From: Joseph A. Rard [rard1@llnl.gov]
Sent: Friday, May 19, 2006 5:44 PM
To: Roberto Pabalan
Subject: RE: tables

Bobby,

The one data set you might be able to model is the NaCl + Ca(NO3)2 + H2O set below, where only a very small amount of precipitate was present. For all of the mixture experiments the very high salt loadings and huge temperature coefficients of solubility for sodium and potassium nitrate made it impossible to remove solution samples at the boiling temperature for molality analysis.

Because of the desperate funding situation, most people are leaving the YMP project at LLNL. I don't know if I will have enough work from them next week to cover my time. I am pretty certain that I will retire from LLNL on Sept. 30, 2007 when the U.C. contract to operate LLNL ends, and then look for part time work. The continual search for accounts is far more stressful than doing actual work. Even if Sandia were to send more work to LLNL next year (which I don't expect), it would be too late to be of much benefit to me and it also would be difficult to lure back the personnel that were let go by them this year.

Joe

Table IV. Boiling Temperatures for Saturated Aqueous Solutions of NaCl + Ca(NO3)2 + H2Oa

x{NaCl}	x{Ca(NO3)2}	p/ bar	t/°C
0	1.0000	0.998	150.2±0.0 b
0.1000	0.9000	0.9980	155.4
0.2000	0.8000	0.9934	161.2
0.3000	0.7000	0.9995	145.8
0.4000	0.6000	1.0022	126.6
0.5000	0.5000	1.0035	119.8
0.6000	0.4000	1.0029	116.1
0.7000	0.3000	0.9978	113.1
0.8181	0.1819	1.0001	111.2
0.9000	0.1000	0.9965	109.7
0.9500	0.0500	0.9943	109.2
1.0000	0	0.991	107.7±0.2c

a The reported compositions are the solute mole fractions (not including water) that were calculated from the mass of each solute component added to the solution. The initially liquid solutions were heated to evaporate solvent until they became faintly opaque (turbid). This corresponds to the beginning of precipitation of a solid phase, and the reported mole fractions should correspond very closely to the actual solution compositions.
b This is the average of two determinations for $Ca(NO_3)_2 + H_2O$ reported in Table I.
c This is the average of ten determinations for $NaCl + H_2O$ reported in Table I

Joe,

Thanks for the data.

It appears a meaningful comparison between StreamAnalyzer values and your data may not be possible for most of the data points. I forgot I also need the amount of water, which is not measured, to do the calculation. Attached is a comparison of experimental data and boiling points calculated using the moles of $NaNO_3$ and KNO_3 you provided and assuming 5.5509 moles (100 mL)of H_2O in the system. The values at low or high X-$NaNO_3$ agree well with measured values, but the calculated values at intermediate X-$NaNO_3$ values are much lower than measured data because of the incorrect assumption about the amount of H_2O. In particular, the calculated points in the vicinity of X-$NaNO_3$ = 0.5 are unsaturated with respect to the solids.

With respect to LLNL YM funding, what is the effect of Sandia taking over the YM Postclosure work?

Regards,

bobby

-----Original Message-----
From: Joseph A. Rard [mailto:rard1@llnl.gov]
Sent: Friday, May 19, 2006 10:46 AM
To: Roberto T Pabalan
Subject: Fwd: tables

Bobby,

I have annotated the $NaNO_3 + KNO_3 + H_2O$ tables to give the number of moles of each solute. You will notice that there are several

experiments with the same number of moles of of NaNO3 but with different number of moles of KNO3. Those experiments were done by adding a large amount of NaNO3 followed by increasing amounts of KNO3. Similarly, some experiments were done by adding a large amount of KNO3 followed by increasing amounts of NaNO3. In other cases the samples were used for a single experiment and then discarded.

There were several cases when the same samples were used for two or more measurements on different days, and the second experiment (with more solid phase from evaporation of water) gave boiling temperatures 1 to 2 degrees C higher. However, when this was done at x(NaNO3) = 0.4568 and 0.4569 larger differences of 6 to 7 degrees C were found.

This was probably the result of the change from NaNO3 + KNO3 being present initially in the solid phase with increasing formation of the solid solution with each reheating.

There was generally a large amount of solid phase present, which can explain why the b.t.s are generally slightly higher that those calculated for minimal precipitation. However, the slight mismatch for x(NaNO3) = 1 suggests to me that the solubilities of NaNO3 in SteamAnalyzer are a bit low.

I will try to get the NaCl + KNO3 data to you next week.

The YMP personnel at LLNL is about 1/3 of the level two years ago, and many of those remaining are only partially covered and looking for work elsewhere at LLNL.

Joe

Date: Thu, 18 May 2006 16:22:10 -0500
From: Roberto T Pabalan <roberto.pabalan@swri.org>
Subject: Re: boiling point measurements
To: "Joseph A. Rard" <rard1@llnl.gov>
X-Accept-Language: en
Priority: normal
X-Scanned-By: MIMEDefang 2.39

Joe,

The NaCl-KNO3 and NaNO3-KNO3 systems are both of interest, but I would say the NaCl-KNO3 system is more interesting because more salts potentially can form. I have attached two files. The NaNO3-KNO3 file compares your experimental boiling points with values calculated using StreamAnalyzer. There is fairly good agreement considering the X-axis is in terms of mole fraction of NaNO3 added, and my assumed moles of NaNO3 and KNO3 may not correspond with actual moles used in the experiments. The file NaCl-KNO3 also compares your data (closed circles) with StreamAnalyzer results. In this file, the curves are calculated by assuming minimal amount of precipitated solids (trial

and error) and the open circles are not constrained with respect to the total amount of salts added. There is more scatter in your data and in the calculated values, likely due to use of X-NaCl(added) to plot the boiling points. Knowing the actual moles of salt used would enable a better comparison of exper
imental and calculated values.

Thanks.

bobby

Attachment converted: Data:NaNO3-KNO3 boiling points.doc (WDBN/MSWD) (00020768)

Hearing Identifier: HLW_YuccaMountain_Hold_EX
Email Number: 1500

Mail Envelope Properties (p06110409c093e729427e)

Subject: RE: tables
Sent Date: 5/19/2006 5:44:25 PM
Received Date: 5/19/2006 6:02:13 PM
From: Joseph A. Rard

Created By: rard1@llnl.gov

Recipients:
"Roberto Pabalan" <rpabalan@cnwra.swri.edu>
Tracking Status: None

Post Office: [128.115.76.86]

Files	**Size**	**Date & Time**
MESSAGE	6305	5/19/2006 6:02:13 PM

Options
Priority: Standard
Return Notification: No
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Sensitivity: Normal
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