Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

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Sensitivity ZAM Modeling Study of Tank 10H VDS Waste Sample (U)

T. Hang

June 2018

SRNL-STI-2018-00215, Revision 0

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Printed in the United States of America

Prepared for
U.S. Department of Energy

SRNL-STI-2018-00215
Revision 0

Keywords: *Ion exchange, cesium removal, crystalline silicotitanate, TCCR, ZAM model*

Retention: *Permanent*

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Savannah River National Laboratory™
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REVIEWS AND APPROVALS

AUTHOR:

_____

T. Hang, Environmental Modeling Date

TECHNICAL REVIEW:

_____

J. L. Wohlwend, Environmental Modeling, Reviewed per E7 2.60 Date

APPROVAL:

_____

D. A. Crowley, Manager Date
Environmental Modeling

_____

B. J. Wiedenman, Manager Date
Advanced Characterization & Processing

_____

L. T. Reid, Director, Environmental Restoration Technology Date

_____

M. T. Keefer, Nuclear Safety & Engineering Integration Date

EXECUTIVE SUMMARY

The objective of this work is to study the sensitivity of cesium loading expected on the Tank Closure Cesium Removal (TCCR) columns. Savannah River National Laboratory (SRNL) utilized ZAM, a computer program developed by the research group of Professor Rayford G. Anthony of Texas A&M University, for prediction of cesium loading on the Crystalline Silicotitanate (CST) resin during the processing of Tank 10H Variable Depth Sample (VDS) waste solution.

The study specifically evaluates cesium loading on CST as a function of:

1. Water additions to Tank 10H. Water dilution ranges from 0% to 20%
2. Temperature in Tank 10H for a prepared batch of salt feed. The temperature range of interest varies from 20°C to 40°C.

Modeling Approach

- Cesium loading on CST in the TCCR ion exchange columns was predicted using ZAM.
- The OLI Studio™ software (Version 9.2) from OLI Systems, Inc., was used to calculate charge balanced feed compositions and to estimate feed solution density which are required as input data to the ZAM program.

Results Summary

Results of the ZAM model predictions are:

- Dilution of the salt waste solution with water increases the cesium loading primarily due to the decreased ionic strength. The cesium loading Q – dilution (%) correlation is essentially linear as indicated by the equation and R^2 value obtained within the dilution range of 0% to 20%.

$$Q(Ci/L_{CST}) = 0.4290 * Dilution(Vol\%) + 357.3847 \qquad (R^2 = 0.998)$$

Table E-1. Dilution Effect on Cesium Loading at 23°C.

Cases[a]	**Q**			**$C_f = C_o$**[b]
	$mmol_{Cs}/g_{CST}$	mg_{Cs}/g_{CST}	Ci/L_{Bed}	$mmol_{Cs}/L$
1 (0% Dilution)	0.0951 (0.1025)	12.75 (13.75)	357.2 (385.1)	0.0157 (0.0157)
2 (1% Dilution)	0.0952	12.77	357.7	0.0155
3 (2% Dilution)	0.0954	12.79	358.2	0.0154
4 (3% Dilution)	0.0955	12.80	358.7	0.0153
5 (4% Dilution)	0.0956	12.82	359.3	0.0151
6 (5% Dilution)	0.0957	12.84	359.6	0.015
7 (10% Dilution)	0.0963	12.91	361.8	0.0143
8 (15% Dilution)	0.0968	12.99	363.8	0.0137
9 (20% Dilution)	0.0974 (0.1050)	13.06 (14.08)	365.9 (394.5)	0.0131 (0.0131)

[a] Volume dilution (%) is the percentage ratio of water addition volume to the waste volume

[b] C_o: initial cesium concentration; C_f: equilibrium cesium concentration

( ) Values at 20°C

- Cesium loading decreases with increasing temperatures. The correlation shows that the behavior is essentially a linear effect as indicated by the equation and R^2 value obtained within the temperature range of 20°C to 40°C.

$$Q(Ci/L_{CST}) = -7.3655 * T(^oC) + 524.2962 \qquad (R^2 = 0.993)$$

Table E-2. Temperature Effect on Cesium Loading for Non-Dilution VDS Sample (Case 1).

Case 1 at T (°C)	Q			$C_f = C_o$ [(a)]
	$mmol_{Cs}/g_{CST}$	mg_{Cs}/g_{CST}	Ci/L_{Bed}	$mmol_{Cs}/L$
20	0.1025	13.75	385.1	0.0157
23	0.0951	12.75	357.2	0.0157
24	0.0927	12.44	348.4	0.0157
25	0.0905	12.13	339.8	0.0157
26	0.0882	11.83	331.5	0.0157
27	0.0861	11.54	323.4	0.0157
28	0.0840	11.26	315.4	0.0157
29	0.0819	10.98	307.7	0.0157
30	0.0799	10.72	300.3	0.0157
31	0.0780	10.46	293.0	0.0157
32	0.0761	10.20	285.9	0.0157
33	0.0743	9.96	278.9	0.0157
34	0.0725	9.72	272.2	0.0157
35	0.0707	9.49	265.7	0.0157
37	0.0674	9.04	253.2	0.0157
39	0.0642	8.61	241.3	0.0157
40	0.0627	8.41	235.6	0.0157

(a) C_o: initial cesium concentration; C_f: equilibrium cesium concentration

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LIST OF ABBREVIATIONS

CST	Crystalline Silicotitanate
SRNL	Savannah River National Laboratory
SRR	Savannah River Remediation
SRS	Savannah River Site
TCCR	Tank Closure Cesium Removal
VDS	Variable Depth Sample

1.0 Introduction

1.1 Background

Currently at the Savannah River Site (SRS), the Tank Closure Cesium Removal (TCCR) is an "at-tank" process designed to remove cesium from aqueous tank waste. Cesium will be removed by ion exchange using engineered IONSIV® R9120 form of the crystalline silicotitanate (CST) resin. The current TCCR design has two columns online in a lead-lag configuration to optimize media usage and achieve the target decontamination. Once the lead column is saturated with cesium, it will be removed from service, the lag column will rotate into the lead position, and a new column will be placed into the lag position. The TCCR process for cesium removal from Tank 10H is detailed in X-SOW-H-00002 (Caldwell, 2017).

A computer model, known as ZAM, was developed by the Texas A&M University to predict the equilibrium condition for a liquid in contact with the CST, allowing the calculation of cesium adsorbed on the media (Zheng et al, 1995; Zheng et al., 1996). Such equilibrium is dependent upon multiple factors, including temperature, ionic strength, and concentrations of cesium, potassium, sodium, hydroxide, rubidium, and strontium. It is important to understand that the CST and the aqueous stream reach an equilibrium condition, not a saturation of the CST. The total cesium capacity of CST is much higher than usually encountered in SRS tank waste, but that total capacity cannot be reached because the loading under any condition is thermodynamically limited by the equilibrium, which depends on the composition of the aqueous stream. The current task calculates the maximum loading of cesium onto CST, given an infinite amount of liquid feed. The maximum loading is then species/composition dependent, not volume dependent. The model accounts for the two types of exchange sites that exist on the CST solid, and the composition of the aqueous phase. The model has been used previously to predict loading on CST for both SRS and Hanford tank waste applications (Aleman et al., 2003; Hamm et al., 2001).

It is also worth noting that there are three isotopes of cesium in the SRS tank waste, ^{133}Cs, ^{135}Cs, and ^{137}Cs (Reboul, 2017). The CST removes all isotopes equally. The primary isotope of concern is ^{137}Cs because it has high specific activity. Although rubidium and strontium are known to impact cesium loading, information on the soluble concentration of these species in this waste is not currently available, so they were not included in the modeling. Assuming that these species are not present is conservative, i.e., ZAM would overestimate the cesium loading due to the absence of these competitors.

1.2 Task Objective

Per request of Savannah River Remediation (SRR) (Fairchild, 2017), the task objective is to utilize ZAM to calculate the maximum cesium loading expected on the TCCR columns during the process of cesium removal from Tank 10H waste. Specifically, this study evaluates the impact of cesium loading on CST as a function of: (1) water additions to Tank 10H; and (2) temperature in Tank 10H for a prepared batch of salt feed (see Appendix A).

2.0 Model Formulations

2.1 Modeling Approach

- Cesium loading on the CST resin in the TCCR ion exchange columns was predicted using a computer program developed by the research group of Professor Rayford G. Anthony of TAMU (Zheng et al., 1997). The ZAM program, named after its developers (i.e., Zheng, Anthony, and Miller), was described in great detail in previous ion exchange studies at SRNL (Hamm et al., 2001; Hang et al., 2017).
- The OLI Studio™ software (Version 9.2) from OLI Systems, Inc., was used to calculate charge balanced feed compositions and to estimate feed solution density (OLI Systems, 2014) required as input data to the ZAM program.

