LSNReviews

From: Roberto Pabalan
Sent: Wednesday, December 05, 2007 4:23 PM
To: Ken Chiang; Lietai Yang; Yi-Ming Pan; Osvaldo Pensado; Pavan Shukla
Cc: Xihua He; James Myers
Subject: carbonate concentration in Na-K-Cl-NO3 mixtures
Attachments: carbonate concentration in Na-K-Cl-NO3 mixtures.xls

Per our meeting yesterday on Ken's proposed stress corrosion cracking experiments at high temperatures in deliquescence brines, I have attached an Excel file showing the results of StreamAnalyzer Version 2.0 calculations at 140 and 160 Celsius for salt mixtures in the system Na-K-Cl-NO3.

1. For Na-K-Cl-NO3 solutions in which atmospheric CO2(g) (pCO2 = 10^-3.5 atm) is the only source of dissolved carbonate, the calculated concentration of HCO3- species is ~5E-7 molal. No SCC is expected under this condition, consistent with experiments.

2. For Na-K-Cl-NO3 solutions in which calcite (present in dusts) is the source of dissolved carbonate and in which the aqueous carbonate concentration is constrained by the atmospheric partial pressure of CO2(g) [i.e., pCO2 = 10^3-5 atm], the concentrations of the dominant aqueous carbonate species, CaCO3(aq) and HCO3-, are as follows:
   CaCO3(aq) = 8E-4 or 9E-4 molal (at 140 or 160 C)
   HCO3- = 8E-4 or 5E-4 molal (at 140 or 160 C)
   These values are above the 1E-4 threshold values assumed for the occurrence of SCC.

--Bobby

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Date: Fri, 19 Jan 2007 09:26:28 -0600
From: Pavan Shukla <pshukla@cnwra.swri.edu>
Subject: Changes to the work plan
To: 'CSPE_Group' <CSPE_Group@cnwra.swri.edu>, gcragnolino@satx.rr.com,
Lietai Yang <ltyang@cnwra.swri.edu>, 'Ken Chiang' <kchiang@cnwra.swri.edu>,
ddunn@swri.edu
Cc: gustavo.cragnolino@swri.org
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Temperature = 140 C

Pressure	0.624971	atm
pH	5.99	
Deliq. RH	17.97%	
log pCO2	-3.502	atm

Stream Inflows

H2O	55.5087	mol
NaCl	20	mol
NaNO3	70	mol
KNO3	100	mol
CO2	1.90E-05	mol

Solids Present:

NaCl
KNO3
NaNO3.KNO3

Species Output (True Species)

	Total mol	Aqueous mol	Vapor mol	Solid mol
H2O	55.5087	55.5087	9.99E-09	0
NaCl	16.3589	0	0	16.3589
KNO3	6.05874	0	0	6.05874
CO2	1.85E-05	1.85E-05	5.04E-12	0
HCl	3.76E-08	3.76E-08	3.02E-16	0
HNO3	3.86E-07	3.86E-07	2.97E-16	0
KOH	4.21E-17	4.21E-17	0	0
N2O5	1.40E-19	1.40E-19	1.97E-28	0
NaNO3.KNO3	15.0893	0	0	15.0893
Cl-1	3.64114	3.64114	0	0
CO3-2	2.09E-20	2.09E-20	0	0
H3O+1	7.68E-08	7.68E-08	0	0
HCO3-1	4.99E-07	**4.99E-07**	0	0
K+1	78.852	78.852	0	0
Na+1	58.5519	58.5519	0	0
NO3-1	133.763	133.763	0	0
OH-1	1.91E-09	1.91E-09	0	0

Temperature = 160 C

Pressure	0.967591	atm
pH	6.19	
Deliq. RH	16.47%	
log pCO2	-3.506	atm

Stream Inflows

H2O	55.5087	mol
NaCl	10	mol
NaNO3	100	mol
KNO3	90	mol
CO2	1.10E-05	mol

Solids Present:

NaNO3.KNO3
NaNO3
NaCl

Species Output (True Species)

