S5-2	8.669e-17	5.687e-17	-16.062	-16.245	-0.183
	S4-2	5.058e-17	3.318e-17	-16.296	-16.479	-0.183
	S6-2	4.487e-17	2.943e-17	-16.348	-16.531	-0.183
	H2S	6.805e-18	6.821e-18	-17.167	-17.166	0.001
	S-2	4.080e-20	2.703e-20	-19.389	-19.568	-0.179
	S3-2	1.782e-20	1.169e-20	-19.749	-19.932	-0.183
	S2-2	1.011e-21	6.635e-22	-20.995	-21.178	-0.183
S(6)	1.856e-03					
	SO4-2	1.471e-03	9.615e-04	-2.832	-3.017	-0.185
	CaSO4	3.846e-04	3.856e-04	-3.415	-3.414	0.001
	NaSO4-	5.920e-07	5.347e-07	-6.228	-6.272	-0.044
	HSO4-	1.934e-10	1.742e-10	-9.714	-9.759	-0.045
	UO2SO4	4.371e-23	4.382e-23	-22.359	-22.358	0.001
	UO2(SO4)2-2	1.913e-24	1.255e-24	-23.718	-23.901	-0.183
	U(SO4)2	1.255e-36	1.258e-36	-35.901	-35.900	0.001
	USO4+2	1.028e-37	6.741e-38	-36.988	-37.171	-0.183
U(3)	0.000e+00					
	U+3	0.000e+00	0.000e+00	-43.932	-44.344	-0.412
U(4)	9.005e-10					
	U(OH)5-	9.004e-10	8.103e-10	-9.046	-9.091	-0.046
	U(OH)4	6.322e-14	6.337e-14	-13.199	-13.198	0.001
	U(OH)3+	4.807e-19	4.326e-19	-18.318	-18.364	-0.046
	U(OH)2+2	5.694e-25	3.735e-25	-24.245	-24.428	-0.183
	UOH+3	7.291e-32	2.824e-32	-31.137	-31.549	-0.412
	U(SO4)2	1.255e-36	1.258e-36	-35.901	-35.900	0.001
	USO4+2	1.028e-37	6.741e-38	-36.988	-37.171	-0.183
	U+4	1.310e-39	2.425e-40	-38.883	-39.615	-0.732
	UCl+3	0.000e+00	0.000e+00	-41.819	-42.230	-0.412
	U6(OH)15+9	0.000e+00	0.000e+00	-120.281	-123.989	-3.708
U(5)	7.041e-16					
	UO2+	7.041e-16	6.336e-16	-15.152	-15.198	-0.046
U(6)	3.415e-13					
	UO2(CO3)3-4	2.877e-13	5.327e-14	-12.541	-13.273	-0.732
	UO2(CO3)2-2	5.373e-14	3.525e-14	-13.270	-13.453	-0.183
	UO2CO3	7.017e-17	7.034e-17	-16.154	-16.153	0.001
	UO2OH+	4.307e-19	3.877e-19	-18.366	-18.412	-0.046
	UO2+2	1.358e-22	8.906e-23	-21.867	-22.050	-0.183
	UO2SO4	4.371e-23	4.382e-23	-22.359	-22.358	0.001
	UO2(SO4)2-2	1.913e-24	1.255e-24	-23.718	-23.901	-0.183
	UO2Cl+	1.829e-26	1.646e-26	-25.738	-25.784	-0.046
	(UO2)2(OH)2+2	7.852e-33	5.151e-33	-32.105	-32.288	-0.183
	(UO2)3(OH)5+	8.824e-39	7.941e-39	-38.054	-38.100	-0.046

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.09	-5.72	-4.64	CaSO4
Aragonite	1.43	-6.91	-8.34	CaCO3
B_UO2(OH)2	-10.14	-4.59	5.54	UO2(OH)2

Calcite	1.57	-6.91	-8.47	CaCO3
CH4(g)	-18.85	-58.95	-40.10	CH4
CO2(g)	-3.50	-21.66	-18.16	CO2
Gummite	-15.00	-4.59	10.40	UO3
Gypsum	-0.88	-5.72	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-18.05	14.75	32.80	CaO
Mirabilite	-9.81	-10.93	-1.11	Na2SO4:10H2O
Natron	-10.80	-12.11	-1.31	Na2CO3:10H2O
O2(g)	-64.47	18.65	83.12	O2
Portlandite	-7.92	14.75	22.68	Ca(OH)2
Rutherfordine	-11.79	-26.25	-14.46	UO2CO3
Schoepite	-10.00	-4.59	5.40	UO2(OH)2:H2O
SULFUR	-12.67	-14.78	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-12.24	-12.11	0.12	Na2CO3:H2O
U3O8(C)	-16.56	4.55	21.11	U3O8
U4O9(C)	-6.09	-9.48	-3.38	U4O9
UO2(am)	-5.63	-4.70	0.93	UO2
UO3(C)	-12.31	-4.59	7.72	UO3
Uraninite	-0.00	-4.70	-4.70	UO2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 6

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

TITLE Run-6 - Equil with U3O8, UO2 and CO2
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 422)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1

U3O8(C) 0.0 10.0
CO2(g) -3.5
Uraninite 0.0 10.0

END

TITLE

Run-6 - Equil with U3O8, UO2 and CO2

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.373e-03	3.373e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.083e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.438e-03
 Total CO2 (mol/kg) = 3.438e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -4.968e-07
 Percent error, $100 * (Cat - |An|) / (Cat + |An|)$ = -0.00
 Iterations = 7.
 Total H = 1.110159e+02
 Total O = 5.552395e+01

-----Distribution of species-----

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	7.068e-07	6.338e-07	-6.151	-6.198	-0.047
	H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)		3.438e-03				
	HCO3-	3.228e-03	2.912e-03	-2.491	-2.536	-0.045
	H2CO3	1.034e-04	1.036e-04	-3.986	-3.984	0.001
	CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
	CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
	CO3-2	1.299e-05	8.600e-06	-4.887	-5.065	-0.179
	NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
	NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
Ca		3.542e-03				
	Ca+2	3.054e-03	2.045e-03	-2.515	-2.689	-0.174
	CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
	CaHCO3+	6.828e-05	6.171e-05	-4.166	-4.210	-0.044
	CaCO3	2.493e-05	2.499e-05	-4.603	-4.602	0.001
	CaOH+	3.603e-08	3.256e-08	-7.443	-7.487	-0.044
Cl		1.242e-04				
	Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
H(0)		8.510e-16				
	H2	4.255e-16	4.266e-16	-15.371	-15.370	0.001
Na		1.240e-04				
	Na+	1.232e-04	1.109e-04	-3.909	-3.955	-0.046
	NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
	NaHCO3	1.813e-07	1.818e-07	-6.742	-6.741	0.001
	NaCO3-	1.960e-08	1.768e-08	-7.708	-7.753	-0.045
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-61.641	-61.640	0.001
S(-2)		1.370e-26				
	HS-	1.012e-26	9.076e-27	-25.995	-26.042	-0.047
	H2S	1.255e-27	1.258e-27	-26.902	-26.900	0.001
	S5-2	2.230e-28	1.455e-28	-27.652	-27.837	-0.185
	S4-2	1.301e-28	8.489e-29	-27.886	-28.071	-0.185

S6-2	1.154e-28	7.532e-29	-27.938	-28.123	-0.185
S-2	1.049e-31	6.916e-32	-30.979	-31.160	-0.181
S3-2	4.584e-32	2.991e-32	-31.339	-31.524	-0.185
S2-2	2.602e-33	1.698e-33	-32.585	-32.770	-0.185
S(6)	1.856e-03				
SO4-2	1.461e-03	9.498e-04	-2.835	-3.022	-0.187
CaSO4	3.947e-04	3.957e-04	-3.404	-3.403	0.001
NaSO4-	5.852e-07	5.280e-07	-6.233	-6.277	-0.045
HSO4-	1.624e-09	1.461e-09	-8.789	-8.835	-0.046

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.07	-5.71	-4.64	CaSO4
Aragonite	0.58	-7.75	-8.34	CaCO3
Calcite	0.72	-7.75	-8.47	CaCO3
CH4(g)	-29.45	-69.55	-40.10	CH4
CO2(g)	-2.51	-20.67	-18.16	CO2
Gypsum	-0.86	-5.71	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-19.89	12.91	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-11.67	-12.98	-1.31	Na2CO3:10H2O
O2(g)	-58.68	24.44	83.12	O2
Portlandite	-9.76	12.91	22.68	Ca(OH)2
SULFUR	-19.51	-21.62	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-13.10	-12.98	0.12	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
CO2(g)	-3.50	-21.66	-18.16	1.000e+01	1.000e+01	3.480e-04
U3O8(C)	0.00	-6.54	-6.54	1.000e+01	1.000e+01	-2.723e-05
Uraninite	0.00	-13.92	-13.92	1.000e+01	1.000e+01	2.723e-05