2.2 Prediction of Cesium Loading

- Use of an isotherm: An isotherm provides the equilibrium relation between the concentration of cesium loaded on the CST surface to the concentration of cesium in the solution. The isotherm covers a wide range of liquid-phase cesium concentrations. ZAM can generate equilibrium cesium loading data at a given temperature. Generally, an excellent fit for the ZAM data would be achieved by use of the Freundlich/Langmuir isotherm model.
- Variation of ZAM phase ratio: A phase ratio ϕ is defined as the ratio of total liquid volume (mL) processed to the mass of CST resin (g_{CST}). To simulate the saturation of cesium loading on a CST bed in the ion exchange column for a specified feed, ZAM calculations are performed at increasing phase ratios until the calculated equilibrium liquid cesium concentration approximates the feed cesium concentration. The corresponding cesium concentration on CST represents the maximum cesium loading (Hang et al., 2017).

The two approaches should deliver practically identical results. In this study, the variation of ZAM phase ratio approach was followed to predict cesium loading. Also, to provide more conservative outcomes, this study uses ZAM without dilution factor to predict equilibrium cesium loading on CST for waste solutions. A detailed description of dilution factor was provided in a previous report (Hang et al., 2017).

3.0 Waste Compositions and Properties

3.1 VDS Sample

The waste composition was obtained from an analysis of a variable depth sample (VDS) recently collected from Tank 10H (Reboul, 2017). The VDS sample was collected in March 2017 following a water addition to the tank, and allowing the saltcake to dissolve for a few weeks. Note that the total Cs concentration was derived from the measured ^{137}Cs. Although the analyzed molar ratio of ^{137}Cs to total Cs is 0.21 in the VDS composition, the ratio of 0.3 was used for consistency with previous calculations.

A VDS composition at 23°C provided by SRR is shown in Table 3-1. The composition was adjusted by leaving out the competitor cations (i.e., K^+ and $SrOH^+$ or Sr^{2+}) and balancing the charges by increasing CO_3^{2-} (See Appendix A).

Table 3-1. Adjusted VDS Tank 10H Composition at 23°C.

Cations	(M)	Anions	(M)
Na^+	3.22	OH^-	0.184
Cs^+	1.57E-05	NO_3^-	1.04
		NO_2^-	0.128
		$Al(OH)_4^-$	0.0631
		SO_4^{2-}	0.381
		CO_3^{2-} [(a)]	0.51
		Cl^-	4.06E-03
		$C_2O_4^{2-}$	9.20E-03
Density[(b)] (g/mL)	1.16		

[(a)] CO_3^{2-} is adjusted for charge balance
[(b)] Density is calculated by OLI

3.2 Water Dilution

The VDS waste composition was adjusted with water to simulate 0% to 5% (in increments of 1%), 10%, 15%, and 20% water dilution. The volume dilution (%) is defined as the percentage ratio of water addition volume to the waste volume. A total of nine case are generated and summarized in Table 3-2. Note that concentration values in Table 3-2 were subjected to rounding. More accurate values are given in the ZAM input files given in Appendix B.

Table 3-2. Water Dilution of VDS Sample at 23°C.

Cases	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
	0% Dilution (M)	1% Dilution (M)	2% Dilution (M)	3% Dilution (M)	4% Dilution (M)	5% Dilution (M)	10% Dilution (M)	15% Dilution (M)	20% Dilution (M)
Na^+	3.22	3.188	3.157	3.126	3.096	3.067	2.927	2.8	2.683
Cs^+	1.57E-05	1.56E-05	1.54E-05	1.53E-05	1.51E-05	1.50E-05	1.43E-05	1.37E-05	1.31E-05
OH^-	0.184	0.182	0.18	0.179	0.177	0.175	0.167	0.16	0.153
NO_3^-	1.04	1.03	1.02	1.01	1	0.99	0.945	0.904	0.867
NO_2^-	0.128	0.127	0.125	0.124	0.123	0.122	0.116	0.111	0.107
$Al(OH)_4^-$	0.0631	0.0625	0.0619	0.0613	0.0607	0.0601	0.0574	0.0549	0.0526
SO_4^{2-}	0.381	0.377	0.374	0.37	0.366	0.363	0.346	0.331	0.318
CO_3^{2-}	0.51	0.505	0.5	0.495	0.491	0.486	0.464	0.444	0.425
Cl^-	4.06E-03	4.02E-03	3.98E-03	3.94E-03	3.90E-03	3.87E-03	3.69E-03	3.53E-03	3.38E-03
$C_2O_4^{2-}$	9.20E-03	9.11E-03	9.02E-03	8.93E-03	8.85E-03	8.76E-03	8.36E-03	8.00E-03	7.67E-03
Density[(a)] (g/mL)	1.16	1.158	1.157	1.156	1.154	1.153	1.146	1.141	1.135

[(a)] Density is calculated by OLI

3.3 Temperature Variation

To determine the change in cesium loading on CST as a function of temperature, the temperature of Case 1 was varied from 23°C to 35°C in increments of 1°C, and then from 35°C to 40°C in increments of 2°C. An additional run of Case 1 at 20°C was also performed. At each temperature, the liquid waste density was calculated by OLI. Predicted densities are given in Table 3-3.

Table 3-3. Temperature Variation of Case 1.

Case 1 at T (°C)	Density[(a)] (g/mL)
20	1.1611
23	1.1599
24	1.1596
25	1.1592
26	1.1588
27	1.1585
28	1.1581
29	1.1577
30	1.1574
31	1.1570
32	1.1567
33	1.1563
34	1.1560
35	1.1556
37	1.1550
39	1.1543
40	1.1539

[(a)] Density is calculated by OLI

3.4 Quality Assurance

This work was performed under a Task Technical and Quality Assurance Plan, SRNL-RP-2017-00204. ZAM and OLI are controlled at Level D, and so are not usable for safety-related calculations. No variability or uncertainty were included in the calculations.

4.0 Results and Discussion

The calculated results of waste compositions specified in Section 3.0 are presented and discussed in this section. Relevant ZAM data (input, output) are provided in Appendix B. In all ZAM results the following estimates are relevant to the conversion of $mmol_{Cs}/g_{CST}$ to mg_{Cs}/g_{CST} and Ci/L_{Bed}:

- $^{137}Cs/Total\ Cs = 0.3$
- $(M_{Cs})_{avg} = 134.1$ g/gmol
- 11926.67 $Ci/mol_{^{137}Cs}$
- CST bed density = 1.05 g/mL (UOP, 2017)

4.1 Dilution of VDS Sample

Table 4-1 summarizes the ZAM results that would be expected to process the diluted Tank 10H saltcake VDS solutions. Cesium loading on CST was calculated for salt solutions varying from 0% to 20% dilution. The ZAM model also calculated the total ionic strength (mol/kg) of the solutions as listed in Table 4-2. Table 4-2 shows a large decrease in the ionic strength with increasing dilution. Zheng et al. (1996) observed that the cesium loading increases with decreasing Na^+ concentrations (i.e., increasing dilution) primarily due to the decreased ionic strength. Table 4-1 confirms cesium loading increases in more diluted salt solutions.

Table 4-1. Dilution Effect on Cesium Loading at 23°C.

Cases	Q			$C_f = C_o$ [(a)]
	$mmol_{Cs}/g_{CST}$	mg_{Cs}/g_{CST}	Ci/L_{Bed}	$mmol_{Cs}/L$
1	0.0951 (0.1025)	12.75 (13.75)	357.2 (385.1)	0.0157 (0.0157)
2	0.0952	12.77	357.7	0.0155
3	0.0954	12.79	358.2	0.0154
4	0.0955	12.80	358.7	0.0153
5	0.0956	12.82	359.3	0.0151
6	0.0957	12.84	359.6	0.015
7	0.0963	12.91	361.8	0.0143
8	0.0968	12.99	363.8	0.0137
9	0.0974 (0.1050)	13.06 (14.08)	365.9 (394.5)	0.0131 (0.0131)

(a) C_o: initial cesium concentration; C_f: equilibrium cesium Concentration

( ) Values at 20°C

Table 4-2. pH and Total Ionic Strength of Diluted Salt Solutions at 23°C.

Cases	pH	Total Ionic Strength (mol/kg)
1	13.23 (13.33)	4.95 (4.95)
2	13.22	4.90
3	13.22	4.85
4	13.21	4.79

5	13.21	4.74
6	13.20	4.70
7	13.17	4.46
8	13.14	4.25
9	13.12 (13.22)	4.06 (4.06)

( ) Values at 20°C

The following calculation demonstrates the temperature effect on cesium loading. The ion exchange reaction involving cesium is represented as follows (Zhang et al., 1997):

$$[Na^+]_S + [Cs^+]_l \overset{K_{eq}}{\longleftrightarrow} [Cs^+]_S + [Na^+]_l \quad \text{Eq. 1}$$

The thermodynamic equilibrium constant K_{eq} is defined as:

$$K_{eq} = K_C K_\gamma \quad \text{Eq. 2}$$

where $$K_C = \frac{Q_{Cs} C_{Na}}{Q_{Na} C_{Cs}} \quad \text{Eq. 3}$$

$$K_\gamma = \frac{\gamma_{Na}}{\gamma_{Cs}} \quad \text{Eq. 4}$$

Q_{Cs}: Equilibrium Cs concentration on the CST resin
Q_{Na}: Equilibrium Na concentration on the CST resin
C_{Cs}: Equilibrium Cs concentration in the solution
C_{Na}: Equilibrium Na concentration in the solution
γ_{Cs}: Activity coefficient of Cs in the solution
γ_{Na}: Activity coefficient of Na in the solution