	Total mol	Aqueous mol	Vapor mol	Solid mol
H2O	55.5087	55.5087	1.00E-08	0
NaCl	5.1961	0	0	5.1961
NaNO3	7.86735	0	0	7.86735
CO2	1.05E-05	1.05E-05	3.22E-12	0
HCl	7.25E-08	7.25E-08	3.70E-16	0
HNO3	4.28E-07	4.28E-07	4.26E-16	0
KOH	7.35E-16	7.35E-16	0	0
N2O5	7.52E-19	7.52E-19	6.97E-28	0
NaNO3.KNO3	21.4768	0	0	21.4768
Cl-1	4.8039	4.8039	0	0
CO3-2	4.39E-21	4.39E-21	0	0
H3O+1	5.08E-08	5.08E-08	0	0
HCO3-1	5.38E-07	**5.38E-07**	0	0
K+1	68.5232	68.5232	0	0
Na+1	75.4598	75.4598	0	0
NO3-1	139.179	139.179	0	0
OH-1	1.36E-08	1.36E-08	0	0

Temperature = 140 C

Pressure	0.632161	atm
pH	9.18	
Deliq. RH	18.17%	
log pCO2	-3.503	atm

Stream Inflows

H2O	55.5087	mol
NaCl	10	mol
NaNO3	100	mol
KNO3	90	mol
CaCO3	1	mol
CO2	4.05E-04	mol

Solids Present:

CaCO3
NaCl
NaNO3
NaNO3.KNO3

Species Output (True Species)

Row Filter Applied: Only Non Zero Values

	Total mol	Aqueous mol	Vapor mol	Solid mol
H2O	55.5083	55.5083	1.00E-08	0
NaCl	6.4709	0	0	6.4709
NaNO3	29.797	0	0	29.797
CaCO3	0.999605	**7.77E-04**	0	0.998828
CO2	1.60E-05	1.60E-05	4.96E-12	0
CaCl2	4.62E-06	4.62E-06	0	0
HCl	2.34E-11	2.34E-11	1.88E-19	0
HNO3	2.48E-10	2.48E-10	1.91E-19	0
KOH	6.69E-14	6.69E-14	0	0
N2O5	5.79E-26	5.79E-26	8.13E-35	0
NaNO3.KNO3	14.5373	0	0	14.5373
Ca+2	3.88E-04	3.88E-04	0	0
CaOH+1	2.78E-06	2.78E-06	0	0
Cl-1	3.52909	3.52909	0	0
CO3-2	5.86E-14	5.86E-14	0	0
H3O+1	4.96E-11	4.96E-11	0	0
HCO3-1	7.84E-04	**7.84E-04**	0	0
K+1	75.4627	7.55E+01	0	0
Na+1	59.1948	5.92E+01	0	0

Temperature = 160 C

Pressure	0.967561	atm
pH	9.19	
Deliq. RH	16.47%	
log pCO2	-3.504	atm

Stream Inflows

H2O	55.5087	mol
NaCl	10	mol
NaNO3	100	mol
KNO3	90	mol
CaCO3	1	mol
CO2	2.70E-04	mol

Solids Present:

CaCO3
NaCl
NaNO3
NaNO3.KNO3

Species Output (True Species)

Row Filter Applied: Only Non Zero Values

	Total mol	Aqueous mol	Vapor mol	Solid mol
H2O	55.5084	55.5084	1.00E-08	0
NaCl	5.19601	0	0	5.19601
NaNO3	7.86783	0	0	7.86783
CaCO3	0.999722	**9.32E-04**	0	0.99879
CO2	1.05E-05	1.05E-05	3.24E-12	0
CaCl2	4.51E-06	4.51E-06	0	0
HCl	7.30E-11	7.30E-11	3.72E-19	0
HNO3	4.31E-10	4.31E-10	4.28E-19	0
KOH	7.30E-13	7.30E-13	0	0
N2O5	7.62E-25	7.62E-25	7.05E-34	0
NaNO3.KNO3	21.4748	0	0	21.4748
Ca+2	2.68E-04	2.68E-04	0	0
CaOH+1	5.37E-06	5.37E-06	0	0
Cl-1	4.80398	4.80398	0	0
CO3-2	4.36E-15	4.36E-15	0	0
H3O+1	5.11E-11	5.11E-11	0	0
HCO3-1	5.38E-04	**5.38E-04**	0	0
K+1	68.5252	68.5252	0	0
Na+1	75.4614	75.4614	0	0

NO3-1	131.128	1.31E+02	0	0	NO3-1	139.183	139.183	0	0
OH-1	3.26E-06	3.26E-06	0	0	OH-1	1.35E-05	1.35E-05	0	0