

**Contract No:**

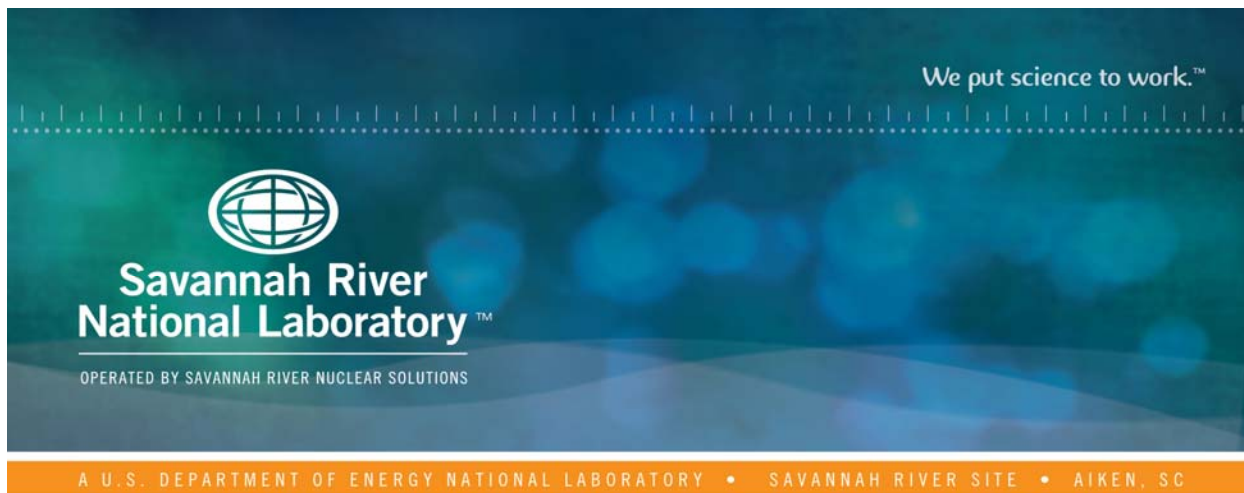
This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

**Disclaimer:**

This work was prepared under an agreement with and funded by the U.S. Government. Neither the U. S. Government or its employees, nor any of its contractors, subcontractors or their employees, makes any express or implied:

- 1 ) warranty or assumes any legal liability for the accuracy, completeness, or for the use or results of such use of any information, product, or process disclosed; or
- 2 ) representation that such use or results of such use would not infringe privately owned rights; or
- 3) endorsement or recommendation of any specifically identified commercial product, process, or service.

Any views and opinions of authors expressed in this work do not necessarily state or reflect those of the United States Government, or its contractors, or subcontractors.



# **ZAM Modeling Study to Support the Tank Closure Cesium Removal (TCCR) 1A Unit**

**T. Hang**

**C. Nash**

August 2020

SRNL-STI-2020-00262, Revision 0



## **DISCLAIMER**

This work was prepared under an agreement with and funded by the U.S. Government. Neither the U.S. Government or its employees, nor any of its contractors, subcontractors or their employees, makes any express or implied:

1. warranty or assumes any legal liability for the accuracy, completeness, or for the use or results of such use of any information, product, or process disclosed; or
2. representation that such use or results of such use would not infringe privately owned rights; or
3. endorsement or recommendation of any specifically identified commercial product, process, or service.

Any views and opinions of authors expressed in this work do not necessarily state or reflect those of the United States Government, or its contractors, or subcontractors.

**Printed in the United States of America**

**Prepared for  
U.S. Department of Energy**

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

**Retention:** *Permanent*

## **ZAM Modeling Study to Support the Tank Closure Cesium Removal (TCCR) 1A Unit**

T. Hang  
C. Nash

August 2020

---

Prepared for the U.S. Department of Energy under contract number DE-AC09-08SR22470.



## REVIEWS AND APPROVALS

### AUTHORS:

---

T. Hang, Environmental Modeling	Date
---------------------------------	------

---

C. Nash, Separation Sciences and Engineering	Date
--	------

### TECHNICAL REVIEW:

---

W. D. King, Separation Sciences and Engineering, Reviewed per E7 2.60	Date
---	------

---

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

### APPROVAL:

---

B. D. Lee, Manager Environmental Sciences	Date
--	------

---

B. J. Wiedenman, Manager Separation Sciences and Engineering	Date
---	------

---

F. M. Pennebaker, Program Manager, Liquid Waste Chemical Processing Sciences	Date
---	------

---

G. C. Arthur, Project Engineering Manager - TCCR Sampling, Isolation and Grouting	Date
--	------

## EXECUTIVE SUMMARY

The objective of this work is to study the sensitivity of cesium loading expected for the Tank Closure Cesium Removal (TCCR) columns. Savannah River National Laboratory (SRNL) utilized the Zheng-Anthony-Miller (ZAM) 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) media during the processing of Savannah River Site (SRS) Tank 10H Variable Depth Sample (VDS) waste solution.

The study specifically evaluates cesium loading on CST as a function of two variables.

1. Water additions to Tank 10H. Water dilution ranges from 0% to 20% by volume.
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 10) from OLI Systems, Inc., was used to calculate charge balanced feed compositions and to estimate feed solution densities which are required as input data to the ZAM program.

### Results Summary

Results of the ZAM model predictions follow.

- Dilution of the salt waste solution with water increases the cesium loading primarily due to the decreased ionic strength. For the Bounding Case, the Case 1 (0% dilution) initial cesium concentration is  $1.52 \times 10^{-4}$  M. Cesium was diluted in the other solutions (Cases 2-9) by the amounts indicated along with the other dissolved species. The results are in Table E-1.

**Table E-1. Dilution Effects on CST Cesium Loading at 20 °C in Diluted and Undiluted ( $1.52 \times 10^{-4}$  M Cs<sup>+</sup>) Tank 10H VDS Waste (Bounding Case)**

Cases <sup>(a)</sup>	Q (mmol <sub>Cs</sub> / g <sub>CST</sub> )
1 (0% Dilution)	0.3917
2 (1% Dilution)	0.3926
3 (2% Dilution)	0.3932
4 (3% Dilution)	0.3930
5 (4% Dilution)	0.3935
6 (5% Dilution)	0.3932
7 (10% Dilution)	0.3946
8 (15% Dilution)	0.3953
9 (20% Dilution)	0.3955

<sup>(a)</sup> Volume dilution (%) is the percentage ratio of water addition volume to the original waste volume

For the Alternate Case, the Case 1a (0% dilution) initial cesium concentration is  $6.7 \times 10^{-5}$  M. The results are in Table E-2. The correlation below shows a linear effect as indicated by the regression equation and R<sup>2</sup> value obtained within the dilution range of interest.

$$Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{CST}}) = 2.5026\text{E-}4 * \text{Dilution}(\text{Vol}\%) + 0.2407 \quad (R^2 = 0.998)$$

**Table E-2. Dilution Effect on Cesium Loading for the Alternate Case ( $6.7 \times 10^{-5} \text{ M Cs}^+$ ) at 20 °C**

Cases <sup>(a)</sup>	Q (mmol <sub>Cs</sub> / g <sub>CST</sub> )
1a (0% Dilution)	0.2406
2a (1% Dilution)	0.2409
3a (2% Dilution)	0.2412
4a (3% Dilution)	0.2415
5a (4% Dilution)	0.2417
6a (5% Dilution)	0.2420
7a (10% Dilution)	0.2433
8a (15% Dilution)	0.2445
9a (20% Dilution)	0.2456

<sup>(a)</sup> Volume dilution (%) is the percentage ratio of water addition volume to the original waste volume

- Cesium loading decreases with increasing temperatures. For the Bounding Case, the results are in Table E-3. The correlation below shows that the behavior is essentially a linear effect as indicated by the regression equation and  $R^2$  value obtained within the temperature range of 20 °C to 40 °C.

$$Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{CST}}) = -3.9280\text{E-}3 * T(^{\circ}\text{C}) + 0.4703 \quad (R^2 = 1.0)$$

**Table E-3. Temperature Effects on Cesium Loading for Undiluted Bounding Case (Case 1)**

Case 1 at T (°C)	Q (mmol <sub>Cs</sub> /g <sub>CST</sub> )
20	0.3917
21	0.3878
22	0.3839
23	0.3800
24	0.3761
25	0.3722
26	0.3682
27	0.3643
28	0.3603
29	0.3564
30	0.3524
31	0.3485
32	0.3446
33	0.3406
34	0.3367
35	0.3328
37	0.3249
39	0.3172
40	0.3133

For the Alternate Case, the temperature effect results are shown in Table E-4. The correlation shown below indicates a linear effect within the temperature range of 20 °C to 40 °C.

$$Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{CST}}) = -3.7436\text{E-}3 * T(^{\circ}\text{C}) + 0.3137 \quad (R^2 = 0.998)$$

**Table E-4. Temperature Effect on Cesium Loading for the Undiluted Alternate Case (Case 1a)**

<b>Case 1 at T (°C)</b>	<b>Q (mmol<sub>Cs</sub>/g<sub>CST</sub>)</b>
20	0.2406
21	0.2363
22	0.2321
23	0.2279
24	0.2238
25	0.2197
26	0.2157
27	0.2118
28	0.2079
29	0.2041
30	0.2003
31	0.1966
32	0.1929
33	0.1893
34	0.1858
35	0.1823
36	0.1789
37	0.1755
38	0.1722
39	0.1689
40	0.1657



## TABLE OF CONTENTS

LIST OF TABLES .....	ix
LIST OF FIGURES .....	x
LIST OF ABBREVIATIONS .....	xi
1.0 Introduction .....	1
1.1 Background .....	1
1.2 Task Objective.....	1
2.0 Model Formulations .....	2
2.1 Modeling Approach.....	2
2.2 Prediction of Cesium Loading.....	2
3.0 Waste Compositions and Properties .....	3
3.1 Tank 10H VDS Sample.....	3
3.2 Water Dilution of Waste Supernates .....	4
3.3 Waste Supernate Temperature Variation.....	7
3.4 Quality Assurance .....	8
4.0 Results and Discussion .....	9
4.1 Bounding Case .....	9
4.1.1 Dilution Effects.....	9
4.1.2 Temperature Effects.....	12
4.2 Alternate Case .....	15
4.2.1 Dilution Effects.....	15
4.2.2 Temperature Effects.....	17
5.0 Conclusions .....	20
6.0 References.....	21
Appendix A. Scope for the Alternate Case .....	22
Appendix B. ZAM Calculations for the Bounding Case .....	23
Appendix C. ZAM Calculations for the Alternate Case .....	51