The cesium-sodium relation on the CST resin is given by the following material balance equation:

$$Q_T = Q_{Cs} + Q_{Na} \quad \text{Eq. 5}$$

Q_T: Total cesium capacity of the CST resin

Cesium loading is obtained by combining the material balance (Eq. 5) and equilibrium constant equations (Eqs 2, 3, and 4):

$$Q_{Cs} = \frac{Q_T C_{Cs}}{C_{Cs} + \left(\frac{K_\gamma}{K_{eq}}\right) C_{Na}} \quad \text{Eq. 6}$$

or $$Q_{Cs} = \frac{Q_T}{1 + \left(\frac{K_\gamma}{K_{eq}}\right)\left(\frac{C_{Na}}{C_{Cs}}\right)} \quad \text{Eq. 7}$$

The equilibrium constant is related to the heat of ion exchange, ΔH°, by the Van't Hoff equation as follows:

$$lnK_{eq,T} = lnK_{eq,25°C} - \frac{\Delta H^\circ}{R}\left(\frac{1}{T} - \frac{1}{T_{25°C}}\right) \quad \text{Eq. 8}$$

with $$K_{eq,25°C} = 4.4x10^4 \quad \text{Eq. 9}$$

$$\Delta H^\circ = -2.18x10^4 \frac{J}{gmole} \quad \text{Eq. 10}$$

As an example, activity coefficients and equilibrium constants calculated for Case 1 and Case 8 are shown below:

Cases	γ_{Cs} (1)	γ_{Na} (1)	K_γ	K_{eq}	K_γ/K_{eq}
1	0.61196	0.45339	0.74089	4.67E+04	1.59E-05
8	0.61022	0.46103	0.75552	4.67E+04	1.62E-05

(1): Calculated from OLI

Note that in Eq. 7 the liquid concentration ratio (C_{Na}/C_{Cs}) remains constant with dilution. Due to the decreased ionic strength, activity coefficient ratios K_γ increase with increasing dilution, making the denominator of the cesium loading Eq. 7 larger, hence reducing cesium sorption.

Figure 4-1 displays the effect of dilution on cesium loading. The correlation in Figure 4-1 shows a linear effect within the dilution range of interest.

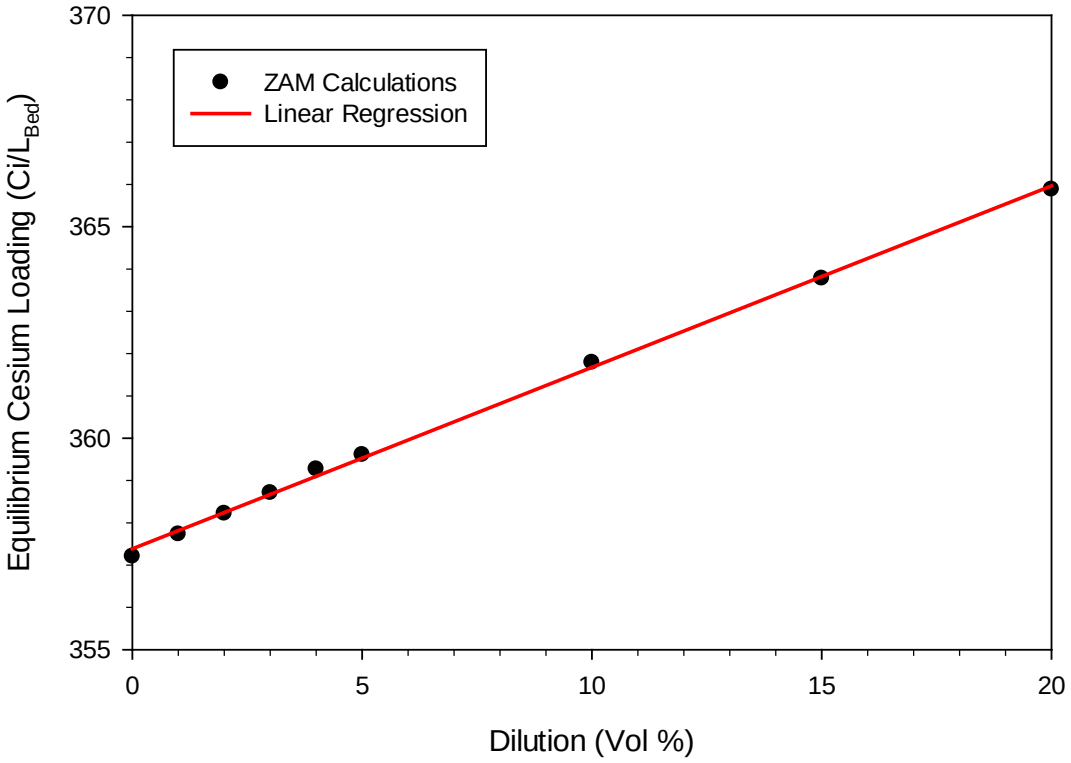

Figure 4-1. Dilution Effect on Cesium Loading at 23°C.

Linear regression: $Q(Ci/L_{CST}) = 0.4290 * Dilution(Vol\%) + 357.3847$ ($R^2 = 0.998$)

Isotherms were also determined for some cases (e.g., cases 1, 2, 3, and 9). Use of the Freundlich/Langmuir model was found to provide an excellent fit for ZAM data. Isotherm parameters are listed in Table 4-3.

Freundlich/Langmuir isotherm:

$$Q = \frac{C_T C_{Cs}}{\beta + C_{Cs}}$$

Q: Equilibrium Cs loading ($mmol/g_{CST}$)
C_{Cs}: Equilibrium Cs concentration in the solution (mol/L)
C_T: Total cesium capacity (~0.58 $mmol/g_{CST}$)
β: Isotherm parameter

Table 4-3. Isotherm Parameters for Dilution Cases at 23°C.

Cases	C_T	β
1	0.5799 (0.5799)	8.0078E-05 (7.3118E-05)
2	0.5799	7.9146E-05
3	0.5799	7.8243E-05
9	0.58 (0.58)	6.4915E-05 (5.9286E-05)

( ) Values at 20°C

Figure 4-2 shows the computed isotherms for the selected cases and confirms that cesium loading increases with more diluted waste solutions.

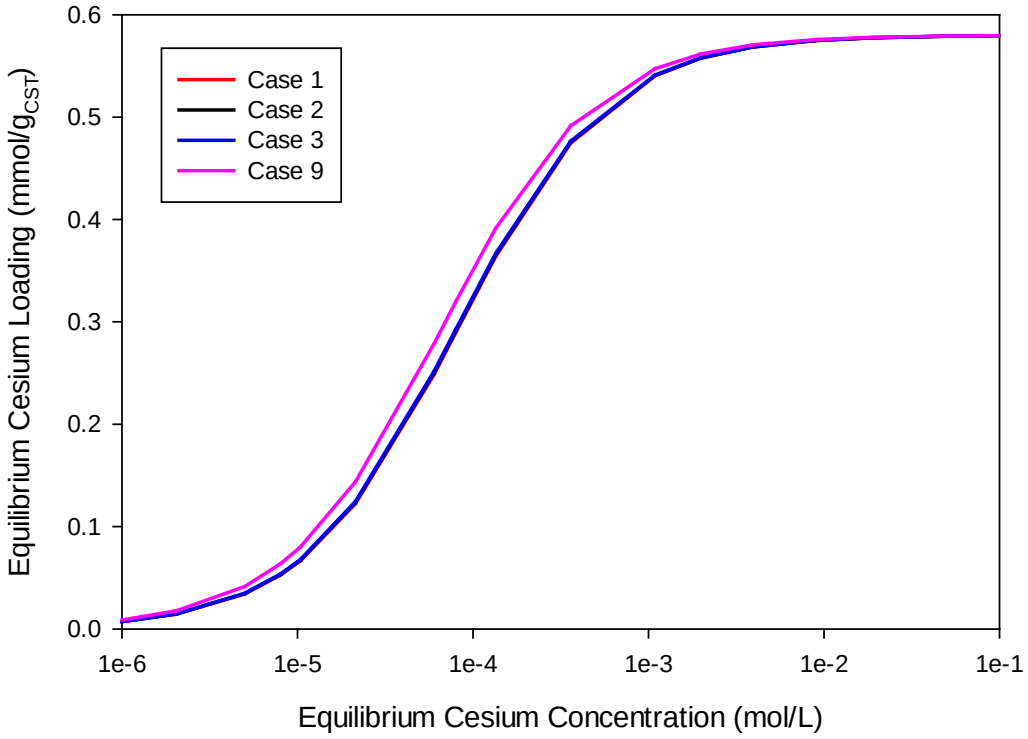

Figure 4-2. Isotherms for Dilution Cases at 23°C.

As discussed in Section 2.2, the two approaches for determination of cesium loading (i.e., use of an isotherm, and variation of ZAM phase ratio) deliver identical results as reaffirmed in Table 4-4.

Table 4-4. Predicted Cesium Loading for Dilution Cases at 23°C.