-----Solution composition-----

Elements	Molality	Moles
C	3.090e-03	3.090e-03

Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
U	5.446e-05	5.446e-05

-----Description of solution-----

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--
                                pH = 8.705      Charge balance
                                pe = 0.096      Adjusted to redox
equilibrium
                                Activity of water = 1.000
                                Ionic strength = 1.086e-02
                                Mass of water (kg) = 1.000e+00
                                Total alkalinity (eq/kg) = 3.482e-03
                                Total CO2 (mol/kg) = 3.090e-03
                                Temperature (deg C) = 25.000
                                Electrical balance (eq) = -4.968e-07
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
                                Iterations = 11
                                Total H = 1.110159e+02
                                Total O = 5.552342e+01

```

-----Distribution of species-----

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	5.684e-06	5.096e-06	-5.245	-5.293	-0.047
	H+	2.164e-09	1.971e-09	-8.665	-8.705	-0.041
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)		3.090e-03				
	HCO3-	2.629e-03	2.371e-03	-2.580	-2.625	-0.045
	CaCO3	1.574e-04	1.578e-04	-3.803	-3.802	0.001
	CO3-2	8.507e-05	5.631e-05	-4.070	-4.249	-0.179
	CaHCO3+	5.364e-05	4.846e-05	-4.271	-4.315	-0.044
	UO2(CO3)3-4	4.520e-05	8.179e-06	-4.345	-5.087	-0.742
	H2CO3	1.047e-05	1.049e-05	-4.980	-4.979	0.001
	UO2(CO3)2-2	9.246e-06	6.030e-06	-5.034	-5.220	-0.186
	NaHCO3	1.475e-07	1.479e-07	-6.831	-6.830	0.001
	NaCO3-	1.282e-07	1.157e-07	-6.892	-6.937	-0.045
	UO2CO3	1.338e-08	1.341e-08	-7.874	-7.873	0.001
Ca		3.542e-03				
	Ca+2	2.947e-03	1.973e-03	-2.531	-2.705	-0.174
	CaSO4	3.835e-04	3.845e-04	-3.416	-3.415	0.001
	CaCO3	1.574e-04	1.578e-04	-3.803	-3.802	0.001
	CaHCO3+	5.364e-05	4.846e-05	-4.271	-4.315	-0.044
	CaOH+	2.795e-07	2.526e-07	-6.554	-6.598	-0.044
Cl		1.242e-04				
	Cl-	1.242e-04	1.112e-04	-3.906	-3.954	-0.048
	UO2Cl+	3.885e-18	3.491e-18	-17.411	-17.457	-0.046
	UCl+3	0.000e+00	0.000e+00	-41.720	-42.137	-0.418
H(0)		3.519e-21				
	H2	1.759e-21	1.764e-21	-20.755	-20.754	0.001
Na		1.240e-04				

	Na+	1.232e-04	1.108e-04	-3.910	-3.955	-0.046
	NaSO4-	5.891e-07	5.313e-07	-6.230	-6.275	-0.045
	NaHCO3	1.475e-07	1.479e-07	-6.831	-6.830	0.001
	NaCO3-	1.282e-07	1.157e-07	-6.892	-6.937	-0.045
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-50.874	-50.873	0.001
S(-2)		0.000e+00				
	HS-	0.000e+00	0.000e+00	-48.431	-48.479	-0.047
	S5-2	0.000e+00	0.000e+00	-49.183	-49.368	-0.186
	S4-2	0.000e+00	0.000e+00	-49.417	-49.602	-0.186
	S6-2	0.000e+00	0.000e+00	-49.469	-49.654	-0.186
	H2S	0.000e+00	0.000e+00	-50.243	-50.242	0.001
	S-2	0.000e+00	0.000e+00	-52.510	-52.691	-0.181
	S3-2	0.000e+00	0.000e+00	-52.870	-53.055	-0.186
	S2-2	0.000e+00	0.000e+00	-54.116	-54.301	-0.186
S(6)		1.856e-03				
	SO4-2	1.472e-03	9.566e-04	-2.832	-3.019	-0.187
	CaSO4	3.835e-04	3.845e-04	-3.416	-3.415	0.001
	NaSO4-	5.891e-07	5.313e-07	-6.230	-6.275	-0.045
	HSO4-	2.034e-10	1.830e-10	-9.692	-9.738	-0.046
	UO2SO4	9.238e-15	9.261e-15	-14.034	-14.033	0.001
	UO2(SO4)2-2	4.046e-16	2.639e-16	-15.393	-15.579	-0.186
	U(SO4)2	1.542e-36	1.546e-36	-35.812	-35.811	0.001
	USO4+2	1.277e-37	8.328e-38	-36.894	-37.079	-0.186
U(3)		0.000e+00				
	U+3	0.000e+00	0.000e+00	-47.996	-48.414	-0.418
U(4)		8.542e-10				
	U(OH)5-	8.542e-10	7.676e-10	-9.068	-9.115	-0.046
	U(OH)4	6.321e-14	6.337e-14	-13.199	-13.198	0.001
	U(OH)3+	5.082e-19	4.567e-19	-18.294	-18.340	-0.046
	U(OH)2+2	6.382e-25	4.162e-25	-24.195	-24.381	-0.186
	UOH+3	8.689e-32	3.322e-32	-31.061	-31.479	-0.418
	U(SO4)2	1.542e-36	1.546e-36	-35.812	-35.811	0.001
	USO4+2	1.277e-37	8.328e-38	-36.894	-37.079	-0.186
	U+4	1.664e-39	3.012e-40	-38.779	-39.521	-0.742
	UC1+3	0.000e+00	0.000e+00	-41.720	-42.137	-0.418
	U6(OH)15+9	0.000e+00	0.000e+00	-120.019	-123.777	-3.759
U(5)		1.028e-11				
	UO2+	1.028e-11	9.235e-12	-10.988	-11.035	-0.046
U(6)		5.446e-05				
	UO2(CO3)3-4	4.520e-05	8.179e-06	-4.345	-5.087	-0.742
	UO2(CO3)2-2	9.246e-06	6.030e-06	-5.034	-5.220	-0.186
	UO2CO3	1.338e-08	1.341e-08	-7.874	-7.873	0.001
	UO2OH+	8.681e-11	7.801e-11	-10.061	-10.108	-0.046
	(UO2)3(OH)5+	6.463e-14	5.808e-14	-13.190	-13.236	-0.046
	UO2+2	2.901e-14	1.892e-14	-13.537	-13.723	-0.186
	UO2SO4	9.238e-15	9.261e-15	-14.034	-14.033	0.001
	UO2(SO4)2-2	4.046e-16	2.639e-16	-15.393	-15.579	-0.186
	(UO2)2(OH)2+2	3.199e-16	2.086e-16	-15.495	-15.681	-0.186
	UO2Cl+	3.885e-18	3.491e-18	-17.411	-17.457	-0.046

-----Saturation indices-----
 --

Phase	SI	log IAP	log KT	
Anhydrite	-1.09	-5.72	-4.64	CaSO4

Aragonite	1.38	-6.95	-8.34	CaCO3
B_UO2(OH)2	-1.86	3.69	5.54	UO2(OH)2
Calcite	1.52	-6.95	-8.47	CaCO3
CH4(g)	-51.97	-92.07	-40.10	CH4
CO2(g)	-3.50	-21.66	-18.16	CO2
Gummite	-6.72	3.69	10.40	UO3
Gypsum	-0.88	-5.72	-4.85	CaSO4:2H2O
Halite	-9.49	-7.91	1.58	NaCl
Lime	-18.09	14.71	32.80	CaO
Mirabilite	-9.82	-10.93	-1.11	Na2SO4:10H2O
Natron	-10.85	-12.16	-1.31	Na2CO3:10H2O
O2(g)	-47.91	35.21	83.12	O2
Portlandite	-7.97	14.71	22.68	Ca(OH)2
Rutherfordine	-3.51	-17.97	-14.46	UO2CO3
Schoepite	-1.72	3.69	5.40	UO2(OH)2:H2O
SULFUR	-37.47	-39.58	-2.11	S
Thenardite	-10.75	-10.93	-0.18	Na2SO4
Thermonatrite	-12.29	-12.16	0.12	Na2CO3:H2O
U3O8(C)	0.00	21.11	21.11	U3O8
U4O9(C)	2.19	-1.20	-3.38	U4O9
UO2(am)	-5.63	-4.70	0.93	UO2
UO3(C)	-4.03	3.69	7.72	UO3
Uraninite	0.00	-4.70	-4.70	UO2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 7

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

TITLE Run-7: LANL well R-15, Depth = 1018.6 ft, Sampled 5/22/01 Equil
with U3O8

SOLUTION 1 Solution
pH 7.87
temp 21.5
units ppm
Alkalinity 34.8 as CO3 # 58.0 as CaCO3
Ca 13.0
Mg 3.5
Na 8.5
K 1.8
Cl 4.7
F 0.14
N 2.4
Si 72.73 as SiO2
S 6.1
Fe 0.06
U 0.000375

EQUILIBRIUM PHASES 1
U3O8(C) 0.0 10.0
END

TITLE

Run-7: LANL well R-15, Depth = 1018.6 ft, Sampled 5/22/01 Equil with U3O8

Beginning of initial solution calculations.

Initial solution 1. Solution

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	5.800e-04	5.800e-04
Ca	3.244e-04	3.244e-04

Cl	1.326e-04	1.326e-04
F	7.370e-06	7.370e-06
Fe	1.075e-06	1.075e-06
K	4.604e-05	4.604e-05
Mg	1.440e-04	1.440e-04
N	1.714e-04	1.714e-04
Na	3.698e-04	3.698e-04
S	6.351e-05	6.351e-05
Si	1.211e-03	1.211e-03
U	1.576e-09	1.576e-09

-----Description of solution-----

--

pH	=	7.870
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	1.692e-03
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	5.769e-04
Total CO2 (mol/kg)	=	5.769e-04
Temperature (deg C)	=	21.500
Electrical balance (eq)	=	6.781e-04
Percent error, 100*(Cat- An)/(Cat+ An)	=	29.01
Iterations	=	11
Total H	=	1.110185e+02
Total O	=	5.551305e+01

-----Distribution of species-----

--

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.966e-07	5.699e-07	-6.224	-6.244	-0.020
H+	1.408e-08	1.349e-08	-7.851	-7.870	-0.019
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)	5.769e-04				
HCO3-	5.562e-04	5.319e-04	-3.255	-3.274	-0.019
H2CO3	1.564e-05	1.564e-05	-4.806	-4.806	0.000
CO3-2	2.049e-06	1.713e-06	-5.689	-5.766	-0.078
CaHCO3+	1.387e-06	1.326e-06	-5.858	-5.877	-0.019
MgHCO3+	7.596e-07	7.258e-07	-6.119	-6.139	-0.020
CaCO3	6.046e-07	6.048e-07	-6.219	-6.218	0.000
MgCO3	1.844e-07	1.845e-07	-6.734	-6.734	0.000
NaHCO3	9.810e-08	9.814e-08	-7.008	-7.008	0.000
NaCO3-	9.810e-09	9.382e-09	-8.008	-8.028	-0.019
UO2(CO3)2-2	1.359e-09	1.133e-09	-8.867	-8.946	-0.079
UO2(CO3)3-4	1.247e-10	6.025e-11	-9.904	-10.220	-0.316
UO2CO3	8.778e-11	8.782e-11	-10.057	-10.056	0.000
Ca	3.244e-04				
Ca+2	3.198e-04	2.679e-04	-3.495	-3.572	-0.077
CaSO4	2.633e-06	2.634e-06	-5.580	-5.579	0.000
CaHCO3+	1.387e-06	1.326e-06	-5.858	-5.877	-0.019
CaCO3	6.046e-07	6.048e-07	-6.219	-6.218	0.000
CaF+	1.578e-08	1.508e-08	-7.802	-7.822	-0.020
CaOH+	3.915e-09	3.745e-09	-8.407	-8.427	-0.019

C1	1.326e-04				
C1-	1.326e-04	1.266e-04	-3.877	-3.897	-0.020
UO2C1+	8.906e-19	8.511e-19	-18.050	-18.070	-0.020
FeCl+2	1.372e-19	1.146e-19	-18.863	-18.941	-0.078
FeCl2+	7.585e-23	7.251e-23	-22.120	-22.140	-0.020
FeCl3	9.178e-28	9.182e-28	-27.037	-27.037	0.000
UC1+3	0.000e+00	0.000e+00	-46.814	-46.992	-0.178
F	7.370e-06				
F-	7.302e-06	6.975e-06	-5.137	-5.156	-0.020
MgF+	5.228e-08	4.997e-08	-7.282	-7.301	-0.020
CaF+	1.578e-08	1.508e-08	-7.802	-7.822	-0.020
NaF	3.994e-10	3.996e-10	-9.399	-9.398	0.000
HF	1.295e-10	1.295e-10	-9.888	-9.888	0.000
UO2F+	3.894e-15	3.721e-15	-14.410	-14.429	-0.020
HF2-	3.518e-15	3.361e-15	-14.454	-14.474	-0.020
FeF+2	4.192e-16	3.503e-16	-15.378	-15.456	-0.078
UO2F2	1.710e-16	1.710e-16	-15.767	-15.767	0.000
FeF2+	9.776e-17	9.346e-17	-16.010	-16.029	-0.020
FeF3	1.020e-18	1.021e-18	-17.991	-17.991	0.000
UO2F3-	3.467e-19	3.312e-19	-18.460	-18.480	-0.020
H2F2	5.187e-20	5.189e-20	-19.285	-19.285	0.000
UO2F4-2	4.874e-23	4.063e-23	-22.312	-22.391	-0.079
SiF6-2	1.150e-35	9.609e-36	-34.939	-35.017	-0.078
UF2+2	0.000e+00	0.000e+00	-40.186	-40.265	-0.079
UF+3	0.000e+00	0.000e+00	-40.710	-40.887	-0.178
UF3+	0.000e+00	0.000e+00	-40.743	-40.763	-0.020
UF4	0.000e+00	0.000e+00	-41.372	-41.372	0.000
UF5-	0.000e+00	0.000e+00	-44.913	-44.933	-0.020
UF6-2	0.000e+00	0.000e+00	-47.517	-47.596	-0.079
Fe (2)	5.386e-08				
Fe+2	5.267e-08	4.410e-08	-7.278	-7.356	-0.077
FeOH+	8.299e-10	7.934e-10	-9.081	-9.100	-0.020
FeSO4	3.653e-10	3.654e-10	-9.437	-9.437	0.000
Fe(OH) 2	3.677e-13	3.679e-13	-12.434	-12.434	0.000
Fe(OH) 3-	1.023e-15	9.785e-16	-14.990	-15.009	-0.020
Fe(HS) 2	0.000e+00	0.000e+00	-144.305	-144.305	0.000
Fe(HS) 3-	0.000e+00	0.000e+00	-215.198	-215.218	-0.020
Fe (3)	1.021e-06				
Fe(OH) 2+	4.119e-07	3.939e-07	-6.385	-6.405	-0.019
Fe(OH) 3	3.429e-07	3.430e-07	-6.465	-6.465	0.000
Fe(OH) 4-	2.659e-07	2.543e-07	-6.575	-6.595	-0.019
FeOH+2	1.559e-11	1.303e-11	-10.807	-10.885	-0.078
FeF+2	4.192e-16	3.503e-16	-15.378	-15.456	-0.078
FeF2+	9.776e-17	9.346e-17	-16.010	-16.029	-0.020
Fe+3	4.927e-17	3.353e-17	-16.307	-16.475	-0.167
FeSO4+	1.341e-17	1.282e-17	-16.873	-16.892	-0.020
FeF3	1.020e-18	1.021e-18	-17.991	-17.991	0.000
FeCl+2	1.372e-19	1.146e-19	-18.863	-18.941	-0.078
Fe(SO4) 2-	2.079e-20	1.987e-20	-19.682	-19.702	-0.020
Fe2(OH) 2+4	1.094e-20	5.287e-21	-19.961	-20.277	-0.316
FeCl2+	7.585e-23	7.251e-23	-22.120	-22.140	-0.020
Fe3(OH) 4+5	1.334e-24	4.281e-25	-23.875	-24.368	-0.494
FeCl3	9.178e-28	9.182e-28	-27.037	-27.037	0.000
H(0)	2.668e-27				
H2	1.334e-27	1.334e-27	-26.875	-26.875	0.000
K	4.604e-05				
K+	4.603e-05	4.395e-05	-4.337	-4.357	-0.020

Mg	KSO4-	1.509e-08	1.443e-08	-7.821	-7.841	-0.019
		1.440e-04				
	Mg+2	1.420e-04	1.191e-04	-3.848	-3.924	-0.076
	MgSO4	1.023e-06	1.024e-06	-5.990	-5.990	0.000
	MgHCO3+	7.596e-07	7.258e-07	-6.119	-6.139	-0.020
	MgCO3	1.844e-07	1.845e-07	-6.734	-6.734	0.000
	MgF+	5.228e-08	4.997e-08	-7.282	-7.301	-0.020
N(-3)	MgOH+	1.113e-08	1.065e-08	-7.954	-7.973	-0.019
		1.714e-04				
	NH4+	1.661e-04	1.585e-04	-3.780	-3.800	-0.020
	NH3	5.212e-06	5.214e-06	-5.283	-5.283	0.000
N(3)	NH4SO4-	1.062e-07	1.015e-07	-6.974	-6.993	-0.020
		2.662e-09				
N(5)	NO2-	2.662e-09	2.543e-09	-8.575	-8.595	-0.020
		1.638e-14				
Na	NO3-	1.638e-14	1.565e-14	-13.786	-13.806	-0.020
		3.698e-04				
	Na+	3.696e-04	3.532e-04	-3.432	-3.452	-0.020
	NaHCO3	9.810e-08	9.814e-08	-7.008	-7.008	0.000
	NaSO4-	8.999e-08	8.605e-08	-7.046	-7.065	-0.019
	NaCO3-	9.810e-09	9.382e-09	-8.008	-8.028	-0.019
	NaF	3.994e-10	3.996e-10	-9.399	-9.398	0.000
O(0)		3.367e-40				
S(-2)	O2	1.683e-40	1.684e-40	-39.774	-39.774	0.000
		0.000e+00				
	HS-	0.000e+00	0.000e+00	-72.930	-72.950	-0.020
	H2S	0.000e+00	0.000e+00	-73.831	-73.831	0.000
	S5-2	0.000e+00	0.000e+00	-74.677	-74.756	-0.079
	S6-2	0.000e+00	0.000e+00	-74.882	-74.961	-0.079
	S4-2	0.000e+00	0.000e+00	-74.914	-74.993	-0.079
	S-2	0.000e+00	0.000e+00	-78.025	-78.103	-0.078
	S3-2	0.000e+00	0.000e+00	-78.373	-78.452	-0.079
	S2-2	0.000e+00	0.000e+00	-79.628	-79.707	-0.079
	Fe(HS)2	0.000e+00	0.000e+00	-144.305	-144.305	0.000
	Fe(HS)3-	0.000e+00	0.000e+00	-215.198	-215.218	-0.020
		6.351e-05				
	SO4-2	5.964e-05	4.971e-05	-4.224	-4.304	-0.079
	CaSO4	2.633e-06	2.634e-06	-5.580	-5.579	0.000
S(6)	MgSO4	1.023e-06	1.024e-06	-5.990	-5.990	0.000
	NH4SO4-	1.062e-07	1.015e-07	-6.974	-6.993	-0.020
	NaSO4-	8.999e-08	8.605e-08	-7.046	-7.065	-0.019
	KSO4-	1.509e-08	1.443e-08	-7.821	-7.841	-0.019
	FeSO4	3.653e-10	3.654e-10	-9.437	-9.437	0.000
	HSO4-	6.180e-11	5.907e-11	-10.209	-10.229	-0.020
	UO2SO4	9.529e-17	9.533e-17	-16.021	-16.021	0.000
	FeSO4+	1.341e-17	1.282e-17	-16.873	-16.892	-0.020
	UO2(SO4)2-2	1.659e-19	1.383e-19	-18.780	-18.859	-0.079
	Fe(SO4)2-	2.079e-20	1.987e-20	-19.682	-19.702	-0.020
	USO4+2	0.000e+00	0.000e+00	-43.142	-43.221	-0.079
	U(SO4)2	0.000e+00	0.000e+00	-43.270	-43.270	0.000
		1.211e-03				
	H4SiO4	1.201e-03	1.202e-03	-2.920	-2.920	0.000
	H3SiO4-	9.166e-06	8.758e-06	-5.038	-5.058	-0.020
Si	H2SiO4-2	1.044e-09	8.731e-10	-8.981	-9.059	-0.078
	UO2H3SiO4+	1.541e-12	1.473e-12	-11.812	-11.832	-0.020
	SiF6-2	1.150e-35	9.609e-36	-34.939	-35.017	-0.078
		0.000e+00				
U(3)		0.000e+00				

U(4)	U+3	0.000e+00	0.000e+00	-57.177	-57.354	-0.178
	4.611e-19					
	U(OH)5-	4.608e-19	4.403e-19	-18.336	-18.356	-0.020
	U(OH)4	2.631e-22	2.632e-22	-21.580	-21.580	0.000
	U(OH)3+	1.417e-26	1.354e-26	-25.848	-25.868	-0.020
	U(OH)2+2	1.118e-31	9.324e-32	-30.951	-31.030	-0.079
	UOH+3	8.694e-38	5.774e-38	-37.061	-37.239	-0.178
	UF2+2	0.000e+00	0.000e+00	-40.186	-40.265	-0.079
	UF+3	0.000e+00	0.000e+00	-40.710	-40.887	-0.178
	UF3+	0.000e+00	0.000e+00	-40.743	-40.763	-0.020
	UF4	0.000e+00	0.000e+00	-41.372	-41.372	0.000
	USO4+2	0.000e+00	0.000e+00	-43.142	-43.221	-0.079
	U(SO4)2	0.000e+00	0.000e+00	-43.270	-43.270	0.000
	U+4	0.000e+00	0.000e+00	-44.030	-44.346	-0.316
	UF5-	0.000e+00	0.000e+00	-44.913	-44.933	-0.020
	UC1+3	0.000e+00	0.000e+00	-46.814	-46.992	-0.178
	UF6-2	0.000e+00	0.000e+00	-47.517	-47.596	-0.079
U(5)	U6(OH)15+9	0.000e+00	0.000e+00	-163.656	-165.255	-1.600
	2.829e-16					
U(6)	UO2+	2.829e-16	2.703e-16	-15.548	-15.568	-0.020
	1.576e-09					
	UO2(CO3)2-2	1.359e-09	1.133e-09	-8.867	-8.946	-0.079
	UO2(CO3)3-4	1.247e-10	6.025e-11	-9.904	-10.220	-0.316
	UO2CO3	8.778e-11	8.782e-11	-10.057	-10.056	0.000
	UO2OH+	2.133e-12	2.038e-12	-11.671	-11.691	-0.020
	UO2H3SiO4+	1.541e-12	1.473e-12	-11.812	-11.832	-0.020
	UO2+2	4.979e-15	4.151e-15	-14.303	-14.382	-0.079
	UO2F+	3.894e-15	3.721e-15	-14.410	-14.429	-0.020
	UO2F2	1.710e-16	1.710e-16	-15.767	-15.767	0.000
	UO2SO4	9.529e-17	9.533e-17	-16.021	-16.021	0.000
	UO2Cl+	8.906e-19	8.511e-19	-18.050	-18.070	-0.020
	UO2F3-	3.467e-19	3.312e-19	-18.460	-18.480	-0.020
	(UO2)2(OH)2+2	2.095e-19	1.747e-19	-18.679	-18.758	-0.079
	UO2(SO4)2-2	1.659e-19	1.383e-19	-18.780	-18.859	-0.079
	(UO2)3(OH)5+	2.587e-20	2.472e-20	-19.587	-19.607	-0.020
	UO2F4-2	4.874e-23	4.063e-23	-22.312	-22.391	-0.079

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Akermanite	-17.83	30.31	48.14	Ca2MgSi2O7
Anhydrite	-3.27	-7.88	-4.60	CaSO4
Aragonite	-1.02	-9.34	-8.31	CaCO3
Artinite	-7.72	2.13	9.85	MgCO3:Mg(OH)2:3H2O
B_UO2(OH)2	-4.31	1.36	5.66	UO2(OH)2
Brucite	-5.20	11.82	17.02	Mg(OH)2
Ca-Olivine	-16.71	21.42	38.13	Ca2SiO4
Ca3SiO5	-41.21	33.58	74.79	Ca3SiO5
Calcite	-0.88	-9.34	-8.45	CaCO3
CH4(g)	-75.84	-116.47	-40.63	CH4
Chalcedony	0.64	-2.92	-3.56	SiO2
Chrysotile	-3.04	29.61	32.64	Mg3Si2O5(OH)4
Clinoenstatite	-2.62	8.90	11.51	MgSiO3
CO2(g)	-3.34	-21.51	-18.16	CO2
Cristobalite	0.71	-2.92	-3.63	SiO2

Diopside	-2.02	18.14	20.17	CaMgSi2O6
Dolomite	-2.10	-19.03	-16.93	CaMg(CO3)2
Epsomite	-6.06	-8.23	-2.16	MgSO4:7H2O
Fe(OH)2.7Cl0.3	6.65	3.61	-3.04	Fe(OH)2.7Cl0.3
Fe2(SO4)3	-49.95	-45.86	4.09	Fe2(SO4)3
Fe3(OH)8	2.43	22.66	20.22	Fe3(OH)8
Ferrihydrite	2.24	7.14	4.89	Fe(OH)3
FeS(ppt)	-68.52	-72.44	-3.92	FeS
Fluorite	-3.24	-13.88	-10.64	CaF2
Forsterite	-8.01	20.71	28.72	Mg2SiO4
Goethite	6.51	7.14	0.63	FeOOH
Greenalite	-1.50	19.31	20.81	Fe3Si2O5(OH)4
Greigite	-255.59	-300.62	-45.03	Fe3S4
Gummite	-9.25	1.36	10.60	UO3
Gypsum	-3.03	-7.88	-4.85	CaSO4:2H2O
Halite	-8.92	-7.35	1.57	NaCl
Hematite	18.01	14.27	-3.74	Fe2O3
Huntite	-8.67	-38.41	-29.74	CaMg3(CO3)4
Hydromagnesite	-18.63	-26.95	-8.31	Mg5(CO3)4(OH)2:4H2O
Jarosite-H	-7.06	-18.68	-11.62	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	-0.64	-15.17	-14.53	KFe3(SO4)2(OH)6
Jarosite-Na	-3.38	-14.26	-10.88	NaFe3(SO4)2(OH)6
Larnite	-18.22	21.42	39.64	Ca2SiO4
Lepidocrocite	5.76	7.14	1.37	FeOOH
Lime	-21.03	12.17	33.20	CaO
Mackinawite	-67.79	-72.44	-4.65	FeS
Magadiite	-1.72	-16.02	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	7.88	14.27	6.39	Fe2O3
Magnesite	-1.72	-9.69	-7.98	MgCO3
Magnetite	18.48	22.66	4.18	Fe3O4
Melanterite	-9.16	-11.66	-2.49	FeSO4:7H2O
Merwinite	-27.00	42.48	69.48	Ca3MgSi2O8
Mg-Ferrite	8.74	26.09	17.35	MgFe2O4
Mirabilite	-9.93	-11.21	-1.28	Na2SO4:10H2O
Monticellite	-9.64	21.06	30.70	CaMgSiO4
Natron	-11.22	-12.67	-1.45	Na2CO3:10H2O
Nesquehonite	-4.12	-9.69	-5.57	MgCO3:3H2O
O2(g)	-36.81	47.48	84.29	O2
P-Wollstanite	-4.78	9.25	14.03	CaSiO3
Periclase	-10.01	11.82	21.82	MgO
Portlandite	-10.77	12.17	22.94	Ca(OH)2
Pyrite	-110.94	-129.52	-18.58	FeS2
Quartz	1.14	-2.92	-4.06	SiO2
Rutherfordine	-5.69	-20.15	-14.45	UO2CO3
Schoepite	-4.15	1.36	5.51	UO2(OH)2:H2O
Sepiolite(a)	-3.91	14.87	18.78	Mg2Si3O7.5OH:3H2O
Sepiolite(c)	-1.28	14.87	16.15	Mg2Si3O7.5OH:3H2O
Siderite	-2.62	-13.12	-10.50	FeCO3
SiO2(a)	0.14	-2.92	-3.06	SiO2
SiO2(am)	-0.18	-2.92	-2.74	SiO2
SULFUR	-55.01	-57.08	-2.07	S
Talc	0.41	23.77	23.36	Mg3Si4O10(OH)2
Thenardite	-11.03	-11.21	-0.17	Na2SO4
Thermonatrite	-12.82	-12.67	0.15	Na2CO3:H2O
Tremolite	2.67	60.05	57.39	Ca2Mg5Si8O22(OH)2
U3O8(C)	-13.24	8.88	22.12	U3O8
U4O9(C)	-25.22	-27.72	-2.50	U4O9

UF4 (C)	-46.53	-64.97	-18.44	UF4
UF4:2.5H2O	-37.41	-64.97	-27.56	UF4:2.5H2O
UO2 (am)	-14.03	-12.87	1.16	UO2
UO2 (NO3) 2	-54.54	-41.99	12.54	UO2 (NO3) 2
UO2 (NO3) 2:2H2O	-46.90	-41.99	4.90	UO2 (NO3) 2:2H2O
UO2 (NO3) 2:3H2O	-45.66	-41.99	3.66	UO2 (NO3) 2:3H2O
UO2 (NO3) 2:6H2O	-44.25	-41.99	2.26	UO2 (NO3) 2:6H2O
UO3 (C)	-6.53	1.36	7.89	UO3
Uraninite	-8.33	-12.87	-4.54	UO2
Uranophane	-8.45	9.04	17.49	Ca (UO2) 2 (SiO3OH) 2
USiO4 (C)	-8.29	-15.79	-7.49	USiO4
Wollastonite	-3.92	9.25	13.17	CaSiO3

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution
Using pure phase assemblage 1.

-----Phase assemblage-----
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Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
U3O8 (C)	-0.00	-6.43	-6.43	1.000e+01	1.000e+01	-4.568e-07

-----Solution composition-----
--

Elements	Molality	Moles
C	5.769e-04	5.769e-04
Ca	3.244e-04	3.244e-04
Cl	1.326e-04	1.326e-04
F	7.370e-06	7.370e-06
Fe	1.075e-06	1.075e-06
K	4.604e-05	4.604e-05
Mg	1.440e-04	1.440e-04
N	1.714e-04	1.714e-04
Na	3.698e-04	3.698e-04
S	6.351e-05	6.351e-05
Si	1.211e-03	1.211e-03
U	1.372e-06	1.372e-06

-----Description of solution-----
--

equilibrium	pH	=	7.890	Charge balance
	pe	=	1.776	Adjusted to redox
	Activity of water	=	1.000	
	Ionic strength	=	1.696e-03	
	Mass of water (kg)	=	1.000e+00	

Total alkalinity (eq/kg) = 5.836e-04
 Total CO2 (mol/kg) = 5.769e-04
 Temperature (deg C) = 21.500
 Electrical balance (eq) = 6.781e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 28.98
 Iterations = 11
 Total H = 1.110185e+02
 Total O = 5.551305e+01

-----Distribution of species-----

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
C(4)	OH-	6.254e-07	5.974e-07	-6.204	-6.224	-0.020
	H+	1.343e-08	1.287e-08	-7.872	-7.890	-0.019
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
		5.769e-04				
	HCO3-	5.541e-04	5.298e-04	-3.256	-3.276	-0.019
	H2CO3	1.486e-05	1.487e-05	-4.828	-4.828	0.000
	CO3-2	2.140e-06	1.789e-06	-5.670	-5.747	-0.078
	CaHCO3+	1.381e-06	1.321e-06	-5.860	-5.879	-0.019
	UO2 (CO3) 2-2	1.182e-06	9.855e-07	-5.927	-6.006	-0.079
	MgHCO3+	7.565e-07	7.228e-07	-6.121	-6.141	-0.020
	CaCO3	6.312e-07	6.314e-07	-6.200	-6.200	0.000
	MgCO3	1.925e-07	1.926e-07	-6.715	-6.715	0.000
	UO2 (CO3) 3-4	1.133e-07	5.471e-08	-6.946	-7.262	-0.316
	NaHCO3	9.772e-08	9.776e-08	-7.010	-7.010	0.000
Ca	UO2CO3	7.310e-08	7.313e-08	-7.136	-7.136	0.000
	NaCO3-	1.024e-08	9.796e-09	-7.990	-8.009	-0.019
		3.244e-04				
	Ca+2	3.197e-04	2.679e-04	-3.495	-3.572	-0.077
	CaSO4	2.632e-06	2.633e-06	-5.580	-5.580	0.000
	CaHCO3+	1.381e-06	1.321e-06	-5.860	-5.879	-0.019
	CaCO3	6.312e-07	6.314e-07	-6.200	-6.200	0.000
Cl	CaF+	1.577e-08	1.508e-08	-7.802	-7.822	-0.020
	CaOH+	4.103e-09	3.925e-09	-8.387	-8.406	-0.019
		1.326e-04				
	Cl-	1.326e-04	1.266e-04	-3.877	-3.898	-0.020
	UO2Cl+	7.102e-16	6.786e-16	-15.149	-15.168	-0.020
	FeCl+2	1.445e-20	1.207e-20	-19.840	-19.918	-0.078
	FeCl2+	7.988e-24	7.636e-24	-23.098	-23.117	-0.020
F	FeCl3	9.665e-29	9.669e-29	-28.015	-28.015	0.000
	UCl+3	2.845e-40	1.889e-40	-39.546	-39.724	-0.178
		7.370e-06				
	F-	7.302e-06	6.974e-06	-5.137	-5.156	-0.020
	MgF+	5.227e-08	4.996e-08	-7.282	-7.301	-0.020
	CaF+	1.577e-08	1.508e-08	-7.802	-7.822	-0.020
	NaF	3.994e-10	3.995e-10	-9.399	-9.398	0.000
	HF	1.235e-10	1.236e-10	-9.908	-9.908	0.000
	UO2F+	3.105e-12	2.967e-12	-11.508	-11.528	-0.020
	UO2F2	1.363e-13	1.364e-13	-12.865	-12.865	0.000
	HF2-	3.356e-15	3.206e-15	-14.474	-14.494	-0.020
	UO2F3-	2.764e-16	2.641e-16	-15.558	-15.578	-0.020
	FeF+2	4.416e-17	3.689e-17	-16.355	-16.433	-0.078
	FeF2+	1.030e-17	9.843e-18	-16.987	-17.007	-0.020

	FeF3	1.075e-19	1.075e-19	-18.969	-18.969	0.000
	H2F2	4.719e-20	4.721e-20	-19.326	-19.326	0.000
	UO2F4-2	3.886e-20	3.239e-20	-19.410	-19.490	-0.079
	UF2+2	1.209e-33	1.008e-33	-32.917	-32.997	-0.079
	UF+3	3.619e-34	2.403e-34	-33.441	-33.619	-0.178
	UF3+	3.351e-34	3.202e-34	-33.475	-33.495	-0.020
	UF4	7.870e-35	7.873e-35	-34.104	-34.104	0.000
	SiF6-2	9.521e-36	7.953e-36	-35.021	-35.099	-0.078
	UF5-	2.266e-38	2.165e-38	-37.645	-37.665	-0.020
	UF6-2	0.000e+00	0.000e+00	-40.248	-40.328	-0.079
Fe (2)		9.514e-07				
	Fe+2	9.296e-07	7.783e-07	-6.032	-6.109	-0.077
	FeOH+	1.535e-08	1.468e-08	-7.814	-7.833	-0.020
	FeSO4	6.444e-09	6.447e-09	-8.191	-8.191	0.000
	Fe(OH)2	7.131e-12	7.134e-12	-11.147	-11.147	0.000
	Fe(OH)3-	2.081e-14	1.989e-14	-13.682	-13.701	-0.020
	Fe(HS)2	0.000e+00	0.000e+00	-107.841	-107.840	0.000
	Fe(HS)3-	0.000e+00	0.000e+00	-161.124	-161.144	-0.020
Fe (3)		1.231e-07				
	Fe(OH)2+	4.767e-08	4.558e-08	-7.322	-7.341	-0.019
	Fe(OH)3	4.160e-08	4.161e-08	-7.381	-7.381	0.000
	Fe(OH)4-	3.382e-08	3.234e-08	-7.471	-7.490	-0.019
	FeOH+2	1.722e-12	1.438e-12	-11.764	-11.842	-0.078
	FeF+2	4.416e-17	3.689e-17	-16.355	-16.433	-0.078
	FeF2+	1.030e-17	9.843e-18	-16.987	-17.007	-0.020
	Fe+3	5.191e-18	3.531e-18	-17.285	-17.452	-0.167
	FeSO4+	1.412e-18	1.350e-18	-17.850	-17.870	-0.020
	FeF3	1.075e-19	1.075e-19	-18.969	-18.969	0.000
	FeCl+2	1.445e-20	1.207e-20	-19.840	-19.918	-0.078
	Fe(SO4)2-	2.189e-21	2.092e-21	-20.660	-20.680	-0.020
	Fe2(OH)2+4	1.335e-22	6.444e-23	-21.875	-22.191	-0.316
	FeCl2+	7.988e-24	7.636e-24	-23.098	-23.117	-0.020
	Fe3(OH)4+5	1.885e-27	6.039e-28	-26.725	-27.219	-0.494
	FeCl3	9.665e-29	9.669e-29	-28.015	-28.015	0.000
H (0)		6.817e-23				
	H2	3.409e-23	3.410e-23	-22.467	-22.467	0.000
K		4.604e-05				
	K+	4.603e-05	4.395e-05	-4.337	-4.357	-0.020
	KSO4-	1.509e-08	1.443e-08	-7.821	-7.841	-0.019
Mg		1.440e-04				
	Mg+2	1.419e-04	1.191e-04	-3.848	-3.924	-0.076
	MgSO4	1.023e-06	1.023e-06	-5.990	-5.990	0.000
	MgHCO3+	7.565e-07	7.228e-07	-6.121	-6.141	-0.020
	MgCO3	1.925e-07	1.926e-07	-6.715	-6.715	0.000
	MgF+	5.227e-08	4.996e-08	-7.282	-7.301	-0.020
	MgOH+	1.166e-08	1.116e-08	-7.933	-7.952	-0.019
N (-3)		1.714e-04				
	NH4+	1.658e-04	1.583e-04	-3.780	-3.801	-0.020
	NH3	5.455e-06	5.458e-06	-5.263	-5.263	0.000
	NH4SO4-	1.060e-07	1.013e-07	-6.975	-6.994	-0.020
N (3)		1.751e-22				
	NO2-	1.751e-22	1.673e-22	-21.757	-21.777	-0.020
N (5)		4.217e-32				
	NO3-	4.217e-32	4.027e-32	-31.375	-31.395	-0.020
Na		3.698e-04				
	Na+	3.696e-04	3.532e-04	-3.432	-3.452	-0.020
	NaHCO3	9.772e-08	9.776e-08	-7.010	-7.010	0.000

	NaSO4-	8.996e-08	8.602e-08	-7.046	-7.065	-0.019
	NaCO3-	1.024e-08	9.796e-09	-7.990	-8.009	-0.019
	NaF	3.994e-10	3.995e-10	-9.399	-9.398	0.000
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-48.589	-48.588	0.000
S(-2)		0.000e+00				
	HS-	0.000e+00	0.000e+00	-55.321	-55.341	-0.020
	H2S	0.000e+00	0.000e+00	-56.243	-56.242	0.000
	S5-2	0.000e+00	0.000e+00	-57.047	-57.126	-0.079
	S6-2	0.000e+00	0.000e+00	-57.252	-57.331	-0.079
	S4-2	0.000e+00	0.000e+00	-57.285	-57.364	-0.079
	S-2	0.000e+00	0.000e+00	-60.396	-60.474	-0.078
	S3-2	0.000e+00	0.000e+00	-60.744	-60.823	-0.079
	S2-2	0.000e+00	0.000e+00	-61.998	-62.078	-0.079
	Fe (HS) 2	0.000e+00	0.000e+00	-107.841	-107.840	0.000
	Fe (HS) 3-	0.000e+00	0.000e+00	-161.124	-161.144	-0.020
S(6)		6.351e-05				
	SO4-2	5.964e-05	4.970e-05	-4.224	-4.304	-0.079
	CaSO4	2.632e-06	2.633e-06	-5.580	-5.580	0.000
	MgSO4	1.023e-06	1.023e-06	-5.990	-5.990	0.000
	NH4SO4-	1.060e-07	1.013e-07	-6.975	-6.994	-0.020
	NaSO4-	8.996e-08	8.602e-08	-7.046	-7.065	-0.019
	KSO4-	1.509e-08	1.443e-08	-7.821	-7.841	-0.019
	FeSO4	6.444e-09	6.447e-09	-8.191	-8.191	0.000
	HSO4-	5.895e-11	5.634e-11	-10.230	-10.249	-0.020
	UO2SO4	7.597e-14	7.600e-14	-13.119	-13.119	0.000
	UO2(SO4) 2-2	1.323e-16	1.103e-16	-15.879	-15.958	-0.079
	FeSO4+	1.412e-18	1.350e-18	-17.850	-17.870	-0.020
	Fe(SO4) 2-	2.189e-21	2.092e-21	-20.660	-20.680	-0.020
	USO4+2	1.338e-36	1.115e-36	-35.874	-35.953	-0.079
	U(SO4) 2	9.942e-37	9.946e-37	-36.003	-36.002	0.000
Si		1.211e-03				
	H4SiO4	1.201e-03	1.202e-03	-2.920	-2.920	0.000
	H3SiO4-	9.605e-06	9.177e-06	-5.018	-5.037	-0.020
	UO2H3SiO4+	1.288e-09	1.230e-09	-8.890	-8.910	-0.020
	H2SiO4-2	1.147e-09	9.590e-10	-8.940	-9.018	-0.078
	SiF6-2	9.521e-36	7.953e-36	-35.021	-35.099	-0.078
U(3)		0.000e+00				
	U+3	0.000e+00	0.000e+00	-47.684	-47.862	-0.178
U(4)		1.082e-11				
	U(OH) 5-	1.082e-11	1.034e-11	-10.966	-10.986	-0.020
	U(OH) 4	5.891e-15	5.894e-15	-14.230	-14.230	0.000
	U(OH) 3+	3.028e-19	2.893e-19	-18.519	-18.539	-0.020
	U(OH) 2+2	2.279e-24	1.900e-24	-23.642	-23.721	-0.079
	UOH+3	1.691e-30	1.122e-30	-29.772	-29.950	-0.178
	UF2+2	1.209e-33	1.008e-33	-32.917	-32.997	-0.079
	UF+3	3.619e-34	2.403e-34	-33.441	-33.619	-0.178
	UF3+	3.351e-34	3.202e-34	-33.475	-33.495	-0.020
	UF4	7.870e-35	7.873e-35	-34.104	-34.104	0.000
	USO4+2	1.338e-36	1.115e-36	-35.874	-35.953	-0.079
	U(SO4) 2	9.942e-37	9.946e-37	-36.003	-36.002	0.000
	U+4	1.732e-37	8.359e-38	-36.761	-37.078	-0.316
	UF5-	2.266e-38	2.165e-38	-37.645	-37.665	-0.020
	UCl+3	2.845e-40	1.889e-40	-39.546	-39.724	-0.178
	UF6-2	0.000e+00	0.000e+00	-40.248	-40.328	-0.079
	U6(OH) 15+9	0.000e+00	0.000e+00	-119.738	-121.339	-1.601
U(5)		3.781e-11				

U(6)	UO2+	3.781e-11	3.612e-11	-10.422	-10.442	-0.020
	1.372e-06					
	UO2(CO3)2-2	1.182e-06	9.855e-07	-5.927	-6.006	-0.079
	UO2(CO3)3-4	1.133e-07	5.471e-08	-6.946	-7.262	-0.316
	UO2CO3	7.310e-08	7.313e-08	-7.136	-7.136	0.000
	UO2OH+	1.783e-09	1.704e-09	-8.749	-8.769	-0.020
	UO2H3SiO4+	1.288e-09	1.230e-09	-8.890	-8.910	-0.020
	(UO2)3(OH)5+	1.661e-11	1.587e-11	-10.780	-10.799	-0.020
	UO2+2	3.972e-12	3.310e-12	-11.401	-11.480	-0.079
	UO2F+	3.105e-12	2.967e-12	-11.508	-11.528	-0.020
	(UO2)2(OH)2+2	1.464e-13	1.221e-13	-12.834	-12.913	-0.079
	UO2F2	1.363e-13	1.364e-13	-12.865	-12.865	0.000
	UO2SO4	7.597e-14	7.600e-14	-13.119	-13.119	0.000
	UO2Cl+	7.102e-16	6.786e-16	-15.149	-15.168	-0.020
	UO2F3-	2.764e-16	2.641e-16	-15.558	-15.578	-0.020
	UO2(SO4)2-2	1.323e-16	1.103e-16	-15.879	-15.958	-0.079
	UO2F4-2	3.886e-20	3.239e-20	-19.410	-19.490	-0.079

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Akermanite	-17.70	30.43	48.14	Ca2MgSi2O7
Anhydrite	-3.27	-7.88	-4.60	CaSO4
Aragonite	-1.00	-9.32	-8.31	CaCO3
Artinite	-7.67	2.18	9.85	MgCO3:Mg(OH)2:3H2O
B_UO2(OH)2	-1.36	4.30	5.66	UO2(OH)2
Brucite	-5.16	11.86	17.02	Mg(OH)2
Ca-Olivine	-16.63	21.50	38.13	Ca2SiO4
Ca3SiO5	-41.09	33.71	74.79	Ca3SiO5
Calcite	-0.87	-9.32	-8.45	CaCO3
CH4(g)	-58.23	-98.86	-40.63	CH4
Chalcedony	0.64	-2.92	-3.56	SiO2