## LIST OF TABLES

Table E-1. Dilution Effects on CST Cesium Loading at 20 °C in Diluted and Undiluted (1.52x10 <sup>-4</sup> M Cs <sup>+</sup> ) Tank 10H VDS Waste (Bounding Case) .....	v
Table E-2. Dilution Effect on Cesium Loading for the Alternate Case (6.7x10 <sup>-5</sup> M Cs <sup>+</sup> ) at 20 °C.....	vi
Table E-3. Temperature Effects on Cesium Loading for Undiluted Bounding Case (Case 1) .....	vi
Table E-4. Temperature Effect on Cesium Loading for the Undiluted Alternate Case (Case 1a) .....	vii
Table 3-1. Adjusted VDS Tank 10H Composition at 20 °C (Bounding Case).....	3
Table 3-2. Composition for Alternate Case at 20 °C .....	4
Table 3-3. Water Dilution of the Tank 10H VDS Sample at 20 °C (Bounding Case).....	5
Table 3-4. Water Dilution for the Alternate Case at 20 °C .....	6
Table 3-5. Predicted Density vs. Temperature for Case 1 (Bounding Case) .....	7
Table 3-6. Predicted Density vs. Temperature for Case 1a (Alternate Case) .....	8
Table 4-1. ZAM Predictions of Dilution Effects on Cesium Loading at 20 °C for Tank 10H VDS (Bounding Case) .....	9
Table 4-2. Isotherm Parameters for Bounding Dilution Cases at 20°C .....	11
Table 4-3. Activity Coefficients and Equilibrium Constants for Bounding Case 1 at 20 °C, 30 °C and 40 °C .....	13
Table 4-4. ZAM Predictions of Temperature Effects on CST Cesium Loading for the Undiluted Tank 10H VDS Sample (Bounding Case 1) .....	13
Table 4-5. Isotherm Parameters for Bounding Case 1 at Different Temperatures.....	14
Table 4-6. ZAM Predictions of Dilution Effects on Cesium Loading at 20 °C for the Alternate Case .....	15
Table 4-7. Isotherm Parameters for Alternate Dilution Cases at 20°C .....	16
Table 4-8. Temperature Effect on Cesium Loading for the Undiluted Alternate Case (Case 1a) .....	18
Table 4-9. Isotherm Parameters for Alternate Case 1a at Different Temperatures.....	19

## LIST OF FIGURES

Figure 4-1. Dilution Effect on CST Cesium Loading at 20 °C.....	10
Figure 4-2. Cesium CST Loading Isotherm at 20 °C (Bounding Case 1).....	10
Figure 4-3. Isotherms for Bounding Dilution Cases at 20°C.....	11
Figure 4-4. Temperature Effect on Cesium Loading for the Bounding Case .....	14
Figure 4-5. Isotherms for Bounding Case 1 at Different Temperatures.....	15
Figure 4-6. Dilution Effect on Cesium Loading for the Alternate Case at 20 °C .....	16
Figure 4-7. Isotherms for Alternate Dilution Cases at 20°C.....	17
Figure 4-8. Temperature Effect on Cesium Loading for the Alternate Case .....	18
Figure 4-9. Isotherms for Alternate Case 1a at Different Temperatures.....	19

## **LIST OF ABBREVIATIONS**

CST	crystalline silicotitanate
SRNL	Savannah River National Laboratory
SRR	Savannah River Remediation
SRS	Savannah River Site
TCCR	Tank Closure Cesium Removal
TTR	Technical Task Request
VDS	Variable Depth Sample
ZAM	ZAM (Zheng, Anthony, and Miller) Computer Program

## 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 the engineered IONSIV® R9120 form of Crystalline Silicotitanate (CST) media. 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 with fresh ion-exchange media 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). Demonstration of the system began in early calendar year 2019 with two batches of salt solution generated by dissolving saltcake in Tank 10H, followed by processing of these batches through the TCCR system. A third TCCR Tank 10H dissolved saltcake batch is scheduled for processing soon. Upon completion of the demonstration with Tank 10H dissolved saltcake, Tank 9H salt solution will be transferred to Tank 10H and subsequently processed through the TCCR unit with new CST media (referred to as R9120-B 30x60) added to new IX columns. The TCCR processing campaign of Tank 9H salt solution is referred to as TCCR-1A (King et al., 2020).

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 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 the concentrations of cesium, potassium, sodium, rubidium, strontium, and anions. It is important to understand that the CST and the aqueous stream reach equilibrium under normal TCCR processing conditions, which is not necessarily a cesium loading saturation for 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 in each solution, given an infinite amount of liquid feed. The maximum loading is then species/composition dependent, not volume or phase ratio 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,  $^{133}\text{Cs}$ ,  $^{135}\text{Cs}$ , and  $^{137}\text{Cs}$  (Reboul, 2017). The stable isotope  $^{133}\text{Cs}$  is the most abundant fission product of the three. The CST removes all isotopes equally. The primary isotope of concern is  $^{137}\text{Cs}$  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 strontium and rubidium species are not present is conservative (i.e., ZAM would overestimate the cesium loading on CST due to the absence of these competitors).

### 1.2 Task Objective

Per the Savannah River Remediation (SRR) need to predict cesium loading on CST (Luzzatti, 2020), 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 predicts cesium loading on CST as a function of: (1) water additions to Tank 10H; and (2) temperature in the TCCR column for a prepared batch of salt feed.

## 2.0 Model Formulations

### 2.1 Modeling Approach

- Cesium loading on the CST media 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 detail in previous ion exchange studies at SRNL (Hamm et al., 2001; Hang et al., 2017).
- The OLI Studio™ software (Version 10) from OLI Systems, Inc., was used to calculate charge balanced feed compositions and to estimate feed solution densities (OLI Systems, 2020) 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 solid 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  $\phi$  is defined as the ratio of total liquid volume (mL) processed to the mass of CST media ( $g_{CST}$ ). 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 in that solution (Hang et al., 2017).

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

### 3.0 Waste Compositions and Properties

#### 3.1 Tank 10H VDS Sample

The waste composition was obtained from an analysis of a variable depth sample (VDS) taken from Tank 10H (Reboul, 2017). The VDS sample was collected in March 2017 following a water addition to the tank after allowing the saltcake to dissolve for a few weeks. Note that the total Cs concentration was derived from the measured  $^{137}\text{Cs}$ . Although the analyzed molar ratio of  $^{137}\text{Cs}$  to total Cs is 0.21 in the VDS composition, the ratio of 0.3 was used as specified in the TTR (Luzzatti, 2020).

The Tank 10H VDS composition used for the analysis is shown in Table 3-1. The composition was adjusted relative to the analysis results reported by Reboul by leaving out the competitor cations (i.e.,  $\text{K}^+$  and  $\text{SrOH}^+$  or  $\text{Sr}^{2+}$ ) and balancing the charges by increasing the  $\text{CO}_3^{2-}$  concentration. Omitting the competitor cations increases the likelihood of producing conservative ZAM cesium loading prediction. With the high cesium concentration of  $1.52 \times 10^{-4} \text{ M}$ , the composition shown in Table 3-1 serves as an upper bounding case for the CST cesium loading.

**Table 3-1. Adjusted VDS Tank 10H Composition at 20 °C (Bounding Case)**

Cations	(M)	Anions	(M)
$\text{Na}^+$	3.22	$\text{OH}^-$	0.184
$\text{Cs}^+$	1.52E-04	$\text{NO}_3^-$	1.04
		$\text{NO}_2^-$	0.128
		$\text{Al}(\text{OH})_4^-$	0.0631
		$\text{SO}_4^{2-}$	0.381
		$\text{CO}_3^{2-}$ (a)	0.512
		$\text{Cl}^-$	1.52E-04
		$\text{C}_2\text{O}_4^{2-}$	9.20E-03
Density <sup>(b)</sup> (g/mL)	1.16		

<sup>(a)</sup>  $\text{CO}_3^{2-}$  adjusted for charge balance

<sup>(b)</sup> Density calculated by OLI

An additional case (i.e., Alternate Case) was requested by SRR (Fellinger, 2020; also see Appendix A). For the Alternate Case, the cesium concentration from Tank 9H Dilution #3 (Taylor-Pashow et al., 2020) was used, and the  $\text{Na}^+$  molarity was changed from 3.22 M to 4 M by increasing the concentrations of all species by the same amount, except cesium. Again, the  $\text{CO}_3^{2-}$  concentration was adjusted for charge balance. The cesium concentration of  $6.7 \times 10^{-5} \text{ M}$  for this case was significantly lower than the Bounding Case. The composition for the Alternate Case is shown in Table 3-2.

**Table 3-2. Composition for Alternate Case at 20 °C**

<b>Cations</b>	<b>(M)</b>	<b>Anions</b>	<b>(M)</b>
Na <sup>+</sup>	4.0	OH <sup>-</sup>	0.229
Cs <sup>+</sup>	6.7E-05	NO <sub>3</sub> <sup>-</sup>	1.29
		NO <sub>2</sub> <sup>-</sup>	0.159
		Al(OH) <sub>4</sub> <sup>-</sup>	0.0784
		SO <sub>4</sub> <sup>2-</sup>	0.473
		CO <sub>3</sub> <sup>2-</sup> (a)	0.636
		Cl <sup>-</sup>	6.7E-05
		C <sub>2</sub> O <sub>4</sub> <sup>2-</sup>	0.0114
Density <sup>(b)</sup> (g/mL)	1.196		

(a) CO<sub>3</sub><sup>2-</sup> adjusted for charge balance

(b) Density calculated by OLI

### 3.2 Water Dilution of Waste Supernates

The Tank 10H 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 original waste volume. A total of nine case were generated and summarized in Table 3-3. Table 3-3 is reproduced from Table 1 of the Technical Task Request (Luzzatti, 2020). Note that concentration values in Table 3-3 were subjected to rounding. More accurate values are given in the ZAM input files given in Appendix B. In this analysis, the cesium concentration is also diluted with water addition, rather than being held constant. Similarly, the Alternate Case was diluted with water and the resulting compositions are shown in Table 3-4.