	Case 1	Case 2	Case 3	Case 9
Initial Cs (M)	1.57E-05	1.56E-05	1.54E-05	1.31E-05
Q (Isotherm) (mmol/g_{CST})	0.0951	0.0952	0.0954	0.0974
Q (ZAM) (mmol/g_{CST})	0.0951	0.0952	0.0954	0.0974

4.2 Temperature Effect

In general, higher temperature discourages the sorption reaction which occurs with evolution of heat (Helfferich, 1995). An increase in temperature decreases the thermodynamic equilibrium constant resulting in a lower cesium sorption.

Based on the equations derived in the previous section, the following calculation demonstrates the temperature effect on cesium loading. Activity coefficients and equilibrium constants are calculated for Case 1 at 25°C and 40°C. Their values are shown below:

T (°C)	γ_{Cs} (1)	γ_{Na} (1)	K_γ	K_{eq}	K_γ/K_{eq}
25	0.61332	0.45642	0.74417	4.40E+04	1.69E-05
40	0.62328	0.47289	0.75871	2.89E+04	2.63E-05

(1): Calculated from OLI

Equilibrium constants K_{eq} decrease with increasing temperatures much more than the increase in activity coefficients. Consequently, the ratio (K_γ/K_{eq}) increases, making the denominator of the cesium loading equation larger, hence reducing cesium sorption.

Table 4-5 shows the ZAM results for Case 1 at different temperatures ranging from 20°C to 40°C. Table 4-5 confirms the decreasing cesium loading with increasing temperatures.

Table 4-5. Temperature Effect on Cesium Loading for Non-Dilution VDS Sample (Case 1).

Case 1 at T (°C)	Q			$C_f = C_o$ (a)
	$mmol_{Cs}/g_{CST}$	mg_{Cs}/g_{CST}	Ci/L_{Bed}	$mmol_{Cs}/L$
20	0.1025	13.75	385.1	0.0157
23	0.0951	12.75	357.2	0.0157
24	0.0927	12.44	348.4	0.0157
25	0.0905	12.13	339.8	0.0157
26	0.0882	11.83	331.5	0.0157
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28	0.0840	11.26	315.4	0.0157
29	0.0819	10.98	307.7	0.0157
30	0.0799	10.72	300.3	0.0157
31	0.0780	10.46	293.0	0.0157
32	0.0761	10.20	285.9	0.0157
33	0.0743	9.96	278.9	0.0157
34	0.0725	9.72	272.2	0.0157
35	0.0707	9.49	265.7	0.0157
37	0.0674	9.04	253.2	0.0157
39	0.0642	8.61	241.3	0.0157
40	0.0627	8.41	235.6	0.0157

(a) C_o: initial cesium concentration; C_f: equilibrium cesium concentration

Figure 4-3 displays the effect of dilution on cesium loading. The correlation in Figure 4-3 shows a linear effect within the temperature range of interest.

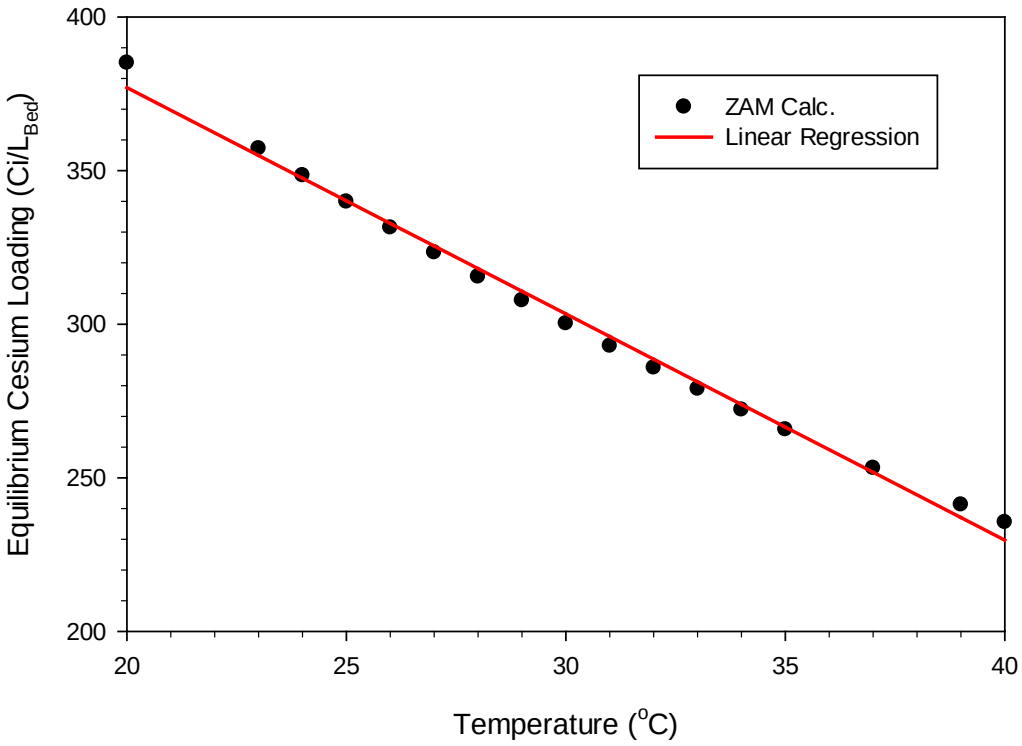

Figure 4-3. Temperature Effect on Cesium Loading.

Linear regression: $Q(Ci/L_{CST}) = -7.3655 * T(^{o}C) + 524.2962$ ($R^2 = 0.993$)

Isotherms were determined for some cases (e.g., at 20°C, 23°C, 30°C, 35°C, and 40°C). Again, the Freundlich/Langmuir model was used to fit ZAM data. Isotherm parameters are listed in Table 4-6.

Table 4-6. Isotherm Parameters for Case 1 at Different Temperatures.

Case 1 at T(°C)	C_T	β
20	0.5799	7.3118E-05
23	0.5799	8.0078E-05
30	0.5800	9.8252E-05
35	0.5799	1.1306E-04
40	0.5799	1.2950E-04

Figure 4-4 shows the computed isotherms for the selected cases and confirms that cesium loading decreases in higher-temperature waste solutions.

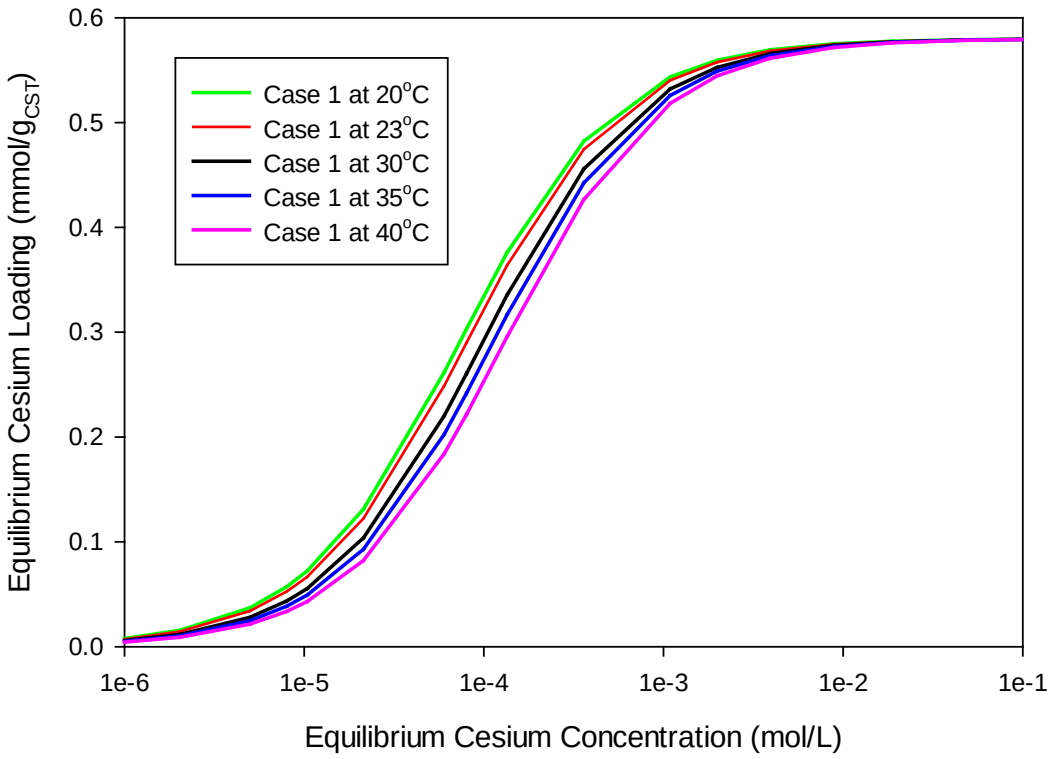

Figure 4-4. Isotherms for Case 1 at Different Temperatures.

Table 4-7 confirms that the two approaches for determination of cesium loading (i.e., use of an isotherm, and variation of ZAM phase ratio) deliver identical results.

Table 4-7. Predicted Cesium Loading for Case 1 at Different Temperatures.

	Case 1 at 20°C	**Case 1 at 23°C**	**Case 1 at 30°C**	**Case 1 at 35°C**	**Case 1 at 40°C**
Q (Isotherm) (mmol/g_{CST})	0.1025	0.0951	0.0799	0.0707	0.0627
Q (ZAM) (mmol/g_{CST})	0.1025	0.0951	0.0799	0.0707	0.0627

5.0 Conclusions

The sensitivity of Tank 10H VDS waste solution to be processed in the TCCR system was studied using the ZAM program. Results of the ZAM model predictions are:

- Dilution of the salt waste solution with water increases the cesium loading primarily due to the decreased ionic strength. The cesium loading – dilution (%) correlation is linear within the dilution range of 0% to 20%.