Chrysotile	-2.92	29.73	32.64	Mg3Si2O5(OH)4
Clinoenstatite	-2.58	8.94	11.51	MgSiO3
CO2(g)	-3.36	-21.53	-18.16	CO2
Cristobalite	0.71	-2.92	-3.63	SiO2
Diopside	-1.94	18.23	20.17	CaMgSi2O6
Dolomite	-2.06	-18.99	-16.93	CaMg(CO3)2
Epsomite	-6.06	-8.23	-2.16	MgSO4:7H2O
Fe(OH)2.7Cl0.3	5.72	2.68	-3.04	Fe(OH)2.7Cl0.3
Fe2(SO4)3	-51.91	-47.82	4.09	Fe2(SO4)3
Fe3(OH)8	1.89	22.11	20.22	Fe3(OH)8
Ferrihydrite	1.33	6.22	4.89	Fe(OH)3
FeS(ppt)	-49.64	-53.56	-3.92	FeS
Fluorite	-3.24	-13.89	-10.64	CaF2
Forsterite	-7.93	20.79	28.72	Mg2SiO4
Goethite	5.59	6.22	0.63	FeOOH
Greenalite	2.37	23.18	20.81	Fe3Si2O5(OH)4
Greigite	-185.78	-230.81	-45.03	Fe3S4
Gummite	-6.30	4.30	10.60	UO3
Gypsum	-3.03	-7.88	-4.85	CaSO4:2H2O
Halite	-8.92	-7.35	1.57	NaCl
Hematite	16.18	12.44	-3.74	Fe2O3
Huntite	-8.59	-38.33	-29.74	CaMg3(CO3)4
Hydromagnesite	-18.52	-26.83	-8.31	Mg5(CO3)4(OH)2:4H2O

Jarosite-H	-9.89	-21.51	-11.62	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	-3.45	-17.98	-14.53	KFe3(SO4)2(OH)6
Jarosite-Na	-6.19	-17.07	-10.88	NaFe3(SO4)2(OH)6
Larnite	-18.14	21.50	39.64	Ca2SiO4
Lepidocrocite	4.85	6.22	1.37	FeOOH
Lime	-20.99	12.21	33.20	CaO
Mackinawite	-48.91	-53.56	-4.65	FeS
Magadiite	-1.70	-16.00	-14.30	NaSi7O13(OH)3·3H2O
Maghemite	6.05	12.44	6.39	Fe2O3
Magnesite	-1.70	-9.67	-7.98	MgCO3
Magnetite	17.93	22.11	4.18	Fe3O4
Melanterite	-7.92	-10.41	-2.49	FeSO4·7H2O
Merwinite	-26.83	42.64	69.48	Ca3MgSi2O8
Mg-Ferrite	6.95	24.30	17.35	MgFe2O4
Mirabilite	-9.93	-11.21	-1.28	Na2SO4·10H2O
Monticellite	-9.56	21.15	30.70	CaMgSiO4
Natron	-11.20	-12.65	-1.45	Na2CO3·10H2O
Nesquehonite	-4.10	-9.67	-5.57	MgCO3·3H2O
O2(g)	-45.62	38.67	84.29	O2
P-Wollstanite	-4.74	9.29	14.03	CaSiO3
Periclase	-9.97	11.86	21.82	MgO
Portlandite	-10.73	12.21	22.94	Ca(OH)2
Pyrite	-78.88	-97.46	-18.58	FeS2
Quartz	1.14	-2.92	-4.06	SiO2
Rutherfordine	-2.77	-17.23	-14.45	UO2CO3
Schoepite	-1.21	4.30	5.51	UO2(OH)2·H2O
Sepiolite(a)	-3.83	14.95	18.78	Mg2Si3O7·5OH·3H2O
Sepiolite(c)	-1.20	14.95	16.15	Mg2Si3O7·5OH·3H2O
Siderite	-1.35	-11.86	-10.50	FeCO3
SiO2(a)	0.14	-2.92	-3.06	SiO2
SiO2(am)	-0.18	-2.92	-2.74	SiO2
SULFUR	-41.83	-43.90	-2.07	S
Talc	0.53	23.89	23.36	Mg3Si4O10(OH)2
Thénardite	-11.03	-11.21	-0.17	Na2SO4
Thermonatrite	-12.80	-12.65	0.15	Na2CO3·H2O
Tremolite	2.95	60.34	57.39	Ca2Mg5Si8O22(OH)2
U3O8(C)	-0.00	22.12	22.12	U3O8
U4O9(C)	-0.23	-2.73	-2.50	U4O9
UF4(C)	-39.26	-57.70	-18.44	UF4
UF4·2.5H2O	-30.14	-57.70	-27.56	UF4·2.5H2O
UO2(am)	-6.68	-5.52	1.16	UO2
UO2(NO3)2	-86.81	-74.27	12.54	UO2(NO3)2
UO2(NO3)2·2H2O	-79.17	-74.27	4.90	UO2(NO3)2·2H2O
UO2(NO3)2·3H2O	-77.93	-74.27	3.66	UO2(NO3)2·3H2O
UO2(NO3)2·6H2O	-76.53	-74.27	2.26	UO2(NO3)2·6H2O
UO3(C)	-3.59	4.30	7.89	UO3
Uraninite	-0.98	-5.52	-4.54	UO2
Uranophane	-2.52	14.97	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	-0.94	-8.44	-7.49	USiO4
Wollastonite	-3.88	9.29	13.17	CaSiO3

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run-8

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
SOLUTION_SPECIES
PHASES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
END

Reading input data for simulation 1.

TITLE Run-8: LANL well R-15, Depth = 1018.6 ft, Sampled 5/22/01 Equil
with U3O8 and CO2

SOLUTION 1 Solution

pH	7.87	
temp	21.5	
units	ppm	
Alkalinity	34.8	as CO3 # 58.0 as CaCO3
Ca	13.0	
Mg	3.5	
Na	8.5	
K	1.8	
Cl	4.7	
F	0.14	
N	2.4	
Si	72.73	as SiO2
S	6.1	
Fe	0.06	
U	0.000375	

EQUILIBRIUM PHASES 1

U3O8 (C)	0.0	10.0
CO2 (g)	-3.5	

END

TITLE

Run-7: LANL well R-15, Depth = 1018.6 ft, Sampled 5/22/01 Equil with U3O8
and CO2

Beginning of initial solution calculations.

Initial solution 1. Solution

-----Solution composition-----
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Elements	Molality	Moles
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Alkalinity	5.800e-04	5.800e-04
Ca	3.244e-04	3.244e-04
Cl	1.326e-04	1.326e-04
F	7.370e-06	7.370e-06
Fe	1.075e-06	1.075e-06
K	4.604e-05	4.604e-05
Mg	1.440e-04	1.440e-04
N	1.714e-04	1.714e-04
Na	3.698e-04	3.698e-04
S	6.351e-05	6.351e-05
Si	1.211e-03	1.211e-03
U	1.576e-09	1.576e-09

-----Description of solution-----

pH = 7.870
 pe = 4.000
 Activity of water = 1.000
 Ionic strength = 1.692e-03
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 5.769e-04
 Total CO2 (mol/kg) = 5.769e-04
 Temperature (deg C) = 21.500
 Electrical balance (eq) = 6.781e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 29.01
 Iterations = 11
 Total H = 1.110185e+02
 Total O = 5.551305e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.966e-07	5.699e-07	-6.224	-6.244	-0.020
H+	1.408e-08	1.349e-08	-7.851	-7.870	-0.019
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)	5.769e-04				
HCO3-	5.562e-04	5.319e-04	-3.255	-3.274	-0.019
H2CO3	1.564e-05	1.564e-05	-4.806	-4.806	0.000
CO3-2	2.049e-06	1.713e-06	-5.689	-5.766	-0.078
CaHCO3+	1.387e-06	1.326e-06	-5.858	-5.877	-0.019
MgHCO3+	7.596e-07	7.258e-07	-6.119	-6.139	-0.020
CaCO3	6.046e-07	6.048e-07	-6.219	-6.218	0.000
MgCO3	1.844e-07	1.845e-07	-6.734	-6.734	0.000
NaHCO3	9.810e-08	9.814e-08	-7.008	-7.008	0.000
NaCO3-	9.810e-09	9.382e-09	-8.008	-8.028	-0.019
UO2(CO3)2-2	1.359e-09	1.133e-09	-8.867	-8.946	-0.079
UO2(CO3)3-4	1.247e-10	6.025e-11	-9.904	-10.220	-0.316
UO2CO3	8.778e-11	8.782e-11	-10.057	-10.056	0.000
Ca	3.244e-04				
Ca+2	3.198e-04	2.679e-04	-3.495	-3.572	-0.077
CaSO4	2.633e-06	2.634e-06	-5.580	-5.579	0.000
CaHCO3+	1.387e-06	1.326e-06	-5.858	-5.877	-0.019
CaCO3	6.046e-07	6.048e-07	-6.219	-6.218	0.000

Cl	CaF+	1.578e-08	1.508e-08	-7.802	-7.822	-0.020
	CaOH+	3.915e-09	3.745e-09	-8.407	-8.427	-0.019
		1.326e-04				
	Cl-	1.326e-04	1.266e-04	-3.877	-3.897	-0.020
	UO2Cl+	8.906e-19	8.511e-19	-18.050	-18.070	-0.020
	FeCl+2	1.372e-19	1.146e-19	-18.863	-18.941	-0.078
	FeCl2+	7.585e-23	7.251e-23	-22.120	-22.140	-0.020
F	FeCl3	9.178e-28	9.182e-28	-27.037	-27.037	0.000
	UCl+3	0.000e+00	0.000e+00	-46.814	-46.992	-0.178
		7.370e-06				
	F-	7.302e-06	6.975e-06	-5.137	-5.156	-0.020
	MgF+	5.228e-08	4.997e-08	-7.282	-7.301	-0.020
	CaF+	1.578e-08	1.508e-08	-7.802	-7.822	-0.020
	NaF	3.994e-10	3.996e-10	-9.399	-9.398	0.000
	HF	1.295e-10	1.295e-10	-9.888	-9.888	0.000
	UO2F+	3.894e-15	3.721e-15	-14.410	-14.429	-0.020
	HF2-	3.518e-15	3.361e-15	-14.454	-14.474	-0.020
	FeF+2	4.192e-16	3.503e-16	-15.378	-15.456	-0.078
	UO2F2	1.710e-16	1.710e-16	-15.767	-15.767	0.000
	FeF2+	9.776e-17	9.346e-17	-16.010	-16.029	-0.020
	FeF3	1.020e-18	1.021e-18	-17.991	-17.991	0.000
	UO2F3-	3.467e-19	3.312e-19	-18.460	-18.480	-0.020
	H2F2	5.187e-20	5.189e-20	-19.285	-19.285	0.000
	UO2F4-2	4.874e-23	4.063e-23	-22.312	-22.391	-0.079
	SiF6-2	1.150e-35	9.609e-36	-34.939	-35.017	-0.078
	UF2+2	0.000e+00	0.000e+00	-40.186	-40.265	-0.079
	UF+3	0.000e+00	0.000e+00	-40.710	-40.887	-0.178
	UF3+	0.000e+00	0.000e+00	-40.743	-40.763	-0.020
	UF4	0.000e+00	0.000e+00	-41.372	-41.372	0.000
	UF5-	0.000e+00	0.000e+00	-44.913	-44.933	-0.020
	UF6-2	0.000e+00	0.000e+00	-47.517	-47.596	-0.079
Fe (2)		5.386e-08				
	Fe+2	5.267e-08	4.410e-08	-7.278	-7.356	-0.077
	FeOH+	8.299e-10	7.934e-10	-9.081	-9.100	-0.020
	FeSO4	3.653e-10	3.654e-10	-9.437	-9.437	0.000
	Fe (OH) 2	3.677e-13	3.679e-13	-12.434	-12.434	0.000
	Fe (OH) 3-	1.023e-15	9.785e-16	-14.990	-15.009	-0.020
	Fe (HS) 2	0.000e+00	0.000e+00	-144.305	-144.305	0.000
	Fe (HS) 3-	0.000e+00	0.000e+00	-215.198	-215.218	-0.020
Fe (3)		1.021e-06				
	Fe (OH) 2+	4.119e-07	3.939e-07	-6.385	-6.405	-0.019
	Fe (OH) 3	3.429e-07	3.430e-07	-6.465	-6.465	0.000
	Fe (OH) 4-	2.659e-07	2.543e-07	-6.575	-6.595	-0.019
	FeOH+2	1.559e-11	1.303e-11	-10.807	-10.885	-0.078
	FeF+2	4.192e-16	3.503e-16	-15.378	-15.456	-0.078
	FeF2+	9.776e-17	9.346e-17	-16.010	-16.029	-0.020
	Fe+3	4.927e-17	3.353e-17	-16.307	-16.475	-0.167
	FeSO4+	1.341e-17	1.282e-17	-16.873	-16.892	-0.020
	FeF3	1.020e-18	1.021e-18	-17.991	-17.991	0.000
	FeCl+2	1.372e-19	1.146e-19	-18.863	-18.941	-0.078
	Fe (SO4) 2-	2.079e-20	1.987e-20	-19.682	-19.702	-0.020
	Fe2 (OH) 2+4	1.094e-20	5.287e-21	-19.961	-20.277	-0.316
	FeCl2+	7.585e-23	7.251e-23	-22.120	-22.140	-0.020
	Fe3 (OH) 4+5	1.334e-24	4.281e-25	-23.875	-24.368	-0.494
	FeCl3	9.178e-28	9.182e-28	-27.037	-27.037	0.000
H (0)		2.668e-27				
	H2	1.334e-27	1.334e-27	-26.875	-26.875	0.000

K		4.604e-05				
	K+	4.603e-05	4.395e-05	-4.337	-4.357	-0.020
	KSO4-	1.509e-08	1.443e-08	-7.821	-7.841	-0.019
Mg		1.440e-04				
	Mg+2	1.420e-04	1.191e-04	-3.848	-3.924	-0.076
	MgSO4	1.023e-06	1.024e-06	-5.990	-5.990	0.000
	MgHCO3+	7.596e-07	7.258e-07	-6.119	-6.139	-0.020
	MgCO3	1.844e-07	1.845e-07	-6.734	-6.734	0.000
	MgF+	5.228e-08	4.997e-08	-7.282	-7.301	-0.020
	MgOH+	1.113e-08	1.065e-08	-7.954	-7.973	-0.019
N(-3)		1.714e-04				
	NH4+	1.661e-04	1.585e-04	-3.780	-3.800	-0.020
	NH3	5.212e-06	5.214e-06	-5.283	-5.283	0.000
	NH4SO4-	1.062e-07	1.015e-07	-6.974	-6.993	-0.020
N(3)		2.662e-09				
	NO2-	2.662e-09	2.543e-09	-8.575	-8.595	-0.020
N(5)		1.638e-14				
	NO3-	1.638e-14	1.565e-14	-13.786	-13.806	-0.020
Na		3.698e-04				
	Na+	3.696e-04	3.532e-04	-3.432	-3.452	-0.020
	NaHCO3	9.810e-08	9.814e-08	-7.008	-7.008	0.000
	NaSO4-	8.999e-08	8.605e-08	-7.046	-7.065	-0.019
	NaCO3-	9.810e-09	9.382e-09	-8.008	-8.028	-0.019
	NaF	3.994e-10	3.996e-10	-9.399	-9.398	0.000
O(0)		3.367e-40				
	O2	1.683e-40	1.684e-40	-39.774	-39.774	0.000
S(-2)		0.000e+00				
	HS-	0.000e+00	0.000e+00	-72.930	-72.950	-0.020
	H2S	0.000e+00	0.000e+00	-73.831	-73.831	0.000
	S5-2	0.000e+00	0.000e+00	-74.677	-74.756	-0.079
	S6-2	0.000e+00	0.000e+00	-74.882	-74.961	-0.079
	S4-2	0.000e+00	0.000e+00	-74.914	-74.993	-0.079
	S-2	0.000e+00	0.000e+00	-78.025	-78.103	-0.078
	S3-2	0.000e+00	0.000e+00	-78.373	-78.452	-0.079
	S2-2	0.000e+00	0.000e+00	-79.628	-79.707	-0.079
	Fe(HS)2	0.000e+00	0.000e+00	-144.305	-144.305	0.000
	Fe(HS)3-	0.000e+00	0.000e+00	-215.198	-215.218	-0.020
S(6)		6.351e-05				
	SO4-2	5.964e-05	4.971e-05	-4.224	-4.304	-0.079
	CaSO4	2.633e-06	2.634e-06	-5.580	-5.579	0.000
	MgSO4	1.023e-06	1.024e-06	-5.990	-5.990	0.000
	NH4SO4-	1.062e-07	1.015e-07	-6.974	-6.993	-0.020
	NaSO4-	8.999e-08	8.605e-08	-7.046	-7.065	-0.019
	KSO4-	1.509e-08	1.443e-08	-7.821	-7.841	-0.019
	FeSO4	3.653e-10	3.654e-10	-9.437	-9.437	0.000
	HSO4-	6.180e-11	5.907e-11	-10.209	-10.229	-0.020
	UO2SO4	9.529e-17	9.533e-17	-16.021	-16.021	0.000
	FeSO4+	1.341e-17	1.282e-17	-16.873	-16.892	-0.020
	UO2(SO4)2-2	1.659e-19	1.383e-19	-18.780	-18.859	-0.079
	Fe(SO4)2-	2.079e-20	1.987e-20	-19.682	-19.702	-0.020
	USO4+2	0.000e+00	0.000e+00	-43.142	-43.221	-0.079
	U(SO4)2	0.000e+00	0.000e+00	-43.270	-43.270	0.000
Si		1.211e-03				
	H4SiO4	1.201e-03	1.202e-03	-2.920	-2.920	0.000
	H3SiO4-	9.166e-06	8.758e-06	-5.038	-5.058	-0.020
	H2SiO4-2	1.044e-09	8.731e-10	-8.981	-9.059	-0.078
	UO2H3SiO4+	1.541e-12	1.473e-12	-11.812	-11.832	-0.020

	SiF6-2	1.150e-35	9.609e-36	-34.939	-35.017	-0.078
U(3)	0.000e+00					
	U+3	0.000e+00	0.000e+00	-57.177	-57.354	-0.178
U(4)	4.611e-19					
	U(OH)5-	4.608e-19	4.403e-19	-18.336	-18.356	-0.020
	U(OH)4	2.631e-22	2.632e-22	-21.580	-21.580	0.000
	U(OH)3+	1.417e-26	1.354e-26	-25.848	-25.868	-0.020
	U(OH)2+2	1.118e-31	9.324e-32	-30.951	-31.030	-0.079
	UOH+3	8.694e-38	5.774e-38	-37.061	-37.239	-0.178
	UF2+2	0.000e+00	0.000e+00	-40.186	-40.265	-0.079
	UF+3	0.000e+00	0.000e+00	-40.710	-40.887	-0.178
	UF3+	0.000e+00	0.000e+00	-40.743	-40.763	-0.020
	UF4	0.000e+00	0.000e+00	-41.372	-41.372	0.000
	USO4+2	0.000e+00	0.000e+00	-43.142	-43.221	-0.079
	U(SO4)2	0.000e+00	0.000e+00	-43.270	-43.270	0.000
	U+4	0.000e+00	0.000e+00	-44.030	-44.346	-0.316
	UF5-	0.000e+00	0.000e+00	-44.913	-44.933	-0.020
	UC1+3	0.000e+00	0.000e+00	-46.814	-46.992	-0.178
	UF6-2	0.000e+00	0.000e+00	-47.517	-47.596	-0.079
	U6(OH)15+9	0.000e+00	0.000e+00	-163.656	-165.255	-1.600
U(5)	2.829e-16					
	UO2+	2.829e-16	2.703e-16	-15.548	-15.568	-0.020
U(6)	1.576e-09					
	UO2(CO3)2-2	1.359e-09	1.133e-09	-8.867	-8.946	-0.079
	UO2(CO3)3-4	1.247e-10	6.025e-11	-9.904	-10.220	-0.316
	UO2CO3	8.778e-11	8.782e-11	-10.057	-10.056	0.000
	UO2OH+	2.133e-12	2.038e-12	-11.671	-11.691	-0.020
	UO2H3SiO4+	1.541e-12	1.473e-12	-11.812	-11.832	-0.020
	UO2+2	4.979e-15	4.151e-15	-14.303	-14.382	-0.079
	UO2F+	3.894e-15	3.721e-15	-14.410	-14.429	-0.020
	UO2F2	1.710e-16	1.710e-16	-15.767	-15.767	0.000
	UO2SO4	9.529e-17	9.533e-17	-16.021	-16.021	0.000
	UO2Cl+	8.906e-19	8.511e-19	-18.050	-18.070	-0.020
	UO2F3-	3.467e-19	3.312e-19	-18.460	-18.480	-0.020
	(UO2)2(OH)2+2	2.095e-19	1.747e-19	-18.679	-18.758	-0.079
	UO2(SO4)2-2	1.659e-19	1.383e-19	-18.780	-18.859	-0.079
	(UO2)3(OH)5+	2.587e-20	2.472e-20	-19.587	-19.607	-0.020
	UO2F4-2	4.874e-23	4.063e-23	-22.312	-22.391	-0.079

-----Saturation indices-----
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Phase	SI	log IAP	log KT	
Akermanite	-17.83	30.31	48.14	Ca2MgSi2O7
Anhydrite	-3.27	-7.88	-4.60	CaSO4
Aragonite	-1.02	-9.34	-8.31	CaCO3
Artinite	-7.72	2.13	9.85	MgCO3:Mg(OH)2:3H2O
B_UO2(OH)2	-4.31	1.36	5.66	UO2(OH)2
Brucite	-5.20	11.82	17.02	Mg(OH)2
Ca-Olivine	-16.71	21.42	38.13	Ca2SiO4
Ca3SiO5	-41.21	33.58	74.79	Ca3SiO5
Calcite	-0.88	-9.34	-8.45	CaCO3
CH4(g)	-75.84	-116.47	-40.63	CH4
Chalcedony	0.64	-2.92	-3.56	SiO2
Chrysotile	-3.04	29.61	32.64	Mg3Si2O5(OH)4
Clinoenstatite	-2.62	8.90	11.51	MgSiO3

CO2(g)	-3.34	-21.51	-18.16	CO2
Cristobalite	0.71	-2.92	-3.63	SiO2
Diopside	-2.02	18.14	20.17	CaMgSi2O6
Dolomite	-2.10	-19.03	-16.93	CaMg(CO3)2
Epsomite	-6.06	-8.23	-2.16	MgSO4:7H2O
Fe(OH)2.7Cl0.3	6.65	3.61	-3.04	Fe(OH)2.7Cl0.3
Fe2(SO4)3	-49.95	-45.86	4.09	Fe2(SO4)3
Fe3(OH)8	2.43	22.66	20.22	Fe3(OH)8
Ferrihydrite	2.24	7.14	4.89	Fe(OH)3
FeS(ppt)	-68.52	-72.44	-3.92	FeS
Fluorite	-3.24	-13.88	-10.64	CaF2
Forsterite	-8.01	20.71	28.72	Mg2SiO4
Goethite	6.51	7.14	0.63	FeOOH
Greenalite	-1.50	19.31	20.81	Fe3Si2O5(OH)4
Greigite	-255.59	-300.62	-45.03	Fe3S4
Gummite	-9.25	1.36	10.60	UO3
Gypsum	-3.03	-7.88	-4.85	CaSO4:2H2O
Halite	-8.92	-7.35	1.57	NaCl
Hematite	18.01	14.27	-3.74	Fe2O3
Huntite	-8.67	-38.41	-29.74	CaMg3(CO3)4
Hydromagnesite	-18.63	-26.95	-8.31	Mg5(CO3)4(OH)2:4H2O
Jarosite-H	-7.06	-18.68	-11.62	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	-0.64	-15.17	-14.53	KFe3(SO4)2(OH)6
Jarosite-Na	-3.38	-14.26	-10.88	NaFe3(SO4)2(OH)6
Larnite	-18.22	21.42	39.64	Ca2SiO4
Lepidocrocite	5.76	7.14	1.37	FeOOH
Lime	-21.03	12.17	33.20	CaO
Mackinawite	-67.79	-72.44	-4.65	FeS
Magadiite	-1.72	-16.02	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	7.88	14.27	6.39	Fe2O3
Magnesite	-1.72	-9.69	-7.98	MgCO3
Magnetite	18.48	22.66	4.18	Fe3O4
Melanterite	-9.16	-11.66	-2.49	FeSO4:7H2O
Merwinite	-27.00	42.48	69.48	Ca3MgSi2O8
Mg-Ferrite	8.74	26.09	17.35	MgFe2O4
Mirabilite	-9.93	-11.21	-1.28	Na2SO4:10H2O
Monticellite	-9.64	21.06	30.70	CaMgSiO4
Natron	-11.22	-12.67	-1.45	Na2CO3:10H2O
Nesquehonite	-4.12	-9.69	-5.57	MgCO3:3H2O
O2(g)	-36.81	47.48	84.29	O2
P-Wollstanite	-4.78	9.25	14.03	CaSiO3
Periclase	-10.01	11.82	21.82	MgO
Portlandite	-10.77	12.17	22.94	Ca(OH)2
Pyrite	-110.94	-129.52	-18.58	FeS2
Quartz	1.14	-2.92	-4.06	SiO2
Rutherfordine	-5.69	-20.15	-14.45	UO2CO3
Schoepite	-4.15	1.36	5.51	UO2(OH)2:H2O
Sepiolite(a)	-3.91	14.87	18.78	Mg2Si3O7.5OH:3H2O
Sepiolite(c)	-1.28	14.87	16.15	Mg2Si3O7.5OH:3H2O
Siderite	-2.62	-13.12	-10.50	FeCO3
SiO2(a)	0.14	-2.92	-3.06	SiO2
SiO2(am)	-0.18	-2.92	-2.74	SiO2
SULFUR	-55.01	-57.08	-2.07	S
Talc	0.41	23.77	23.36	Mg3Si4O10(OH)2
Thenardite	-11.03	-11.21	-0.17	Na2SO4
Thermonatrite	-12.82	-12.67	0.15	Na2CO3:H2O
Tremolite	2.67	60.05	57.39	Ca2Mg5Si8O22(OH)2

U3O8 (C)	-13.24	8.88	22.12	U3O8
U4O9 (C)	-25.22	-27.72	-2.50	U4O9
UF4 (C)	-46.53	-64.97	-18.44	UF4
UF4:2.5H2O	-37.41	-64.97	-27.56	UF4:2.5H2O
UO2(am)	-14.03	-12.87	1.16	UO2
UO2(NO3)2	-54.54	-41.99	12.54	UO2(NO3)2
UO2(NO3)2:2H2O	-46.90	-41.99	4.90	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-45.66	-41.99	3.66	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-44.25	-41.99	2.26	UO2(NO3)2:6H2O
UO3(C)	-6.53	1.36	7.89	UO3
Uraninite	-8.33	-12.87	-4.54	UO2
Uranophane	-8.45	9.04	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	-8.29	-15.79	-7.49	USiO4
Wollastonite	-3.92	9.25	13.17	CaSiO3

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution
Using pure phase assemblage 1.

-----Phase assemblage-----
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Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
CO2(g)	-3.50	-21.66	-18.16	1.000e+01	1.000e+01	1.059e-05
U3O8(C)	0.00	-6.43	-6.43	1.000e+01	1.000e+01	-4.240e-07

-----Solution composition-----
--

Elements	Molality	Moles
C	5.663e-04	5.663e-04
Ca	3.244e-04	3.244e-04
Cl	1.326e-04	1.326e-04
F	7.370e-06	7.370e-06
Fe	1.075e-06	1.075e-06
K	4.604e-05	4.604e-05
Mg	1.440e-04	1.440e-04
N	1.714e-04	1.714e-04
Na	3.698e-04	3.698e-04
S	6.351e-05	6.351e-05
Si	1.211e-03	1.211e-03
U	1.273e-06	1.273e-06

-----Description of solution-----
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	pH =	8.021	Charge balance
	pe =	1.606	Adjusted to redox
equilibrium			

Activity of water = 1.000
 Ionic strength = 1.694e-03
 Mass of water (kg) = 1.000e+00
 Total alkalinity (eq/kg) = 5.834e-04
 Total CO2 (mol/kg) = 5.663e-04
 Temperature (deg C) = 21.500
 Electrical balance (eq) = 6.781e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 29.04
 Iterations = 12
 Total H = 1.110185e+02
 Total O = 5.551303e+01

-----Distribution of species-----

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	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	8.445e-07	8.067e-07	-6.073	-6.093	-0.020
	H+	9.947e-09	9.530e-09	-8.002	-8.021	-0.019
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000
C(4)		5.663e-04				
	HCO3-	5.467e-04	5.228e-04	-3.262	-3.282	-0.019
	H2CO3	1.086e-05	1.086e-05	-4.964	-4.964	0.000
	CO3-2	2.850e-06	2.383e-06	-5.545	-5.623	-0.078
	CaHCO3+	1.362e-06	1.303e-06	-5.866	-5.885	-0.019
	UO2(CO3)2-2	1.083e-06	9.026e-07	-5.965	-6.045	-0.079
	CaCO3	8.405e-07	8.408e-07	-6.075	-6.075	0.000
	MgHCO3+	7.462e-07	7.130e-07	-6.127	-6.147	-0.020
	MgCO3	2.564e-07	2.565e-07	-6.591	-6.591	0.000
	UO2(CO3)3-4	1.382e-07	6.675e-08	-6.859	-7.176	-0.316
	NaHCO3	9.642e-08	9.646e-08	-7.016	-7.016	0.000
	UO2CO3	5.025e-08	5.027e-08	-7.299	-7.299	0.000
	NaCO3-	1.365e-08	1.305e-08	-7.865	-7.884	-0.019
Ca		3.244e-04				
	Ca+2	3.195e-04	2.677e-04	-3.495	-3.572	-0.077
	CaSO4	2.631e-06	2.632e-06	-5.580	-5.580	0.000
	CaHCO3+	1.362e-06	1.303e-06	-5.866	-5.885	-0.019
	CaCO3	8.405e-07	8.408e-07	-6.075	-6.075	0.000
	CaF+	1.576e-08	1.507e-08	-7.802	-7.822	-0.020
	CaOH+	5.537e-09	5.297e-09	-8.257	-8.276	-0.019
Cl		1.326e-04				
	Cl-	1.326e-04	1.266e-04	-3.877	-3.897	-0.020
	UO2Cl+	3.664e-16	3.501e-16	-15.436	-15.456	-0.020
	FeCl+2	9.037e-21	7.550e-21	-20.044	-20.122	-0.078
	FeCl2+	4.997e-24	4.777e-24	-23.301	-23.321	-0.020
	FeCl3	6.047e-29	6.049e-29	-28.218	-28.218	0.000
	UCl+3	0.000e+00	0.000e+00	-40.015	-40.193	-0.178
F		7.370e-06				
	F-	7.302e-06	6.975e-06	-5.137	-5.156	-0.020
	MgF+	5.225e-08	4.994e-08	-7.282	-7.302	-0.020
	CaF+	1.576e-08	1.507e-08	-7.802	-7.822	-0.020
	NaF	3.994e-10	3.996e-10	-9.399	-9.398	0.000
	HF	9.148e-11	9.151e-11	-10.039	-10.039	0.000
	UO2F+	1.602e-12	1.531e-12	-11.795	-11.815	-0.020
	UO2F2	7.033e-14	7.036e-14	-13.153	-13.153	0.000
	HF2-	2.485e-15	2.374e-15	-14.605	-14.624	-0.020

	UO2F3-	1.426e-16	1.363e-16	-15.846	-15.866	-0.020
	FeF+2	2.762e-17	2.308e-17	-16.559	-16.637	-0.078
	FeF2+	6.441e-18	6.158e-18	-17.191	-17.211	-0.020
	FeF3	6.723e-20	6.726e-20	-19.172	-19.172	0.000
	H2F2	2.588e-20	2.589e-20	-19.587	-19.587	0.000
	UO2F4-2	2.005e-20	1.672e-20	-19.698	-19.777	-0.079
	UF2+2	4.110e-34	3.426e-34	-33.386	-33.465	-0.079
	UF+3	1.230e-34	8.166e-35	-33.910	-34.088	-0.178
	UF3+	1.139e-34	1.088e-34	-33.943	-33.963	-0.020
	UF4	2.675e-35	2.676e-35	-34.573	-34.573	0.000
	SiF6-2	2.856e-36	2.386e-36	-35.544	-35.622	-0.078
	UF5-	7.702e-39	7.359e-39	-38.113	-38.133	-0.020
	UF6-2	0.000e+00	0.000e+00	-40.717	-40.796	-0.079
Fe (2)		8.857e-07				
	Fe+2	8.606e-07	7.206e-07	-6.065	-6.142	-0.077
	FeOH+	1.919e-08	1.835e-08	-7.717	-7.736	-0.020
	FeSO4	5.967e-09	5.969e-09	-8.224	-8.224	0.000
	Fe (OH) 2	1.204e-11	1.204e-11	-10.919	-10.919	0.000
	Fe (OH) 3-	4.743e-14	4.534e-14	-13.324	-13.343	-0.020
	Fe (HS) 2	0.000e+00	0.000e+00	-107.498	-107.498	0.000
	Fe (HS) 3-	0.000e+00	0.000e+00	-160.594	-160.614	-0.020
Fe (3)		1.888e-07				
	Fe (OH) 4-	7.033e-08	6.726e-08	-7.153	-7.172	-0.019
	Fe (OH) 3	6.407e-08	6.410e-08	-7.193	-7.193	0.000
	Fe (OH) 2+	5.437e-08	5.200e-08	-7.265	-7.284	-0.019
	FeOH+2	1.454e-12	1.215e-12	-11.837	-11.915	-0.078
	FeF+2	2.762e-17	2.308e-17	-16.559	-16.637	-0.078
	FeF2+	6.441e-18	6.158e-18	-17.191	-17.211	-0.020
	Fe+3	3.247e-18	2.209e-18	-17.489	-17.656	-0.167
	FeSO4+	8.832e-19	8.443e-19	-18.054	-18.073	-0.020
	FeF3	6.723e-20	6.726e-20	-19.172	-19.172	0.000
	FeCl+2	9.037e-21	7.550e-21	-20.044	-20.122	-0.078
	Fe (SO4) 2-	1.370e-21	1.309e-21	-20.863	-20.883	-0.020
	Fe2 (OH) 2+4	9.522e-23	4.598e-23	-22.021	-22.337	-0.316
	FeCl2+	4.997e-24	4.777e-24	-23.301	-23.321	-0.020
	Fe3 (OH) 4+5	1.533e-27	4.916e-28	-26.814	-27.308	-0.494
	FeCl3	6.047e-29	6.049e-29	-28.218	-28.218	0.000
H (0)		8.188e-23				
	H2	4.094e-23	4.096e-23	-22.388	-22.388	0.000
K		4.604e-05				
	K+	4.603e-05	4.395e-05	-4.337	-4.357	-0.020
	KSO4-	1.509e-08	1.443e-08	-7.821	-7.841	-0.019
Mg		1.440e-04				
	Mg+2	1.419e-04	1.190e-04	-3.848	-3.924	-0.076
	MgSO4	1.023e-06	1.023e-06	-5.990	-5.990	0.000
	MgHCO3+	7.462e-07	7.130e-07	-6.127	-6.147	-0.020
	MgCO3	2.564e-07	2.565e-07	-6.591	-6.591	0.000
	MgF+	5.225e-08	4.994e-08	-7.282	-7.302	-0.020
	MgOH+	1.574e-08	1.506e-08	-7.803	-7.822	-0.019
N (-3)		1.714e-04				
	NH4+	1.640e-04	1.565e-04	-3.785	-3.805	-0.020
	NH3	7.286e-06	7.288e-06	-5.138	-5.137	0.000
	NH4SO4-	1.048e-07	1.002e-07	-6.979	-6.999	-0.020
N (3)		1.822e-22				
	NO2-	1.822e-22	1.741e-22	-21.739	-21.759	-0.020
N (5)		3.654e-32				
	NO3-	3.654e-32	3.489e-32	-31.437	-31.457	-0.020

Na		3.698e-04				
	Na+	3.696e-04	3.532e-04	-3.432	-3.452	-0.020
	NaHCO3	9.642e-08	9.646e-08	-7.016	-7.016	0.000
	NaSO4-	8.998e-08	8.604e-08	-7.046	-7.065	-0.019
	NaCO3-	1.365e-08	1.305e-08	-7.865	-7.884	-0.019
	NaF	3.994e-10	3.996e-10	-9.399	-9.398	0.000
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-48.748	-48.748	0.000
S(-2)		0.000e+00				
	HS-	0.000e+00	0.000e+00	-55.133	-55.153	-0.020
	H2S	0.000e+00	0.000e+00	-56.185	-56.185	0.000
	S5-2	0.000e+00	0.000e+00	-56.729	-56.808	-0.079
	S6-2	0.000e+00	0.000e+00	-56.934	-57.013	-0.079
	S4-2	0.000e+00	0.000e+00	-56.966	-57.045	-0.079
	S-2	0.000e+00	0.000e+00	-60.077	-60.155	-0.078
	S3-2	0.000e+00	0.000e+00	-60.425	-60.504	-0.079
	S2-2	0.000e+00	0.000e+00	-61.680	-61.759	-0.079
	Fe(HS)2	0.000e+00	0.000e+00	-107.498	-107.498	0.000
	Fe(HS)3-	0.000e+00	0.000e+00	-160.594	-160.614	-0.020
S(6)		6.351e-05				
	SO4-2	5.964e-05	4.970e-05	-4.224	-4.304	-0.079
	CaSO4	2.631e-06	2.632e-06	-5.580	-5.580	0.000
	MgSO4	1.023e-06	1.023e-06	-5.990	-5.990	0.000
	NH4SO4-	1.048e-07	1.002e-07	-6.979	-6.999	-0.020
	NaSO4-	8.998e-08	8.604e-08	-7.046	-7.065	-0.019
	KSO4-	1.509e-08	1.443e-08	-7.821	-7.841	-0.019
	FeSO4	5.967e-09	5.969e-09	-8.224	-8.224	0.000
	HSO4-	4.366e-11	4.173e-11	-10.360	-10.380	-0.020
	UO2SO4	3.920e-14	3.921e-14	-13.407	-13.407	0.000
	UO2(SO4)2-2	6.826e-17	5.690e-17	-16.166	-16.245	-0.079
	FeSO4+	8.832e-19	8.443e-19	-18.054	-18.073	-0.020
	Fe(SO4)2-	1.370e-21	1.309e-21	-20.863	-20.883	-0.020
	USO4+2	4.546e-37	3.790e-37	-36.342	-36.421	-0.079
	U(SO4)2	3.380e-37	3.381e-37	-36.471	-36.471	0.000
Si		1.211e-03				
	H4SiO4	1.198e-03	1.198e-03	-2.922	-2.921	0.000
	H3SiO4-	1.293e-05	1.236e-05	-4.888	-4.908	-0.020
	H2SiO4-2	2.086e-09	1.744e-09	-8.681	-8.758	-0.078
	UO2H3SiO4+	8.947e-10	8.549e-10	-9.048	-9.068	-0.020
	SiF6-2	2.856e-36	2.386e-36	-35.544	-35.622	-0.078
U(3)		0.000e+00				
	U+3	0.000e+00	0.000e+00	-47.983	-48.161	-0.178
U(4)		1.651e-11				
	U(OH)5-	1.650e-11	1.577e-11	-10.782	-10.802	-0.020
	U(OH)4	6.657e-15	6.660e-15	-14.177	-14.177	0.000
	U(OH)3+	2.534e-19	2.421e-19	-18.596	-18.616	-0.020
	U(OH)2+2	1.412e-24	1.177e-24	-23.850	-23.929	-0.079
	UOH+3	7.757e-31	5.151e-31	-30.110	-30.288	-0.178
	UF2+2	4.110e-34	3.426e-34	-33.386	-33.465	-0.079
	UF+3	1.230e-34	8.166e-35	-33.910	-34.088	-0.178
	UF3+	1.139e-34	1.088e-34	-33.943	-33.963	-0.020
	UF4	2.675e-35	2.676e-35	-34.573	-34.573	0.000
	USO4+2	4.546e-37	3.790e-37	-36.342	-36.421	-0.079
	U(SO4)2	3.380e-37	3.381e-37	-36.471	-36.471	0.000
	U+4	5.883e-38	2.841e-38	-37.230	-37.547	-0.316
	UF5-	7.702e-39	7.359e-39	-38.113	-38.133	-0.020
	UC1+3	0.000e+00	0.000e+00	-40.015	-40.193	-0.178

	UF6-2	0.000e+00	0.000e+00	-40.717	-40.796	-0.079
	U6(OH)15+9	0.000e+00	0.000e+00	-120.594	-122.195	-1.600
U(5)	2.887e-11					
	UO2+	2.887e-11	2.758e-11	-10.540	-10.559	-0.020
U(6)	1.273e-06					
	UO2(CO3)2-2	1.083e-06	9.026e-07	-5.965	-6.045	-0.079
	UO2(CO3)3-4	1.382e-07	6.675e-08	-6.859	-7.176	-0.316
	UO2CO3	5.025e-08	5.027e-08	-7.299	-7.299	0.000
	UO2OH+	1.242e-09	1.187e-09	-8.906	-8.926	-0.020
	UO2H3SiO4+	8.947e-10	8.549e-10	-9.048	-9.068	-0.020
	(UO2)3(OH)5+	1.024e-11	9.784e-12	-10.990	-11.009	-0.020
	UO2+2	2.049e-12	1.708e-12	-11.688	-11.768	-0.079
	UO2F+	1.602e-12	1.531e-12	-11.795	-11.815	-0.020
	(UO2)2(OH)2+2	7.107e-14	5.924e-14	-13.148	-13.227	-0.079
	UO2F2	7.033e-14	7.036e-14	-13.153	-13.153	0.000
	UO2SO4	3.920e-14	3.921e-14	-13.407	-13.407	0.000
	UO2Cl+	3.664e-16	3.501e-16	-15.436	-15.456	-0.020
	UO2F3-	1.426e-16	1.363e-16	-15.846	-15.866	-0.020
	UO2(SO4)2-2	6.826e-17	5.690e-17	-16.166	-16.245	-0.079
	UO2F4-2	2.005e-20	1.672e-20	-19.698	-19.777	-0.079

-----Saturation indices-----
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Phase	SI	log IAP	log KT	
Akermanite	-16.92	31.21	48.14	Ca2MgSi2O7
Anhydrite	-3.27	-7.88	-4.60	CaSO4
Aragonite	-0.88	-9.20	-8.31	CaCO3
Artinite	-7.28	2.57	9.85	MgCO3:Mg(OH)2:3H2O
B_UO2(OH)2	-1.39	4.27	5.66	UO2(OH)2
Brucite	-4.90	12.12	17.02	Mg(OH)2
Ca-Olivine	-16.11	22.02	38.13	Ca2SiO4
Ca3SiO5	-40.31	34.49	74.79	Ca3SiO5
Calcite	-0.74	-9.20	-8.45	CaCO3
CH4(g)	-58.05	-98.68	-40.63	CH4
Chalcedony	0.64	-2.92	-3.56	SiO2
Chrysotile	-2.14	30.51	32.64	Mg3Si2O5(OH)4
Clinoenstatite	-2.32	9.20	11.51	MgSiO3
CO2(g)	-3.50	-21.66	-18.16	CO2
Cristobalite	0.71	-2.92	-3.63	SiO2
Diopside	-1.42	18.74	20.17	CaMgSi2O6
Dolomite	-1.81	-18.74	-16.93	CaMg(CO3)2
Epsomite	-6.06	-8.23	-2.16	MgSO4:7H2O
Fe(OH)2.7Cl0.3	5.87	2.83	-3.04	Fe(OH)2.7Cl0.3
Fe2(SO4)3	-52.32	-48.22	4.09	Fe2(SO4)3
Fe3(OH)8	2.49	22.71	20.22	Fe3(OH)8
Ferrihydrite	1.52	6.41	4.89	Fe(OH)3
FeS(ppt)	-49.36	-53.27	-3.92	FeS
Fluorite	-3.24	-13.89	-10.64	CaF2
Forsterite	-7.41	21.31	28.72	Mg2SiO4
Goethite	5.78	6.41	0.63	FeOOH
Greenalite	3.05	23.86	20.81	Fe3Si2O5(OH)4
Greigite	-184.95	-229.98	-45.03	Fe3S4
Gummite	-6.33	4.27	10.60	UO3
Gypsum	-3.03	-7.88	-4.85	CaSO4:2H2O
Halite	-8.92	-7.35	1.57	NaCl

Hematite	16.55	12.81	-3.74	Fe2O3
Huntite	-8.09	-37.84	-29.74	CaMg3(CO3)4
Hydromagnesite	-17.76	-26.07	-8.31	Mg5(CO3)4(OH)2:4H2O
Jarosite-H	-9.85	-21.47	-11.62	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	-3.28	-17.81	-14.53	KFe3(SO4)2(OH)6
Jarosite-Na	-6.02	-16.90	-10.88	NaFe3(SO4)2(OH)6
Larnite	-17.62	22.02	39.64	Ca2SiO4
Lepidocrocite	5.04	6.41	1.37	FeOOH
Lime	-20.73	12.47	33.20	CaO
Mackinawite	-48.63	-53.27	-4.65	FeS
Magadiite	-1.58	-15.88	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	6.43	12.81	6.39	Fe2O3
Magnesite	-1.57	-9.55	-7.98	MgCO3
Magnetite	18.54	22.71	4.18	Fe3O4
Melanterite	-7.95	-10.45	-2.49	FeSO4:7H2O
Merwinite	-25.79	43.68	69.48	Ca3MgSi2O8
Mg-Ferrite	7.59	24.93	17.35	MgFe2O4
Mirabilite	-9.93	-11.21	-1.28	Na2SO4:10H2O
Monticellite	-9.04	21.67	30.70	CaMgSiO4
Natron	-11.08	-12.53	-1.45	Na2CO3:10H2O
Nesquehonite	-3.98	-9.55	-5.57	MgCO3:3H2O
O2(g)	-45.78	38.51	84.29	O2
P-Wollstanite	-4.48	9.55	14.03	CaSiO3
Periclase	-9.71	12.12	21.82	MgO
Portlandite	-10.47	12.47	22.94	Ca(OH)2
Pyrite	-78.62	-97.19	-18.58	FeS2
Quartz	1.14	-2.92	-4.06	SiO2
Rutherfordine	-2.94	-17.39	-14.45	UO2CO3
Schoepite	-1.23	4.27	5.51	UO2(OH)2:H2O
Sepiolite(a)	-3.31	15.47	18.78	Mg2Si3O7.5OH:3H2O
Sepiolite(c)	-0.68	15.47	16.15	Mg2Si3O7.5OH:3H2O
Siderite	-1.26	-11.77	-10.50	FeCO3
SiO2(a)	0.14	-2.92	-3.06	SiO2