**Table 3-3. Water Dilution of the Tank 10H VDS Sample at 20 °C (Bounding Case)**

<b>Cases</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>	<b>9</b>
	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 <sup>+</sup>	3.22	3.188	3.157	3.126	3.096	3.067	2.927	2.8	2.683
Cs <sup>+</sup>	1.52E-04	1.50E-04	1.49E-04	1.47E-04	1.46E-04	1.44E-04	1.38E-04	1.32E-04	1.26E-04
OH <sup>-</sup>	0.184	0.182	0.18	0.179	0.177	0.175	0.167	0.16	0.153
NO <sub>3</sub> <sup>-</sup>	1.04	1.03	1.02	1.01	1.00	0.99	0.945	0.904	0.867
NO <sub>2</sub> <sup>-</sup>	0.128	0.127	0.125	0.124	0.123	0.122	0.116	0.111	0.107
Al(OH) <sub>4</sub> <sup>-</sup>	0.0631	0.0625	0.0619	0.0613	0.0607	0.0601	0.0574	0.0549	0.0526
SO <sub>4</sub> <sup>2-</sup>	0.381	0.377	0.374	0.37	0.366	0.363	0.346	0.331	0.318
CO <sub>3</sub> <sup>2-</sup> (a)	0.512	0.507	0.502	0.497	0.493	0.488	0.466	0.445	0.427
Cl <sup>-</sup>	1.52E-04	1.50E-04	1.49E-04	1.47E-04	1.46E-04	1.44E-04	1.38E-04	1.32E-04	1.26E-04
C <sub>2</sub> O <sub>4</sub> <sup>2-</sup>	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 <sup>(b)</sup> (g/mL)	1.1611	1.1596	1.1582	1.1568	1.1554	1.1541	1.1476	1.1417	1.1362

<sup>(a)</sup> adjusted for charge balance<sup>(b)</sup> calculated by OLI

**Table 3-4. Water Dilution for the Alternate Case at 20 °C**

<b>Cases</b>	<b>1a</b>	<b>2a</b>	<b>3a</b>	<b>4a</b>	<b>5a</b>	<b>6a</b>	<b>7a</b>	<b>8a</b>	<b>9a</b>
	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 <sup>+</sup>	4.00	3.9604	3.9216	3.8835	3.8462	3.8095	3.6364	3.4783	3.3333
Cs <sup>+</sup>	6.70E-05	6.6337E-05	6.5686E-05	6.5049E-05	6.4423E-05	6.381E-05	6.0909E-05	5.8261E-05	5.5833E-05
OH <sup>-</sup>	0.229	0.2267	0.2245	0.2223	0.2202	0.2181	0.2082	0.1991	0.1908
NO <sub>3</sub> <sup>-</sup>	1.29	1.2772	1.2647	1.2524	1.2404	1.2286	1.1727	1.1217	1.075
NO <sub>2</sub> <sup>-</sup>	0.159	0.1574	0.1559	0.1544	0.1529	0.1514	0.1445	0.1383	0.1325
Al(OH) <sub>4</sub> <sup>-</sup>	0.0784	0.0776	0.0769	0.0761	0.0754	0.0747	0.0713	0.0682	0.0653
SO <sub>4</sub> <sup>2-</sup>	0.473	0.4683	0.4637	0.4592	0.4548	0.4505	0.4300	0.4113	0.3942
CO <sub>3</sub> <sup>2-</sup> (a)	0.6374	0.63115	0.6249	0.61885	0.61285	0.606965	0.57945	0.5543	0.53115
Cl <sup>-</sup>	6.70E-05	6.6337E-05	6.5686E-05	6.5049E-05	6.4423E-05	6.3810E-05	6.0909E-05	5.8261E-05	5.5833E-05
C <sub>2</sub> O <sub>4</sub> <sup>2-</sup>	0.0114	0.0113	0.0112	0.0111	0.0110	0.0109	0.0104	0.0099	0.0095
Density <sup>(b)</sup> (g/mL)	1.196	1.1943	1.1926	1.1909	1.1892	1.1876	1.1799	1.1728	1.1663

<sup>(a)</sup> adjusted for charge balance<sup>(b)</sup> calculated by OLI

### 3.3 Waste Supernate Temperature Variation

To determine the change in cesium loading on CST as a function of temperature, the Bounding Case 1 (undiluted supernate) temperature was varied from 20 °C to 40 °C in increments as shown in Table 3-5. At each temperature, the liquid waste density was calculated by OLI. Predicted densities for each temperature are given in Table 3-5. For the undiluted supernate Case 1a (Alternate Case), predicted densities are shown in Table 3-6.

**Table 3-5. Predicted Density vs. Temperature for Case 1 (Bounding Case)**

<b>Case 1 at T (°C)</b>	<b>Density<sup>(a)</sup> (g/mL)</b>
20	1.1611
21	1.1607
22	1.1604
23	1.1600
24	1.1596
25	1.1592
26	1.1589
27	1.1585
28	1.1582
29	1.1578
30	1.1575
31	1.1571
32	1.1568
33	1.1564
34	1.1561
35	1.1557
37	1.1550
39	1.1543
40	1.1540

(a) Density calculated by OLI

**Table 3-6. Predicted Density vs. Temperature for Case 1a (Alternate Case)**

Case 1 at T (°C)	Density <sup>(a)</sup> (g/mL)
20	1.1961
21	1.1957
22	1.1953
23	1.1949
24	1.1946
25	1.1942
26	1.1939
27	1.1936
28	1.1932
29	1.1929
30	1.1926
31	1.1923
32	1.1919
33	1.1916
34	1.1912
35	1.1909
36	1.1906
37	1.1902
38	1.1899
39	1.1896
40	1.1892

(a) Density calculated by OLI

### 3.4 Quality Assurance

The Customer requests that a Functional Classification of Safety Class apply to the TCCR 1A Unit work (Luzzatti, 2020). This work was performed under a Task Technical and Quality Assurance Plan (King et al., 2020). Computer modeling using the ZAM CST isotherm program will be conducted as specified in Tasks 5-7 and Table 1 of SRR's Technical Task Request (Luzzatti, 2020).

Both ZAM and OLI software are controlled at Level D, and so their calculations are for production support purposes only. The functional requirements placed on ZAM Version 4 were verified and validated (Hamm et al., 2001). All the activities related to the verification and validation of the OLI software database and the resulting models were documented in accordance with Manual E7 Section 5.0 Software Engineering and Control (Choi, 2019).

This report received technical review by design verification (E7 Manual Procedure 2.60, Section 5.3). Signatures of E7 technical reviewers on the final document signifies completion of the design verification review.

## 4.0 Results and Discussion

The calculated ZAM cesium loading results for the waste compositions specified in the previous section are presented and discussed in this section.

### 4.1 Bounding Case

#### 4.1.1 Dilution Effects

Table 4-1 summarizes the ZAM modeling cesium loading predictions for the undiluted and diluted Tank 10H saltcake VDS solutions. Cesium loading on CST was calculated for salt solutions varying from 0% to 20% volume dilution. Table 4-1 also provides pH and the total ionic strength (mol/kg) calculated by OLI for each solution.

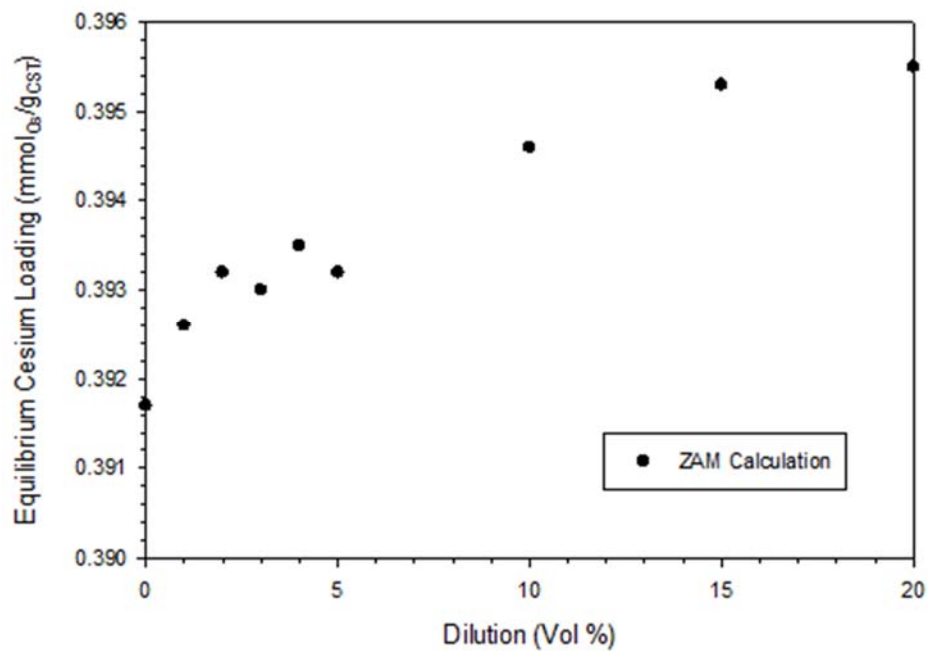
Table 4-1 shows a large decrease in the ionic strength with increasing dilution. Zheng et al. (1996) observed that the CST cesium loading increases with decreasing  $\text{Na}^+$  concentrations (i.e., increasing dilution) primarily due to the decreased ionic strength. Table 4-1 confirms cesium loading increases in more diluted salt solutions even though the initial liquid-phase cesium concentration is decreasing with dilution.