  $Q(Ci/L_{CST}) = 0.4290 * Dilution(Vol\%) + 357.3847$ $(R^2 = 0.998)$

- Cesium loading decreases with increasing temperatures. The correlation shows a linear effect within the temperature range of 23°C to 40°C.

  $Q(Ci/L_{CST}) = -7.3655 * T(°C) + 524.2962$ $(R^2 = 0.993)$

6.0 References

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Appendix A. ZAM Model Run Scope

Original Scope

From: Terri Fellinger
To: Thong Hang
Cc: Boyd Wiedenman; Mark Keefer; Joshua Segura; Peter02 Fairchild; David02 Martin; William02 King; Charles Nash; Gregory Arthur; David Harris; Robert Voegtlen; Blake Mckibbin; Selina Guardiano
Subject: Zam Model
Date: Tuesday, March 27, 2018 11:34:22 AM
Attachments: image001.png

Thong,

Per the scope written in TTR, X-TTR-H-00065, Rev. 1, ZAM model runs are being requested. Please see the scope below. If you have any questions, please let me know.

ZAM Model Run Scope:

Background:

A basis is needed to evaluate the impact of Cs loading on CST as a function of water additions to Tank 10 and as a function of temperature in Tank 10 for a prepared batch of salt feed. SRNL is being requested to perform the following tasks:

Tasks:

- Using the Tank 10 variable depth sample results reported in SRNL-STI-2017-00392, a starting composition was calculated. The composition was adjusted by leaving the competitors (K and Sr) out of the composition and reconciling the cation/anion balance by increasing the molarity of the carbonate. The compositions were then adjusted with water to simulate 0% to 5% (in increments of 1%) 10%, 15%, and 20% water dilution. A total of 9 cases have been generated. Perform ZAM model runs for Case 1 through Case 9 at 23°C. Document the results (input/output ZAM model) in an E7, 2.60 technically reviewed (design verification) document.

- Using the "0% Dilution – Balanced" case (Case 1), complete ZAM Model runs to determine the change in Cs loading expected on CST as a function of temperature. Temperature range of interest is 23°C to 35°C in increments of 1°C, then from 35°C to 40°C in increments of 2°C. Document the results (input/output ZAM model) in an E7, 2.60 technically reviewed (design verification) document.

Cases	1	2	3	4	5	6	7	8	9
	0% Dilution - Balanced (M)	1% Dilution (M)	2% Dilution (M)	3% Dilution (M)	4% Dilution (M)	5% Dilution (M)	10% Dilution (M)	15% Dilution (M)	20% Dilution (M)
Na	3.22E+00	3.188	3.157	3.126	3.096	3.067	2.927	2.800	2.683
Cs	1.57E-05	1.56E-05	1.54E-05	1.53E-05	1.51E-05	1.50E-05	1.43E-05	1.37E-05	1.31E-05
Hydroxide	0.184	1.82E-01	1.80E-01	1.79E-01	1.77E-01	1.75E-01	1.67E-01	1.60E-01	1.53E-01
Nitrate	1.04E+00	1.03E+00	1.02E+00	1.01E+00	1.00E+00	9.90E-01	9.45E-01	9.04E-01	8.67E-01
Nitrite	1.28E-01	1.27E-01	1.25E-01	1.24E-01	1.23E-01	1.22E-01	1.16E-01	1.11E-01	1.07E-01
Aluminate	6.31E-02	6.25E-02	6.19E-02	6.13E-02	6.07E-02	6.01E-02	5.74E-02	5.49E-02	5.26E-02
Sulfate	3.81E-01	3.77E-01	3.74E-01	3.70E-01	3.66E-01	3.63E-01	3.46E-01	3.31E-01	3.18E-01
Carbonate	5.10E-01	5.05E-01	5.00E-01	4.95E-01	4.91E-01	4.86E-01	4.64E-01	4.44E-01	4.25E-01
Chloride	4.06E-03	4.02E-03	3.98E-03	3.94E-03	3.90E-03	3.87E-03	3.69E-03	3.53E-03	3.38E-03
Oxalate	9.20E-03	9.11E-03	9.02E-03	8.93E-03	8.85E-03	8.76E-03	8.36E-03	8.00E-03	7.67E-03

Thanks in Advance,
Terri

Additional Scope

From: Terri Fellinger
To: Thong Hang
Cc: Mark Keefer; Joshua Segura; Peter02 Fairchild; David Harris; David02 Martin; Boyd Wiedenman; Gregory Arthur
Subject: RE: Zam Model
Date: Monday, May 14, 2018 2:15:11 PM
Attachments: image001.png
SRNL-STI-2018-00215_draft1 - TLF.docm

Thong,

Attached are my comments on the report. I have an additional request for three more case runs….see below. Please add these cases to the report.

Per the scope written in TTR, X-TTR-H-00065, Rev. 1, I am making additional request of ZAM model runs performed at 20˚C for the bullets listed below.

- Using the "0% Dilution – Balanced" case (Case 1), complete a ZAM Model run at 20˚C.
- Complete two additional ZAM model runs. The first is rerunning Case 1 (0% Dilution) at 20˚C. The second is re-running Case 9 (20% Dilution) at 20˚C

Thanks in Advance,
Terri

Appendix B. ZAM Calculations

1) Water Dilution

- Case 1 (0% Dilution)

ZAM input

```
1, 296.15                                                              Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 23C                                           Title
7, 8                                                                   Number of Cations & Anions
1159.92                                                                Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                            Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                         Names of Anions (Add C2O4--)
88.02                                                                  C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                                 Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092           Concentrations of Anions
1, 0.000001                                                            Liquid (L), Solid (g)
0                                                                      Initial Solid Form (Na+ (0); H- (1))
1                                                                      Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 23C
**********************INPUT************************

  Density=  .1160E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .3220E+01
Cs+.....        132.9054          1.       .1570E-04
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********************OUTPUT***********************

 Ionic Strength=           4.952460086776033 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .9508E-01      .1570E-01      .6056E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 2 (1% Dilution)

```
1, 296.15                                                              Activity Coeff. Model, Temperature
Case 2 Maximum Loading @ 23C                                           Title
7, 8                                                                   Number of Cations & Anions
1158.46                                                                Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                            Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                         Names of Anions (Add C2O4--)
```

```
88.02                                                                          C2O4-2 MW
3.18812, 1.55446E-05, 5.4891E-14, 0, 0 , 0, 0                                  Concentrations of Cations
0.18218, 1.02969, 0.12673, 0.06248, 0.37723, 0.50518, 0.00402, 9.10891E-03   Concentrations of Anions
1, 0.000001                                                                    Liquid (L), Solid (g)
0                                                                              Initial Solid Form (Na+ (0); H- (1))
1                                                                              Calculation Adjustment
```

ZAM ouput

```
   Solution:  Case 2 Maximum Loading @ 23C
  **********************INPUT************************

    Density=  .1158E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898          1.       .3188E+01
  Cs+.....        132.9054          1.       .1554E-04
  H+......          1.0079          1.       .5489E-13
  Rb+.....         85.4678          1.       .0000E+00
  K+......         39.0983          1.       .0000E+00
  SrOH+...        105.0000          1.       .0000E+00
  Sr++....         87.6200          2.       .0000E+00
  OH-.....         17.0073         -1.       .1822E+00
  NO3-....         62.0049         -1.       .1030E+01
  NO2-....         46.0000         -1.       .1267E+00
  Al(OH)4-         95.0000         -1.       .6248E-01
  SO4--...         96.0636         -2.       .3772E+00
  CO3--...         60.0092         -2.       .5052E+00
  Cl-.....         35.4527         -1.       .4020E-02
  Other--.         88.0200         -2.       .9109E-02

  Liquid(L)= .1000E+01   Solid(g)= .1000E-05

   Material: Na Form


  **********************OUTPUT************************

   Ionic Strength=           4.898727916833204 mol/kg

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .9522E-01      .1554E-01      .6125E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .0000E+00      .0000E+00      .0000E+00
```

- Case 3 (2% Dilution)

```
1, 296.15                                                                      Activity Coeff. Model, Temperature
Case 3 Maximum Loading @ 23C                                                   Title
7, 8                                                                           Number of Cations & Anions
1157.03                                                                        Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                                    Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                                 Names of Anions (Add C2O4--)
88.02                                                                          C2O4-2 MW
3.15686, 1.53922E-05, 5.5435E-14, 0, 0, 0, 0                                   Concentrations of Cations
0.18039, 1.01961, 0.12549, 0.06186, 0.37353, 0.50023, 0.00398, 9.01961E-03   Concentrations of Anions
1, 0.000001                                                                    Liquid (L), Solid (g)
0                                                                              Initial Solid Form (Na+ (0); H- (1))
1                                                                              Calculation Adjustment
```

ZAM ouput

```
   Solution:  Case 3 Maximum Loading @ 23C
  **********************INPUT************************