SiO2(am)	-0.18	-2.92	-2.74	SiO2
SULFUR	-41.85	-43.92	-2.07	S
Talc	1.31	24.67	23.36	Mg3Si4O10(OH)2
Thenardite	-11.03	-11.21	-0.17	Na2SO4
Thermonatrite	-12.68	-12.53	0.15	Na2CO3:H2O
Tremolite	4.77	62.15	57.39	Ca2Mg5Si8O22(OH)2
U3O8(C)	0.00	22.12	22.12	U3O8
U4O9(C)	-0.10	-2.60	-2.50	U4O9
UF4(C)	-39.73	-58.17	-18.44	UF4
UF4:2.5H2O	-30.61	-58.17	-27.56	UF4:2.5H2O
UO2(am)	-6.63	-5.46	1.16	UO2
UO2(NO3)2	-87.23	-74.68	12.54	UO2(NO3)2
UO2(NO3)2:2H2O	-79.59	-74.68	4.90	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-78.35	-74.68	3.66	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-76.94	-74.68	2.26	UO2(NO3)2:6H2O
UO3(C)	-3.61	4.27	7.89	UO3
Uraninite	-0.93	-5.46	-4.54	UO2
Uranophane	-2.31	15.18	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	-0.89	-8.38	-7.49	USiO4
Wollastonite	-3.62	9.55	13.17	CaSiO3

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Attachment 5

Run 9

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 9 # Equil with RaSO4 only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1
RaSO4 0.0 10.0
END

TITLE

Run 9

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
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Elements	Molality	Moles
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Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

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pH	=	7.800
pe	=	-1.690
Activity of water	=	1.000
Ionic strength	=	1.113e-02
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	3.427e-03
Total CO2 (mol/kg)	=	3.427e-03
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-1.908e-06
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.01
Iterations	=	4
Total H	=	1.110539e+02
Total O	=	5.554293e+01

-----Distribution of species-----

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Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000

Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				
ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048
Cl(7)	0.000e+00				
ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H(0)	9.537e-16				
H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na	1.240e-04				
Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)	0.000e+00				
S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(-2)	1.368e-26				
HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(2)	3.392e-32				
S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S(3)	0.000e+00				
S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S(4)	2.664e-19				
SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S(5)	0.000e+00				
S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S(6)	1.856e-03				
SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)	0.000e+00				
S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189

S(8) 0.000e+00
 HSO5- 0.000e+00 0.000e+00 -58.790 -58.836 -0.047

-----Saturation indices-----
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Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

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Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
RaSO4	0.00	-10.46	-10.46	1.000e+01	1.000e+01	-5.229e-08

-----Solution composition-----

--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
Ra	5.229e-08	5.229e-08
S	1.856e-03	1.856e-03

-----Description of solution-----

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equilibrium	pH	=	7.800	Charge balance
	pe	=	-1.855	Adjusted to redox
	Activity of water	=	1.000	
	Ionic strength	=	1.113e-02	
	Mass of water (kg)	=	1.000e+00	
	Total alkalinity (eq/kg)	=	3.374e-03	
	Total CO2 (mol/kg)	=	3.427e-03	
	Temperature (deg C)	=	25.000	
	Electrical balance (eq)	=	-1.908e-06	
	Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	-0.01	
	Iterations	=	6	
	Total H	=	1.110539e+02	
	Total O	=	5.554293e+01	

-----Distribution of species-----

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Species	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-88.459	-88.459	0.000
C(-3)	6.899e-32				

C(-4)	C2H6	3.450e-32	3.450e-32	-31.462	-31.462	0.000
		9.883e-31				
C(2)	CH4	9.883e-31	9.883e-31	-30.005	-30.005	0.000
		1.233e-21				
C(4)	CO	1.233e-21	1.233e-21	-20.909	-20.909	0.000
		3.427e-03				
	HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
	CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
		3.542e-03				
Ca	Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
		1.242e-04				
Cl(-1)	Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
	HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)		0.000e+00				
	ClO-	0.000e+00	0.000e+00	-50.126	-50.173	-0.047
Cl(3)	HClO	0.000e+00	0.000e+00	-50.404	-50.404	0.000
		0.000e+00				
Cl(5)	ClO2-	0.000e+00	0.000e+00	-89.239	-89.286	-0.047
	HClO2	0.000e+00	0.000e+00	-93.916	-93.916	0.000
Cl(7)		0.000e+00				
	ClO3-	0.000e+00	0.000e+00	-114.499	-114.546	-0.048
H(0)	ClO4-	0.000e+00	0.000e+00	-144.061	-144.109	-0.048
		2.038e-15				
Na	H2	1.019e-15	1.022e-15	-14.992	-14.991	0.001
		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-46.964	-47.153	-0.189
	S3O6-2	0.000e+00	0.000e+00	-61.568	-61.757	-0.189
	O2	0.000e+00	0.000e+00	-62.216	-62.215	0.001
	S3-2	0.000e+00	0.000e+00	-64.380	-64.569	-0.189
	S4O6-2	0.000e+00	0.000e+00	-65.562	-65.751	-0.189
	S4-2	0.000e+00	0.000e+00	-82.024	-82.213	-0.189
	S5O6-2	0.000e+00	0.000e+00	-98.435	-98.624	-0.189
	S5-2	0.000e+00	0.000e+00	-99.884	-100.073	-0.189
		5.229e-08				
Ra		5.229e-08	3.427e-08	-7.282	-7.465	-0.183
	Ra+2	5.229e-08	3.427e-08	-7.282	-7.465	-0.183

S(-2)	2.851e-25					
HS-	2.489e-25	2.230e-25	-24.604	-24.652	-0.048	
H2S	3.614e-26	3.614e-26	-25.442	-25.442	0.000	
S-2	2.546e-30	1.669e-30	-29.594	-29.778	-0.183	
S2-2	0.000e+00	0.000e+00	-46.964	-47.153	-0.189	
S3-2	0.000e+00	0.000e+00	-64.380	-64.569	-0.189	
S4-2	0.000e+00	0.000e+00	-82.024	-82.213	-0.189	
S5-2	0.000e+00	0.000e+00	-99.884	-100.073	-0.189	
S(2)	7.067e-31					
S2O3-2	3.533e-31	2.286e-31	-30.452	-30.641	-0.189	
HS2O3-	4.168e-38	3.741e-38	-37.380	-37.427	-0.047	
S(3)	0.000e+00					
S2O4-2	0.000e+00	0.000e+00	-48.989	-49.173	-0.183	
S(4)	5.691e-19					
SO3-2	4.758e-19	3.099e-19	-18.323	-18.509	-0.186	
HSO3-	9.327e-20	8.372e-20	-19.030	-19.077	-0.047	
H2SO3	1.272e-25	1.272e-25	-24.896	-24.896	0.000	
SO2	1.010e-25	1.010e-25	-24.996	-24.996	0.000	
S2O5-2	0.000e+00	0.000e+00	-42.795	-42.984	-0.189	
S3O6-2	0.000e+00	0.000e+00	-61.568	-61.757	-0.189	
S4O6-2	0.000e+00	0.000e+00	-65.562	-65.751	-0.189	
S5O6-2	0.000e+00	0.000e+00	-98.435	-98.624	-0.189	
S(5)	0.000e+00					
S2O6-2	0.000e+00	0.000e+00	-41.669	-41.858	-0.189	
S(6)	1.856e-03					
SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189	
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000	
NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047	
HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047	
H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000	
S(7)	0.000e+00					
S2O8-2	0.000e+00	0.000e+00	-74.970	-75.159	-0.189	
S(8)	0.000e+00					
HSO5-	0.000e+00	0.000e+00	-59.119	-59.166	-0.047	

-----Saturation indices-----

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Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.27	51.87	64.15	C
C(g)	-129.89	51.87	181.77	C
Ca	-95.81	44.02	139.83	Ca
Ca(g)	-121.05	44.02	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
CH4(g)	-27.16	-30.01	-2.84	CH4
Cl2(g)	-57.61	-54.62	2.99	Cl2
CO(g)	-17.91	-20.91	-3.00	CO
CO2(g)	-2.51	-10.34	-7.83	CO2

Gaylussite	-11.25	-0.09	11.16	CaNa ₂ (CO ₃) ₂ :5H ₂ O
Glauberite	-11.13	-16.60	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-1.15	-5.68	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-11.89	-14.99	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
H ₂ S(g)	-24.46	-32.45	-7.99	H ₂ S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na ₂ SO ₄ :10H ₂ O
Monohydrocalcite	-0.10	2.57	2.68	CaCO ₃ :H ₂ O
Na	-47.98	19.40	67.37	Na
Na(g)	-61.46	19.40	80.86	Na
Na ₂ CO ₃	-13.82	-2.66	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-12.60	-2.66	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-59.73	7.68	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-24.78	-25.67	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-21.62	-27.51	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-6.36	-6.50	-0.14	NaHCO ₃
Natron	-12.25	-2.66	9.59	Na ₂ CO ₃ :10H ₂ O
O ₂ (g)	-59.32	-62.21	-2.89	O ₂
Pirssonite	-11.41	-0.09	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Portlandite	-9.63	12.92	22.55	Ca(OH) ₂
Ra	-102.13	39.24	141.37	Ra
RaCl ₂ :2H ₂ O	-14.60	-15.37	-0.77	RaCl ₂ :2H ₂ O
RaSO ₄	0.00	-10.46	-10.46	RaSO ₄
S	-18.45	-63.56	-45.11	S
S ₂ (g)	-50.79	-57.98	-7.19	S ₂
SO ₂ (g)	-25.17	-25.00	0.18	SO ₂
Thenardite	-10.56	-10.91	-0.36	Na ₂ SO ₄
Thermonatrite	-13.59	-2.66	10.94	Na ₂ CO ₃ :H ₂ O

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 10

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 10 # Equil with Ra(NO3)2 only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 $\# = -100$ mV, $pe = eh/0.059$ (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1
Ra(NO3)2 0.0 10.0
END

TITLE

Run 10

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04

S

1.856e-03 1.856e-03

-----Description of solution-----

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.113e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.427e-03
 Total CO2 (mol/kg) = 3.427e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -1.908e-06
 Percent error, $100 * (Cat - |An|) / (Cat + |An|)$ = -0.01
 Iterations = 4
 Total H = 1.110539e+02
 Total O = 5.554293e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				

	ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048
Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H(0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S(4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----

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Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

--

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
Ra(NO3)2	0.00	205.06	205.06	1.000e+01	9.733e+00	-2.668e-01

-----Solution composition-----

--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
N	5.335e-01	5.335e-01
Na	1.240e-04	1.240e-04
Ra	2.668e-01	2.668e-01
S	1.856e-03	1.856e-03

-----Description of solution-----

--

	pH =	7.691	Charge balance
	pe =	12.129	Adjusted to redox
equilibrium	Activity of water =	0.986	
	Ionic strength =	8.102e-01	
	Mass of water (kg) =	1.000e+00	
	Total alkalinity (eq/kg) =	3.374e-03	
	Total CO2 (mol/kg) =	3.427e-03	
	Temperature (deg C) =	25.000	
	Electrical balance (eq) =	-1.908e-06	
	Percent error, 100*(Cat- An)/(Cat+ An) =	-0.00	
	Iterations =	27	
	Total H =	1.110539e+02	
	Total O =	5.714350e+01	

-----Distribution of species-----

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Species	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
OH-	7.271e-07	4.664e-07	-6.138	-6.331	-0.193
H+	2.521e-08	2.038e-08	-7.598	-7.691	-0.092
H2O	5.553e+01	9.863e-01	1.744	-0.006	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-254.940	-254.940	0.000
C(-3)	0.000e+00				
C2H6	0.000e+00	0.000e+00	-225.693	-225.693	0.000
C(-4)	0.000e+00				

	CH4	0.000e+00	0.000e+00	-140.995	-140.995	0.000
C(2)		0.000e+00				
	CO	0.000e+00	0.000e+00	-48.656	-48.656	0.000
C(4)		3.427e-03				
	HCO3-	3.287e-03	2.184e-03	-2.483	-2.661	-0.178
	CO2	8.701e-05	1.047e-04	-4.060	-3.980	0.080
	CO3-2	2.714e-05	4.755e-06	-4.566	-5.323	-0.756
	CaHCO3+	2.020e-05	1.342e-05	-4.695	-4.872	-0.178
	CaCO3	5.716e-06	5.716e-06	-5.243	-5.243	0.000
	NaHCO3	2.564e-07	2.564e-07	-6.591	-6.591	0.000
	NaCO3-	2.055e-09	1.366e-09	-8.687	-8.865	-0.178
	SCN-	0.000e+00	0.000e+00	-199.969	-200.162	-0.193
Ca		3.542e-03				
	Ca+2	2.213e-03	5.186e-04	-2.655	-3.285	-0.630
	CaNO3+	1.282e-03	8.518e-04	-2.892	-3.070	-0.178
	CaSO4	2.153e-05	2.153e-05	-4.667	-4.667	0.000
	CaHCO3+	2.020e-05	1.342e-05	-4.695	-4.872	-0.178
	CaCO3	5.716e-06	5.716e-06	-5.243	-5.243	0.000
	CaCl+	1.265e-08	8.403e-09	-7.898	-8.076	-0.178
	CaOH+	5.337e-09	3.546e-09	-8.273	-8.450	-0.178
	CaCl2	7.556e-13	7.556e-13	-12.122	-12.122	0.000
Cl(-1)		1.242e-04				
	Cl-	1.242e-04	7.645e-05	-3.906	-4.117	-0.211
	CaCl+	1.265e-08	8.403e-09	-7.898	-8.076	-0.178
	NaCl	1.103e-09	1.103e-09	-8.957	-8.957	0.000
	CaCl2	7.556e-13	7.556e-13	-12.122	-12.122	0.000
	HCl	3.499e-13	3.499e-13	-12.456	-12.456	0.000
Cl(1)		5.797e-23				
	ClO-	3.860e-23	2.564e-23	-22.413	-22.591	-0.178
	HClO	1.938e-23	1.938e-23	-22.713	-22.713	0.000
Cl(3)		1.650e-34				
	ClO2-	1.650e-34	1.096e-34	-33.782	-33.960	-0.178
	HClO2	3.303e-39	3.303e-39	-38.481	-38.481	0.000
Cl(5)		5.201e-32				
	ClO3-	5.201e-32	3.336e-32	-31.284	-31.477	-0.193
Cl(7)		7.899e-34				
	ClO4-	7.899e-34	5.066e-34	-33.102	-33.295	-0.193
H(0)		0.000e+00				
	H2	0.000e+00	0.000e+00	-42.821	-42.741	0.080
N(-03)		0.000e+00				
	N3-	0.000e+00	0.000e+00	-79.002	-79.179	-0.178
	HN3	0.000e+00	0.000e+00	-82.168	-82.168	0.000
N(-3)		0.000e+00				
	NH4+	0.000e+00	0.000e+00	-55.015	-55.247	-0.231
	NH3	0.000e+00	0.000e+00	-56.796	-56.796	0.000
	NH4SO4-	0.000e+00	0.000e+00	-66.915	-67.093	-0.178
	SCN-	0.000e+00	0.000e+00	-199.969	-200.162	-0.193
N(-5)		0.000e+00				
	HCN	0.000e+00	0.000e+00	-110.560	-110.560	0.000
	CN-	0.000e+00	0.000e+00	-111.918	-112.128	-0.211
N(0)		1.247e-07				
	N2	6.237e-08	6.237e-08	-7.205	-7.205	0.000
N(3)		7.187e-13				
	NO2-	7.187e-13	4.425e-13	-12.143	-12.354	-0.211
	HNO2	1.539e-17	1.539e-17	-16.813	-16.813	0.000
N(5)		5.335e-01				
	NO3-	5.322e-01	3.277e-01	-0.274	-0.485	-0.211

	CaNO3+	1.282e-03	8.518e-04	-2.892	-3.070	-0.178
	HNO3	3.492e-10	3.492e-10	-9.457	-9.457	0.000
Na		1.240e-04				
	Na+	1.235e-04	8.208e-05	-3.908	-4.086	-0.178
	NaHCO3	2.564e-07	2.564e-07	-6.591	-6.591	0.000
	NaSO4-	2.320e-07	1.541e-07	-6.635	-6.812	-0.178
	NaCO3-	2.055e-09	1.366e-09	-8.687	-8.865	-0.178
	NaCl	1.103e-09	1.103e-09	-8.957	-8.957	0.000
	NaOH	6.604e-12	6.604e-12	-11.180	-11.180	0.000
O(0)		3.119e-07				
	O2	1.559e-07	1.875e-07	-6.807	-6.727	0.080
	S306-2	0.000e+00	0.000e+00	-173.119	-173.929	-0.810
	S2-2	0.000e+00	0.000e+00	-241.422	-242.232	-0.810
	S406-2	0.000e+00	0.000e+00	-260.668	-261.478	-0.810
	S3-2	0.000e+00	0.000e+00	-342.394	-343.204	-0.810
	S506-2	0.000e+00	0.000e+00	-377.097	-377.907	-0.810
	S4-2	0.000e+00	0.000e+00	-443.593	-444.403	-0.810
	S5-2	0.000e+00	0.000e+00	-545.009	-545.819	-0.810
Ra		2.668e-01				
	Ra+2	2.668e-01	5.210e-02	-0.574	-1.283	-0.709
S(-2)		0.000e+00				
	HS-	0.000e+00	0.000e+00	-135.873	-136.066	-0.193
	H2S	0.000e+00	0.000e+00	-136.747	-136.747	0.000
	S-2	0.000e+00	0.000e+00	-140.592	-141.301	-0.709
	SCN-	0.000e+00	0.000e+00	-199.969	-200.162	-0.193
	S2-2	0.000e+00	0.000e+00	-241.422	-242.232	-0.810
	S3-2	0.000e+00	0.000e+00	-342.394	-343.204	-0.810
	S4-2	0.000e+00	0.000e+00	-443.593	-444.403	-0.810
	S5-2	0.000e+00	0.000e+00	-545.009	-545.819	-0.810
S(2)		0.000e+00				
	S203-2	0.000e+00	0.000e+00	-141.679	-142.488	-0.810
	HS203-	0.000e+00	0.000e+00	-148.988	-149.165	-0.178
S(3)		0.000e+00				
	S204-2	0.000e+00	0.000e+00	-132.567	-133.277	-0.709
S(4)		0.000e+00				
	SO3-2	0.000e+00	0.000e+00	-46.044	-46.801	-0.756
	HSO3-	0.000e+00	0.000e+00	-47.082	-47.260	-0.178
	H2SO3	0.000e+00	0.000e+00	-52.969	-52.969	0.000
	SO2	0.000e+00	0.000e+00	-53.064	-53.064	0.000
	S205-2	0.000e+00	0.000e+00	-98.534	-99.344	-0.810
	S306-2	0.000e+00	0.000e+00	-173.119	-173.929	-0.810
	S406-2	0.000e+00	0.000e+00	-260.668	-261.478	-0.810
	S506-2	0.000e+00	0.000e+00	-377.097	-377.907	-0.810
S(5)		0.000e+00				
	S206-2	0.000e+00	0.000e+00	-69.664	-70.474	-0.810
S(6)		1.856e-03				
	SO4-2	1.835e-03	2.842e-04	-2.736	-3.546	-0.810
	CaSO4	2.153e-05	2.153e-05	-4.667	-4.667	0.000
	NaSO4-	2.320e-07	1.541e-07	-6.635	-6.812	-0.178
	HSO4-	8.804e-10	5.850e-10	-9.055	-9.233	-0.178
	H2SO4	1.124e-20	1.124e-20	-19.949	-19.949	0.000
	NH4SO4-	0.000e+00	0.000e+00	-66.915	-67.093	-0.178
S(7)		0.000e+00				
	S208-2	0.000e+00	0.000e+00	-47.477	-48.287	-0.810
S(8)		2.071e-32				
	HSO5-	2.071e-32	1.376e-32	-31.684	-31.861	-0.178

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-2.48	-6.83	-4.35	CaSO ₄
Antarcticite	-15.65	-11.55	4.09	CaCl ₂ :6H ₂ O
Aragonite	-0.23	1.74	1.97	CaCO ₃
Bassanite	-3.13	-6.83	-3.71	CaSO ₄ :0.5H ₂ O
Burkeite	-36.06	-26.58	9.49	Na ₆ CO ₃ (SO ₄) ₂
C	-67.76	-3.62	64.15	C
C(g)	-185.38	-3.62	181.77	C
Ca	-124.38	15.45	139.83	Ca
Ca(g)	-149.62	15.45	165.07	Ca
Ca ₂ Cl ₂ (OH) ₂ :H ₂ O	-25.73	0.56	26.29	Ca ₂ Cl ₂ (OH) ₂ :H ₂ O
Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O	-43.67	24.66	68.33	Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O
Calcite	-0.08	1.74	1.82	CaCO ₃
CaSO ₄ :0.5H ₂ O(beta)	-3.30	-6.83	-3.54	CaSO ₄ :0.5H ₂ O
CH ₄ (g)	-138.15	-141.00	-2.84	CH ₄
Cl ₂ (g)	-29.97	-26.97	2.99	Cl ₂
CO(g)	-45.66	-48.66	-3.00	CO
CO ₂ (g)	-2.52	-10.35	-7.83	CO ₂
Gaylussite	-12.59	-1.43	11.16	CaNa ₂ (CO ₃) ₂ :5H ₂ O
Glauberite	-13.08	-18.55	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-2.31	-6.84	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-39.64	-42.74	-3.10	H ₂
H ₂ O(g)	-1.59	-0.01	1.59	H ₂ O
H ₂ S(g)	-135.76	-143.76	-7.99	H ₂ S
Halite	-9.77	-8.20	1.56	NaCl
HCl(g)	-18.11	-11.81	6.30	HCl
Hydrophilite	-23.26	-11.52	11.75	CaCl ₂
Ice	-0.14	-0.01	0.14	H ₂ O
Lime	-20.48	12.09	32.57	CaO
Mirabilite	-10.62	-11.78	-1.15	Na ₂ SO ₄ :10H ₂ O
Monohydrocalcite	-0.94	1.74	2.68	CaCO ₃ :H ₂ O
N ₂ (g)	-4.03	-7.21	-3.18	N ₂
Na	-62.09	5.28	67.37	Na
Na(g)	-75.58	5.28	80.86	Na
Na ₂ CO ₃	-14.30	-3.14	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-13.12	-3.18	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-60.21	7.20	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-26.15	-27.04	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-24.39	-30.28	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-6.60	-6.75	-0.14	NaHCO ₃
Natron	-12.79	-3.20	9.59	Na ₂ CO ₃ :10H ₂ O
NH ₃ (g)	-58.59	-56.80	1.80	NH ₃
NO(g)	-19.10	-18.36	0.74	NO
NO ₂ (g)	-14.84	-6.49	8.35	NO ₂
O ₂ (g)	-3.83	-6.73	-2.89	O ₂
Pirssonite	-12.73	-1.41	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Portlandite	-10.46	12.08	22.55	Ca(OH) ₂
Ra	-123.91	17.46	141.37	Ra
Ra(NO ₃) ₂	0.00	-2.25	-2.25	Ra(NO ₃) ₂
RaCl ₂ :2H ₂ O	-8.75	-9.53	-0.77	RaCl ₂ :2H ₂ O
RaSO ₄	5.63	-4.83	-10.46	RaSO ₄
S	-102.00	-147.11	-45.11	S
S ₂ (g)	-217.90	-225.09	-7.19	S ₂

SO2(g)	-53.24	-53.06	0.18	SO2
Thenardite	-11.36	-11.72	-0.36	Na2SO4
Thermonatrite	-14.08	-3.15	10.94	Na2CO3:H2O

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 11

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 11 # Equil with RaCl2:2H2O only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1

RaCl2:2H2O 0.0 10.0

END

TITLE

Run 9

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

--

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.113e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.427e-03
 Total CO2 (mol/kg) = 3.427e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -1.908e-06
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.01
 Iterations = 4
 Total H = 1.110539e+02
 Total O = 5.554293e+01

-----Distribution of species-----

--

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				
ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048

Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H(0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S(4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----
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Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----
--

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
RaCl ₂ :2H ₂ O	0.00	-0.77	-0.77	1.000e+01	9.057e+00	-9.435e-01

-----Solution composition-----
--

Elements	Molality	Moles
C	3.315e-03	3.427e-03
Ca	3.426e-03	3.542e-03
Cl	1.825e+00	1.887e+00
Na	1.200e-04	1.240e-04
Ra	9.125e-01	9.435e-01
S	1.795e-03	1.856e-03

-----Description of solution-----
--

equilibrium	pH	=	7.552	Charge balance
	pe	=	-1.778	Adjusted to redox
	Activity of water	=	0.953	
	Ionic strength	=	2.748e+00	
	Mass of water (kg)	=	1.034e+00	
	Total alkalinity (eq/kg)	=	3.263e-03	
	Total CO ₂ (mol/kg)	=	3.315e-03	
	Temperature (deg C)	=	25.000	
	Electrical balance (eq)	=	-1.908e-06	
	Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.00	
	Iterations	=	17	
	Total H	=	1.148278e+02	
	Total O	=	5.742986e+01	

-----Distribution of species-----
--

Species	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
OH-	4.948e-07	3.277e-07	-6.306	-6.484	-0.179
H+	3.009e-08	2.803e-08	-7.522	-7.552	-0.031
H ₂ O	5.553e+01	9.533e-01	1.744	-0.021	0.000
C(-2)	0.000e+00				
C ₂ H ₄	0.000e+00	0.000e+00	-86.012	-86.012	0.000
C(-3)	4.238e-29				
C ₂ H ₆	2.119e-29	2.119e-29	-28.674	-28.674	0.000
C(-4)	3.628e-29				
CH ₄	3.628e-29	3.628e-29	-28.440	-28.440	0.000
C(2)	4.089e-21				
CO	4.089e-21	4.089e-21	-20.388	-20.388	0.000

C(4)	3.315e-03					
HCO3-	3.177e-03	2.229e-03	-2.498	-2.652	-0.154	
CO2	8.346e-05	1.520e-04	-4.079	-3.818	0.260	
CO3-2	2.612e-05	3.528e-06	-4.583	-5.452	-0.869	
CaHCO3+	2.330e-05	1.635e-05	-4.633	-4.786	-0.154	
CaCO3	5.062e-06	5.062e-06	-5.296	-5.296	0.000	
NaHCO3	2.348e-07	2.348e-07	-6.629	-6.629	0.000	
NaCO3-	1.296e-09	9.094e-10	-8.887	-9.041	-0.154	
Ca	3.426e-03					
Ca+2	2.973e-03	6.191e-04	-2.527	-3.208	-0.681	
CaCl+	2.108e-04	1.479e-04	-3.676	-3.830	-0.154	
CaCl2	1.962e-04	1.962e-04	-3.707	-3.707	0.000	
CaHCO3+	2.330e-05	1.635e-05	-4.633	-4.786	-0.154	
CaSO4	1.788e-05	1.788e-05	-4.748	-4.748	0.000	
CaCO3	5.062e-06	5.062e-06	-5.296	-5.296	0.000	
CaOH+	4.240e-09	2.975e-09	-8.373	-8.527	-0.154	
Cl(-1)	1.825e+00					
Cl-	1.824e+00	1.127e+00	0.261	0.052	-0.209	
CaCl+	2.108e-04	1.479e-04	-3.676	-3.830	-0.154	
CaCl2	1.962e-04	1.962e-04	-3.707	-3.707	0.000	
NaCl	1.460e-05	1.460e-05	-4.836	-4.836	0.000	
HCl	7.097e-09	7.097e-09	-8.149	-8.149	0.000	
Cl(1)	0.000e+00					
ClO-	0.000e+00	0.000e+00	-46.374	-46.528	-0.154	
HClO	0.000e+00	0.000e+00	-46.511	-46.511	0.000	
Cl(3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-85.849	-86.003	-0.154	
HClO2	0.000e+00	0.000e+00	-90.385	-90.385	0.000	
Cl(5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-111.446	-111.625	-0.179	
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-141.370	-141.549	-0.179	
H(0)	2.461e-15					
H2	1.230e-15	2.240e-15	-14.910	-14.650	0.260	
Na	1.200e-04					
Na+	1.050e-04	7.366e-05	-3.979	-4.133	-0.154	
NaCl	1.460e-05	1.460e-05	-4.836	-4.836	0.000	
NaHCO3	2.348e-07	2.348e-07	-6.629	-6.629	0.000	
NaSO4-	1.372e-07	9.625e-08	-6.863	-7.017	-0.154	
NaCO3-	1.296e-09	9.094e-10	-8.887	-9.041	-0.154	
NaOH	4.165e-12	4.165e-12	-11.380	-11.380	0.000	
O(0)	0.000e+00					
S2-2	0.000e+00	0.000e+00	-44.562	-45.516	-0.954	
S3O6-2	0.000e+00	0.000e+00	-60.442	-61.395	-0.954	
S3-2	0.000e+00	0.000e+00	-61.084	-62.037	-0.954	
O2	0.000e+00	0.000e+00	-63.198	-62.938	0.260	
S4O6-2	0.000e+00	0.000e+00	-63.540	-64.494	-0.954	
S4-2	0.000e+00	0.000e+00	-77.832	-78.785	-0.954	
S5-2	0.000e+00	0.000e+00	-94.797	-95.750	-0.954	
S5O6-2	0.000e+00	0.000e+00	-95.518	-96.471	-0.954	
Ra	9.125e-01					
Ra+2	9.125e-01	1.454e-01	-0.040	-0.837	-0.798	
S(-2)	3.906e-24					
HS-	3.283e-24	2.174e-24	-23.484	-23.663	-0.179	
H2S	6.229e-25	6.229e-25	-24.206	-24.206	0.000	
S-2	5.773e-29	9.201e-30	-28.239	-29.036	-0.798	
S2-2	0.000e+00	0.000e+00	-44.562	-45.516	-0.954	

	S3-2	0.000e+00	0.000e+00	-61.084	-62.037	-0.954
	S4-2	0.000e+00	0.000e+00	-77.832	-78.785	-0.954
	S5-2	0.000e+00	0.000e+00	-94.797	-95.750	-0.954
S (2)		1.463e-29				
	S2O3-2	7.316e-30	8.141e-31	-29.136	-30.089	-0.954
	HS2O3-	3.357e-37	2.356e-37	-36.474	-36.628	-0.154
S (3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-48.185	-48.983	-0.798
S (4)		1.135e-18				
	SO3-2	1.039e-18	1.404e-19	-17.983	-18.853	-0.869
	HSO3-	9.559e-20	6.707e-20	-19.020	-19.173	-0.154
	H2SO3	1.802e-25	1.802e-25	-24.744	-24.744	0.000
	SO2	1.500e-25	1.500e-25	-24.824	-24.824	0.000
	S2O5-2	0.000e+00	0.000e+00	-42.203	-43.156	-0.954
	S3O6-2	0.000e+00	0.000e+00	-60.442	-61.395	-0.954
	S4O6-2	0.000e+00	0.000e+00	-63.540	-64.494	-0.954
	S5O6-2	0.000e+00	0.000e+00	-95.518	-96.471	-0.954
S (5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.438	-42.391	-0.954
S (6)		1.795e-03				
	SO4-2	1.777e-03	1.978e-04	-2.750	-3.704	-0.954
	CaSO4	1.788e-05	1.788e-05	-4.748	-4.748	0.000
	NaSO4-	1.372e-07	9.625e-08	-6.863	-7.017	-0.154
	HSO4-	7.979e-10	5.599e-10	-9.098	-9.252	-0.154
	H2SO4	1.480e-20	1.480e-20	-19.830	-19.830	0.000
S (7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-75.462	-76.416	-0.954
S (8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-59.832	-59.986	-0.154

-----Saturation indices-----

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Phase	SI	log IAP	log KT	
Anhydrite	-2.56	-6.91	-4.35	CaSO4
Antarcticite	-7.32	-3.23	4.09	CaCl2:6H2O
Aragonite	-0.28	1.69	1.97	CaCO3
Bassanite	-3.22	-6.92	-3.71	CaSO4:0.5H2O
Burkeite	-36.79	-27.30	9.49	Na6CO3(SO4)2
C	-11.39	52.75	64.15	C
C(g)	-129.01	52.75	181.77	C
Ca	-96.49	43.34	139.83	Ca
Ca(g)	-121.73	43.34	165.07	Ca
Ca2Cl2(OH)2:H2O	-17.56	8.73	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-36.14	32.19	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-0.13	1.69	1.82	CaCO3
CaSO4:0.5H2O(beta)	-3.39	-6.92	-3.54	CaSO4:0.5H2O
CH4(g)	-25.60	-28.44	-2.84	CH4
Cl2(g)	-49.44	-46.45	2.99	Cl2
CO(g)	-17.39	-20.39	-3.00	CO
CO2(g)	-2.35	-10.18	-7.83	CO2
Gaylussite	-12.94	-1.78	11.16	CaNa2(CO3)2:5H2O
Glauberite	-13.41	-18.88	-5.47	Na2Ca(SO4)2
Gypsum	-2.42	-6.95	-4.53	CaSO4:2H2O
H2(g)	-11.55	-14.65	-3.10	H2
H2O(g)	-1.61	-0.02	1.59	H2O

H2S(g)	-23.22	-31.22	-7.99	H2S
Halite	-5.64	-4.08	1.56	NaCl
HCl(g)	-13.80	-7.50	6.30	HCl
Hydrophilite	-14.85	-3.10	11.75	CaCl2
Ice	-0.16	-0.02	0.14	H2O
Lime	-20.69	11.88	32.57	CaO
Mirabilite	-11.02	-12.18	-1.15	Na2SO4:10H2O
Monohydrocalcite	-1.01	1.67	2.68	CaCO3:H2O
Na	-48.23	19.14	67.37	Na
Na(g)	-61.72	19.14	80.86	Na
Na2CO3	-14.53	-3.36	11.16	Na2CO3
Na2CO3:7H2O	-13.45	-3.51	9.94	Na2CO3:7H2O
Na2O	-60.60	6.82	67.42	Na2O
Na3H(SO4)2	-26.47	-27.36	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-25.00	-30.89	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.64	-6.78	-0.14	NaHCO3
Natron	-13.16	-3.57	9.59	Na2CO3:10H2O
O2(g)	-60.05	-62.94	-2.89	O2
Pirssonite	-13.04	-1.71	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-10.69	11.86	22.55	Ca(OH)2
Ra	-95.65	45.72	141.37	Ra
RaCl2:2H2O	0.00	-0.77	-0.77	RaCl2:2H2O
RaSO4	5.92	-4.54	-10.46	RaSO4
S	-17.55	-62.66	-45.11	S
S2(g)	-49.00	-56.19	-7.19	S2
SO2(g)	-25.00	-24.82	0.18	SO2
Thenardite	-11.61	-11.97	-0.36	Na2SO4
Thermonatrite	-14.32	-3.39	10.94	Na2CO3:H2O

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 12

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 12 # Equil with Th(NO3)4:5H2O only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 #=-100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1

Th(NO3)4:5H2O 0.0 10.0

END

TITLE

Run 12

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

--

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.113e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.427e-03
 Total CO2 (mol/kg) = 3.427e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -1.908e-06
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.01
 Iterations = 4
 Total H = 1.110539e+02
 Total O = 5.554293e+01

-----Distribution of species-----

--

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				
ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048

Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H(0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S(4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----
 --

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

Numerical method failed with this set of convergence parameters.
 WARNING: Trying smaller step size, pe step size 10, 5 ...

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----
 --

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
Th(NO3)4·5H2O	0.00	416.39	416.39	1.000e+01	8.463e+00	-1.537e+00

-----Solution composition-----