**Table 4-1. ZAM Predictions of Dilution Effects on Cesium Loading at 20 °C for Tank 10H VDS (Bounding Case)**

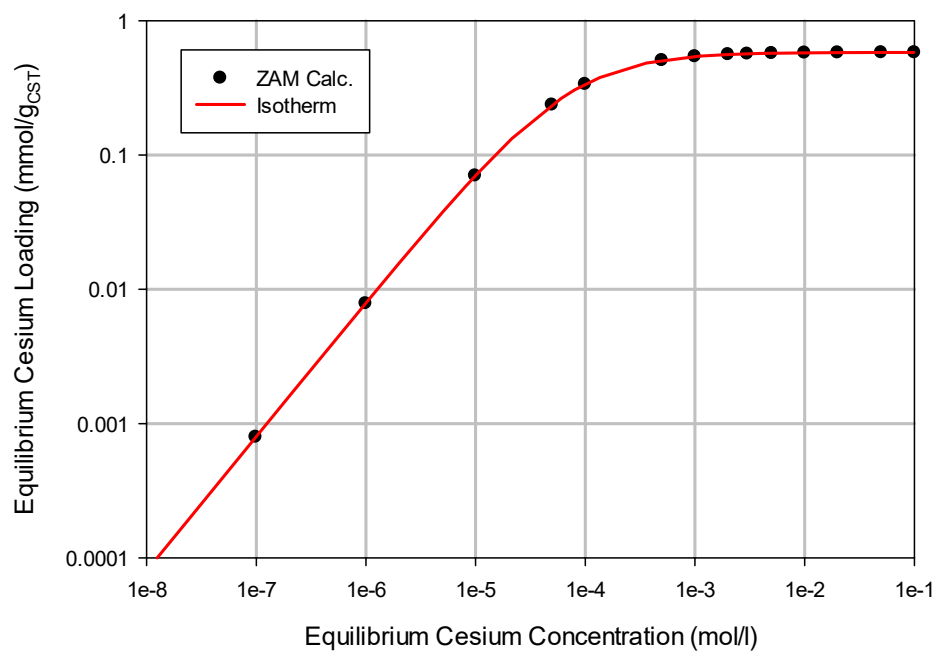
Cases	Q mmol <sub>Cs</sub> /g <sub>CST</sub>	pH <sup>(a)</sup>	Total Ionic Strength <sup>(a)</sup> (mol/kg)
1	0.3917	13.3292	4.3665
2	0.3926	13.3225	4.3198
3	0.3932	13.3157	4.2753
4	0.3930	13.3109	4.2298
5	0.3935	13.3043	4.1865
6	0.3932	13.2977	4.1451
7	0.3946	13.2691	3.9437
8	0.3953	13.2432	3.7619
9	0.3955	13.2177	3.5953

<sup>(a)</sup> Calculated by OLI

Figure 4-1 displays the effect of dilution on cesium loading. Unlike the VDS sample studied previously (Hang, 2018), in which the cesium concentration is one order of magnitude smaller (i.e.,  $1.57 \times 10^{-5}$  M), dilution of the current VDS sample has a non-linear effect on cesium loading. Figure 4-2 exhibits the isotherm for the specified Case 1 at 20 °C. The equilibrium CST cesium loading shows a linear correlation with the equilibrium cesium concentration in the liquid phase across a large range of solution cesium concentrations. When the cesium concentration approaches  $1 \times 10^{-4}$  M, the relationship becomes non-linear. The deviation from the linear relationship eventually occurs as the CST begins to run out of selective cesium sites. The CST cesium loading was predicted to increase by 1% when the Tank 10H VDS was diluted by 20%.



**Figure 4-1. Dilution Effect on CST Cesium Loading at 20 °C.**



**Figure 4-2. Cesium CST Loading Isotherm at 20 °C (Bounding Case 1)**

Isotherms were also determined for some cases (e.g., cases 1, 3, 5, and 9). Use of the Freundlich/Langmuir model was found to provide an excellent fit for ZAM data. Isotherm parameters are listed in Table 4-2.

Freundlich/Langmuir isotherm:

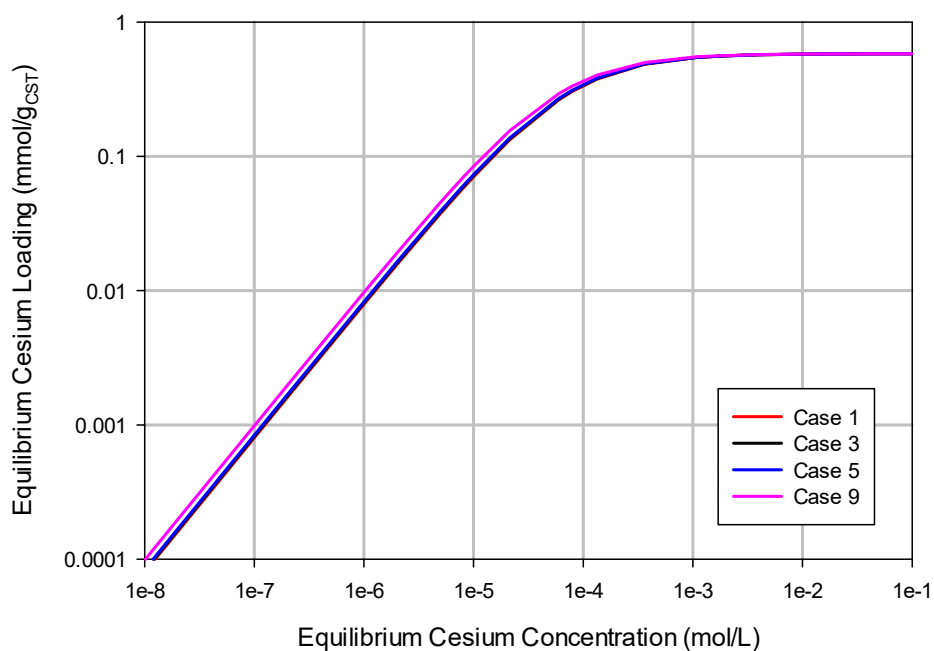
$$Q = \frac{C_T C_{Cs}}{\beta + C_{Cs}}$$

Q: Equilibrium Cs loading (mmol/g<sub>CST</sub>)  
 C<sub>Cs</sub>: Equilibrium Cs concentration in the solution (mol/L)  
 C<sub>T</sub>: Total cesium capacity (~0.58 mmol/g<sub>CST</sub>)  
 β: Isotherm parameter

**Table 4-2. Isotherm Parameters for Bounding Dilution Cases at 20°C**

Cases	C <sub>T</sub>	β
1	0.58	7.2363E-05
3	0.58	7.0735E-05
5	0.58	6.9157E-05
9	0.58	5.8777E-05

Figure 4-3 shows the computed isotherms for the selected cases and confirms that cesium loading increases with more diluted waste solutions.



**Figure 4-3. Isotherms for Bounding Dilution Cases at 20°C**

#### 4.1.2 Temperature Effects

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

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



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

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

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

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

$K_{eq}$ :	Thermodynamic equilibrium constant
$K_C$ :	Concentration-related equilibrium parameter
$K_\gamma$ :	Activity coefficient-related equilibrium parameter
$Q_{Cs}$ :	Equilibrium Cs concentration on the CST media,
$Q_{Na}$ :	Equilibrium Na concentration on the CST media,
$C_{Cs}$ :	Equilibrium Cs concentration in the solution,
$C_{Na}$ :	Equilibrium Na concentration in the solution,
$\gamma_{Cs}$ :	Activity coefficient of Cs in the solution, and
$\gamma_{Na}$ :	Activity coefficient of Na in the solution

The solid phase was found to be ideal along the binary ion exchange isotherms of  $Cs^+/Na^+$ ,  $Rb^+/Na^+$ , and  $K^+/N^+$  systems (Zheng et al., 1997). Therefore, no activity coefficients for the solid phase are included in Eq. 4.

The cesium-sodium relation on the CST media 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 media

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,  $\Delta H^\circ$ , by the Van't Hoff equation as follows.

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

with  $K_{eq,25^\circ C} = 4.4 \times 10^4 \quad \text{Eq. 9}$

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



For illustration, activity coefficients and equilibrium constants calculated for Case 1 at 20 °C, 30 °C, and 40 °C are shown in Table 4-3.

**Table 4-3. Activity Coefficients and Equilibrium Constants for Bounding Case 1 at 20 °C, 30 °C and 40 °C**

T (°C)	$\gamma_{Cs}^{(a)}$	$\gamma_{Na}^{(a)}$	$K_{\gamma}$	$K_{eq}$	$K_{\gamma}/K_{eq}$
20	0.5517	0.4053	0.7346	5.1120E+04	1.4370E-05
30	0.5576	0.4183	0.7502	3.8059E+04	1.9712E-05
40	0.5633	0.4270	0.7580	2.8874E+04	2.6251E-05

<sup>(a)</sup>: Calculated by OLI

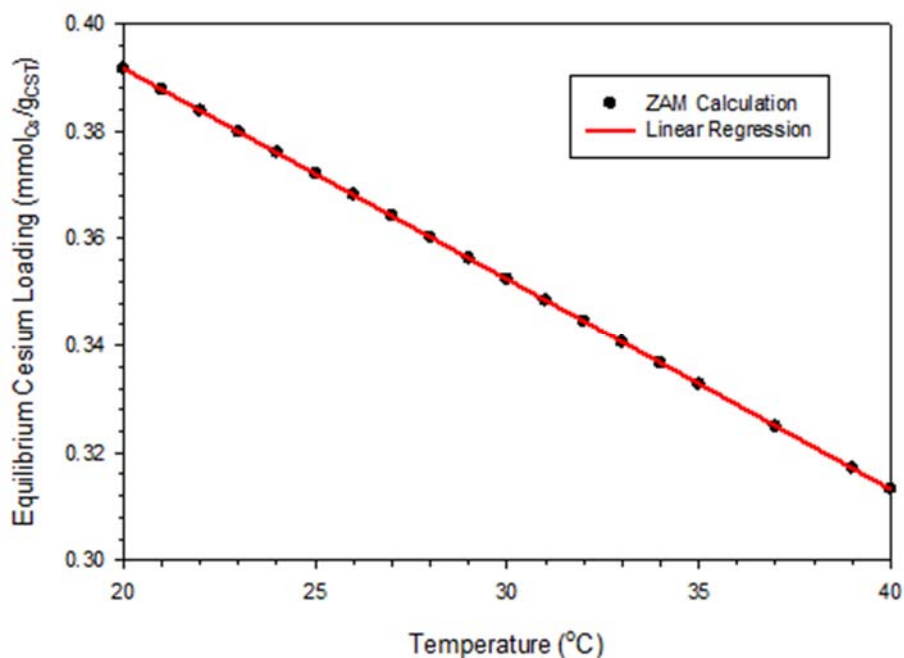
Equilibrium constants  $K_{eq}$  decrease with increasing temperatures much more than the increase in activity coefficients. Consequently, the ratio ( $K_{\gamma}/K_{eq}$ ) increases, making the denominator of the cesium loading equation (Eq. 7) larger, therefore reducing cesium sorption.