    Density=  .1157E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898          1.       .3157E+01
  Cs+.....        132.9054          1.       .1539E-04
```

```
H+......          1.0079          1.       .5544E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1804E+00
NO3-....         62.0049         -1.       .1020E+01
NO2-....         46.0000         -1.       .1255E+00
Al(OH)4-         95.0000         -1.       .6186E-01
SO4--...         96.0636         -2.       .3735E+00
CO3--...         60.0092         -2.       .5002E+00
Cl-.....         35.4527         -1.       .3980E-02
Other--.         88.0200         -2.       .9020E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.846130741638794 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .9535E-01      .1539E-01      .6195E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 4 (3% Dilution)

```
1, 296.15                                                                    Activity Coeff. Model, Temperature
Case 4 Maximum Loading @ 23C                                                 Title
7, 8                                                                         Number of Cations & Anions
1155.62                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                                  Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                               Names of Anions (Add C2O4--)
88.02                                                                        C2O4-2 MW
3.12621, 1.52427E-05, 5.5978E-14, 0, 0, 0, 0                                 Concentrations of Cations
0.17864, 1.00971, 0.12427, 0.06126, 0.36990, 0.49537, 0.00394, 8.93204E-03   Concentrations of Anions
1, 0.0000001                                                                 Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 4 Maximum Loading @ 23C
**********INPUT**********

  Density=  .1156E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .3126E+01
Cs+.....        132.9054          1.       .1524E-04
H+......          1.0079          1.       .5598E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1786E+00
NO3-....         62.0049         -1.       .1010E+01
NO2-....         46.0000         -1.       .1243E+00
Al(OH)4-         95.0000         -1.       .6126E-01
SO4--...         96.0636         -2.       .3699E+00
CO3--...         60.0092         -2.       .4954E+00
Cl-.....         35.4527         -1.       .3940E-02
Other--.         88.0200         -2.       .8932E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form


**********OUTPUT**********
```

```
 Ionic Strength=           4.794679711727707 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .9548E-01      .1524E-01      .6264E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 5 (4% Dilution)

```
1, 296.15                                                          Activity Coeff. Model, Temperature
Case 5 Maximum Loading @ 23C                                       Title
7, 8                                                               Number of Cations & Anions
1154.22                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.096, 1.51E-05, 5.6497E-14, 0, 0, 0, 0                            Concentrations of Cations
0.177, 1.0, 0.123, 0.0607, 0.366, 0.49086, 0.0039, 8.85E-03        Concentrations of Anions
1, 0.0000001                                                       Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 5 Maximum Loading @ 23C
**********INPUT**********

  Density=  .1154E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3096E+01
Cs+.....       132.9054          1.       .1510E-04
H+......         1.0079          1.       .5650E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1770E+00
NO3-....        62.0049         -1.       .1000E+01
NO2-....        46.0000         -1.       .1230E+00
Al(OH)4-        95.0000         -1.       .6070E-01
SO4--...        96.0636         -2.       .3660E+00
CO3--...        60.0092         -2.       .4909E+00
Cl-.....        35.4527         -1.       .3900E-02
Other--.        88.0200         -2.       .8850E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.743996930373317 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .9563E-01      .1510E-01      .6333E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 6 (5% Dilution)

```
1, 296.15                                                          Activity Coeff. Model, Temperature
Case 6 Maximum Loading @ 23C                                       Title
7, 8                                                               Number of Cations & Anions
1152.88                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.06667, 1.49524E-05, 5.7065E-14, 0, 0, 0, 0                       Concentrations of Cations
```

```
0.17524, 0.99048, 0.12190, 0.06010, 0.36286, 0.48593, 0.00387, 8.76190E-03   Concentrations of Anions
1, 0.0000001                                                                  Liquid (L), Solid (g)
0                                                                             Initial Solid Form (Na+ (0); H- (1))
1                                                                             Calculation Adjustment
```

ZAM ouput

```
  Solution:  Case 6 Maximum Loading @ 23C
 **********************INPUT************************

   Density=  .1153E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898          1.       .3067E+01
 Cs+.....        132.9054          1.       .1495E-04
 H+......          1.0079          1.       .5706E-13
 Rb+.....         85.4678          1.       .0000E+00
 K+......         39.0983          1.       .0000E+00
 SrOH+...        105.0000          1.       .0000E+00
 Sr++....         87.6200          2.       .0000E+00
 OH-.....         17.0073         -1.       .1752E+00
 NO3-....         62.0049         -1.       .9905E+00
 NO2-....         46.0000         -1.       .1219E+00
 Al(OH)4-         95.0000         -1.       .6010E-01
 SO4--...         96.0636         -2.       .3629E+00
 CO3--...         60.0092         -2.       .4859E+00
 Cl-.....         35.4527         -1.       .3870E-02
 Other--.         88.0200         -2.       .8762E-02

 Liquid(L)= .1000E+01   Solid(g)= .1000E-06

  Material: Na Form


 **********************OUTPUT************************

  Ionic Strength=           4.695033288975175 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs        .9572E-01      .1495E-01      .6402E+04
 Rb        .0000E+00      .0000E+00      .0000E+00
 Sr        .0000E+00      .0000E+00      .0000E+00
 K         .0000E+00      .0000E+00      .0000E+00
```

- Case 7 (10% Dilution)

```
1, 296.15                                                                     Activity Coeff. Model, Temperature
Case 7 Maximum Loading @ 23C                                                  Title
7, 8                                                                          Number of Cations & Anions
1146.44                                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                                   Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                                Names of Anions (Add C2O4--)
88.02                                                                         C2O4-2 MW
2.92727, 1.42727E-05, 5.9783E-14, 0, 0, 0, 0                                  Concentrations of Cations
0.16727, 0.94545, 0.11636, 0.05736, 0.34636, 0.46385, 0.00369, 8.36364E-03   Concentrations of Anions
1, 0.0000001                                                                  Liquid (L), Solid (g)
0                                                                             Initial Solid Form (Na+ (0); H- (1))
1                                                                             Calculation Adjustment
```

ZAM ouput

```
  Solution:  Case 7 Maximum Loading @ 23C
 **********************INPUT************************

   Density=  .1146E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898          1.       .2927E+01
 Cs+.....        132.9054          1.       .1427E-04
 H+......          1.0079          1.       .5978E-13
 Rb+.....         85.4678          1.       .0000E+00
```

```
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1673E+00
NO3-....         62.0049         -1.       .9455E+00
NO2-....         46.0000         -1.       .1164E+00
Al(OH)4-         95.0000         -1.       .5736E-01
SO4--...         96.0636         -2.       .3464E+00
CO3--...         60.0092         -2.       .4639E+00
Cl-.....         35.4527         -1.       .3690E-02
Other--.         88.0200         -2.       .8364E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.463220820137013 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .9630E-01      .1427E-01      .6747E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 8 (15% Dilution)

```
1, 296.15                                                                  Activity Coeff. Model, Temperature
Case 8 Maximum Loading @ 23C                                               Title
7, 8                                                                       Number of Cations & Anions
1140.52                                                                    Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                                Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                             Names of Anions (Add C2O4--)
88.02                                                                      C2O4-2 MW
2.8, 1.36522E-05, 6.2500E-14, 0, 0, 0, 0                                   Concentrations of Cations
0.16, 0.90435, 0.11130, 0.05487, 0.33130, 0.44368, 0.00353, 8.0E-03        Concentrations of Anions
1, 0.0000001                                                              Liquid (L), Solid (g)
0                                                                          Initial Solid Form (Na+ (0); H- (1))
1                                                                          Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 8 Maximum Loading @ 23C
**********INPUT**********

  Density=  .1141E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .2800E+01
Cs+.....        132.9054          1.       .1365E-04
H+......          1.0079          1.       .6250E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1600E+00
NO3-....         62.0049         -1.       .9044E+00
NO2-....         46.0000         -1.       .1113E+00
Al(OH)4-         95.0000         -1.       .5487E-01
SO4--...         96.0636         -2.       .3313E+00
CO3--...         60.0092         -2.       .4437E+00
Cl-.....         35.4527         -1.       .3530E-02
Other--.         88.0200         -2.       .8000E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.253413663413609 mol/kg
```

```
         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .9683E-01      .1365E-01      .7092E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .0000E+00      .0000E+00      .0000E+00
```

- Case 9 (20% Dilution) at 20°C

```
1, 293.15                                                              Activity Coeff. Model, Temperature
Case 9 Maximum Loading @ 20C                                           Title
7, 8                                                                   Number of Cations & Anions
1136.16                                                                Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                            Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                         Names of Anions (Add C2O4--)
88.02                                                                  C2O4-2 MW
2.683, 1.31E-05, 6.5359E-14, 0, 0, 0, 0                                Concentrations of Cations
0.153, 0.867, 0.107, 0.0526, 0.318, 0.424345, 0.00338, 7.67E-03        Concentrations of Anions
1, 0.0000001                                                           Liquid (L), Solid (g)
0                                                                      Initial Solid Form (Na+ (0); H- (1))
1                                                                      Calculation Adjustment
```

ZAM ouput

```
   Solution:  Case 9 Maximum Loading @ 20C
  **********************INPUT************************