 --

Elements	Molality	Moles
C	3.024e-03	3.427e-03
Ca	3.126e-03	3.542e-03
Cl	1.096e-04	1.242e-04
N	5.423e+00	6.146e+00
Na	1.094e-04	1.240e-04
S	1.638e-03	1.856e-03
Th	1.356e+00	1.537e+00

-----Description of solution-----
 --

equilibrium	pH	=	0.506	Charge balance
	pe	=	20.648	Adjusted to redox
	Activity of water	=	0.885	
	Ionic strength	=	1.379e+01	
	Mass of water (kg)	=	1.133e+00	
	Total alkalinity (eq/kg)	=	4.388e-03	
	Total CO2 (mol/kg)	=	3.024e-03	
	Temperature (deg C)	=	25.000	
	Electrical balance (eq)	=	-1.908e-06	
	Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.00	
	Iterations	=	64	
	Total H	=	1.264198e+02	
	Total O	=	8.166489e+01	

-----Distribution of species-----
 --

Species	Molality	Activity	Log	Log	Log Gamma
			Molality	Activity	
H+	1.222e-01	3.121e-01	-0.913	-0.506	0.407
OH-	1.702e-14	2.731e-14	-13.769	-13.564	0.205
H2O	5.553e+01	8.847e-01	1.744	-0.053	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-265.298	-265.298	0.000

C(-3)		0.000e+00				
	C2H6	0.000e+00	0.000e+00	-238.718	-238.718	0.000
C(-4)		0.000e+00				
	CH4	0.000e+00	0.000e+00	-148.841	-148.841	0.000
C(2)		0.000e+00				
	CO	0.000e+00	0.000e+00	-48.549	-48.549	0.000
C(4)		3.024e-03				
	CO2	3.024e-03	5.572e-02	-2.519	-1.254	1.265
	HCO3-	3.894e-08	6.810e-08	-7.410	-7.167	0.243
	CaHCO3+	5.993e-11	1.048e-10	-10.222	-9.980	0.243
	NaHCO3	1.865e-11	1.865e-11	-10.729	-10.729	0.000
	CO3-2	3.891e-17	9.681e-18	-16.410	-17.014	-0.604
	CaCO3	2.914e-18	2.914e-18	-17.535	-17.535	0.000
	NaCO3-	3.707e-21	6.484e-21	-20.431	-20.188	0.243
	SCN-	0.000e+00	0.000e+00	-206.508	-206.303	0.205
Ca		3.126e-03				
	CaNO3+	2.837e-03	4.962e-03	-2.547	-2.304	0.243
	Ca+2	2.886e-04	1.299e-04	-3.540	-3.886	-0.347
	CaSO4	1.087e-09	1.087e-09	-8.964	-8.964	0.000
	CaCl+	8.125e-11	1.421e-10	-10.090	-9.847	0.243
	CaHCO3+	5.993e-11	1.048e-10	-10.222	-9.980	0.243
	CaCl2	8.628e-16	8.628e-16	-15.064	-15.064	0.000
	CaOH+	2.974e-17	5.201e-17	-16.527	-16.284	0.243
	CaCO3	2.914e-18	2.914e-18	-17.535	-17.535	0.000
Cl(-1)		1.096e-04				
	ThCl+3	1.056e-04	1.526e-06	-3.976	-5.816	-1.840
	Cl-	3.585e-06	5.162e-06	-5.445	-5.287	0.158
	HCl	3.618e-07	3.618e-07	-6.442	-6.442	0.000
	NaCl	1.737e-10	1.737e-10	-9.760	-9.760	0.000
	CaCl+	8.125e-11	1.421e-10	-10.090	-9.847	0.243
	ThCl2+2	1.615e-11	4.018e-12	-10.792	-11.396	-0.604
	CaCl2	8.628e-16	8.628e-16	-15.064	-15.064	0.000
	ThCl3+	7.865e-17	1.376e-16	-16.104	-15.861	0.243
	ThCl4	2.672e-22	2.672e-22	-21.573	-21.573	0.000
Cl(1)		8.342e-15				
	HClO	8.342e-15	8.342e-15	-14.079	-14.079	0.000
	ClO-	4.121e-22	7.208e-22	-21.385	-21.142	0.243
Cl(3)		5.927e-28				
	HClO2	5.920e-28	5.920e-28	-27.228	-27.228	0.000
	ClO2-	7.336e-31	1.283e-30	-30.135	-29.892	0.243
Cl(5)		1.013e-25				
	ClO3-	1.013e-25	1.625e-25	-24.995	-24.789	0.205
Cl(7)		6.402e-25				
	ClO4-	6.402e-25	1.027e-24	-24.194	-23.988	0.205
H(0)		0.000e+00				
	H2	0.000e+00	0.000e+00	-46.673	-45.407	1.265
N(-03)		0.000e+00				
	HN3	0.000e+00	0.000e+00	-77.421	-77.421	0.000
	N3-	0.000e+00	0.000e+00	-81.860	-81.617	0.243
N(-3)		0.000e+00				
	NH4+	0.000e+00	0.000e+00	-50.131	-50.035	0.097
	NH3	0.000e+00	0.000e+00	-58.769	-58.769	0.000
	NH4SO4-	0.000e+00	0.000e+00	-65.819	-65.576	0.243
	SCN-	0.000e+00	0.000e+00	-206.508	-206.303	0.205
N(-5)		0.000e+00				
	HCN	0.000e+00	0.000e+00	-112.380	-112.380	0.000
	CN-	0.000e+00	0.000e+00	-121.291	-121.132	0.158

N(0)		1.411e-03				
	N2	7.057e-04	7.057e-04	-3.151	-3.151	0.000
N(3)		1.319e-11				
	HNO2	1.317e-11	1.317e-11	-10.880	-10.880	0.000
	NO2-	1.717e-14	2.473e-14	-13.765	-13.607	0.158
N(5)		5.422e+00				
	NO3-	5.295e+00	7.623e+00	0.724	0.882	0.158
	HNO3	1.244e-01	1.244e-01	-0.905	-0.905	0.000
	CaNO3+	2.837e-03	4.962e-03	-2.547	-2.304	0.243
Na		1.094e-04				
	Na+	1.094e-04	1.914e-04	-3.961	-3.718	0.243
	NaCl	1.737e-10	1.737e-10	-9.760	-9.760	0.000
	NaSO4-	4.143e-11	7.246e-11	-10.383	-10.140	0.243
	NaHCO3	1.865e-11	1.865e-11	-10.729	-10.729	0.000
	NaOH	9.021e-19	9.021e-19	-18.045	-18.045	0.000
	NaCO3-	3.707e-21	6.484e-21	-20.431	-20.188	0.243
O(0)		3.528e-03				
	O2	1.764e-03	3.250e-02	-2.753	-1.488	1.265
	S306-2	0.000e+00	0.000e+00	-165.932	-166.658	-0.725
	S406-2	0.000e+00	0.000e+00	-250.618	-251.344	-0.725
	S2-2	0.000e+00	0.000e+00	-252.816	-253.542	-0.725
	S3-2	0.000e+00	0.000e+00	-350.924	-351.650	-0.725
	S506-2	0.000e+00	0.000e+00	-364.183	-364.909	-0.725
	S4-2	0.000e+00	0.000e+00	-449.260	-449.985	-0.725
	S5-2	0.000e+00	0.000e+00	-547.812	-548.538	-0.725
S(-2)		0.000e+00				
	H2S	0.000e+00	0.000e+00	-136.550	-136.550	0.000
	HS-	0.000e+00	0.000e+00	-143.260	-143.054	0.205
	S-2	0.000e+00	0.000e+00	-154.971	-155.474	-0.504
	SCN-	0.000e+00	0.000e+00	-206.508	-206.303	0.205
	S2-2	0.000e+00	0.000e+00	-252.816	-253.542	-0.725
	S3-2	0.000e+00	0.000e+00	-350.924	-351.650	-0.725
	S4-2	0.000e+00	0.000e+00	-449.260	-449.985	-0.725
	S5-2	0.000e+00	0.000e+00	-547.812	-548.538	-0.725
S(2)		0.000e+00				
	S203-2	0.000e+00	0.000e+00	-145.214	-145.940	-0.725
	HS203-	0.000e+00	0.000e+00	-145.674	-145.432	0.243
S(3)		0.000e+00				
	S204-2	0.000e+00	0.000e+00	-133.605	-134.108	-0.504
S(4)		0.000e+00				
	H2SO3	0.000e+00	0.000e+00	-44.914	-44.914	0.000
	SO2	0.000e+00	0.000e+00	-44.961	-44.961	0.000
	HSO3-	0.000e+00	0.000e+00	-46.633	-46.390	0.243
	SO3-2	0.000e+00	0.000e+00	-52.512	-53.116	-0.604
	S205-2	0.000e+00	0.000e+00	-96.831	-97.557	-0.725
	S306-2	0.000e+00	0.000e+00	-165.932	-166.658	-0.725
	S406-2	0.000e+00	0.000e+00	-250.618	-251.344	-0.725
	S506-2	0.000e+00	0.000e+00	-364.183	-364.909	-0.725
S(5)		0.000e+00				
	S206-2	0.000e+00	0.000e+00	-65.341	-66.067	-0.725
S(6)		1.638e-03				
	ThSO4+2	1.636e-03	4.070e-04	-2.786	-3.390	-0.604
	HSO4-	1.033e-06	1.806e-06	-5.986	-5.743	0.243
	Th(SO4)2	4.631e-07	4.631e-07	-6.334	-6.334	0.000
	SO4-2	3.045e-07	5.729e-08	-6.516	-7.242	-0.725
	CaSO4	1.087e-09	1.087e-09	-8.964	-8.964	0.000
	H2SO4	5.318e-10	5.318e-10	-9.274	-9.274	0.000

	NaSO4-	4.143e-11	7.246e-11	-10.383	-10.140	0.243
	Th(SO4)3-2	8.013e-13	1.508e-13	-12.096	-12.822	-0.725
	Th(SO4)4-4	3.419e-18	8.616e-23	-17.466	-22.065	-4.599
	NH4SO4-	0.000e+00	0.000e+00	-65.819	-65.576	0.243
S (7)		2.429e-38				
	S2O8-2	1.214e-38	2.285e-39	-37.916	-38.641	-0.725
S (8)		1.011e-26				
	HSO5-	1.011e-26	1.769e-26	-25.995	-25.752	0.243
Th		1.356e+00				
	Th+4	1.103e+00	3.181e-02	0.043	-1.497	-1.540
	Th2(OH)2+6	1.251e-01	2.828e-09	-0.903	-8.549	-7.646
	ThSO4+2	1.636e-03	4.070e-04	-2.786	-3.390	-0.604
	ThOH+3	8.052e-04	1.164e-05	-3.094	-4.934	-1.840
	ThCl+3	1.056e-04	1.526e-06	-3.976	-5.816	-1.840
	Th(SO4)2	4.631e-07	4.631e-07	-6.334	-6.334	0.000
	Th(OH)2+2	7.978e-08	1.985e-08	-7.098	-7.702	-0.604
	Th4(OH)8+8	8.140e-11	7.553e-25	-10.089	-24.122	-14.033
	ThCl2+2	1.615e-11	4.018e-12	-10.792	-11.396	-0.604
	Th(SO4)3-2	8.013e-13	1.508e-13	-12.096	-12.822	-0.725
	Th(OH)3+	5.690e-13	9.952e-13	-12.245	-12.002	0.243
	Th(OH)4	1.988e-16	1.988e-16	-15.702	-15.702	0.000
	ThCl3+	7.865e-17	1.376e-16	-16.104	-15.861	0.243
	Th(SO4)4-4	3.419e-18	8.616e-23	-17.466	-22.065	-4.599
	ThCl4	2.672e-22	2.672e-22	-21.573	-21.573	0.000
	Th6(OH)15+9	1.077e-22	1.325e-40	-21.968	-39.878	-17.910

-----Saturation indices-----
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Phase	SI	log IAP	log KT	
Anhydrite	-6.78	-11.13	-4.35	CaSO4
Antarcticite	-18.87	-14.78	4.09	CaCl2·6H2O
Aragonite	-12.52	-10.55	1.97	CaCO3
Bassanite	-7.45	-11.15	-3.71	CaSO4·0.5H2O
Burkeite	-52.94	-43.45	9.49	Na6CO3(SO4)2
C	-70.28	-6.13	64.15	C
C(g)	-187.90	-6.13	181.77	C
Ca	-142.02	-2.18	139.83	Ca
Ca(g)	-167.26	-2.18	165.07	Ca
Ca2Cl2(OH)2·H2O	-43.79	-17.50	26.29	Ca2Cl2(OH)2·H2O
Ca4Cl2(OH)6·13H2O	-92.42	-24.10	68.33	Ca4Cl2(OH)6·13H2O
Calcite	-12.37	-10.55	1.82	CaCO3
CaSO4·0.5H2O(beta)	-7.62	-11.15	-3.54	CaSO4·0.5H2O
CH4(g)	-146.00	-148.84	-2.84	CH4
Cl2(g)	-15.27	-12.28	2.99	Cl2
CO(g)	-45.55	-48.55	-3.00	CO
CO2(g)	0.21	-7.62	-7.83	CO2
Gaylussite	-36.07	-24.91	11.16	CaNa2(CO3)2·5H2O
Glauberite	-20.34	-25.81	-5.47	Na2Ca(SO4)2
Gypsum	-6.70	-11.23	-4.53	CaSO4·2H2O
H2(g)	-42.31	-45.41	-3.10	H2
H2O(g)	-1.64	-0.05	1.59	H2O
H2S(g)	-135.57	-143.56	-7.99	H2S
Halite	-10.57	-9.01	1.56	NaCl
HCl(g)	-12.09	-5.79	6.30	HCl
Hydrophilite	-26.21	-14.46	11.75	CaCl2

Ice	-0.19	-0.05	0.14	H2O
Lime	-35.50	-2.93	32.57	CaO
Mirabilite	-14.06	-15.21	-1.15	Na2SO4:10H2O
Monohydrocalcite	-13.28	-10.60	2.68	CaCO3:H2O
N2(g)	0.03	-3.15	-3.18	N2
Na	-70.24	-2.87	67.37	Na
Na(g)	-83.73	-2.87	80.86	Na
Na2CO3	-25.26	-14.10	11.16	Na2CO3
Na2CO3:7H2O	-24.41	-14.47	9.94	Na2CO3:7H2O
Na2O	-73.90	-6.48	67.42	Na2O
Na3H(SO4)2	-25.25	-26.14	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-34.70	-40.59	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-10.74	-10.88	-0.14	NaHCO3
Natron	-24.22	-14.63	9.59	Na2CO3:10H2O
NH3(g)	-60.56	-58.77	1.80	NH3
NO(g)	-14.45	-13.71	0.74	NO
NO2(g)	-7.57	0.77	8.35	NO2
O2(g)	1.40	-1.49	-2.89	O2
Pirssonite	-36.07	-24.75	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-25.53	-2.98	22.55	Ca(OH)2
S	-99.14	-144.25	-45.11	S
S2(g)	-212.17	-219.36	-7.19	S2
SO2(g)	-45.14	-44.96	0.18	SO2
Th	-207.68	1.91	209.59	Th
Th(g)	-305.94	1.91	307.84	Th
Th(NO3)4:5H2O	0.00	1.77	1.77	Th(NO3)4:5H2O
Th(OH)4	-9.35	0.31	9.66	Th(OH)4
Th(SO4)2	4.34	-15.98	-20.32	Th(SO4)2
Th2S3	-524.11	-428.94	95.17	Th2S3
Th7S12	-1921.71	-1717.66	204.06	Th7S12
ThCl4	-46.48	-22.65	23.84	ThCl4
Thenardite	-14.32	-14.68	-0.36	Na2SO4
Thermonatrite	-25.09	-14.15	10.94	Na2CO3:H2O
Thorianite	-1.44	0.42	1.86	ThO2
ThS	-238.38	-142.34	96.04	ThS
ThS2	-297.38	-286.59	10.78	ThS2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 13

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 13 # Equil with Th(OH)4 only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM PHASES 1
Th(OH)4 0.0 10.0
END

TITLE

Run 13

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.113e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.427e-03
 Total CO2 (mol/kg) = 3.427e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -1.908e-06
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.01
 Iterations = 4
 Total H = 1.110539e+02
 Total O = 5.554293e+01

-----Distribution of species-----

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
	H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
	H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)		3.427e-03				
	HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
	CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca		3.542e-03				
	Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)		1.242e-04				
	Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
	HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)		0.000e+00				
	ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
	HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)		0.000e+00				
	ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
	HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)		0.000e+00				
	ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048

Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H(0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S(4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----
 --

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1..

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----
--

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
Th(OH)4	0.00	9.66	9.66	1.000e+01	1.000e+01	-4.473e-07

-----Solution composition-----
--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
Th	4.473e-07	4.473e-07

-----Description of solution-----
--

	pH =	7.800	Charge balance
	pe =	9.978	Adjusted to redox
equilibrium	Activity of water =	1.000	
	Ionic strength =	1.113e-02	
	Mass of water (kg) =	1.000e+00	
	Total alkalinity (eq/kg) =	3.376e-03	
	Total CO2 (mol/kg) =	3.427e-03	
	Temperature (deg C) =	25.000	
	Electrical balance (eq) =	-1.908e-06	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.01	
	Iterations =	18	
	Total H =	1.110539e+02	
	Total O =	5.554293e+01	

-----Distribution of species-----
--

Species	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-230.450	-230.450	0.000
C(-3)	0.000e+00				
C2H6	0.000e+00	0.000e+00	-197.118	-197.118	0.000
C(-4)	0.000e+00				
CH4	0.000e+00	0.000e+00	-124.666	-124.666	0.000
C(2)	0.000e+00				
CO	0.000e+00	0.000e+00	-44.574	-44.574	0.000

C(4)	3.427e-03					
	HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
	CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03					
	Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04					
	Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
	HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
	ThCl+3	7.801e-25	3.012e-25	-24.108	-24.521	-0.413
	ThCl2+2	2.618e-29	1.705e-29	-28.582	-28.768	-0.186
	ThCl3+	1.399e-32	1.256e-32	-31.854	-31.901	-0.047
	ThCl4	5.247e-37	5.247e-37	-36.280	-36.280	0.000
Cl(1)	5.288e-27					
	ClO-	3.461e-27	3.107e-27	-26.461	-26.508	-0.047
	HClO	1.826e-27	1.826e-27	-26.738	-26.738	0.000
Cl(3)	0.000e+00					
	ClO2-	0.000e+00	0.000e+00	-41.908	-41.955	-0.047
	HClO2	0.000e+00	0.000e+00	-46.586	-46.586	0.000
Cl(5)	0.000e+00					
	ClO3-	0.000e+00	0.000e+00	-43.503	-43.551	-0.048
Cl(7)	0.000e+00					
	ClO4-	0.000e+00	0.000e+00	-49.400	-49.448	-0.048
H(0)	4.405e-39					
	H2	2.203e-39	2.208e-39	-38.657	-38.656	0.001
Na	1.240e-04					
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)	2.604e-15					
	O2	1.302e-15	1.305e-15	-14.885	-14.884	0.001
	S3O6-2	0.000e+00	0.000e+00	-156.229	-156.418	-0.189
	S2-2	0.000e+00	0.000e+00	-212.620	-212.809	-0.189
	S4O6-2	0.000e+00	0.000e+00	-231.218	-231.407	-0.189
	S3-2	0.000e+00	0.000e+00	-301.032	-301.221	-0.189
	S5O6-2	0.000e+00	0.000e+00	-335.087	-335.276	-0.189
	S4-2	0.000e+00	0.000e+00	-389.671	-389.860	-0.189
	S5-2	0.000e+00	0.000e+00	-478.527	-478.716	-0.189
S(-2)	0.000e+00					
	HS-	0.000e+00	0.000e+00	-119.265	-119.312	-0.048
	H2S	0.000e+00	0.000e+00	-120.103	-120.103	0.000

	S-2	0.000e+00	0.000e+00	-124.255	-124.438	-0.183
	S2-2	0.000e+00	0.000e+00	-212.620	-212.809	-0.189
	S3-2	0.000e+00	0.000e+00	-301.032	-301.221	-0.189
	S4-2	0.000e+00	0.000e+00	-389.671	-389.860	-0.189
	S5-2	0.000e+00	0.000e+00	-478.527	-478.716	-0.189
S(2)		0.000e+00				
	S2O3-2	0.000e+00	0.000e+00	-125.112	-125.302	-0.189
	HS2O3-	0.000e+00	0.000e+00	-132.041	-132.088	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-119.985	-120.168	-0.183
S(4)		0.000e+00				
	SO3-2	0.000e+00	0.000e+00	-41.988	-42.174	-0.186
	HSO3-	0.000e+00	0.000e+00	-42.695	-42.742	-0.047
	H2SO3	0.000e+00	0.000e+00	-48.561	-48.561	0.000
	SO2	0.000e+00	0.000e+00	-48.661	-48.661	0.000
	S2O5-2	0.000e+00	0.000e+00	-90.126	-90.315	-0.189
	S3O6-2	0.000e+00	0.000e+00	-156.229	-156.418	-0.189
	S4O6-2	0.000e+00	0.000e+00	-231.218	-231.407	-0.189
	S5O6-2	0.000e+00	0.000e+00	-335.087	-335.276	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-65.334	-65.523	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	Th(SO4)2	1.305e-18	1.305e-18	-17.885	-17.885	0.000
	ThSO4+2	1.005e-19	6.543e-20	-18.998	-19.184	-0.186
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
	Th(SO4)3-2	1.150e-20	7.444e-21	-19.939	-20.128	-0.189
	Th(SO4)4-4	4.267e-25	7.456e-26	-24.370	-25.128	-0.758
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-51.305	-51.494	-0.189
S(8)		3.515e-36				
	HSO5-	3.515e-36	3.155e-36	-35.454	-35.501	-0.047
Th		4.473e-07				
	Th(OH)4	4.472e-07	4.472e-07	-6.350	-6.350	0.000
	Th(OH)3+	1.121e-10	1.006e-10	-9.950	-9.997	-0.047
	Th(OH)2+2	1.384e-13	9.017e-14	-12.859	-13.045	-0.186
	ThOH+3	6.153e-18	2.375e-18	-17.211	-17.624	-0.413
	Th(SO4)2	1.305e-18	1.305e-18	-17.885	-17.885	0.000
	ThSO4+2	1.005e-19	6.543e-20	-18.998	-19.184	-0.186
	Th(SO4)3-2	1.150e-20	7.444e-21	-19.939	-20.128	-0.189
	Th+4	1.229e-21	2.918e-22	-20.911	-21.535	-0.624
	ThCl+3	7.801e-25	3.012e-25	-24.108	-24.521	-0.413
	Th(SO4)4-4	4.267e-25	7.456e-26	-24.370	-25.128	-0.758
	ThCl2+2	2.618e-29	1.705e-29	-28.582	-28.768	-0.186
	ThCl3+	1.399e-32	1.256e-32	-31.854	-31.901	-0.047
	Th2(OH)2+6	4.770e-33	1.178e-34	-32.321	-33.929	-1.607
	ThCl4	5.247e-37	5.247e-37	-36.280	-36.280	0.000
	Th4(OH)8+8	0.000e+00	0.000e+00	-42.635	-45.493	-2.858
	Th6(OH)15+9	0.000e+00	0.000e+00	-46.275	-49.892	-3.617

-----Saturation indices-----
 --

Phase

SI log IAP log KT

Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2·6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4·0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-59.60	4.54	64.15	C
C(g)	-177.22	4.54	181.77	C
Ca	-119.47	20.36	139.83	Ca
Ca(g)	-144.71	20.36	165.07	Ca
Ca2Cl2(OH)2·H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2·H2O
Ca4Cl2(OH)6·13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6·13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4·0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4·0.5H2O
CH4(g)	-121.82	-124.67	-2.84	CH4
Cl2(g)	-33.95	-30.95	2.99	Cl2
CO(g)	-41.58	-44.57	-3.00	CO
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2·5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4·2H2O
H2(g)	-35.55	-38.66	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-119.12	-127.11	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4·10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3·H2O
Na	-59.81	7.56	67.37	Na
Na(g)	-73.30	7.56	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3·7H2O	-12.60	-2.66	9.94	Na2CO3·7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3·2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3·2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3·10H2O
O2(g)	-11.99	-14.88	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2·2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-89.44	-134.55	-45.11	S
S2(g)	-192.78	-199.97	-7.19	S2
SO2(g)	-48.84	-48.66	0.18	SO2
Th	-185.04	24.55	209.59	Th
Th(g)	-283.29	24.55	307.84	Th
Th(OH)4	-0.00	9.66	9.66	Th(OH)4
Th(SO4)2	-7.21	-27.53	-20.32	Th(SO4)2
Th2S3	-449.74	-354.56	95.17	Th2S3
Th7S12	-1646.86	-1442.81	204.06	Th7S12
ThCl4	-61.19	-37.35	23.84	ThCl4
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3·H2O
Thorianite	7.80	9.66	1.86	ThO2
ThS	-206.04	-110.01	96.04	ThS

ThS2 -255.34 -244.56 10.78 ThS2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 14

Reading data base.

LLNL AQUEOUS MODEL PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 14 # Equil with Th(SO4)2 only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.
pH 7.8
temp 25.0
pe -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2
EQUILIBRIUM_PHASES 1
Th(SO4)2 0.0 10.0
END

TITLE

Run 14

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.113e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.427e-03
 Total CO2 (mol/kg) = 3.427e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -1.908e-06
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.01
 Iterations = 4
 Total H = 1.110539e+02
 Total O = 5.554293e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				
ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048

Cl (7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H (0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O (0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S (-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S (2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S (3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S (4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S (5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S (6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S (7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S (8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----
--

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
Th(SO4)2	0.00	-20.32	-20.32	1.000e+01	1.000e+01	-2.250e-04

-----Solution composition-----
--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	2.307e-03	2.307e-03
Th	2.250e-04	2.250e-04

-----Description of solution-----
--

	pH =	6.718	Charge balance
	pe =	-0.765	Adjusted to redox
equilibrium	Activity of water	=	1.000
	Ionic strength	=	1.144e-02
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	3.374e-03
	Total CO2 (mol/kg)	=	3.427e-03
	Temperature (deg C)	=	25.000
	Electrical balance (eq)	=	-1.908e-06
Percent error, 100*(Cat- An)/(Cat+ An)		=	-0.01
	Iterations	=	15
	Total H	=	1.110539e+02
	Total O	=	5.554473e+01

-----Distribution of species-----
--

Species	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
H+	2.103e-07	1.913e-07	-6.677	-6.718	-0.041
OH-	5.626e-08	5.035e-08	-7.250	-7.298	-0.048
H2O	5.553e+01	9.998e-01	1.744	-0.000	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-86.635	-86.635	0.000
C(-3)	4.443e-30				
C2H6	2.222e-30	2.222e-30	-29.653	-29.653	0.000
C(-4)	7.790e-30				
CH4	7.790e-30	7.790e-30	-29.108	-29.108	0.000
C(2)	1.082e-20				
CO	1.082e-20	1.082e-20	-19.966	-19.966	0.000

C(4)	3.427e-03					
HCO3-	2.409e-03	2.160e-03	-2.618	-2.666	-0.047	
CO2	9.560e-04	9.587e-04	-3.020	-3.018	0.001	
CaHCO3+	5.861e-05	5.254e-05	-4.232	-4.280	-0.047	
CaCO3	2.382e-06	2.382e-06	-5.623	-5.623	0.000	
CO3-2	7.728e-07	5.008e-07	-6.112	-6.300	-0.188	
NaHCO3	3.397e-07	3.397e-07	-6.469	-6.469	0.000	
NaCO3-	2.150e-10	1.927e-10	-9.668	-9.715	-0.047	
Ca	3.542e-03					
Ca+2	3.108e-03	2.053e-03	-2.507	-2.688	-0.180	
CaSO4	3.730e-04	3.730e-04	-3.428	-3.428	0.000	
CaHCO3+	5.861e-05	5.254e-05	-4.232	-4.280	-0.047	
CaCO3	2.382e-06	2.382e-06	-5.623	-5.623	0.000	
CaCl+	5.381e-08	4.824e-08	-7.269	-7.317	-0.047	
CaOH+	1.690e-09	1.515e-09	-8.772	-8.820	-0.047	
CaCl2	6.291e-12	6.291e-12	-11.201	-11.201	0.000	
Cl(-1)	1.242e-04					
Cl-	1.241e-04	1.109e-04	-3.906	-3.955	-0.049	
CaCl+	5.381e-08	4.824e-08	-7.269	-7.317	-0.047	
NaCl	2.143e-09	2.143e-09	-8.669	-8.669	0.000	
CaCl2	6.291e-12	6.291e-12	-11.201	-11.201	0.000	
HCl	4.765e-12	4.765e-12	-11.322	-11.322	0.000	
ThCl+3	8.396e-18	3.205e-18	-17.076	-17.494	-0.418	
ThCl2+2	2.797e-22	1.812e-22	-21.553	-21.742	-0.188	
ThCl3+	1.487e-25	1.333e-25	-24.828	-24.875	-0.047	
ThCl4	5.561e-30	5.561e-30	-29.255	-29.255	0.000	
Cl(1)	0.000e+00					
HClO	0.000e+00	0.000e+00	-49.307	-49.307	0.000	
ClO-	0.000e+00	0.000e+00	-50.110	-50.158	-0.047	
Cl(3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-89.208	-89.255	-0.047	
HClO2	0.000e+00	0.000e+00	-92.804	-92.804	0.000	
Cl(5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-114.452	-114.500	-0.048	
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-143.999	-144.047	-0.048	
H(0)	1.966e-15					
H2	9.828e-16	9.855e-16	-15.008	-15.006	0.001	
Na	1.240e-04					
Na+	1.227e-04	1.100e-04	-3.911	-3.959	-0.047	
NaSO4-	1.008e-06	9.038e-07	-5.996	-6.044	-0.047	
NaHCO3	3.397e-07	3.397e-07	-6.469	-6.469	0.000	
NaCl	2.143e-09	2.143e-09	-8.669	-8.669	0.000	
NaCO3-	2.150e-10	1.927e-10	-9.668	-9.715	-0.047	
NaOH	9.553e-13	9.553e-13	-12.020	-12.020	0.000	
O(0)	0.000e+00					
S2-2	0.000e+00	0.000e+00	-44.721	-44.912	-0.191	
S3O6-2	0.000e+00	0.000e+00	-57.022	-57.213	-0.191	
S4O6-2	0.000e+00	0.000e+00	-58.806	-58.997	-0.191	
S3-2	0.000e+00	0.000e+00	-59.928	-60.119	-0.191	
O2	0.000e+00	0.000e+00	-62.185	-62.183	0.001	
S4-2	0.000e+00	0.000e+00	-75.362	-75.553	-0.191	
S5O6-2	0.000e+00	0.000e+00	-89.469	-89.660	-0.191	
S5-2	0.000e+00	0.000e+00	-91.012	-91.203	-0.191	
S(-2)	8.881e-24					
H2S	5.652e-24	5.652e-24	-23.248	-23.248	0.000	
HS-	3.229e-24	2.890e-24	-23.491	-23.539	-0.048	

	S-2	2.746e-30	1.791e-30	-29.561	-29.747	-0.186
	S2-2	0.000e+00	0.000e+00	-44.721	-44.912	-0.191
	S3-2	0.000e+00	0.000e+00	-59.928	-60.119	-0.191
	S4-2	0.000e+00	0.000e+00	-75.362	-75.553	-0.191
	S5-2	0.000e+00	0.000e+00	-91.012	-91.203	-0.191
S(2)		1.376e-28				
	S2O3-2	6.882e-29	4.430e-29	-28.162	-28.354	-0.191
	HS2O3-	9.762e-35	8.751e-35	-34.010	-34.058	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-46.684	-46.870	-0.186
S(4)		1.919e-18				
	HSO3-	1.347e-18	1.208e-18	-17.870	-17.918	-0.047
	SO3-2	5.716e-19	3.704e-19	-18.243	-18.431	-0.188
	H2SO3	2.215e-23	2.215e-23	-22.655	-22.655	0.000
	SO2	1.759e-23	1.759e-23	-22.755	-22.755	0.000
	S2O5-2	0.000e+00	0.000e+00	-40.475	-40.666	-0.191
	S3O6-2	0.000e+00	0.000e+00	-57.022	-57.213	-0.191
	S4O6-2	0.000e+00	0.000e+00	-58.806	-58.997	-0.191
	S5O6-2	0.000e+00	0.000e+00	-89.469	-89.660	-0.191
S(5)		9.303e-40				
	S2O6-2	4.652e-40	2.994e-40	-39.332	-39.524	-0.191
S(6)		2.307e-03				
	SO4-2	1.933e-03	1.244e-03	-2.714	-2.905	-0.191
	CaSO4	3.730e-04	3.730e-04	-3.428	-3.428	0.000
	NaSO4-	1.008e-06	9.038e-07	-5.996	-6.044	-0.047
	HSO4-	2.682e-08	2.404e-08	-7.572	-7.619	-0.047
	Th(SO4)2	2.134e-11	2.134e-11	-10.671	-10.671	0.000
	ThSO4+2	1.333e-12	8.638e-13	-11.875	-12.064	-0.188
	Th(SO4)3-2	2.343e-13	1.508e-13	-12.630	-12.822	-0.191
	Th(SO4)4-4	1.094e-17	1.871e-18	-16.961	-17.728	-0.767
	H2SO4	4.340e-18	4.340e-18	-17.363	-17.363	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-72.602	-72.794	-0.191
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-57.928	-57.976	-0.047
Th		2.250e-04				
	Th(OH)4	2.244e-04	2.244e-04	-3.649	-3.649	0.000
	Th(OH)3+	6.797e-07	6.093e-07	-6.168	-6.215	-0.047
	Th(OH)2+2	1.018e-08	6.593e-09	-7.992	-8.181	-0.188
	Th(SO4)2	2.134e-11	2.134e-11	-10.671	-10.671	0.000
	ThOH+3	5.493e-12	2.097e-12	-11.260	-11.678	-0.418
	ThSO4+2	1.333e-12	8.638e-13	-11.875	-12.064	-0.188
	Th(SO4)3-2	2.343e-13	1.508e-13	-12.630	-12.822	-0.191
	Th+4	1.329e-14	3.110e-15	-13.877	-14.507	-0.631
	Th(SO4)4-4	1.094e-17	1.871e-18	-16.961	-17.728	-0.767
	ThCl+3	8.396e-18	3.205e-18	-17.076	-17.494	-0.418
	Th6(OH)15+9	5.073e-21	1.114e-24	-20.295	-23.953	-3.658
	Th2(OH)2+6	3.878e-21	9.182e-23	-20.411	-22.037	-1.626
	ThCl2+2	2.797e-22	1.812e-22	-21.553	-21.742	-0.188
	Th4(OH)8+8	7.143e-24	9.193e-27	-23.146	-26.037	-2.890
	ThCl3+	1.487e-25	1.333e-25	-24.828	-24.875	-0.047
	ThCl4	5.561e-30	5.561e-30	-29.255	-29.255	0.000

-----Saturation indices-----
 --

Phase SI log IAP log KT

Anhydrite	-1.24	-5.59	-4.35	CaSO4
Antarcticite	-14.69	-10.60	4.09	CaCl2:6H2O
Aragonite	-0.61	1.36	1.97	CaCO3
Bassanite	-1.89	-5.59	-3.71	CaSO4:0.5H2O
Burkeite	-35.00	-25.51	9.49	Na6CO3(SO4)2
C	-11.35	52.80	64.15	C
C(g)	-128.97	52.80	181.77	C
Ca	-97.99	41.84	139.83	Ca
Ca(g)	-123.23	41.84	165.07	Ca
Ca2Cl2(OH)2:H2O	-26.14	0.15	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-46.68	21.65	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-0.46	1.36	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.06	-5.59	-3.54	CaSO4:0.5H2O
CH4(g)	-26.27	-29.11	-2.84	CH4
Cl2(g)	-55.43	-52.44	2.99	Cl2
CO(g)	-16.97	-19.97	-3.00	CO
CO2(g)	-1.56	-9.38	-7.83	CO2
Gaylussite	-13.66	-2.50	11.16	CaNa2(CO3)2:5H2O
Glauberite	-10.95	-16.42	-5.47	Na2Ca(SO4)2
Gypsum	-1.06	-5.59	-4.53	CaSO4:2H2O
H2(g)	-11.91	-15.01	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-22.26	-30.26	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-16.98	-10.67	6.30	HCl
Hydrophilite	-22.34	-10.60	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-21.82	10.75	32.57	CaO
Mirabilite	-9.67	-10.82	-1.15	Na2SO4:10H2O
Monohydrocalcite	-1.31	1.36	2.68	CaCO3:H2O
Na	-49.07	18.31	67.37	Na
Na(g)	-62.55	18.31	80.86	Na
Na2CO3	-15.03	-3.86	11.16	Na2CO3
Na2CO3:7H2O	-13.80	-3.87	9.94	Na2CO3:7H2O
Na2O	-61.90	5.52	67.42	Na2O
Na3H(SO4)2	-23.51	-24.40	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.34	-27.24	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.48	-6.62	-0.14	NaHCO3
Natron	-13.45	-3.87	9.59	Na2CO3:10H2O
O2(g)	-59.29	-62.18	-2.89	O2
Pirssonite	-13.82	-2.50	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-11.80	10.75	22.55	Ca(OH)2
S	-16.24	-61.35	-45.11	S
S2(g)	-46.37	-53.56	-7.19	S2
SO2(g)	-22.93	-22.75	0.18	SO2
Th	-135.04	74.55	209.59	Th
Th(g)	-233.29	74.55	307.84	Th
Th(OH)4	2.70	12.37	9.66	Th(OH)4
Th(SO4)2	0.00	-20.32	-20.32	Th(SO4)2
Th2S3	-130.12	-34.95	95.17	Th2S3
Th7S12	-418.40	-214.35	204.06	Th7S12
ThCl4	-54.17	-30.33	23.84	ThCl4
Thenardite	-10.47	-10.82	-0.36	Na2SO4
Thermonatrite	-14.80	-3.86	10.94	Na2CO3:H2O
Thorianite	10.50	12.37	1.86	ThO2
ThS	-82.84	13.20	96.04	ThS

ThS2 -58.93 -48.15 .10.78 ThS2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Attachment 6

Run 15

Reading data base.