Table 4-4 shows the ZAM results for Case 1 at different temperatures ranging from 20 to 40 °C. Table 4-4 confirms the decrease in cesium loading with increasing temperatures. The cesium loading on CST was predicted to decrease by 20% when the temperature was increased from 20 to 40 °C.

**Table 4-4. ZAM Predictions of Temperature Effects on CST Cesium Loading for the Undiluted Tank 10H VDS Sample (Bounding Case 1)**

Case 1 at T (°C)	Q mmol <sub>Cs</sub> / g <sub>CST</sub>
20	0.3917
21	0.3878
22	0.3839
23	0.3800
24	0.3761
25	0.3722
26	0.3682
27	0.3643
28	0.3603
29	0.3564
30	0.3524
31	0.3485
32	0.3446
33	0.3406
34	0.3367
35	0.3328
37	0.3249
39	0.3172
40	0.3133

Figure 4-4 displays the effect of temperature on cesium loading as predicted by the ZAM model. The correlation in Figure 4-4 is linear within the temperature range of interest. The linear regression of the plotted calculation results yields the equation below the figure.



**Figure 4-4. Temperature Effect on Cesium Loading for the Bounding Case**

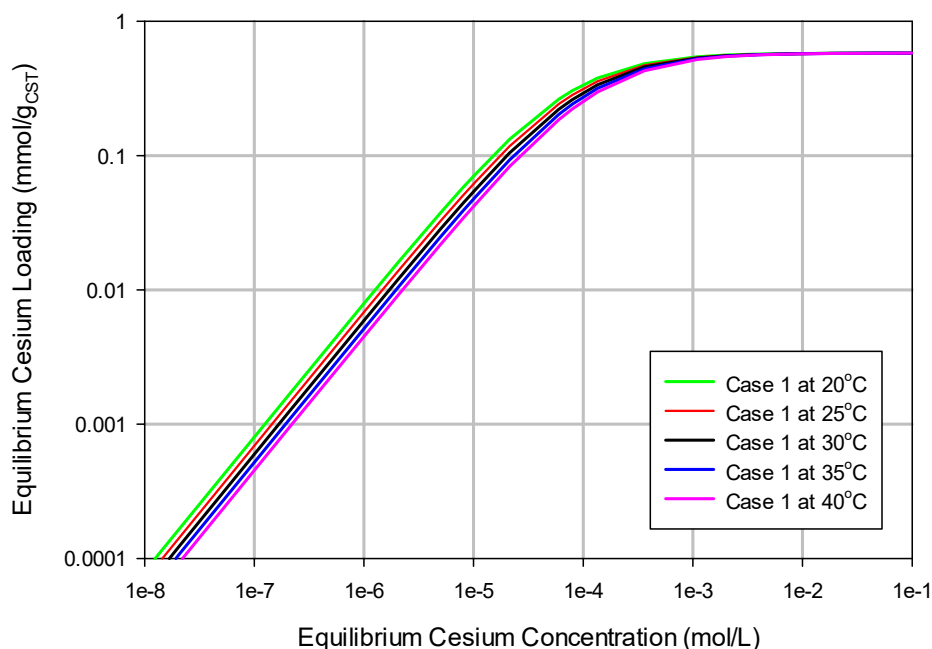
Linear regression:  $Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{cst}}) = -3.9280\text{E-}3 * T(^{\circ}\text{C}) + 0.4703$  ( $R^2 = 1$ )

Isotherms were determined for some cases (e.g., at 20°C, 25°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 4-5.

**Table 4-5. Isotherm Parameters for Bounding Case 1 at Different Temperatures**

Case 1 at T(°C)	C <sub>T</sub>	β
20	0.58	7.2363E-05
25	0.58	8.4079E-05
30	0.58	9.7242E-05
35	0.58	1.1189E-04
40	0.58	1.2819E-04

Figure 4-5 shows the isotherms for the selected cases and confirms that cesium loading decreases with increasing temperatures.



**Figure 4-5. Isotherms for Bounding Case 1 at Different Temperatures**

## 4.2 Alternate Case

### 4.2.1 Dilution Effects

Table 4-6 shows the ZAM modeling CST cesium loading predictions for the undiluted and diluted supernate solutions of the Alternate Case. Table 4-6 also provides pH and the total ionic strength (mol/kg) calculated by OLI. Similarly to the results for the Bounding Case, Table 4-6 confirms cesium loading increases in more diluted salt solutions.

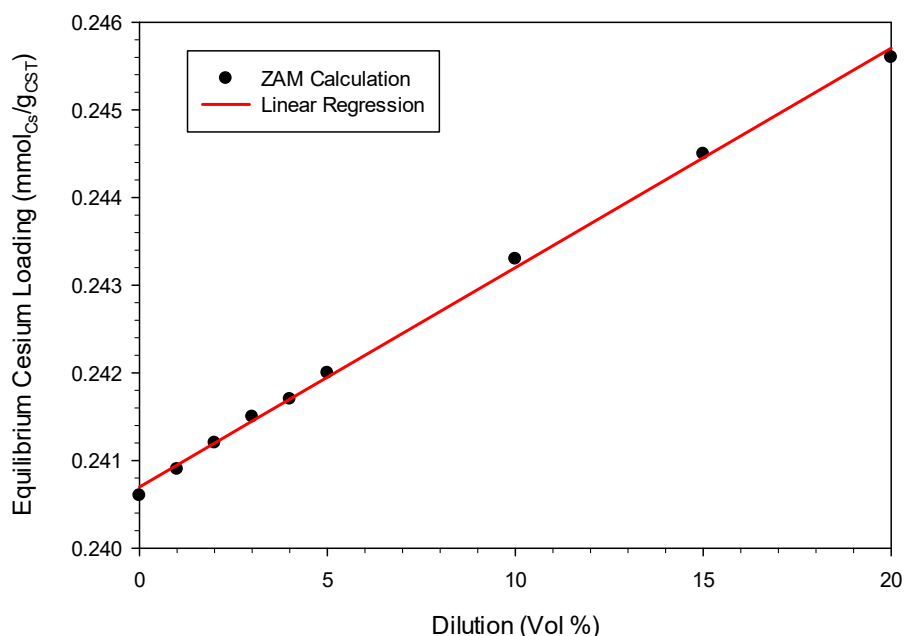
**Table 4-6. ZAM Predictions of Dilution Effects on Cesium Loading at 20 °C for the Alternate Case**

Cases	Q mmol <sub>Cs</sub> /g <sub>CST</sub>	pH <sup>(a)</sup>	Total Ionic Strength <sup>(a)</sup> (mol/kg)
1a	0.2406	13.4825	5.5061
2a	0.2409	13.4748	5.4472
3a	0.2412	13.4674	5.3896
4a	0.2415	13.4600	5.3333
5a	0.2417	13.4529	5.2781
6a	0.2420	13.4458	5.2241
7a	0.2433	13.4122	4.9708
8a	0.2445	13.3813	4.7420
9a	0.2456	13.3525	4.5321

(a) calculated by OLI

Figure 4-6 exhibits the effect of dilution on cesium loading. As was the case for the Bounding Case discussed in Section 4.1.1 above, since the initial cesium concentration for the Alternate Case is below

$1 \times 10^{-4}$  M, a linear relationship of the equilibrium CST cesium loading and the equilibrium cesium concentration in the liquid phase would be expected assuming a similar loading isotherm for this supernate composition. Figure 4-6 confirms this linear correlation. The linear regression of the calculated results produces the equation shown below. The CST cesium loading was predicted to increase by ~2% when the Alternate supernate was diluted by 20%.



**Figure 4-6. Dilution Effect on Cesium Loading for the Alternate Case at 20 °C**

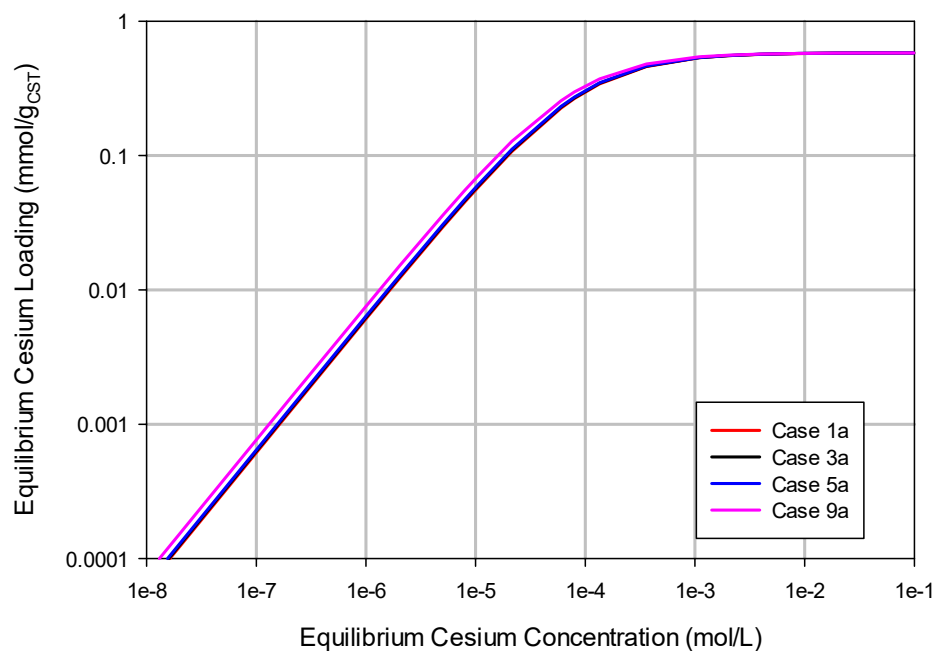
Linear regression:  $Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{CST}}) = 2.5026\text{E-}4 * \text{Dilution}(\text{Vol}\%) + 0.2407$  ( $R^2 = 0.998$ )

Isotherms were determined for some cases (e.g., cases 1, 3, 5, and 9). The Freundlich/Langmuir model was used to fit ZAM data. Table 4-7 shows the isotherm parameters for these cases.

**Table 4-7. Isotherm Parameters for Alternate Dilution Cases at 20°C**

Cases	$C_T$	$\beta$
1a	0.58	9.4527E-05
3a	0.58	9.2266E-05
5a	0.58	9.0122E-05
9a	0.58	7.6014E-05

Figure 4-7 shows the computed isotherms for the selected cases and confirms that cesium loading increases with more diluted waste solutions.