    Density=  .1136E+04 kg/m3

                 Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....          22.9898          1.       .2683E+01
  Cs+.....         132.9054          1.       .1310E-04
  H+......           1.0079          1.       .6536E-13
  Rb+.....          85.4678          1.       .0000E+00
  K+......          39.0983          1.       .0000E+00
  SrOH+...         105.0000          1.       .0000E+00
  Sr++....          87.6200          2.       .0000E+00
  OH-.....          17.0073         -1.       .1530E+00
  NO3-....          62.0049         -1.       .8670E+00
  NO2-....          46.0000         -1.       .1070E+00
  Al(OH)4-          95.0000         -1.       .5260E-01
  SO4--...          96.0636         -2.       .3180E+00
  CO3--...          60.0092         -2.       .4243E+00
  Cl-.....          35.4527         -1.       .3380E-02
  Other--.          88.0200         -2.       .7670E-02

  Liquid(L)= .1000E+01   Solid(g)= .1000E-06

   Material: Na Form


  **********************OUTPUT************************

   Ionic Strength=           4.057000202175339 mol/kg

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .1050E+00      .1310E-01      .8012E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .0000E+00      .0000E+00      .0000E+00
```

- Case 9 (20% Dilution) at 23°C

```
1, 296.15                                                              Activity Coeff. Model, Temperature
Case 9 Maximum Loading @ 23C                                           Title
7, 8                                                                   Number of Cations & Anions
1135                                                                   Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                            Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                         Names of Anions (Add C2O4--)
88.02                                                                  C2O4-2 MW
2.683, 1.31E-05, 6.5359E-14, 0, 0, 0, 0                                Concentrations of Cations
0.153, 0.867, 0.107, 0.0526, 0.318, 0.424345, 0.00338, 7.67E-03        Concentrations of Anions
```

```
1, 0.0000001                                                    Liquid (L), Solid (g)
0                                                               Initial Solid Form (Na+ (0); H- (1))
1                                                               Calculation Adjustment
```

ZAM ouput

```
   Solution:  Case 9 Maximum Loading @ 23C
  **********************INPUT************************

    Density=  .1135E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898          1.       .2683E+01
  Cs+.....        132.9054          1.       .1310E-04
  H+......          1.0079          1.       .6536E-13
  Rb+.....         85.4678          1.       .0000E+00
  K+......         39.0983          1.       .0000E+00
  SrOH+...        105.0000          1.       .0000E+00
  Sr++....         87.6200          2.       .0000E+00
  OH-.....         17.0073         -1.       .1530E+00
  NO3-....         62.0049         -1.       .8670E+00
  NO2-....         46.0000         -1.       .1070E+00
  Al(OH)4-         95.0000         -1.       .5260E-01
  SO4--...         96.0636         -2.       .3180E+00
  CO3--...         60.0092         -2.       .4243E+00
  Cl-.....         35.4527         -1.       .3380E-02
  Other--.         88.0200         -2.       .7670E-02

  Liquid(L)= .1000E+01   Solid(g)= .1000E-06

   Material: Na Form


  **********************OUTPUT************************

   Ionic Strength=           4.062020315600587 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .9739E-01      .1310E-01      .7435E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .0000E+00      .0000E+00      .0000E+00
```

2) Temperature Variation of Case 1

- Case 1 at 20°C

```
1, 293.15                                                       Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 20C                                    Title
7, 8                                                            Number of Cations & Anions
1161.06                                                         Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                     Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                  Names of Anions (Add C2O4--)
88.02                                                           C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                          Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092    Concentrations of Anions
1, 0.000001                                                     Liquid (L), Solid (g)
0                                                               Initial Solid Form (Na+ (0); H- (1))
1                                                               Calculation Adjustment
```

ZAM ouput

```
   Solution:  Case 1 Maximum Loading @ 20C
  **********************INPUT************************

    Density=  .1161E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
```

```
Na+.....         22.9898          1.       .3220E+01
Cs+.....        132.9054          1.       .1570E-04
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.946349911962168 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .1025E+00      .1570E-01      .6530E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 23°C

```
1, 296.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 23C                                       Title
7, 8                                                               Number of Cations & Anions
1159.92                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                             Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092       Concentrations of Anions
1, 0.000001                                                        Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 23C
**********INPUT**********

  Density=  .1160E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .3220E+01
Cs+.....        132.9054          1.       .1570E-04
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form
```

```
**********OUTPUT**********

 Ionic Strength=           4.952460086776033 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .9508E-01      .1570E-01      .6056E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 24°C

```
1, 297.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 24C                                       Title
7, 8                                                               Number of Cations & Anions
1159.55                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                             Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092       Concentrations of Anions
1, 0.0000001                                                       Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 24C
**********INPUT**********

  Density=  .1160E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
H+......         1.0079          1.       .5435E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1840E+00
NO3-....        62.0049         -1.       .1040E+01
NO2-....        46.0000         -1.       .1280E+00
Al(OH)4-        95.0000         -1.       .6310E-01
SO4--...        96.0636         -2.       .3810E+00
CO3--...        60.0092         -2.       .5102E+00
Cl-.....        35.4527         -1.       .4060E-02
Other--.        88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.954446176385449 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .9274E-01      .1570E-01      .5907E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 25°C

```
1, 298.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 25C                                       Title
7, 8                                                               Number of Cations & Anions
1159.55                                                            Density(kg/m3)
```

```
 3,  6,  1,   5,  4, 40, 13                                          Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                       Names of Anions (Add C2O4--)
88.02                                                                C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                               Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092         Concentrations of Anions
1, 0.0000001                                                         Liquid (L), Solid (g)
0                                                                    Initial Solid Form (Na+ (0); H- (1))
1                                                                    Calculation Adjustment
```

ZAM ouput

```
  Solution:  Case 1 Maximum Loading @ 25C
 **********************INPUT************************

   Density=  .1160E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898          1.       .3220E+01
 Cs+.....        132.9054          1.       .1570E-04
 H+......          1.0079          1.       .5435E-13
 Rb+.....         85.4678          1.       .0000E+00
 K+......         39.0983          1.       .0000E+00
 SrOH+...        105.0000          1.       .0000E+00
 Sr++....         87.6200          2.       .0000E+00
 OH-.....         17.0073         -1.       .1840E+00
 NO3-....         62.0049         -1.       .1040E+01
 NO2-....         46.0000         -1.       .1280E+00
 Al(OH)4-         95.0000         -1.       .6310E-01
 SO4--...         96.0636         -2.       .3810E+00
 CO3--...         60.0092         -2.       .5102E+00
 Cl-.....         35.4527         -1.       .4060E-02
 Other--.         88.0200         -2.       .9200E-02

 Liquid(L)= .1000E+01   Solid(g)= .1000E-06

  Material: Na Form



 **********************OUTPUT************************

  Ionic Strength=           4.954446176385449 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs        .9046E-01      .1570E-01      .5762E+04
 Rb        .0000E+00      .0000E+00      .0000E+00
 Sr        .0000E+00      .0000E+00      .0000E+00
 K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 26°C

```
1, 299.15                                                            Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 26C                                         Title
7, 8                                                                 Number of Cations & Anions
1158.82                                                              Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                          Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                       Names of Anions (Add C2O4--)
88.02                                                                C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                               Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092         Concentrations of Anions
1, 0.0000001                                                         Liquid (L), Solid (g)
0                                                                    Initial Solid Form (Na+ (0); H- (1))
1                                                                    Calculation Adjustment
```

ZAM ouput

```
  Solution:  Case 1 Maximum Loading @ 26C
 **********************INPUT************************

   Density=  .1159E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
```

```
Na+.....         22.9898          1.       .3220E+01
Cs+.....        132.9054          1.       .1570E-04
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form


**********************OUTPUT************************

 Ionic Strength=           4.958370236566812 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .8823E-01      .1570E-01      .5620E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 27°C

```
1, 300.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 27C                                       Title
7, 8                                                               Number of Cations & Anions
1158.46                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                             Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092       Concentrations of Anions
1, 0.000001                                                        Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 27C
**********************INPUT************************

  Density=  .1158E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .3220E+01
Cs+.....        132.9054          1.       .1570E-04
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form
```

```
**********OUTPUT**********

 Ionic Strength=           4.960307485406172 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .8607E-01      .1570E-01      .5482E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 28°C

```
1, 301.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 28C                                       Title
7, 8                                                               Number of Cations & Anions
1158.1                                                             Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                             Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092       Concentrations of Anions
1, 0.000001                                                        Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 28C
**********INPUT**********

  Density=  .1158E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
H+......         1.0079          1.       .5435E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1840E+00
NO3-....        62.0049         -1.       .1040E+01
NO2-....        46.0000         -1.       .1280E+00
Al(OH)4-        95.0000         -1.       .6310E-01
SO4--...        96.0636         -2.       .3810E+00
CO3--...        60.0092         -2.       .5102E+00
Cl-.....        35.4527         -1.       .4060E-02
Other--.        88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.962245927671440 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .8396E-01      .1570E-01      .5348E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 29°C

```
1, 302.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 29C                                       Title
7, 8                                                               Number of Cations & Anions
1157.75                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
```

```
13,  9, 27,  28, 15, 19, 2, 25                                   Names of Anions (Add C2O4--)
88.02                                                            C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                           Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092     Concentrations of Anions
1, 0.000001                                                      Liquid (L), Solid (g)
0                                                                Initial Solid Form (Na+ (0); H- (1))
1                                                                Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 29C
**********INPUT**********

  Density=  .1158E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
H+......         1.0079          1.       .5435E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1840E+00
NO3-....        62.0049         -1.       .1040E+01
NO2-....        46.0000         -1.       .1280E+00
Al(OH)4-        95.0000         -1.       .6310E-01
SO4--...        96.0636         -2.       .3810E+00
CO3--...        60.0092         -2.       .5102E+00
Cl-.....        35.4527         -1.       .4060E-02
Other--.        88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.964132218395968 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .8191E-01      .1570E-01      .5217E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 30°C