```
-----  
LLNL_AQUEOUS_MODEL_PARAMETERS  
SOLUTION_MASTER_SPECIES  
SOLUTION_SPECIES  
PHASES  
EXCHANGE_MASTER_SPECIES  
EXCHANGE_SPECIES  
SURFACE_MASTER_SPECIES  
SURFACE_SPECIES  
RATES  
END
```

Reading input data for simulation 1.

```
-----  
TITLE Run 15 # Equil with RaSO4 only - using Llnl database  
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.
```

```
pH      7.8  
temp    25.0  
pe      -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)  
units   ppm  
Alkalinity      205.7 as HCO3  
Ca             141.9  
Cl             4.4  
Na             2.85  
S             178.2
```

```
EQUILIBRIUM_PHASES 1  
RaSO4      0.0  1.46E-5
```

END

TITLE

Run 15

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03

Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03

-----Description of solution-----

```

pH = 7.800
pe = -1.690
Activity of water = 1.000
Ionic strength = 1.113e-02
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 3.427e-03
Total CO2 (mol/kg) = 3.427e-03
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.908e-06
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.01
Iterations = 4
Total H = 1.110539e+02
Total O = 5.554293e+01

```

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047

	HC1O2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl (5)		0.000e+00				
	ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048
Cl (7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H (0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O (0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S (-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S (2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S (3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S (4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S (5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S (6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S (7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S (8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

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Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
RaSO4	0.00	-10.46	-10.46	1.460e-05	1.455e-05	-5.229e-08

-----Solution composition-----

--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
Ra	5.229e-08	5.229e-08
S	1.856e-03	1.856e-03

-----Description of solution-----

--

equilibrium	pH	=	7.800	Charge balance
	pe	=	-1.855	Adjusted to redox
	Activity of water	=	1.000	
	Ionic strength	=	1.113e-02	
	Mass of water (kg)	=	1.000e+00	
	Total alkalinity (eq/kg)	=	3.374e-03	
	Total CO2 (mol/kg)	=	3.427e-03	
	Temperature (deg C)	=	25.000	
	Electrical balance (eq)	=	-1.908e-06	
	Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.01	
	Iterations	=	6	
	Total H	=	1.110539e+02	
	Total O	=	5.554293e+01	

-----Distribution of species-----

--

Species	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-88.459	-88.459	0.000
C(-3)	6.899e-32				
C2H6	3.450e-32	3.450e-32	-31.462	-31.462	0.000
C(-4)	9.883e-31				

	CH4	9.883e-31	9.883e-31	-30.005	-30.005	0.000
C(2)		1.233e-21				
	CO	1.233e-21	1.233e-21	-20.909	-20.909	0.000
C(4)		3.427e-03				
	HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
	CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca		3.542e-03				
	Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)		1.242e-04				
	Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
	HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)		0.000e+00				
	ClO-	0.000e+00	0.000e+00	-50.126	-50.173	-0.047
	HClO	0.000e+00	0.000e+00	-50.404	-50.404	0.000
Cl(3)		0.000e+00				
	ClO2-	0.000e+00	0.000e+00	-89.239	-89.286	-0.047
	HClO2	0.000e+00	0.000e+00	-93.916	-93.916	0.000
Cl(5)		0.000e+00				
	ClO3-	0.000e+00	0.000e+00	-114.499	-114.546	-0.048
Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-144.061	-144.109	-0.048
H(0)		2.038e-15				
	H2	1.019e-15	1.022e-15	-14.992	-14.991	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-46.964	-47.153	-0.189
	S3O6-2	0.000e+00	0.000e+00	-61.568	-61.757	-0.189
	O2	0.000e+00	0.000e+00	-62.216	-62.215	0.001
	S3-2	0.000e+00	0.000e+00	-64.380	-64.569	-0.189
	S4O6-2	0.000e+00	0.000e+00	-65.562	-65.751	-0.189
	S4-2	0.000e+00	0.000e+00	-82.024	-82.213	-0.189
	S5O6-2	0.000e+00	0.000e+00	-98.435	-98.624	-0.189
	S5-2	0.000e+00	0.000e+00	-99.884	-100.073	-0.189
Ra		5.229e-08				
	Ra+2	5.229e-08	3.427e-08	-7.282	-7.465	-0.183
S(-2)		2.851e-25				
	HS-	2.489e-25	2.230e-25	-24.604	-24.652	-0.048

	H2S	3.614e-26	3.614e-26	-25.442	-25.442	0.000
	S-2	2.546e-30	1.669e-30	-29.594	-29.778	-0.183
	S2-2	0.000e+00	0.000e+00	-46.964	-47.153	-0.189
	S3-2	0.000e+00	0.000e+00	-64.380	-64.569	-0.189
	S4-2	0.000e+00	0.000e+00	-82.024	-82.213	-0.189
	S5-2	0.000e+00	0.000e+00	-99.884	-100.073	-0.189
S(2)		7.067e-31				
	S2O3-2	3.533e-31	2.286e-31	-30.452	-30.641	-0.189
	HS2O3-	4.168e-38	3.741e-38	-37.380	-37.427	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-48.989	-49.173	-0.183
S(4)		5.691e-19				
	SO3-2	4.758e-19	3.099e-19	-18.323	-18.509	-0.186
	HSO3-	9.327e-20	8.372e-20	-19.030	-19.077	-0.047
	H2SO3	1.272e-25	1.272e-25	-24.896	-24.896	0.000
	SO2	1.010e-25	1.010e-25	-24.996	-24.996	0.000
	S2O5-2	0.000e+00	0.000e+00	-42.795	-42.984	-0.189
	S3O6-2	0.000e+00	0.000e+00	-61.568	-61.757	-0.189
	S4O6-2	0.000e+00	0.000e+00	-65.562	-65.751	-0.189
	S5O6-2	0.000e+00	0.000e+00	-98.435	-98.624	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.669	-41.858	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.970	-75.159	-0.189
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-59.119	-59.166	-0.047

-----Saturation indices-----

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Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.27	51.87	64.15	C
C(g)	-129.89	51.87	181.77	C
Ca	-95.81	44.02	139.83	Ca
Ca(g)	-121.05	44.02	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
CH4(g)	-27.16	-30.01	-2.84	CH4
Cl2(g)	-57.61	-54.62	2.99	Cl2
CO(g)	-17.91	-20.91	-3.00	CO
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2

Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-11.89	-14.99	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-24.46	-32.45	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-47.98	19.40	67.37	Na
Na(g)	-61.46	19.40	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-59.32	-62.21	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
Ra	-102.13	39.24	141.37	Ra
RaCl2:2H2O	-14.60	-15.37	-0.77	RaCl2:2H2O
RaSO4	0.00	-10.46	-10.46	RaSO4
S	-18.45	-63.56	-45.11	S
S2(g)	-50.79	-57.98	-7.19	S2
SO2(g)	-25.17	-25.00	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 16

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 10 # Equil with Ra(NO3)2 only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 $\# = -100$ mV, $pe = eh/0.059$ (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM PHASES 1

Ra(NO3)2 0.0 1.46E-5

END

TITLE

Run 16

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04

S

1.856e-03 1.856e-03

-----Description of solution-----