**Figure 4-7. Isotherms for Alternate Dilution Cases at 20°C**

#### 4.2.2 Temperature Effects

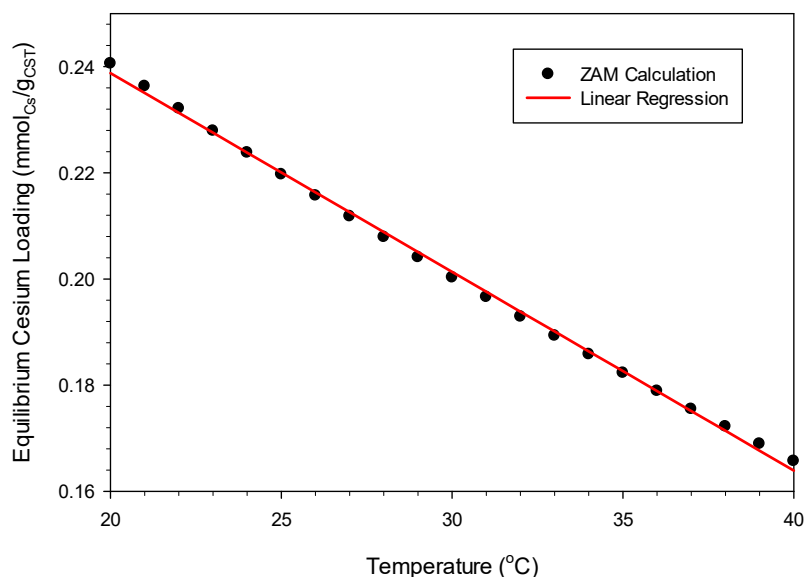
Table 4-8 provides the ZAM results for the Alternate Case 1a at temperatures varying from 20 °C to 40 °C, showing the decrease in cesium loading with increasing temperatures. The CST cesium loading was predicted to decrease by 31% when the temperature was increased from 20 °C to 40 °C.

**Table 4-8. Temperature Effect on Cesium Loading for the Undiluted Alternate Case (Case 1a)**

Case 1a at T (°C)	Density <sup>(a)</sup> (g/mL)	Q mmol <sub>Cs</sub> /g <sub>CST</sub>
20	1.1961	0.2406
21	1.1957	0.2363
22	1.1953	0.2321
23	1.1949	0.2279
24	1.1946	0.2238
25	1.1942	0.2197
26	1.1939	0.2157
27	1.1936	0.2118
28	1.1932	0.2079
29	1.1929	0.2041
30	1.1926	0.2003
31	1.1923	0.1966
32	1.1919	0.1929
33	1.1916	0.1893
34	1.1912	0.1858
35	1.1909	0.1823
36	1.1906	0.1789
37	1.1902	0.1755
38	1.1899	0.1722
39	1.1896	0.1689
40	1.1892	0.1657

<sup>(a)</sup> calculated by OLI

Figure 4-8 displays the effect of temperature on CST cesium loading as predicted by the ZAM model. The correlation in Figure 4-8 is linear within the temperature range of interest. The linear regression of the calculated results yields the equation shown below.



**Figure 4-8. Temperature Effect on Cesium Loading for the Alternate Case**

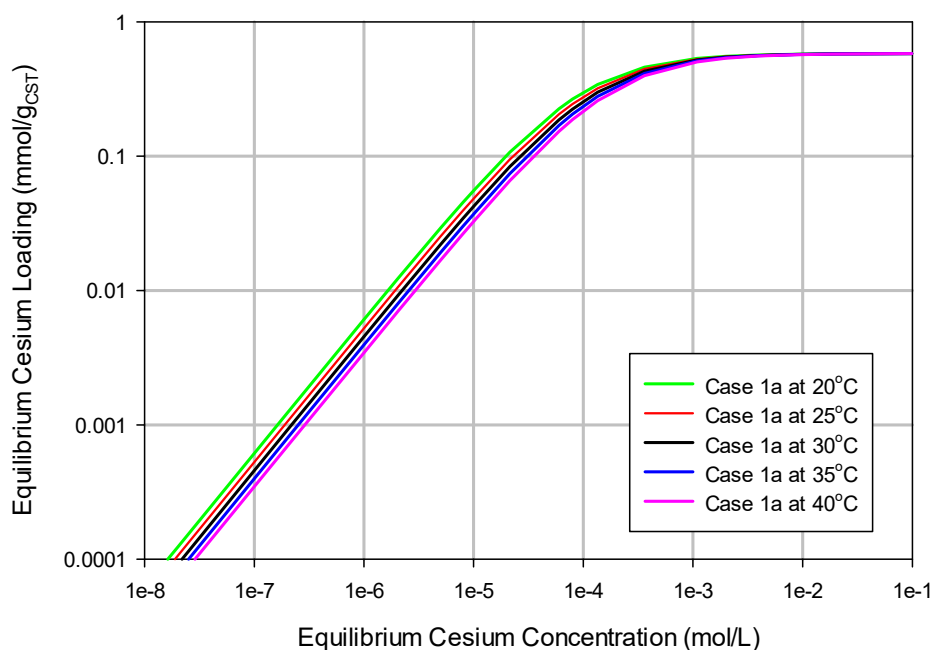
Linear regression:  $Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{CST}}) = -3.7436\text{E-}3 * T(^{\circ}\text{C}) + 0.3137$  ( $R^2 = 0.9983$ )

Isotherms were determined for some cases (e.g., at 20°C, 25°C, 30°C, 35°C, and 40°C). The Freundlich/Langmuir model was used to fit ZAM data. Isotherm parameters are listed in Table 4-9.

**Table 4-9. Isotherm Parameters for Alternate Case 1a at Different Temperatures**

Case 1a at T(°C)	C <sub>T</sub>	β
20	0.58	9.4527E-05
25	0.58	1.0982E-04
30	0.58	1.2699E-04
35	0.58	1.4613E-04
40	0.58	1.6741E-04

Figure 4-9 shows the isotherms for the selected cases and confirms that cesium loading decreases with increasing temperatures.



**Figure 4-9. Isotherms for Alternate Case 1a at Different Temperatures**

## 5.0 Conclusions

The sensitivity of Tank 10H VDS waste solution to be processed in the TCCR 1A Unit was studied using the ZAM program. Results of the ZAM model predictions follow.

- Dilution of the salt waste solution with water increases the cesium loading primarily due to the decreased ionic strength. For the Bounding Case, dilution has a non-linear effect on cesium loading within the dilution range of 0% to 20% by volume. For the Alternate Case, the dilution effect on cesium loading is linear with the following correlation equation:

$$Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{CST}}) = 2.5026\text{E-}4 * \text{Dilution}(\text{Vol}\%) + 0.2407 \quad (R^2 = 0.998)$$

Diluting either supernate by 20% results in a 1-2% increase in cesium loading.

- Cesium loading decreases with increasing temperatures. For the Bounding Case, the correlation shows a linear effect within the temperature range of 20 to 40 °C. The cesium loading on CST was predicted to decrease by 20% when the temperature was increased from 20 to 40 °C.

$$Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{CST}}) = -3.9280\text{E-}3 * T(^{\circ}\text{C}) + 0.4703 \quad (R^2 = 1)$$

For the Alternate Case, the temperature effect on the CST cesium loading is also linear within the temperature range of 20 to 40 °C. The cesium loading on CST was predicted to decrease by 31% when the temperature was increased from 20 to 40 °C.

$$Q(\text{mmol}_{\text{Cs}}/\text{g}_{\text{CST}}) = -3.7436\text{E-}3 * T(^{\circ}\text{C}) + 0.3137 \quad (R^2 = 0.998)$$

Across the ranges evaluated, temperature effects on CST cesium loading are much greater than ionic strength or dilution effects.



## 6.0 References

- Aleman, S. E., and L. L. Hamm, 2003. "Small Column Ion Exchange Analysis for Removal of Cesium from SRS Low Curie Salt Solutions Using Crystalline Silicotitanate (CST) Resin," WSRC-TR-2003-00430, December 2003.
- Caldwell, T. B., 2017. "Tank Closure Cesium Removal (TCCR) System," X-SOW-H-00002, Rev. 4.
- Choi, A. S., 2019. "Software Quality Assurance Plan for the OLI Platform Software Used at the Savannah River Site", X-SQP-A-00001, Rev. 0, September 2019.
- Fellinger, T. L., 2020. "New Case for Penalty Document," email dated 22 July 2020, ELN A2341-00117-15.
- Hamm, L. L., T. Hang, D. J. McCabe, and W. D. King, 2001. "Preliminary Ion Exchange Modeling for Removal of Cesium from Hanford Waste Using Hydrous Crystalline Silicotitanate Material," WSRC-TR-2001-00400, July 2001.
- Hang, T., D. J. McCabe, L. L. Hamm, and J. L. Wohlwend, 2017. "Modeling Ion Exchange Performance of Crystalline Silicotitanate to Support SRS Tank 10H Closure," SRNL-STI-2017-00336, Rev. 0, July 2017.
- Hang, T., 2018. "Sensitivity ZAM Modeling Study of Tank 10H VDS Waste Sample," SRNL-STI-2018-00215, Rev. 0, June 2018.
- Helfferrich, F., 1995. "Ion Exchange," pp. 166-167, Dover Publications, Inc., Mineola, NY.
- King, W. D., C. A. Nash, and T. Hang, 2020. "Task Technical and Quality Assurance Plan to support the Tank Closure Cesium Removal (TCCR) 1A Project", SRNL-RP-2020-00376, Rev. 0.
- Luzzatti, A. M., 2020. "In-Tank Batch Contact Test Sample Vessel Fabrication and Procedure for the CST Pretreatment Process, the Sample Dissolution, and Reporting the Results for the Tank Closure Cesium Removal (TCCR) 1A Unit," Liquid Waste Technical Task Request, X-TTR-H-00100, Rev. 0.
- OLI Systems, Inc., 2020. "An Introduction to OLI Studio V10" ([www.olisystems.com](http://www.olisystems.com)).
- Reboul, S. H., 2017. "Characterization of the March 2017 Tank 10 Surface Sample (combination of HTF-10-17-30 and HTF-10-17-31) and Variable Depth Sample (combination of HTF-10-17-32 and HTF-10-17-33)," SRNL-STI-2017-00392, Rev. 0, July 2017.
- Taylor-Pashow, K. M. L., W. D. King, T. Hang, and F. F. Fondeur, 2020. "Characterization and CST Batch Contact Equilibrium Testing of Modified Tank 9H Process Supernate Samples in Support of TCCR," SRNL-STI-2020-00128, Rev. 0, April 2020.
- UOP Certificate of Analysis for IONSIV R9120-B, May 2017.
- Zheng, Z., R. G. Anthony, and J. E. Miller, 1997. "Modeling Multicomponent Ion Exchange Equilibrium Utilizing Hydrous Crystalline Silicotitanates by a Multiple Interactive Ion Exchange Site Model," Ind. Eng. Chem. Res., Vol. 36(6), 2427-2434 (1997).
- Zheng, Z., D. Gu, and R. G. Anthony, 1995. "Estimation of Cesium Ion Exchange Distribution Coefficients for Concentrated Electrolytic Solutions When Using Crystalline Silicotitanates," Ind. Eng. Chem. Res., **34**(6), 2142-2147 (1995).
- Zheng, Z., C. V. Philip, R. G. Anthony, J. L. Krumhansl, D. E. Trudell, and J. E. Miller, 1996. "Ion Exchange of Group I Metals by Hydrous Crystalline Silicotitanates," Ind. Eng. Chem. Res., **35**(11), 4246-4256 (1996).