```
1, 303.15                                                        Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 30C                                     Title
7, 8                                                             Number of Cations & Anions
1157.4                                                           Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                      Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                   Names of Anions (Add C2O4--)
88.02                                                            C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                           Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092     Concentrations of Anions
1, 0.000001                                                      Liquid (L), Solid (g)
0                                                                Initial Solid Form (Na+ (0); H- (1))
1                                                                Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 30C
**********INPUT**********

  Density=  .1157E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
```

```
Cs+.....        132.9054          1.       .1570E-04
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.966019943731275 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .7992E-01      .1570E-01      .5090E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 31°C

```
1, 304.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 31C                                       Title
7, 8                                                               Number of Cations & Anions
1157                                                               Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                             Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092       Concentrations of Anions
1, 0.0000001                                                       Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 31C
**********INPUT**********

  Density=  .1157E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .3220E+01
Cs+.....        132.9054          1.       .1570E-04
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form
```

```
**********OUTPUT**********

 Ionic Strength=           4.968179149034341 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .7798E-01      .1570E-01      .4967E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 32°C

```
1, 305.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 32C                                       Title
7, 8                                                               Number of Cations & Anions
1156.69                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                             Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092       Concentrations of Anions
1, 0.000001                                                        Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 32C
**********INPUT**********

  Density=  .1157E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
H+......         1.0079          1.       .5435E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1840E+00
NO3-....        62.0049         -1.       .1040E+01
NO2-....        46.0000         -1.       .1280E+00
Al(OH)4-        95.0000         -1.       .6310E-01
SO4--...        96.0636         -2.       .3810E+00
CO3--...        60.0092         -2.       .5102E+00
Cl-.....        35.4527         -1.       .4060E-02
Other--.        88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.969854138778498 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .7609E-01      .1570E-01      .4846E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 33°C

```
1, 306.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 33C                                       Title
7, 8                                                               Number of Cations & Anions
1156.34                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
```

```
88.02                                                                  C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                                 Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092           Concentrations of Anions
1, 0.000001                                                            Liquid (L), Solid (g)
0                                                                      Initial Solid Form (Na+ (0); H- (1))
1                                                                      Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 33C
**********INPUT**********

  Density=  .1156E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
H+......         1.0079          1.       .5435E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1840E+00
NO3-....        62.0049         -1.       .1040E+01
NO2-....        46.0000         -1.       .1280E+00
Al(OH)4-        95.0000         -1.       .6310E-01
SO4--...        96.0636         -2.       .3810E+00
CO3--...        60.0092         -2.       .5102E+00
Cl-.....        35.4527         -1.       .4060E-02
Other--.        88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.971746219234586 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .7425E-01      .1570E-01      .4729E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 34°C

```
1, 307.15                                                              Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 34C                                           Title
7, 8                                                                   Number of Cations & Anions
1156                                                                   Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                            Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                         Names of Anions (Add C2O4--)
88.02                                                                  C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                                 Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092           Concentrations of Anions
1, 0.000001                                                            Liquid (L), Solid (g)
0                                                                      Initial Solid Form (Na+ (0); H- (1))
1                                                                      Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 34C
**********INPUT**********

  Density=  .1156E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
```

```
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.973585223962764 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .7246E-01      .1570E-01      .4616E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 35°C

```
1, 308.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 35C                                       Title
7, 8                                                               Number of Cations & Anions
1155.65                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                             Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092       Concentrations of Anions
1, 0.0000001                                                       Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 35C
**********INPUT**********

  Density=  .1156E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .3220E+01
Cs+.....        132.9054          1.       .1570E-04
H+......          1.0079          1.       .5435E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1840E+00
NO3-....         62.0049         -1.       .1040E+01
NO2-....         46.0000         -1.       .1280E+00
Al(OH)4-         95.0000         -1.       .6310E-01
SO4--...         96.0636         -2.       .3810E+00
CO3--...         60.0092         -2.       .5102E+00
Cl-.....         35.4527         -1.       .4060E-02
Other--.         88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form


**********OUTPUT**********
```

```
 Ionic Strength=           4.975480147131139 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .7073E-01      .1570E-01      .4505E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 37°C

```
1, 310.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 37C                                       Title
7, 8                                                               Number of Cations & Anions
1154.95                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                             Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092       Concentrations of Anions
1, 0.000001                                                        Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 37C
**********INPUT**********

  Density=  .1155E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
H+......         1.0079          1.       .5435E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1840E+00
NO3-....        62.0049         -1.       .1040E+01
NO2-....        46.0000         -1.       .1280E+00
Al(OH)4-        95.0000         -1.       .6310E-01
SO4--...        96.0636         -2.       .3810E+00
CO3--...        60.0092         -2.       .5102E+00
Cl-.....        35.4527         -1.       .4060E-02
Other--.        88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.979274651344523 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .6739E-01      .1570E-01      .4292E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 39°C

```
1, 312.15                                                          Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 39C                                       Title
7, 8                                                               Number of Cations & Anions
1154.26                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                        Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                     Names of Anions (Add C2O4--)
88.02                                                              C2O4-2 MW
```

```
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                                  Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092            Concentrations of Anions
1, 0.000001                                                             Liquid (L), Solid (g)
0                                                                       Initial Solid Form (Na+ (0); H- (1))
1                                                                       Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 39C
**********INPUT**********

  Density=  .1154E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
H+......         1.0079          1.       .5435E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1840E+00
NO3-....        62.0049         -1.       .1040E+01
NO2-....        46.0000         -1.       .1280E+00
Al(OH)4-        95.0000         -1.       .6310E-01
SO4--...        96.0636         -2.       .3810E+00
CO3--...        60.0092         -2.       .5102E+00
Cl-.....        35.4527         -1.       .4060E-02
Other--.        88.0200         -2.       .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-05

 Material: Na Form


**********OUTPUT**********

 Ionic Strength=           4.983019900039656 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .6422E-01      .1570E-01      .4091E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

- Case 1 at 40°C

```
1, 313.15                                                               Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 40C                                            Title
7, 8                                                                    Number of Cations & Anions
1153.91                                                                 Density(kg/m3)
 3,  6,  1,   5,  4, 40, 13                                             Names of Cations
13,  9, 27,  28, 15, 19, 2, 25                                          Names of Anions (Add C2O4--)
88.02                                                                   C2O4-2 MW
3.22, 1.57E-05, 5.4348E-14, 0, 0, 0, 0                                  Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.510230, 0.00406, 0.0092            Concentrations of Anions
1, 0.0000001                                                            Liquid (L), Solid (g)
0                                                                       Initial Solid Form (Na+ (0); H- (1))
1                                                                       Calculation Adjustment
```

ZAM ouput

```
 Solution:  Case 1 Maximum Loading @ 40C
**********INPUT**********

  Density=  .1154E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .3220E+01
Cs+.....       132.9054          1.       .1570E-04
H+......         1.0079          1.       .5435E-13
```

```
Rb+.....          85.4678           1.        .0000E+00
K+......          39.0983           1.        .0000E+00
SrOH+...         105.0000           1.        .0000E+00
Sr++....          87.6200           2.        .0000E+00
OH-.....          17.0073          -1.        .1840E+00
NO3-....          62.0049          -1.        .1040E+01
NO2-....          46.0000          -1.        .1280E+00
Al(OH)4-          95.0000          -1.        .6310E-01
SO4--...          96.0636          -2.        .3810E+00
CO3--...          60.0092          -2.        .5102E+00
Cl-.....          35.4527          -1.        .4060E-02
Other--.          88.0200          -2.        .9200E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-06

 Material: Na Form


**********************OUTPUT************************

 Ionic Strength=            4.984922020575817 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .6271E-01      .1570E-01      .3994E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .0000E+00      .0000E+00      .0000E+00
```

Distribution:

sebastian.aleman@srnl.doe.gov
dave.crowley@srnl.doe.gov
David.Dooley@srnl.doe.gov
luther.hamm@srnl.doe.gov
thong.hang@srnl.doe.gov
michael.hay@srnl.doe.gov
william02.king@srnl.doe.gov
si.lee@srnl.doe.gov
john.mayer@srnl.doe.gov
daniel.mccabe@srnl.doe.gov
charles.nash@srnl.doe.gov
frank.pennebaker@srnl.doe.gov
scott.reboul@srnl.doe.gov
luke.reid@srnl.doe.gov
Boyd.Wiedenman@srnl.doe.gov
bill.wilmarth@srnl.doe.gov
Jennifer.Wohlwend@srnl.doe.gov

Drew.Fairchild@srs.gov
terri.fellinger@srs.gov
mark.keefer@srs.gov
Joshua.Segura@srs.gov

Terry.Foster@srnl.doe.gov
Records Administration (EDWS)