```

pH = 7.800
pe = -1.690
Activity of water = 1.000
Ionic strength = 1.113e-02
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 3.427e-03
Total CO2 (mol/kg) = 3.427e-03
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.908e-06
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.01
Iterations = 4
Total H = 1.110539e+02
Total O = 5.554293e+01

```

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				

	ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048
Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H(0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S(4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----
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Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
Ra(NO3)2	-11.94	193.12	205.06	1.460e-05		-1.460e-05

-----Solution composition-----
--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
N	2.920e-05	2.920e-05
Na	1.240e-04	1.240e-04
Ra	1.460e-05	1.460e-05
S	1.856e-03	1.856e-03

-----Description of solution-----
--

	pH =	7.800	Charge balance
	pe =	11.409	Adjusted to redox
equilibrium	Activity of water =	1.000	
	Ionic strength =	1.118e-02	
	Mass of water (kg) =	1.000e+00	
	Total alkalinity (eq/kg) =	3.374e-03	
	Total CO2 (mol/kg) =	3.427e-03	
	Temperature (deg C) =	25.000	
	Electrical balance (eq) =	-1.908e-06	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.01	
	Iterations =	25	
	Total H =	1.110539e+02	
	Total O =	5.554302e+01	

-----Distribution of species-----
--

Species	Molality	Activity	Log		Log Gamma
			Molality	Activity	
OH-	6.785e-07	6.078e-07	-6.168	-6.216	-0.048
H+	1.741e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-247.629	-247.629	0.000
C(-3)	0.000e+00				
C2H6	0.000e+00	0.000e+00	-217.160	-217.160	0.000
C(-4)	0.000e+00				

	CH4	0.000e+00	0.000e+00	-136.118	-136.118	0.000
C(2)		0.000e+00				
	CO	0.000e+00	0.000e+00	-47.437	-47.437	0.000
C(4)		3.427e-03				
	HCO3-	3.193e-03	2.865e-03	-2.496	-2.543	-0.047
	CO2	1.051e-04	1.053e-04	-3.979	-3.977	0.001
	CaHCO3+	7.831e-05	7.028e-05	-4.106	-4.153	-0.047
	CaCO3	3.848e-05	3.848e-05	-4.415	-4.415	0.000
	CO3-2	1.232e-05	8.021e-06	-4.909	-5.096	-0.187
	NaHCO3	4.515e-07	4.515e-07	-6.345	-6.345	0.000
	NaCO3-	3.445e-09	3.092e-09	-8.463	-8.510	-0.047
	SCN-	0.000e+00	0.000e+00	-194.166	-194.214	-0.048
Ca		3.542e-03				
	Ca+2	3.122e-03	2.070e-03	-2.506	-2.684	-0.178
	CaSO4	3.034e-04	3.034e-04	-3.518	-3.518	0.000
	CaHCO3+	7.831e-05	7.028e-05	-4.106	-4.153	-0.047
	CaCO3	3.848e-05	3.848e-05	-4.415	-4.415	0.000
	CaNO3+	2.988e-07	2.681e-07	-6.525	-6.572	-0.047
	CaCl+	5.426e-08	4.870e-08	-7.265	-7.312	-0.047
	CaOH+	2.055e-08	1.845e-08	-7.687	-7.734	-0.047
	CaCl2	6.358e-12	6.358e-12	-11.197	-11.197	0.000
Cl(-1)		1.242e-04				
	Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.049
	CaCl+	5.426e-08	4.870e-08	-7.265	-7.312	-0.047
	NaCl	2.149e-09	2.149e-09	-8.668	-8.668	0.000
	CaCl2	6.358e-12	6.358e-12	-11.197	-11.197	0.000
	HCl	3.951e-13	3.951e-13	-12.403	-12.403	0.000
Cl(1)		3.857e-24				
	ClO-	2.525e-24	2.266e-24	-23.598	-23.645	-0.047
	HClO	1.332e-24	1.332e-24	-23.876	-23.876	0.000
Cl(3)		6.572e-37				
	ClO2-	6.572e-37	5.898e-37	-36.182	-36.229	-0.047
	HClO2	0.000e+00	0.000e+00	-40.860	-40.860	0.000
Cl(5)		1.219e-35				
	ClO3-	1.219e-35	1.092e-35	-34.914	-34.962	-0.048
Cl(7)		1.127e-38				
	ClO4-	1.127e-38	1.010e-38	-37.948	-37.996	-0.048
H(0)		0.000e+00				
	H2	0.000e+00	0.000e+00	-41.520	-41.519	0.001
N(-03)		0.000e+00				
	N3-	0.000e+00	0.000e+00	-81.941	-81.988	-0.047
	HN3	0.000e+00	0.000e+00	-85.085	-85.085	0.000
N(-3)		0.000e+00				
	NH4+	0.000e+00	0.000e+00	-54.650	-54.699	-0.049
	NH3	0.000e+00	0.000e+00	-56.139	-56.139	0.000
	NH4SO4-	0.000e+00	0.000e+00	-65.951	-65.998	-0.047
	SCN-	0.000e+00	0.000e+00	-194.166	-194.214	-0.048
N(-5)		0.000e+00				
	HCN	0.000e+00	0.000e+00	-108.692	-108.692	0.000
	CN-	0.000e+00	0.000e+00	-110.102	-110.150	-0.049
N(0)		5.543e-10				
	N2	2.772e-10	2.772e-10	-9.557	-9.557	0.000
N(3)		6.412e-16				
	NO2-	6.412e-16	5.734e-16	-15.193	-15.242	-0.049
	HNO2	1.551e-20	1.551e-20	-19.809	-19.809	0.000
N(5)		2.920e-05				
	NO3-	2.890e-05	2.585e-05	-4.539	-4.588	-0.049

	CaNO3+	2.988e-07	2.681e-07	-6.525	-6.572	-0.047
	HNO3	2.142e-14	2.142e-14	-13.669	-13.669	0.000
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.140e-07	7.305e-07	-6.089	-6.136	-0.047
	NaHCO3	4.515e-07	4.515e-07	-6.345	-6.345	0.000
	NaCO3-	3.445e-09	3.092e-09	-8.463	-8.510	-0.047
	NaCl	2.149e-09	2.149e-09	-8.668	-8.668	0.000
	NaOH	1.155e-11	1.155e-11	-10.937	-10.937	0.000
O(0)		1.386e-09				
	O2	6.929e-10	6.948e-10	-9.159	-9.158	0.001
	S3O6-2	0.000e+00	0.000e+00	-167.681	-167.871	-0.189
	S2-2	0.000e+00	0.000e+00	-232.662	-232.851	-0.189
	S4O6-2	0.000e+00	0.000e+00	-251.260	-251.450	-0.189
	S3-2	0.000e+00	0.000e+00	-329.663	-329.852	-0.189
	S5O6-2	0.000e+00	0.000e+00	-363.718	-363.908	-0.189
	S4-2	0.000e+00	0.000e+00	-426.892	-427.081	-0.189
	S5-2	0.000e+00	0.000e+00	-524.337	-524.526	-0.189
Ra		1.460e-05				
	Ra+2	1.460e-05	9.563e-06	-4.836	-5.019	-0.184
S(-2)		0.000e+00				
	HS-	0.000e+00	0.000e+00	-130.717	-130.765	-0.048
	H2S	0.000e+00	0.000e+00	-131.555	-131.555	0.000
	S-2	0.000e+00	0.000e+00	-135.707	-135.891	-0.184
	SCN-	0.000e+00	0.000e+00	-194.166	-194.214	-0.048
	S2-2	0.000e+00	0.000e+00	-232.662	-232.851	-0.189
	S3-2	0.000e+00	0.000e+00	-329.663	-329.852	-0.189
	S4-2	0.000e+00	0.000e+00	-426.892	-427.081	-0.189
	S5-2	0.000e+00	0.000e+00	-524.337	-524.526	-0.189
S(2)		0.000e+00				
	S2O3-2	0.000e+00	0.000e+00	-136.565	-136.754	-0.189
	HS2O3-	0.000e+00	0.000e+00	-143.493	-143.540	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-128.574	-128.758	-0.184
S(4)		0.000e+00				
	SO3-2	0.000e+00	0.000e+00	-44.851	-45.037	-0.187
	HSO3-	0.000e+00	0.000e+00	-45.559	-45.606	-0.047
	H2SO3	0.000e+00	0.000e+00	-51.424	-51.424	0.000
	SO2	0.000e+00	0.000e+00	-51.524	-51.524	0.000
	S2O5-2	0.000e+00	0.000e+00	-95.852	-96.041	-0.189
	S3O6-2	0.000e+00	0.000e+00	-167.681	-167.871	-0.189
	S4O6-2	0.000e+00	0.000e+00	-251.260	-251.450	-0.189
	S5O6-2	0.000e+00	0.000e+00	-363.718	-363.908	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-68.197	-68.386	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.034e-04	3.034e-04	-3.518	-3.518	0.000
	NaSO4-	8.140e-07	7.305e-07	-6.089	-6.136	-0.047
	HSO4-	1.790e-09	1.607e-09	-8.747	-8.794	-0.047
	H2SO4	2.402e-20	2.402e-20	-19.619	-19.619	0.000
	NH4SO4-	0.000e+00	0.000e+00	-65.951	-65.998	-0.047
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-48.442	-48.631	-0.189
S(8)		2.563e-33				
	HSO5-	2.563e-33	2.300e-33	-32.591	-32.638	-0.047

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO ₄
Antarcticite	-14.69	-10.59	4.09	CaCl ₂ :6H ₂ O
Aragonite	0.60	2.57	1.97	CaCO ₃
Bassanite	-1.98	-5.68	-3.71	CaSO ₄ :0.5H ₂ O
Burkeite	-33.97	-24.49	9.49	Na ₆ CO ₃ (SO ₄) ₂
C	-65.33	-1.18	64.15	C
C(g)	-182.95	-1.18	181.77	C
Ca	-122.34	17.49	139.83	Ca
Ca(g)	-147.58	17.49	165.07	Ca
Ca ₂ Cl ₂ (OH) ₂ :H ₂ O	-23.97	2.32	26.29	Ca ₂ Cl ₂ (OH) ₂ :H ₂ O
Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O	-40.17	28.15	68.33	Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O
Calcite	0.75	2.57	1.82	CaCO ₃
CaSO ₄ :0.5H ₂ O(beta)	-2.15	-5.68	-3.54	CaSO ₄ :0.5H ₂ O
CH ₄ (g)	-133.28	-136.12	-2.84	CH ₄
Cl ₂ (g)	-31.08	-28.09	2.99	Cl ₂
CO(g)	-44.44	-47.44	-3.00	CO
CO ₂ (g)	-2.51	-10.34	-7.83	CO ₂
Gaylussite	-11.25	-0.09	11.16	CaNa ₂ (CO ₃) ₂ :5H ₂ O
Glauberite	-11.13	-16.60	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-1.15	-5.68	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-38.42	-41.52	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
H ₂ S(g)	-130.57	-138.56	-7.99	H ₂ S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na ₂ SO ₄ :10H ₂ O
Monohydrocalcite	-0.10	2.57	2.68	CaCO ₃ :H ₂ O
N ₂ (g)	-6.38	-9.56	-3.18	N ₂
Na	-61.24	6.13	67.37	Na
Na(g)	-74.73	6.13	80.86	Na
Na ₂ CO ₃	-13.82	-2.66	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-12.60	-2.66	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-59.73	7.68	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-24.78	-25.67	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-21.62	-27.51	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-6.36	-6.50	-0.14	NaHCO ₃
Natron	-12.25	-2.66	9.59	Na ₂ CO ₃ :10H ₂ O
NH ₃ (g)	-57.94	-56.14	1.80	NH ₃
NO(g)	-21.49	-20.75	0.74	NO
NO ₂ (g)	-18.45	-10.10	8.35	NO ₂
O ₂ (g)	-6.27	-9.16	-2.89	O ₂
Pirssonite	-11.41	-0.09	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Portlandite	-9.63	12.92	22.55	Ca(OH) ₂
Ra	-126.21	15.16	141.37	Ra
Ra(NO ₃) ₂	-11.94	-14.19	-2.25	Ra(NO ₃) ₂
RaCl ₂ :2H ₂ O	-12.15	-12.93	-0.77	RaCl ₂ :2H ₂ O
RaSO ₄	2.45	-8.02	-10.46	RaSO ₄
S	-98.03	-143.14	-45.11	S
S ₂ (g)	-209.96	-217.15	-7.19	S ₂

SO2(g)	-51.70	-51.52	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.60	-2.66	10.94	Na2CO3:H2O

 End of simulation.

 Reading input data for simulation 2.

 End of run.

No memory leaks

Run 17

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 11 # Equil with RaCl2:2H2O only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1
RaCl2:2H2O 0.0 1.46E-5
END

TITLE

Run 11

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12..

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04

S

1.856e-03 1.856e-03

-----Description of solution-----

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.113e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.427e-03
 Total CO2 (mol/kg) = 3.427e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -1.908e-06
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = -0.01
 Iterations = 4
 Total H = 1.110539e+02
 Total O = 5.554293e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				

	ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048
Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H(0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S(4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO ₄
Antarcticite	-14.69	-10.59	4.09	CaCl ₂ :6H ₂ O
Aragonite	0.60	2.57	1.97	CaCO ₃
Bassanite	-1.98	-5.68	-3.71	CaSO ₄ :0.5H ₂ O
Burkeite	-33.97	-24.49	9.49	Na ₆ CO ₃ (SO ₄) ₂
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca ₂ Cl ₂ (OH) ₂ :H ₂ O	-23.97	2.32	26.29	Ca ₂ Cl ₂ (OH) ₂ :H ₂ O
Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O	-40.17	28.15	68.33	Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O
Calcite	0.75	2.57	1.82	CaCO ₃
CaSO ₄ :0.5H ₂ O(beta)	-2.15	-5.68	-3.54	CaSO ₄ :0.5H ₂ O
Cl ₂ (g)	-57.28	-54.29	2.99	Cl ₂
CO ₂ (g)	-2.51	-10.34	-7.83	CO ₂
Gaylussite	-11.25	-0.09	11.16	CaNa ₂ (CO ₃) ₂ :5H ₂ O
Glauberite	-11.13	-16.60	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-1.15	-5.68	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-12.22	-15.32	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
H ₂ S(g)	-25.78	-33.77	-7.99	H ₂ S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na ₂ SO ₄ :10H ₂ O
Monohydrocalcite	-0.10	2.57	2.68	CaCO ₃ :H ₂ O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na ₂ CO ₃	-13.82	-2.66	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-12.60	-2.66	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-59.73	7.68	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-24.78	-25.67	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-21.62	-27.51	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-6.36	-6.50	-0.14	NaHCO ₃
Natron	-12.25	-2.66	9.59	Na ₂ CO ₃ :10H ₂ O
O ₂ (g)	-58.66	-61.56	-2.89	O ₂
Pirssonite	-11.41	-0.09	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Portlandite	-9.63	12.92	22.55	Ca(OH) ₂
S	-19.44	-64.55	-45.11	S
S ₂ (g)	-52.77	-59.95	-7.19	S ₂
SO ₂ (g)	-25.50	-25.33	0.18	SO ₂
Thenardite	-10.56	-10.91	-0.36	Na ₂ SO ₄
Thermonatrite	-13.59	-2.66	10.94	Na ₂ CO ₃ :H ₂ O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----
--

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
RaCl ₂ :2H ₂ O	-11.97	-12.75	-0.77	1.460e-05		-1.460e-05

-----Solution composition-----
--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.534e-04	1.534e-04
Na	1.240e-04	1.240e-04
Ra	1.460e-05	1.460e-05
S	1.856e-03	1.856e-03

-----Description of solution-----
--

	pH =	7.800	Charge balance
	pe =	-1.863	Adjusted to redox
equilibrium	Activity of water =	1.000	
	Ionic strength =	1.118e-02	
	Mass of water (kg) =	1.000e+00	
	Total alkalinity (eq/kg) =	3.374e-03	
	Total CO ₂ (mol/kg) =	3.427e-03	
	Temperature (deg C) =	25.000	
	Electrical balance (eq) =	-1.908e-06	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.01	
	Iterations =	11	
	Total H =	1.110540e+02	
	Total O =	5.554296e+01	

-----Distribution of species-----
--

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.785e-07	6.078e-07	-6.168	-6.216	-0.048
H+	1.741e-08	1.585e-08	-7.759	-7.800	-0.041
H ₂ O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(-2)	0.000e+00				
C ₂ H ₄	0.000e+00	0.000e+00	-88.356	-88.356	0.000
C(-3)	9.099e-32				
C ₂ H ₆	4.549e-32	4.549e-32	-31.342	-31.342	0.000
C(-4)	1.158e-30				
CH ₄	1.158e-30	1.158e-30	-29.936	-29.936	0.000

C(2)		1.282e-21				
	CO	1.282e-21	1.282e-21	-20.892	-20.892	0.000
C(4)		3.427e-03				
	HCO3-	3.193e-03	2.865e-03	-2.496	-2.543	-0.047
	CO2	1.051e-04	1.053e-04	-3.979	-3.977	0.001
	CaHCO3+	7.832e-05	7.028e-05	-4.106	-4.153	-0.047
	CaCO3	3.848e-05	3.848e-05	-4.415	-4.415	0.000
	CO3-2	1.232e-05	8.021e-06	-4.909	-5.096	-0.187
	NaHCO3	4.515e-07	4.515e-07	-6.345	-6.345	0.000
	NaCO3-	3.445e-09	3.092e-09	-8.463	-8.510	-0.047
Ca		3.542e-03				
	Ca+2	3.122e-03	2.070e-03	-2.506	-2.684	-0.178
	CaSO4	3.034e-04	3.034e-04	-3.518	-3.518	0.000
	CaHCO3+	7.832e-05	7.028e-05	-4.106	-4.153	-0.047
	CaCO3	3.848e-05	3.848e-05	-4.415	-4.415	0.000
	CaCl+	6.703e-08	6.015e-08	-7.174	-7.221	-0.047
	CaOH+	2.056e-08	1.845e-08	-7.687	-7.734	-0.047
	CaCl2	9.701e-12	9.701e-12	-11.013	-11.013	0.000
Cl(-1)		1.534e-04				
	Cl-	1.533e-04	1.371e-04	-3.814	-3.863	-0.049
	CaCl+	6.703e-08	6.015e-08	-7.174	-7.221	-0.047
	NaCl	2.655e-09	2.655e-09	-8.576	-8.576	0.000
	CaCl2	9.701e-12	9.701e-12	-11.013	-11.013	0.000
	HCl	4.880e-13	4.880e-13	-12.312	-12.312	0.000
Cl(1)		0.000e+00				
	ClO-	0.000e+00	0.000e+00	-50.051	-50.098	-0.047
	HClO	0.000e+00	0.000e+00	-50.329	-50.329	0.000
Cl(3)		0.000e+00				
	ClO2-	0.000e+00	0.000e+00	-89.181	-89.228	-0.047
	HClO2	0.000e+00	0.000e+00	-93.859	-93.859	0.000
Cl(5)		0.000e+00				
	ClO3-	0.000e+00	0.000e+00	-114.458	-114.506	-0.048
Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-144.038	-144.086	-0.048
H(0)		2.120e-15				
	H2	1.060e-15	1.063e-15	-14.975	-14.974	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.140e-07	7.305e-07	-6.089	-6.136	-0.047
	NaHCO3	4.515e-07	4.515e-07	-6.345	-6.345	0.000
	NaCO3-	3.445e-09	3.092e-09	-8.463	-8.510	-0.047
	NaCl	2.655e-09	2.655e-09	-8.576	-8.576	0.000
	NaOH	1.155e-11	1.155e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-46.844	-47.033	-0.189
	S3O6-2	0.000e+00	0.000e+00	-61.500	-61.689	-0.189
	O2	0.000e+00	0.000e+00	-62.250	-62.249	0.001
	S3-2	0.000e+00	0.000e+00	-64.209	-64.398	-0.189
	S4O6-2	0.000e+00	0.000e+00	-65.442	-65.632	-0.189
	S4-2	0.000e+00	0.000e+00	-81.801	-81.991	-0.189
	S5O6-2	0.000e+00	0.000e+00	-98.264	-98.453	-0.189
	S5-2	0.000e+00	0.000e+00	-99.610	-99.800	-0.189
Ra		1.460e-05				
	Ra+2	1.460e-05	9.562e-06	-4.836	-5.019	-0.184
S(-2)		3.338e-25				
	HS-	2.915e-25	2.612e-25	-24.535	-24.583	-0.048
	H2S	4.231e-26	4.231e-26	-25.374	-25.374	0.000

	S-2	2.983e-30	1.954e-30	-29.525	-29.709	-0.184
	S2-2	0.000e+00	0.000e+00	-46.844	-47.033	-0.189
	S3-2	0.000e+00	0.000e+00	-64.209	-64.398	-0.189
	S4-2	0.000e+00	0.000e+00	-81.801	-81.991	-0.189
	S5-2	0.000e+00	0.000e+00	-99.610	-99.800	-0.189
S (2)		8.275e-31				
	S2O3-2	4.138e-31	2.675e-31	-30.383	-30.573	-0.189
	HS2O3-	4.878e-38	4.378e-38	-37.312	-37.359	-0.047
S (3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-48.938	-49.122	-0.184
S (4)		5.921e-19				
	SO3-2	4.951e-19	3.222e-19	-18.305	-18.492	-0.187
	HSO3-	9.700e-20	8.705e-20	-19.013	-19.060	-0.047
	H2SO3	1.322e-25	1.322e-25	-24.879	-24.879	0.000
	SO2	1.050e-25	1.050e-25	-24.979	-24.979	0.000
	S2O5-2	0.000e+00	0.000e+00	-42.761	-42.951	-0.189
	S3O6-2	0.000e+00	0.000e+00	-61.500	-61.689	-0.189
	S4O6-2	0.000e+00	0.000e+00	-65.442	-65.632	-0.189
	S5O6-2	0.000e+00	0.000e+00	-98.264	-98.453	-0.189
S (5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.652	-41.841	-0.189
S (6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.034e-04	3.034e-04	-3.518	-3.518	0.000
	NaSO4-	8.140e-07	7.305e-07	-6.089	-6.136	-0.047
	HSO4-	1.790e-09	1.607e-09	-8.747	-8.794	-0.047
	H2SO4	2.402e-20	2.402e-20	-19.619	-19.619	0.000
S (7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.987	-75.176	-0.189
S (8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-59.137	-59.184	-0.047

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.50	-10.41	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.24	51.91	64.15	C
C(g)	-129.86	51.91	181.77	C
Ca	-95.79	44.04	139.83	Ca
Ca(g)	-121.03	44.04	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.78	2.51	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-39.99	28.34	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
CH4(g)	-27.09	-29.94	-2.84	CH4
Cl2(g)	-57.44	-54.45	2.99	Cl2
CO(g)	-17.89	-20.89	-3.00	CO
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O

H2(g)	-11.87	-14.97	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-24.39	-32.38	-7.99	H2S
Halite	-9.38	-7.82	1.56	NaCl
HCl(g)	-17.96	-11.66	6.30	HCl
Hydrophilite	-22.16	-10.41	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-47.97	19.40	67.37	Na
Na(g)	-61.45	19.40	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-59.36	-62.25	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
Ra	-99.66	41.71	141.37	Ra
RaCl2:2H2O	-11.97	-12.75	-0.77	RaCl2:2H2O
RaSO4	2.45	-8.02	-10.46	RaSO4
S	-18.40	-63.51	-45.11	S
S2(g)	-50.69	-57.87	-7.19	S2
SO2(g)	-25.15	-24.98	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.60	-2.66	10.94	Na2CO3:H2O

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 18

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 18 # Equil with Th(NO3)4:5H2O only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1
Th(NO3)4:5H2O 0.0 6.47E-4
END

TITLE

Run 18

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04

S

1.856e-03 1.856e-03

-----Description of solution-----

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.113e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.427e-03
 Total CO2 (mol/kg) = 3.427e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -1.908e-06
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = -0.01
 Iterations = 4
 Total H = 1.110539e+02
 Total O = 5.554293e+01

-----Distribution of species-----

	Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
	OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
	H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
	H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)		3.427e-03				
	HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
	CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca		3.542e-03				
	Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)		1.242e-04				
	Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
	HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)		0.000e+00				
	ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
	HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)		0.000e+00				
	ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
	HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)		0.000e+00				

	ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048
Cl (7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H (0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O (0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S306-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S406-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S506-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S (-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S (2)		3.392e-32				
	S203-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS203-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S (3)		0.000e+00				
	S204-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S (4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S205-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S306-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S406-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S506-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S (5)		0.000e+00				
	S206-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S (6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S (7)		0.000e+00				
	S208-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S (8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----
 --

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

--

Phase	SI	log IAP	log KT	Moles in assemblage		Delta
				Initial	Final	
Th(NO3)4:5H2O	-22.70	393.69	416.39	6.470e-04		-6.470e-04

-----Solution composition-----

--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
N	2.588e-03	2.588e-03
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
Th	6.470e-04	6.470e-04

-----Description of solution-----

--

equilibrium	pH	=	5.796	Charge balance
	pe	=	13.978	Adjusted to redox
	Activity of water	=	1.000	
	Ionic strength	=	1.131e-02	
	Mass of water (kg)	=	1.000e+00	
	Total alkalinity (eq/kg)	=	3.374e-03	
	Total CO2 (mol/kg)	=	3.427e-03	
	Temperature (deg C)	=	25.000	
	Electrical balance (eq)	=	-1.908e-06	
	Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.01	
	Iterations	=	27	
	Total H	=	1.110604e+02	
	Total O	=	5.555393e+01	

-----Distribution of species-----

--

Species	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
H+	1.758e-06	1.600e-06	-5.755	-5.796	-0.041
OH-	6.722e-09	6.019e-09	-8.172	-8.220	-0.048
H2O	5.553e+01	9.998e-01	1.744	-0.000	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-251.609	-251.609	0.000
C(-3)	0.000e+00				
C2H6	0.000e+00	0.000e+00	-222.270	-222.270	0.000
C(-4)	0.000e+00				

C(2)	CH4	0.000e+00	0.000e+00	-139.237	-139.237	0.000
		0.000e+00				
C(4)	CO	0.000e+00	0.000e+00	-47.170	-47.170	0.000
		3.427e-03				
	CO2	2.619e-03	2.626e-03	-2.582	-2.581	0.001
	HCO3-	7.886e-04	7.073e-04	-3.103	-3.150	-0.047
	CaHCO3+	1.971e-05	1.768e-05	-4.705	-4.753	-0.047
	NaHCO3	1.117e-07	1.117e-07	-6.952	-6.952	0.000
	CaCO3	9.586e-08	9.586e-08	-7.018	-7.018	0.000
	CO3-2	3.019e-08	1.961e-08	-7.520	-7.708	-0.187
	NaCO3-	8.445e-12	7.574e-12	-11.073	-11.121	-0.047
	SCN-	0.000e+00	0.000e+00	-195.848	-195.896	-0.048
Ca		3.542e-03				
	Ca+2	3.188e-03	2.109e-03	-2.497	-2.676	-0.179
	CaSO4	3.076e-04	3.076e-04	-3.512	-3.512	0.000
	CaNO3+	2.698e-05	2.420e-05	-4.569	-4.616	-0.047
	CaHCO3+	1.971e-05	1.768e-05	-4.705	-4.753	-0.047
	CaCO3	9.586e-08	9.586e-08	-7.018	-7.018	0.000
	CaCl+	5.530e-08	4.960e-08	-7.257	-7.305	-0.047
	CaOH+	2.075e-10	1.862e-10	-9.683	-9.730	-0.047
	CaCl2	6.472e-12	6.472e-12	-11.189	-11.189	0.000
Cl(-1)		1.242e-04				
	Cl-	1.241e-04	1.109e-04	-3.906	-3.955	-0.049
	CaCl+	5.530e-08	4.960e-08	-7.257	-7.305	-0.047
	NaCl	2.153e-09	2.153e-09	-8.667	-8.667	0.000
	HCl	3.987e-11	3.987e-11	-10.399	-10.399	0.000
	CaCl2	6.472e-12	6.472e-12	-11.189	-11.189	0.000
	ThCl+3	1.147e-13	4.400e-14	-12.940	-13.357	-0.416
	ThCl2+2	3.832e-18	2.489e-18	-17.417	-17.604	-0.187
	ThCl3+	2.042e-21	1.831e-21	-20.690	-20.737	-0.047
	ThCl4	7.646e-26	7.646e-26	-25.117	-25.117	0.000
Cl(1)		1.843e-21				
	HClO	1.809e-21	1.809e-21	-20.743	-20.743	0.000
	ClO-	3.398e-23	3.048e-23	-22.469	-22.516	-0.047
Cl(3)		1.193e-34				
	ClO2-	1.190e-34	1.068e-34	-33.924	-33.972	-0.047
	HClO2	2.526e-37	2.526e-37	-36.598	-36.598	0.000
Cl(5)		2.971e-32				
	ClO3-	2.971e-32	2.661e-32	-31.527	-31.575	-0.048
Cl(7)		3.696e-34				
	ClO4-	3.696e-34	3.310e-34	-33.432	-33.480	-0.048
H(0)		0.000e+00				
	H2	0.000e+00	0.000e+00	-42.649	-42.648	0.001
N(-03)		0.000e+00				
	N3-	0.000e+00	0.000e+00	-81.122	-81.170	-0.047
	HN3	0.000e+00	0.000e+00	-82.263	-82.263	0.000
N(-3)		0.000e+00				
	NH4+	0.000e+00	0.000e+00	-53.210	-53.260	-0.050
	NH3	0.000e+00	0.000e+00	-56.704	-56.704	0.000
	NH4SO4-	0.000e+00	0.000e+00	-64.513	-64.561	-0.047
	SCN-	0.000e+00	0.000e+00	-195.848	-195.896	-0.048
N(-5)		0.000e+00				
	HCN	0.000e+00	0.000e+00	-108.988	-108.988	0.000
	CN-	0.000e+00	0.000e+00	-112.403	-112.451	-0.049
N(0)		1.004e-07				
	N2	5.020e-08	5.020e-08	-7.299	-7.299	0.000
N(3)		4.232e-15				

N(5)	NO2-	4.221e-15	3.773e-15	-14.375	-14.423	-0.049
	HNO2	1.031e-17	1.031e-17	-16.987	-16.987	0.000
		2.588e-03				
Na	NO3-	2.561e-03	2.289e-03	-2.592	-2.640	-0.049
	CaNO3+	2.698e-05	2.420e-05	-4.569	-4.616	-0.047
	HNO3	1.916e-10	1.916e-10	-9.718	-9.718	0.000
O(0)		1.240e-04				
	Na+	1.231e-04	1.104e-04	-3.910	-3.957	-0.047
	NaSO4-	8.119e-07	7.282e-07	-6.091	-6.138	-0.047
	NaHCO3	1.117e-07	1.117e-07	-6.952	-6.952	0.000
	NaCl	2.153e-09	2.153e-09	-8.667	-8.667	0.000
	NaCO3-	8.445e-12	7.574e-12	-11.073	-11.121	-0.047
	NaOH	1.147e-13	1.147e-13	-12.941	-12.941	0.000
S(-2)		2.510e-07				
	O2	1.255e-07	1.258e-07	-6.901	-6.900	0.001
	S3O6-2	0.000e+00	0.000e+00	-164.186	-164.377	-0.190
	S2-2	0.000e+00	0.000e+00	-236.560	-236.750	-0.190
	S4O6-2	0.000e+00	0.000e+00	-247.146	-247.336	-0.190
	S3-2	0.000e+00	0.000e+00	-332.942	-333.132	-0.190
	S5O6-2	0.000e+00	0.000e+00	-358.985	-359.175	-0.190
	S4-2	0.000e+00	0.000e+00	-429.551	-429.742	-0.190
	S5-2	0.000e+00	0.000e+00	-526.378	-526.568	-0.190
S(2)		0.000e+00				
	H2S	0.000e+00	0.000e+00	-132.065	-132.065	0.000
	HS-	0.000e+00	0.000e+00	-133.231	-133.279	-0.048
	S-2	0.000e+00	0.000e+00	-140.224	-140.409	-0.185
	SCN-	0.000e+00	0.000e+00	-195.848	-195.896	-0.048
	S2-2	0.000e+00	0.000e+00	-236.560	-236.750	-0.190
	S3-2	0.000e+00	0.000e+00	-332.942	-333.132	-0.190
	S4-2	0.000e+00	0.000e+00	-429.551	-429.742	-0.190
	S5-2	0.000e+00	0.000e+00	-526.378	-526.568	-0.190
S(3)		0.000e+00				
	S2O3-2	0.000e+00	0.000e+00	-137.076	-137.266	-0.190
S(4)	HS2O3-	0.000e+00	0.000e+00	-142.001	-142.048	-0.047
		0.000e+00				
S(5)	S2O4-2	0.000e+00	0.000e+00	-127.956	-128.141	-0.185
		0.000e+00				
	HSO3-	0.000e+00	0.000e+00	-44.685	-44.733	-0.047
	SO3-2	0.000e+00	0.000e+00	-45.981	-46.169	-0.187
	H2SO3	0.000e+00	0.000e+00	-48.547	-48.547	0.000
	SO2	0.000e+00	0.000e+00	-48.647	-48.647	0.000
	S2O5-2	0.000e+00	0.000e+00	-94.105	-94.296	-0.190
	S3O6-2	0.000e+00	0.000e+00	-164.186	-164.377	-0.190
	S4O6-2	0.000e+00	0.000e+00	-247.146	-247.336	-0.190
S(6)	S5O6-2	0.000e+00	0.000e+00	-358.985	-359.175	-0.190
		0.000e+00				
S(6)	S2O6-2	0.000e+00	0.000e+00	-65.321	-65.512	-0.190
		1.856e-03				
	SO4-2	1.547e-03	9.982e-04	-2.810	-3.001	-0.190
	CaSO4	3.076e-04	3.076e-04	-3.512	-3.512	0.000
	NaSO4-	8.119e-07	7.282e-07	-6.091	-6.138	-0.047
	Th(SO4)2	1.885e-07	1.885e-07	-6.725	-6.725	0.000
	HSO4-	1.799e-07	1.614e-07	-6.745	-6.792	-0.047
	ThSO4+2	1.465e-08	9.511e-09	-7.834	-8.022	-0.187
	Th(SO4)3-2	1.658e-09	1.069e-09	-8.780	-8.971	-0.190
	Th(SO4)4-4	6.168e-14	1.065e-14	-13.210	-13.973	-0.763
	H2SO4	2.436e-16	2.436e-16	-15.613	-15.613	0.000

S(7)	NH4SO4-	0.000e+00	0.000e+00	-64.513	-64.561	-0.047
	0.000e+00					
S(8)	S2O8-2	0.000e+00	0.000e+00	-43.308	-43.498	-0.190
	3.467e-30					
Th	HSO5-	3.467e-30	3.110e-30	-29.460	-29.507	-0.047
	6.470e-04					
	Th(OH)4	6.288e-04	6.288e-04	-3.201	-3.201	0.000
	Th(OH)3+	1.593e-05	1.428e-05	-4.798	-4.845	-0.047
	Th(OH)2+2	1.991e-06	1.293e-06	-5.701	-5.888	-0.187
	Th(SO4)2	1.885e-07	1.885e-07	-6.725	-6.725	0.000
	ThSO4+2	1.465e-08	9.511e-09	-7.834	-8.022	-0.187
	ThOH+3	8.965e-09	3.439e-09	-8.047	-8.464	-0.416
	Th(SO4)3-2	1.658e-09	1.069e-09	-8.780	-8.971	-0.190
	Th6(OH)15+9	4.728e-10	1.082e-13	-9.325	-12.966	-3.640
	Th+4	1.811e-10	4.267e-11	-9.742	-10.370	-0.628
	ThCl+3	1.147e-13	4.400e-14	-12.940	-13.357	-0.416
	Th(SO4)4-4	6.168e-14	1.065e-14	-13.210	-13.973	-0.763
	Th2(OH)2+6	1.024e-14	2.470e-16	-13.990	-15.607	-1.618
	Th4(OH)8+8	1.022e-14	1.359e-17	-13.991	-16.867	-2.876
	ThCl2+2	3.832e-18	2.489e-18	-17.417	-17.604	-0.187
	ThCl3+	2.042e-21	1.831e-21	-20.690	-20.737	-0.047
	ThCl4	7.646e-26	7.646e-26	-25.117	-25.117	0.000

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.68	-10.59	4.09	CaCl2:6H2O
Aragonite	-2.00	-0.03	1.97	CaCO3
Bassanite	-1.97	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-36.58	-27.10	9.49	Na6CO3(SO4)2
C	-66.19	-2.05	64.15	C
C(g)	-183.81	-2.05	181.77	C
Ca	-127.47	12.37	139.83	Ca
Ca(g)	-152.71	12.37	165.07	Ca
Ca2Cl2(OH)2:H2O	-27.96	-1.67	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-52.17	16.16	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-1.86	-0.03	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.14	-5.68	-3.54	CaSO4:0.5H2O
CH4(g)	-136.39	-139.24	-2.84	CH4
Cl2(g)	-25.95	-22.95	2.99	Cl2
CO(g)	-44.17	-47.17	-3.00	CO
CO2(g)	-1.12	-8.95	-7.83	CO2
Gaylussite	-16.46	-5.30	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.12	-16.59	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-39.55	-42.65	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-131.08	-139.07	-7.99	H2S
Halite	-9.47	-7.91	1.56	NaCl
HCl(g)	-16.05	-9.75	6.30	HCl
Hydrophilite	-22.33	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-23.65	8.92	32.57	CaO
Mirabilite	-9.76	-10.92	-1.15	Na2SO4:10H2O

Monohydrocalcite	-2.71	-0.03	2.68	CaCO3:H2O
N2(g)	-4.12	-7.30	-3.18	N2
Na	-63.81	3.56	67.37	Na
Na(g)	-77.30	3.56	80.86	Na
Na2CO3	-16.43	-5.27	11.16	Na2CO3
Na2CO3:7H2O	-15.21	-5.27	9.94	Na2CO3:7H2O
Na2O	-63.74	3.68	67.42	Na2O
Na3H(SO4)2	-22.78	-23.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.61	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.97	-7.11	-0.14	NaHCO3
Natron	-14.86	-5.27	9.59	Na2CO3:10H2O
NH3(g)	-58.50	-56.70	1.80	NH3
NO(g)	-19.23	-18.49	0.74	NO
NO2(g)	-15.06	-6.71	8.35	NO2
O2(g)	-4.01	-6.90	-2.89	O2
Pirssonite	-16.62	-5.30	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-13.63	8.92	22.55	Ca(OH)2
S	-97.41	-142.52	-45.11	S
S2(g)	-208.72	-215.91	-7.19	S2
SO2(g)	-48.82	-48.65	0.18	SO2
Th	-189.88	19.71	209.59	Th
Th(g)	-288.13	19.71	307.84	Th
Th(NO3)4:5H2O	-22.70	-20.93	1.77	Th(NO3)4:5H2O
Th(OH)4	3.15	12.81	9.66	Th(OH)4
Th(SO4)2	3.95	-16.37	-20.32	Th(SO4)2
Th2S3	-483.32	-388.15	95.17	Th2S3
Th7S12	-1776.36	-1572.30	204.06	Th7S12
ThCl4	-50.03	-26.19	23.84	ThCl4
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-16.20	-5.27	10.94	Na2CO3:H2O
Thorianite	10.95	12.81	1.86	ThO2
ThS	-218.85	-122.81	96.04	ThS
ThS2	-276.12	-265.34	10.78	ThS2

End of simulation.

Reading input data for simulation 2.

End of run.

No memory leaks

Run 19

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 19 # Equil with Th(OH)4 only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 #= -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1
Th(OH)4 0.0 6.47E-4
END

TITLE

Run 19

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04

S

1.856e-03 1.856e-03

-----Description of solution-----

pH = 7.800
 pe = -1.690
 Activity of water = 1.000
 Ionic strength = 1.113e-02
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 3.427e-03
 Total CO2 (mol/kg) = 3.427e-03
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -1.908e-06
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = -0.01
 Iterations = 4
 Total H = 1.110539e+02
 Total O = 5.554293e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				

Cl (7)	ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048
		0.000e+00				
H (0)	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
		9.537e-16				
Na	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
		0.000e+00				
O (0)	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
		1.368e-26				
S (-2)	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
		3.392e-32				
S (2)	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S (3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S (4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
		0.000e+00				
S (5)	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
		1.856e-03				
S (6)	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
		0.000e+00				
S (7)	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
		0.000e+00				
S (8)	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----
--

Phase	SI log IAP	log KT	Moles in assemblage		
			Initial	Final	Delta
Th(OH)4	0.00	9.66	9.66	6.470e-04	6.466e-04 -4.473e-07

-----Solution composition-----
--

Elements	Molality	Moles
C	3.427e-03	3.427e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04
S	1.856e-03	1.856e-03
Th	4.473e-07	4.473e-07

-----Description of solution-----
--

equilibrium	pH	=	7.800	Charge balance
	pe	=	9.978	Adjusted to redox
	Activity of water	=	1.000	
	Ionic strength	=	1.113e-02	
	Mass of water (kg)	=	1.000e+00	
	Total alkalinity (eq/kg)	=	3.376e-03	
	Total CO2 (mol/kg)	=	3.427e-03	
	Temperature (deg C)	=	25.000	
	Electrical balance (eq)	=	-1.908e-06	
	Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.01	
	Iterations	=	18	
	Total H	=	1.110539e+02	
	Total O	=	5.554293e+01	

-----Distribution of species-----
--

Species	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(-2)	0.000e+00				
C2H4	0.000e+00	0.000e+00	-230.450	-230.450	0.000
C(-3)	0.000e+00				
C2H6	0.000e+00	0.000e+00	-197.118	-197.118	0.000
C(-4)	0.000e+00				
CH4	0.000e+00	0.000e+00	-124.666	-124.666	0.000

C(2)		0.000e+00				
	CO	0.000e+00	0.000e+00	-44.574	-44.574	0.000
C(4)		3.427e-03				
	HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
	CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca		3.542e-03				
	Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
	CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)		1.242e-04				
	Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
	CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
	HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
	ThCl+3	7.801e-25	3.012e-25	-24.108	-24.521	-0.413
	ThCl2+2	2.618e-29	1.705e-29	-28.582	-28.768	-0.186
	ThCl3+	1.399e-32	1.256e-32	-31.854	-31.901	-0.047
	ThCl4	5.247e-37	5.247e-37	-36.280	-36.280	0.000
Cl(1)		5.288e-27				
	ClO-	3.461e-27	3.107e-27	-26.461	-26.508	-0.047
	HClO	1.826e-27	1.826e-27	-26.738	-26.738	0.000
Cl(3)		0.000e+00				
	ClO2-	0.000e+00	0.000e+00	-41.908	-41.955	-0.047
	HClO2	0.000e+00	0.000e+00	-46.586	-46.586	0.000
Cl(5)		0.000e+00				
	ClO3-	0.000e+00	0.000e+00	-43.503	-43.551	-0.048
Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-49.400	-49.448	-0.048
H(0)		4.405e-39				
	H2	2.203e-39	2.208e-39	-38.657	-38.656	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		2.604e-15				
	O2	1.302e-15	1.305e-15	-14.885	-14.884	0.001
	S3O6-2	0.000e+00	0.000e+00	-156.229	-156.418	-0.189
	S2-2	0.000e+00	0.000e+00	-212.620	-212.809	-0.189
	S4O6-2	0.000e+00	0.000e+00	-231.218	-231.407	-0.189
	S3-2	0.000e+00	0.000e+00	-301.032	-301.221	-0.189
	S5O6-2	0.000e+00	0.000e+00	-335.087	-335.276	-0.189
	S4-2	0.000e+00	0.000e+00	-389.671	-389.860	-0.189
	S5-2	0.000e+00	0.000e+00	-478.527	-478.716	-0.189
S(-2)		0.000e+00				

	HS-	0.000e+00	0.000e+00	-119.265	-119.312	-0.048
	H2S	0.000e+00	0.000e+00	-120.103	-120.103	0.000
	S-2	0.000e+00	0.000e+00	-124.255	-124.438	-0.183
	S2-2	0.000e+00	0.000e+00	-212.620	-212.809	-0.189
	S3-2	0.000e+00	0.000e+00	-301.032	-301.221	-0.189
	S4-2	0.000e+00	0.000e+00	-389.671	-389.860	-0.189
	S5-2	0.000e+00	0.000e+00	-478.527	-478.716	-0.189
S (2)		0.000e+00				
	S2O3-2	0.000e+00	0.000e+00	-125.112	-125.302	-0.189
	HS2O3-	0.000e+00	0.000e+00	-132.041	-132.088	-0.047
S (3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-119.985	-120.168	-0.183
S (4)		0.000e+00				
	SO3-2	0.000e+00	0.000e+00	-41.988	-42.174	-0.186
	HSO3-	0.000e+00	0.000e+00	-42.695	-42.742	-0.047
	H2SO3	0.000e+00	0.000e+00	-48.561	-48.561	0.000
	SO2	0.000e+00	0.000e+00	-48.661	-48.661	0.000
	S2O5-2	0.000e+00	0.000e+00	-90.126	-90.315	-0.189
	S3O6-2	0.000e+00	0.000e+00	-156.229	-156.418	-0.189
	S4O6-2	0.000e+00	0.000e+00	-231.218	-231.407	-0.189
	S5O6-2	0.000e+00	0.000e+00	-335.087	-335.276	-0.189
S (5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-65.334	-65.523	-0.189
S (6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	Th(SO4)2	1.305e-18	1.305e-18	-17.885	-17.885	0.000
	ThSO4+2	1.005e-19	6.543e-20	-18.998	-19.184	-0.186
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
	Th(SO4)3-2	1.150e-20	7.444e-21	-19.939	-20.128	-0.189
	Th(SO4)4-4	4.267e-25	7.456e-26	-24.370	-25.128	-0.758
S (7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-51.305	-51.494	-0.189
S (8)		3.515e-36				
	HSO5-	3.515e-36	3.155e-36	-35.454	-35.501	-0.047
Th		4.473e-07				
	Th(OH)4	4.472e-07	4.472e-07	-6.350	-6.350	0.000
	Th(OH)3+	1.121e-10	1.006e-10	-9.950	-9.997	-0.047
	Th(OH)2+2	1.384e-13	9.017e-14	-12.859	-13.045	-0.186
	ThOH+3	6.153e-18	2.375e-18	-17.211	-17.624	-0.413
	Th(SO4)2	1.305e-18	1.305e-18	-17.885	-17.885	0.000
	ThSO4+2	1.005e-19	6.543e-20	-18.998	-19.184	-0.186
	Th(SO4)3-2	1.150e-20	7.444e-21	-19.939	-20.128	-0.189
	Th+4	1.229e-21	2.918e-22	-20.911	-21.535	-0.624
	ThCl+3	7.801e-25	3.012e-25	-24.108	-24.521	-0.413
	Th(SO4)4-4	4.267e-25	7.456e-26	-24.370	-25.128	-0.758
	ThCl2+2	2.618e-29	1.705e-29	-28.582	-28.768	-0.186
	ThCl3+	1.399e-32	1.256e-32	-31.854	-31.901	-0.047
	Th2(OH)2+6	4.770e-33	1.178e-34	-32.321	-33.929	-1.607
	ThCl4	5.247e-37	5.247e-37	-36.280	-36.280	0.000
	Th4(OH)8+8	0.000e+00	0.000e+00	-42.635	-45.493	-2.858
	Th6(OH)15+9	0.000e+00	0.000e+00	-46.275	-49.892	-3.617

-----Saturation indices-----

--

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2·6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4·0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-59.60	4.54	64.15	C
C(g)	-177.22	4.54	181.77	C
Ca	-119.47	20.36	139.83	Ca
Ca(g)	-144.71	20.36	165.07	Ca
Ca2Cl2(OH)2·H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2·H2O
Ca4Cl2(OH)6·13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6·13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4·0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4·0.5H2O
CH4(g)	-121.82	-124.67	-2.84	CH4
Cl2(g)	-33.95	-30.95	2.99	Cl2
CO(g)	-41.58	-44.57	-3.00	CO
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2·5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4·2H2O
H2(g)	-35.55	-38.66	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-119.12	-127.11	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4·10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3·H2O
Na	-59.81	7.56	67.37	Na
Na(g)	-73.30	7.56	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3·7H2O	-12.60	-2.66	9.94	Na2CO3·7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3·2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3·2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3·10H2O
O2(g)	-11.99	-14.88	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2·2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-89.44	-134.55	-45.11	S
S2(g)	-192.78	-199.97	-7.19	S2
SO2(g)	-48.84	-48.66	0.18	SO2
Th	-185.04	24.55	209.59	Th
Th(g)	-283.29	24.55	307.84	Th
Th(OH)4	-0.00	9.66	9.66	Th(OH)4
Th(SO4)2	-7.21	-27.53	-20.32	Th(SO4)2
Th2S3	-449.74	-354.56	95.17	Th2S3
Th7Si12	-1646.86	-1442.81	204.06	Th7Si12
ThCl4	-61.19	-37.35	23.84	ThCl4
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3·H2O

Thorianite	7.80	9.66	1.86	ThO2
ThS	-206.04	-110.01	96.04	ThS
ThS2	-255.34	-244.56	10.78	ThS2

 End of simulation.

 Reading input data for simulation 2.

 End of run.

No memory leaks

Run 20

Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

TITLE Run 20 # Equil with Th(SO4)2 only - using Llnl database
SOLUTION 1 Solution Information Provided by LES: Claiborne EIS pg A-12.

pH 7.8
temp 25.0
pe -1.69 # = -100 mV, pe=eh/0.059 (Stumm & Morgan, pg 423)
units ppm
Alkalinity 205.7 as HCO3
Ca 141.9
Cl 4.4
Na 2.85
S 178.2

EQUILIBRIUM_PHASES 1
Th(SO4)2 0.0 6.47E-4
END

TITLE

Run 20

Beginning of initial solution calculations.

Initial solution 1. Solution Information Provided by LES: Claiborne EIS
pg A-12.

-----Solution composition-----
--

Elements	Molality	Moles
Alkalinity	3.374e-03	3.374e-03
Ca	3.542e-03	3.542e-03
Cl	1.242e-04	1.242e-04
Na	1.240e-04	1.240e-04

S

1.856e-03 1.856e-03

-----Description of solution-----