## Appendix A. Scope for the Alternate Case

**From:** Terri Fellingner  
**Sent:** Wednesday, July 22, 2020 6:47 AM  
**To:** Thong Hang  
**Cc:** Charles Nash; Boyd Wiedenman; Aubrey Silker; David02 Martin; Kurtis Miklia; Pen Mayson; Gregory Arthur  
**Subject:** New Case for Penalty Document

Thong,

Per TTR X-TTR-H-00100, SRR Engineering is invoking the email clause in the TTR. Please run the following scenarios for the composition outlined below using the ZAM model. Please record this request in a laboratory notebook and attach a copy of the request to the final technical report.

As I indicated earlier, please leave the bounding case in the report and add this case run to it. Also, because the penalty we will have to apply is large, I am asking for a refinement in the increments for the temperature range. I have highlighted the change in yellow below.

Composition for Alternate Case:

Na	4.00E+00	M
Cs	6.70E-05	M
Hydroxide	2.29E-01	M
Nitrate	1.29E+00	M
Nitrite	1.59E-01	M
Aluminate	7.84E-02	M
Sulfate	4.73E-01	M
Carbonate	6.36E-01	M
Chloride	6.70E-05	M
Oxalate	1.14E-02	M
Check of Anions	4.00E+00	M
Check of Cations	4.00E+00	M

Scenarios:

a.) Using the Tank 10 variable depth sample results reported in SRNL-STI-2017-00392, a starting composition was calculated by adjusting the Cs molarity to match the Cs molarity reported in SRNL-STI-2020-00128 (Tank 9H Case 3) and adjusting the minimum Na molarity from 3.22M to 4M. The composition was also 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. Adjust the provided composition with water to simulate 0% to 5% (in increments of 1%) 10%, 15%, and 20% water dilution. Perform ZAM model runs for these adjusted cases at 20°C.

b.) 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 20°C to 40°C in increments of 1°C.

c.) Add these additional ZAM model runs to draft report SRNL-STI-2020-00262 along with the associated data produced from OLI (ionic strength, density, etc.).

If you have any questions, please call me (803-643-3589 or 803-215-7513). Also, can you provide an estimate of when you might be able to complete this additional scope? As always, I appreciate the support!

Thanks in Advance,  
Terri

## Appendix B. ZAM Calculations for the Bounding Case

### 1) Cases 1 to 9, Water Dilution at 20 °C

- Case 1 (0% Dilution)

#### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1161.12	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

#### ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.949644289095292 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3917E+00	.1520E+00	.2577E+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)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 2 Maximum Loading @ 20C	Title
6, 8	Number of Cations & Anions
1159.64	Density(kg/m3)
3, 6, 1, 5, 4, 13	Names of Cations
13, 9, 27, 28, 15, 19, 2, 25	Names of Anions (Add C2O4--)
88.02	C2O4-2 MW
3.188, 1.5E-04, 5.4945E-14, 0, 0, 0	Concentrations of Cations
0.182, 1.03, 0.127, 0.0625, 0.377, 0.50714, 1.50E-04, 9.11E-3	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

Solution: Case 2 Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1160E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.3188E+01
Cs+.....	132.9054	1.	.1500E-03
H+.....	1.0079	1.	.5495E-13
Rb+.....	85.4678	1.	.0000E+00
K+.....	39.0983	1.	.0000E+00
Sr++.....	87.6200	2.	.0000E+00
OH-.....	17.0073	-1.	.1820E+00
NO3-....	62.0049	-1.	.1030E+01
NO2-....	46.0000	-1.	.1270E+00
Al(OH)4-	95.0000	-1.	.6250E-01
SO4--...	96.0636	-2.	.3770E+00
CO3--...	60.0092	-2.	.5071E+00
Cl-.....	35.4527	-1.	.1500E-03
Other--.	88.0200	-2.	.9110E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 5.126559723553072 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3926E+00	.1500E+00	.2618E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.1820E+03	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 3 (2% Dilution)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 3 Maximum Loading @ 20C	Title
6, 8	Number of Cations & Anions
1158.23	Density(kg/m3)
3, 6, 1, 5, 4, 13	Names of Cations
13, 9, 27, 28, 15, 19, 2, 25	Names of Anions (Add C2O4--)
88.02	C2O4-2 MW
3.157, 1.49E-04, 5.5556E-14, 0, 0, 0	Concentrations of Cations
0.180, 1.02, 0.125, 0.06190, 0.374, 0.50203, 1.49E-04, 9.02E-03	Concentrations of Anions
1, 0.0000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

Solution: Case 3 Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1158E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3157E+01
Cs+....	132.9054	1.	.1490E-03
H+.....	1.0079	1.	.5556E-13
Rb+....	85.4678	1.	.0000E+00
K+.....	39.0983	1.	.0000E+00
Sr++....	87.6200	2.	.0000E+00
OH-....	17.0073	-1.	.1800E+00
NO3-....	62.0049	-1.	.1020E+01
NO2-....	46.0000	-1.	.1250E+00
Al(OH)4-	95.0000	-1.	.6190E-01
SO4--...	96.0636	-2.	.3740E+00
CO3--...	60.0092	-2.	.5020E+00
Cl-....	35.4527	-1.	.1490E-03
Other--.	88.0200	-2.	.9020E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 5.072194800246161 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3932E+00	.1490E+00	.2639E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.1800E+03	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 4 (3% Dilution)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 4 Maximum Loading @ 20C	Title
6, 8	Number of Cations & Anions
1156.79	Density(kg/m3)
3, 6, 1, 5, 4, 13	Names of Cations
13, 9, 27, 28, 15, 19, 2, 25	Names of Anions (Add C2O4--)
88.02	C2O4-2 MW
3.126, 1.47E-04, 5.5866E-14, 0, 0, 0	Concentrations of Cations
0.179, 1.01, 0.124, 0.0613, 0.37, 0.49692, 1.47E-04, 8.93E-03	Concentrations of Anions
1, 0.0000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

Solution: Case 4 Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1157E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.3126E+01
Cs+.....	132.9054	1.	.1470E-03
H+.....	1.0079	1.	.5587E-13
Rb+.....	85.4678	1.	.0000E+00
K+.....	39.0983	1.	.0000E+00
Sr++.....	87.6200	2.	.0000E+00
OH-.....	17.0073	-1.	.1790E+00
NO3-....	62.0049	-1.	.1010E+01
NO2-....	46.0000	-1.	.1240E+00
Al(OH)4-	95.0000	-1.	.6130E-01
SO4--...	96.0636	-2.	.3700E+00
CO3--...	60.0092	-2.	.4969E+00
Cl-.....	35.4527	-1.	.1470E-03
Other--.	88.0200	-2.	.8930E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 5.017468578546675 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3930E+00	.1470E+00	.2673E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.1790E+03	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 5 (4% Dilution)

ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 5 Maximum Loading @ 20C	Title
6, 8	Number of Cations & Anions
1155.4	Density(kg/m3)
3, 6, 1, 5, 4, 13	Names of Cations
13, 9, 27, 28, 15, 19, 2, 25	Names of Anions (Add C2O4--)
88.02	C2O4-2 MW
3.096, 1.46E-04, 5.6497E-14, 0, 0, 0	Concentrations of Cations
0.177, 1.0, 0.123, 0.0607, 0.366, 0.4928, 1.46E-04, 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 output

Solution: Case 5 Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1155E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3096E+01
Cs+....	132.9054	1.	.1460E-03
H+.....	1.0079	1.	.5650E-13
Rb+....	85.4678	1.	.0000E+00
K+.....	39.0983	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.	.4928E+00
Cl-....	35.4527	-1.	.1460E-03
Other--.	88.0200	-2.	.8850E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.964475572981345 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3935E+00	.1460E+00	.2695E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.1770E+03	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 6 (5% Dilution)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 6 Maximum Loading @ 20C	Title
6, 8	Number of Cations & Anions
1154.07	Density(kg/m3)
3, 6, 1, 5, 4, 13	Names of Cations
13, 9, 27, 28, 15, 19, 2, 25	Names of Anions (Add C2O4--)
88.02	C2O4-2 MW
3.067, 1.44E-04, 5.7143E-14, 0, 0, 0	Concentrations of Cations
0.175, 0.099, 0.122, 0.0601, 0.363, 0.48819, 1.44E-04, 8.76E-03	Concentrations of Anions
1, 0.0000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

---

Solution: Case 6 Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1154E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3067E+01
Cs+....	132.9054	1.	.1440E-03
H+.....	1.0079	1.	.5714E-13
Rb+....	85.4678	1.	.0000E+00
K+.....	39.0983	1.	.0000E+00
Sr++....	87.6200	2.	.0000E+00
OH-.....	17.0073	-1.	.1750E+00
NO3-....	62.0049	-1.	.9900E+00
NO2-....	46.0000	-1.	.1220E+00
Al(OH)4-	95.0000	-1.	.6010E-01
SO4--...	96.0636	-2.	.3630E+00
CO3--...	60.0092	-2.	.4882E+00
Cl-.....	35.4527	-1.	.1440E-03
Other--.	88.0200	-2.	.8760E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.913680651599114 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3932E+00	.1440E+00	.2730E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.1750E+03	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