```

pH = 7.800
pe = -1.690
Activity of water = 1.000
Ionic strength = 1.113e-02
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 3.427e-03
Total CO2 (mol/kg) = 3.427e-03
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.908e-06
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.01
Iterations = 4
Total H = 1.110539e+02
Total O = 5.554293e+01

```

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.783e-07	6.078e-07	-6.169	-6.216	-0.048
H+	1.740e-08	1.585e-08	-7.759	-7.800	-0.041
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000
C(4)	3.427e-03				
HCO3-	3.193e-03	2.866e-03	-2.496	-2.543	-0.047
CO2	1.051e-04	1.054e-04	-3.978	-3.977	0.001
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CO3-2	1.232e-05	8.022e-06	-4.909	-5.096	-0.186
NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
Ca	3.542e-03				
Ca+2	3.122e-03	2.071e-03	-2.506	-2.684	-0.178
CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
CaHCO3+	7.836e-05	7.034e-05	-4.106	-4.153	-0.047
CaCO3	3.851e-05	3.851e-05	-4.414	-4.414	0.000
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
CaOH+	2.056e-08	1.846e-08	-7.687	-7.734	-0.047
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
Cl(-1)	1.242e-04				
Cl-	1.241e-04	1.110e-04	-3.906	-3.955	-0.048
CaCl+	5.430e-08	4.874e-08	-7.265	-7.312	-0.047
NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
CaCl2	6.365e-12	6.365e-12	-11.196	-11.196	0.000
HCl	3.952e-13	3.952e-13	-12.403	-12.403	0.000
Cl(1)	0.000e+00				
ClO-	0.000e+00	0.000e+00	-49.796	-49.843	-0.047
HClO	0.000e+00	0.000e+00	-50.074	-50.074	0.000
Cl(3)	0.000e+00				
ClO2-	0.000e+00	0.000e+00	-88.579	-88.626	-0.047
HClO2	0.000e+00	0.000e+00	-93.256	-93.256	0.000
Cl(5)	0.000e+00				

	ClO3-	0.000e+00	0.000e+00	-113.510	-113.557	-0.048
Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-142.742	-142.790	-0.048
H(0)		9.537e-16				
	H2	4.768e-16	4.781e-16	-15.322	-15.320	0.001
Na		1.240e-04				
	Na+	1.228e-04	1.102e-04	-3.911	-3.958	-0.047
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	NaHCO3	4.517e-07	4.517e-07	-6.345	-6.345	0.000
	NaCO3-	3.446e-09	3.093e-09	-8.463	-8.510	-0.047
	NaCl	2.150e-09	2.150e-09	-8.668	-8.668	0.000
	NaOH	1.156e-11	1.156e-11	-10.937	-10.937	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	O2	0.000e+00	0.000e+00	-61.556	-61.555	0.001
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(-2)		1.368e-26				
	HS-	1.195e-26	1.071e-26	-25.923	-25.970	-0.048
	H2S	1.734e-27	1.734e-27	-26.761	-26.761	0.000
	S-2	1.222e-31	8.010e-32	-30.913	-31.096	-0.183
	S2-2	0.000e+00	0.000e+00	-49.272	-49.461	-0.189
	S3-2	0.000e+00	0.000e+00	-67.677	-67.866	-0.189
	S4-2	0.000e+00	0.000e+00	-86.310	-86.499	-0.189
	S5-2	0.000e+00	0.000e+00	-105.160	-105.349	-0.189
S(2)		3.392e-32				
	S2O3-2	1.696e-32	1.097e-32	-31.771	-31.960	-0.189
	HS2O3-	2.000e-39	1.796e-39	-38.699	-38.746	-0.047
S(3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-49.978	-50.162	-0.183
S(4)		2.664e-19				
	SO3-2	2.227e-19	1.451e-19	-18.652	-18.838	-0.186
	HSO3-	4.366e-20	3.919e-20	-19.360	-19.407	-0.047
	H2SO3	5.953e-26	5.953e-26	-25.225	-25.225	0.000
	SO2	4.726e-26	4.726e-26	-25.325	-25.325	0.000
	S2O5-2	0.000e+00	0.000e+00	-43.455	-43.644	-0.189
	S3O6-2	0.000e+00	0.000e+00	-62.887	-63.076	-0.189
	S4O6-2	0.000e+00	0.000e+00	-67.870	-68.059	-0.189
	S5O6-2	0.000e+00	0.000e+00	-101.732	-101.921	-0.189
S(5)		0.000e+00				
	S2O6-2	0.000e+00	0.000e+00	-41.998	-42.187	-0.189
S(6)		1.856e-03				
	SO4-2	1.552e-03	1.004e-03	-2.809	-2.998	-0.189
	CaSO4	3.038e-04	3.038e-04	-3.517	-3.517	0.000
	NaSO4-	8.144e-07	7.310e-07	-6.089	-6.136	-0.047
	HSO4-	1.791e-09	1.608e-09	-8.747	-8.794	-0.047
	H2SO4	2.404e-20	2.404e-20	-19.619	-19.619	0.000
S(7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-74.640	-74.829	-0.189
S(8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-58.790	-58.836	-0.047

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.33	-5.68	-4.35	CaSO4
Antarcticite	-14.69	-10.59	4.09	CaCl2:6H2O
Aragonite	0.60	2.57	1.97	CaCO3
Bassanite	-1.98	-5.68	-3.71	CaSO4:0.5H2O
Burkeite	-33.97	-24.49	9.49	Na6CO3(SO4)2
C	-12.93	51.21	64.15	C
C(g)	-130.55	51.21	181.77	C
Ca	-96.14	43.69	139.83	Ca
Ca(g)	-121.38	43.69	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.97	2.32	26.29	Ca2Cl2(OH)2:H2O
Ca4Cl2(OH)6:13H2O	-40.17	28.15	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.75	2.57	1.82	CaCO3
CaSO4:0.5H2O(beta)	-2.15	-5.68	-3.54	CaSO4:0.5H2O
Cl2(g)	-57.28	-54.29	2.99	Cl2
CO2(g)	-2.51	-10.34	-7.83	CO2
Gaylussite	-11.25	-0.09	11.16	CaNa2(CO3)2:5H2O
Glauberite	-11.13	-16.60	-5.47	Na2Ca(SO4)2
Gypsum	-1.15	-5.68	-4.53	CaSO4:2H2O
H2(g)	-12.22	-15.32	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-25.78	-33.77	-7.99	H2S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-18.06	-11.75	6.30	HCl
Hydrophilite	-22.34	-10.59	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Lime	-19.65	12.92	32.57	CaO
Mirabilite	-9.76	-10.91	-1.15	Na2SO4:10H2O
Monohydrocalcite	-0.10	2.57	2.68	CaCO3:H2O
Na	-48.14	19.23	67.37	Na
Na(g)	-61.63	19.23	80.86	Na
Na2CO3	-13.82	-2.66	11.16	Na2CO3
Na2CO3:7H2O	-12.60	-2.66	9.94	Na2CO3:7H2O
Na2O	-59.73	7.68	67.42	Na2O
Na3H(SO4)2	-24.78	-25.67	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-21.62	-27.51	-5.89	Na4Ca(SO4)3:2H2O
Nahcolite	-6.36	-6.50	-0.14	NaHCO3
Natron	-12.25	-2.66	9.59	Na2CO3:10H2O
O2(g)	-58.66	-61.56	-2.89	O2
Pirssonite	-11.41	-0.09	11.32	Na2Ca(CO3)2:2H2O
Portlandite	-9.63	12.92	22.55	Ca(OH)2
S	-19.44	-64.55	-45.11	S
S2(g)	-52.77	-59.95	-7.19	S2
SO2(g)	-25.50	-25.33	0.18	SO2
Thenardite	-10.56	-10.91	-0.36	Na2SO4
Thermonatrite	-13.59	-2.66	10.94	Na2CO3:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1. Solution Information Provided by LES: Claiborne EIS pg A-12.

Using pure phase assemblage 1.

-----Phase assemblage-----

C(2)		1.082e-20				
	CO	1.082e-20	1.082e-20	-19.966	-19.966	0.000
C(4)		3.427e-03				
	HCO3-	2.409e-03	2.160e-03	-2.618	-2.666	-0.047
	CO2	9.560e-04	9.587e-04	-3.020	-3.018	0.001
	CaHCO3+	5.861e-05	5.254e-05	-4.232	-4.280	-0.047
	CaCO3	2.382e-06	2.382e-06	-5.623	-5.623	0.000
	CO3-2	7.728e-07	5.008e-07	-6.112	-6.300	-0.188
	NaHCO3	3.397e-07	3.397e-07	-6.469	-6.469	0.000
	NaCO3-	2.150e-10	1.927e-10	-9.668	-9.715	-0.047
Ca		3.542e-03				
	Ca+2	3.108e-03	2.053e-03	-2.507	-2.688	-0.180
	CaSO4	3.730e-04	3.730e-04	-3.428	-3.428	0.000
	CaHCO3+	5.861e-05	5.254e-05	-4.232	-4.280	-0.047
	CaCO3	2.382e-06	2.382e-06	-5.623	-5.623	0.000
	CaCl+	5.381e-08	4.824e-08	-7.269	-7.317	-0.047
	CaOH+	1.690e-09	1.515e-09	-8.772	-8.820	-0.047
	CaCl2	6.291e-12	6.291e-12	-11.201	-11.201	0.000
Cl(-1)		1.242e-04				
	Cl-	1.241e-04	1.109e-04	-3.906	-3.955	-0.049
	CaCl+	5.381e-08	4.824e-08	-7.269	-7.317	-0.047
	NaCl	2.143e-09	2.143e-09	-8.669	-8.669	0.000
	CaCl2	6.291e-12	6.291e-12	-11.201	-11.201	0.000
	HCl	4.765e-12	4.765e-12	-11.322	-11.322	0.000
	ThCl+3	8.396e-18	3.205e-18	-17.076	-17.494	-0.418
	ThCl2+2	2.797e-22	1.812e-22	-21.553	-21.742	-0.188
	ThCl3+	1.487e-25	1.333e-25	-24.828	-24.875	-0.047
	ThCl4	5.561e-30	5.561e-30	-29.255	-29.255	0.000
Cl(1)		0.000e+00				
	HClO	0.000e+00	0.000e+00	-49.307	-49.307	0.000
	ClO-	0.000e+00	0.000e+00	-50.110	-50.158	-0.047
Cl(3)		0.000e+00				
	ClO2-	0.000e+00	0.000e+00	-89.208	-89.255	-0.047
	HClO2	0.000e+00	0.000e+00	-92.804	-92.804	0.000
Cl(5)		0.000e+00				
	ClO3-	0.000e+00	0.000e+00	-114.452	-114.500	-0.048
Cl(7)		0.000e+00				
	ClO4-	0.000e+00	0.000e+00	-143.999	-144.047	-0.048
H(0)		1.966e-15				
	H2	9.828e-16	9.855e-16	-15.008	-15.006	0.001
Na		1.240e-04				
	Na+	1.227e-04	1.100e-04	-3.911	-3.959	-0.047
	NaSO4-	1.008e-06	9.038e-07	-5.996	-6.044	-0.047
	NaHCO3	3.397e-07	3.397e-07	-6.469	-6.469	0.000
	NaCl	2.143e-09	2.143e-09	-8.669	-8.669	0.000
	NaCO3-	2.150e-10	1.927e-10	-9.668	-9.715	-0.047
	NaOH	9.553e-13	9.553e-13	-12.020	-12.020	0.000
O(0)		0.000e+00				
	S2-2	0.000e+00	0.000e+00	-44.721	-44.912	-0.191
	S3O6-2	0.000e+00	0.000e+00	-57.022	-57.213	-0.191
	S4O6-2	0.000e+00	0.000e+00	-58.806	-58.997	-0.191
	S3-2	0.000e+00	0.000e+00	-59.928	-60.119	-0.191
	O2	0.000e+00	0.000e+00	-62.185	-62.183	0.001
	S4-2	0.000e+00	0.000e+00	-75.362	-75.553	-0.191
	S5O6-2	0.000e+00	0.000e+00	-89.469	-89.660	-0.191
	S5-2	0.000e+00	0.000e+00	-91.012	-91.203	-0.191
S(-2)		8.881e-24				

	H2S	5.652e-24	5.652e-24	-23.248	-23.248	0.000
	HS-	3.229e-24	2.890e-24	-23.491	-23.539	-0.048
	S-2	2.746e-30	1.791e-30	-29.561	-29.747	-0.186
	S2-2	0.000e+00	0.000e+00	-44.721	-44.912	-0.191
	S3-2	0.000e+00	0.000e+00	-59.928	-60.119	-0.191
	S4-2	0.000e+00	0.000e+00	-75.362	-75.553	-0.191
	S5-2	0.000e+00	0.000e+00	-91.012	-91.203	-0.191
S (2)		1.376e-28				
	S2O3-2	6.882e-29	4.430e-29	-28.162	-28.354	-0.191
	HS2O3-	9.762e-35	8.751e-35	-34.010	-34.058	-0.047
S (3)		0.000e+00				
	S2O4-2	0.000e+00	0.000e+00	-46.684	-46.870	-0.186
S (4)		1.919e-18				
	HSO3-	1.347e-18	1.208e-18	-17.870	-17.918	-0.047
	SO3-2	5.716e-19	3.704e-19	-18.243	-18.431	-0.188
	H2SO3	2.215e-23	2.215e-23	-22.655	-22.655	0.000
	SO2	1.759e-23	1.759e-23	-22.755	-22.755	0.000
	S2O5-2	0.000e+00	0.000e+00	-40.475	-40.666	-0.191
	S3O6-2	0.000e+00	0.000e+00	-57.022	-57.213	-0.191
	S4O6-2	0.000e+00	0.000e+00	-58.806	-58.997	-0.191
	S5O6-2	0.000e+00	0.000e+00	-89.469	-89.660	-0.191
S (5)		9.303e-40				
	S2O6-2	4.652e-40	2.994e-40	-39.332	-39.524	-0.191
S (6)		2.307e-03				
	SO4-2	1.933e-03	1.244e-03	-2.714	-2.905	-0.191
	CaSO4	3.730e-04	3.730e-04	-3.428	-3.428	0.000
	NaSO4-	1.008e-06	9.038e-07	-5.996	-6.044	-0.047
	HSO4-	2.682e-08	2.404e-08	-7.572	-7.619	-0.047
	Th(SO4) 2	2.134e-11	2.134e-11	-10.671	-10.671	0.000
	ThSO4+2	1.333e-12	8.638e-13	-11.875	-12.064	-0.188
	Th(SO4) 3-2	2.343e-13	1.508e-13	-12.630	-12.822	-0.191
	Th(SO4) 4-4	1.094e-17	1.871e-18	-16.961	-17.728	-0.767
	H2SO4	4.340e-18	4.340e-18	-17.363	-17.363	0.000
S (7)		0.000e+00				
	S2O8-2	0.000e+00	0.000e+00	-72.602	-72.794	-0.191
S (8)		0.000e+00				
	HSO5-	0.000e+00	0.000e+00	-57.928	-57.976	-0.047
Th		2.250e-04				
	Th(OH) 4	2.244e-04	2.244e-04	-3.649	-3.649	0.000
	Th(OH) 3+	6.797e-07	6.093e-07	-6.168	-6.215	-0.047
	Th(OH) 2+2	1.018e-08	6.593e-09	-7.992	-8.181	-0.188
	Th(SO4) 2	2.134e-11	2.134e-11	-10.671	-10.671	0.000
	ThOH+3	5.493e-12	2.097e-12	-11.260	-11.678	-0.418
	ThSO4+2	1.333e-12	8.638e-13	-11.875	-12.064	-0.188
	Th(SO4) 3-2	2.343e-13	1.508e-13	-12.630	-12.822	-0.191
	Th+4	1.329e-14	3.110e-15	-13.877	-14.507	-0.631
	Th(SO4) 4-4	1.094e-17	1.871e-18	-16.961	-17.728	-0.767
	ThCl+3	8.396e-18	3.205e-18	-17.076	-17.494	-0.418
	Th6(OH) 15+9	5.073e-21	1.114e-24	-20.295	-23.953	-3.658
	Th2(OH) 2+6	3.878e-21	9.182e-23	-20.411	-22.037	-1.626
	ThCl2+2	2.797e-22	1.812e-22	-21.553	-21.742	-0.188
	Th4(OH) 8+8	7.143e-24	9.193e-27	-23.146	-26.037	-2.890
	ThCl3+	1.487e-25	1.333e-25	-24.828	-24.875	-0.047
	ThCl4	5.561e-30	5.561e-30	-29.255	-29.255	0.000

-----Saturation indices-----

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Phase	SI	log IAP	log KT	
Anhydrite	-1.24	-5.59	-4.35	CaSO ₄
Antarcticite	-14.69	-10.60	4.09	CaCl ₂ :6H ₂ O
Aragonite	-0.61	1.36	1.97	CaCO ₃
Bassanite	-1.89	-5.59	-3.71	CaSO ₄ :0.5H ₂ O
Burkeite	-35.00	-25.51	9.49	Na ₆ CO ₃ (SO ₄) ₂
C	-11.35	52.80	64.15	C
C(g)	-128.97	52.80	181.77	C
Ca	-97.99	41.84	139.83	Ca
Ca(g)	-123.23	41.84	165.07	Ca
Ca ₂ Cl ₂ (OH) ₂ :H ₂ O	-26.14	0.15	26.29	Ca ₂ Cl ₂ (OH) ₂ :H ₂ O
Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O	-46.68	21.65	68.33	Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O
Calcite	-0.46	1.36	1.82	CaCO ₃
CaSO ₄ :0.5H ₂ O(beta)	-2.06	-5.59	-3.54	CaSO ₄ :0.5H ₂ O
CH ₄ (g)	-26.27	-29.11	-2.84	CH ₄
Cl ₂ (g)	-55.43	-52.44	2.99	Cl ₂
CO(g)	-16.97	-19.97	-3.00	CO
CO ₂ (g)	-1.56	-9.38	-7.83	CO ₂
Gaylussite	-13.66	-2.50	11.16	CaNa ₂ (CO ₃) ₂ :5H ₂ O
Glauberite	-10.95	-16.42	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-1.06	-5.59	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-11.91	-15.01	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
H ₂ S(g)	-22.26	-30.26	-7.99	H ₂ S
Halite	-9.48	-7.91	1.56	NaCl
HCl(g)	-16.98	-10.67	6.30	HCl
Hydrophilite	-22.34	-10.60	11.75	CaCl ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Lime	-21.82	10.75	32.57	CaO
Mirabilite	-9.67	-10.82	-1.15	Na ₂ SO ₄ :10H ₂ O
Monohydrocalcite	-1.31	1.36	2.68	CaCO ₃ :H ₂ O
Na	-49.07	18.31	67.37	Na
Na(g)	-62.55	18.31	80.86	Na
Na ₂ CO ₃	-15.03	-3.86	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-13.80	-3.87	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-61.90	5.52	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-23.51	-24.40	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-21.34	-27.24	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-6.48	-6.62	-0.14	NaHCO ₃
Natron	-13.45	-3.87	9.59	Na ₂ CO ₃ :10H ₂ O
O ₂ (g)	-59.29	-62.18	-2.89	O ₂
Pirssonite	-13.82	-2.50	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Portlandite	-11.80	10.75	22.55	Ca(OH) ₂
S	-16.24	-61.35	-45.11	S
S ₂ (g)	-46.37	-53.56	-7.19	S ₂
SO ₂ (g)	-22.93	-22.75	0.18	SO ₂
Th	-135.04	74.55	209.59	Th
Th(g)	-233.29	74.55	307.84	Th
Th(OH) ₄	2.70	12.37	9.66	Th(OH) ₄
Th(SO ₄) ₂	0.00	-20.32	-20.32	Th(SO ₄) ₂
Th ₂ S ₃	-130.12	-34.95	95.17	Th ₂ S ₃
Th ₇ S ₁₂	-418.40	-214.35	204.06	Th ₇ S ₁₂
ThCl ₄	-54.17	-30.33	23.84	ThCl ₄
Thenardite	-10.47	-10.82	-0.36	Na ₂ SO ₄
Thermonatrite	-14.80	-3.86	10.94	Na ₂ CO ₃ :H ₂ O

Thorianite	10.50	12.37	1.86	ThO2
ThS	-82.84	13.20	96.04	ThS
ThS2	-58.93	-48.15	10.78	ThS2

 End of simulation.

 Reading input data for simulation 2.

 End of run.

No memory leaks

12.