---



• Case 7 (10% Dilution)

ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 7 Maximum Loading @ 20C	Title
6, 8	Number of Cations & Anions
1147.58	Density(kg/m3)
3, 6, 1, 5, 4, 13	Names of Cations
13, 9, 27, 28, 15, 19, 2, 25	Names of Anions (Add C2O4--)
88.02	C2O4-2 MW
2.927, 1.38E-04, 5.9880E-14, 0, 0, 0	Concentrations of Cations
0.167, 0.945, 0.116, 0.0574, 0.346, 0.46644, 1.38E-04, 8.36E-03	Concentrations of Anions
1, 0.0000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

---

Solution: Case 7 Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1148E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.2927E+01
Cs+....	132.9054	1.	.1380E-03
H+.....	1.0079	1.	.5988E-13
Rb+....	85.4678	1.	.0000E+00
K+.....	39.0983	1.	.0000E+00
Sr++....	87.6200	2.	.0000E+00
OH-.....	17.0073	-1.	.1670E+00
NO3-....	62.0049	-1.	.9450E+00
NO2-....	46.0000	-1.	.1160E+00
Al(OH)4-	95.0000	-1.	.5740E-01
SO4--...	96.0636	-2.	.3460E+00
CO3--...	60.0092	-2.	.4664E+00
Cl-.....	35.4527	-1.	.1380E-03
Other--.	88.0200	-2.	.8360E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.668789322949483 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3946E+00	.1380E+00	.2859E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.1670E+03	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

---

- Case 8 (15% Dilution)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 8 Maximum Loading @ 20C	Title
6, 8	Number of Cations & Anions
1141.67	Density(kg/m3)
3, 6, 1, 5, 4, 13	Names of Cations
13, 9, 27, 28, 15, 19, 2, 25	Names of Anions (Add C2O4--)
88.02	C2O4-2 MW
2.8, 1.32E-04, 6.2500E-14, 0, 0, 0	Concentrations of Cations
0.16, 0.904, 0.111, 0.0549, 0.331, 0.44605, 1.32E-04, 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 output

Solution: Case 8 Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1142E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.2800E+01
Cs+.....	132.9054	1.	.1320E-03
H+.....	1.0079	1.	.6250E-13
Rb+.....	85.4678	1.	.0000E+00
K+.....	39.0983	1.	.0000E+00
Sr++.....	87.6200	2.	.0000E+00
OH-.....	17.0073	-1.	.1600E+00
NO3-....	62.0049	-1.	.9040E+00
NO2-....	46.0000	-1.	.1110E+00
Al(OH)4-	95.0000	-1.	.5490E-01
SO4--...	96.0636	-2.	.3310E+00
CO3--...	60.0092	-2.	.4461E+00
Cl-.....	35.4527	-1.	.1320E-03
Other--.	88.0200	-2.	.8000E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.448579781525522 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3953E+00	.1320E+00	.2995E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.1600E+03	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 9 (20% Dilution)

ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 9 Maximum Loading @ 20C	Title
6, 8	Number of Cations & Anions
1136.2	Density(kg/m3)
3, 6, 1, 5, 4, 13	Names of Cations
13, 9, 27, 28, 15, 19, 2, 25	Names of Anions (Add C2O4--)
88.02	C2O4-2 MW
2.683, 1.26E-04, 6.5359E-14, 0, 0, 0	Concentrations of Cations
0.153, 0.867, 0.107, 0.0526, 0.318, 0.42603, 1.26E-04, 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 output

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.	.1260E-03
H+.....	1.0079	1.	.6536E-13
Rb+....	85.4678	1.	.0000E+00
K+.....	39.0983	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.	.4260E+00
Cl-.....	35.4527	-1.	.1260E-03
Other--.	88.0200	-2.	.7670E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.246311806077563 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3955E+00	.1260E+00	.3139E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.1530E+03	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

## 2) Temperature Variation of Case 1

- Case 1 at 20°C

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1161.12	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 C204--)
88.02	C204-2 MW
3.22, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02
Liquid(L)= .1000E+01 Solid(g)= .1000E-05			
Material: Na Form			
*****OUTPUT*****			
Ionic Strength= 4.949644289095292 mol/kg			
	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3917E+00	.1520E+00	.2577E+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 21 °C

## ZAM input

1, 294.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 21C	Title
7, 8	Number of Cations & Anions
1160.73	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1 Maximum Loading @ 21C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1161E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3220E+01
Cs+....	132.9054	1.	.1520E-03
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.	.5123E+00
Cl-....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.951734106938101 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3878E+00	.1520E+00	.2552E+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 22 °C

## ZAM input

1, 295.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 22C	Title
7, 8	Number of Cations & Anions
1160.35	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1 Maximum Loading @ 22C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1160E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.3220E+01
Cs+.....	132.9054	1.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.953772283817894 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3839E+00	.1520E+00	.2526E+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

## ZAM input

1, 296.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 23C	Title
7, 8	Number of Cations & Anions
1159.98	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.955758049891398 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3800E+00	.1520E+00	.2500E+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

ZAM input

1, 297.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 24C	Title
7, 8	Number of Cations & Anions
1159.61	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.957745728937899 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3761E+00	.1520E+00	.2474E+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

### ZAM input

1, 298.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 25C	Title
7, 8	Number of Cations & Anions
1159.24	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

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

Density= .1159E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.3220E+01
Cs+.....	132.9054	1.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.959734682513975 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3722E+00	.1520E+00	.2448E+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

ZAM input

1, 299.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 26C	Title
7, 8	Number of Cations & Anions
1158.88	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
3.22, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.961671655712632 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3682E+00	.1520E+00	.2423E+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

## ZAM input

1, 300.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 27C	Title
7, 8	Number of Cations & Anions
1158.52	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
3.22, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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

Density= .1159E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.3220E+01
Cs+.....	132.9054	1.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.963609821365289 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3643E+00	.1520E+00	.2397E+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

## ZAM input

1, 301.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 28C	Title
7, 8	Number of Cations & Anions
1158.16	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
3.22, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.965549823129335 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3603E+00	.1520E+00	.2371E+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

## ZAM input

1, 302.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 29C	Title
7, 8	Number of Cations & Anions
1157.8	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.967491020396874 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3564E+00	.1520E+00	.2345E+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

## ZAM input

1, 303.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 30C	Title
7, 8	Number of Cations & Anions
1157.45	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.969380636161126 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3524E+00	.1520E+00	.2319E+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

## ZAM input

1, 304.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 31C	Title
7, 8	Number of Cations & Anions
1157.1	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.971271045960994 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3485E+00	.1520E+00	.2293E+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

## ZAM input

1, 305.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 32C	Title
7, 8	Number of Cations & Anions
1156.75	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.973162572271766 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3446E+00	.1520E+00	.2267E+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

## ZAM input

1, 306.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 33C	Title
7, 8	Number of Cations & Anions
1156.4	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.975055861099047 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3406E+00	.1520E+00	.2241E+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

ZAM input

1, 307.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 34C	Title
7, 8	Number of Cations & Anions
1156.05	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.976950269234869 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3367E+00	.1520E+00	.2215E+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

## ZAM input

1, 308.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 35C	Title
7, 8	Number of Cations & Anions
1155.7	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.978847089753680 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3328E+00	.1520E+00	.2189E+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

## ZAM input

1, 310.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 37C	Title
7, 8	Number of Cations & Anions
1155.01	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.982589100832413 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3249E+00	.1520E+00	.2138E+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

ZAM input

1, 312.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 39C	Title
7, 8	Number of Cations & Anions
1154.31	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.986391499919001 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3172E+00	.1520E+00	.2087E+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

## ZAM input

1, 313.15	Activity Coeff. Model, Temperature
Case 1 Maximum Loading @ 40C	Title
7, 8	Number of Cations & Anions
1153.97	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, 1.52E-04, 5.4348E-14, 0, 0, 0, 0	Concentrations of Cations
0.184, 1.04, 0.128, 0.0631, 0.381, 0.51225, 1.52E-4, 0.0092	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

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.	.1520E-03
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.	.5123E+00
Cl-.....	35.4527	-1.	.1520E-03
Other--.	88.0200	-2.	.9200E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 4.988240724395293 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.3133E+00	.1520E+00	.2061E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

## Appendix C. ZAM Calculations for the Alternate Case

### 1) Cases 1 to 9, Water Dilution at 20 °C

- Case 1a (0% Dilution)

#### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1196.07	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

#### ZAM output

Solution: Case 1a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1196E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4--...	96.0636	-2.	.4730E+00
CO3--...	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.302380125585418 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2406E+00	.6700E-01	.3591E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 2a (1% Dilution)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 2a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1194.31	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
3.9604, 6.6337E-05, 4.4111E-14, 0, 0, 0, 0	Concentrations of Cations
0.2267, 1.2772, 0.1574, 0.0776, 0.4683, 0.63115, 6.6337E-05, 0.0113	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

Solution: Case 2a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1194E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.3960E+01
Cs+.....	132.9054	1.	.6634E-04
H+.....	1.0079	1.	.4411E-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.	.2267E+00
NO3-....	62.0049	-1.	.1277E+01
NO2-....	46.0000	-1.	.1574E+00
Al(OH)4-	95.0000	-1.	.7760E-01
SO4-....	96.0636	-2.	.4683E+00
CO3-....	60.0092	-2.	.6312E+00
Cl-.....	35.4527	-1.	.6634E-04
Other--.	88.0200	-2.	.1130E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.232087751188554 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2409E+00	.6634E-01	.3631E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00



- Case 3a (2% Dilution)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 3a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1192.58	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
3.9216, 6.5686E-05, 4.4543E-14, 0, 0, 0, 0	Concentrations of Cations
0.2245, 1.2647, 0.1559, 0.0769, 0.4637, 0.6249, 6.5686E-05, 0.0112	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

Solution: Case 3a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1193E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3922E+01
Cs+....	132.9054	1.	.6569E-04
H+....	1.0079	1.	.4454E-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.	.2245E+00
NO3-....	62.0049	-1.	.1265E+01
NO2-....	46.0000	-1.	.1559E+00
Al(OH)4-	95.0000	-1.	.7690E-01
SO4--...	96.0636	-2.	.4637E+00
CO3--...	60.0092	-2.	.6249E+00
Cl-....	35.4527	-1.	.6569E-04
Other--.	88.0200	-2.	.1120E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.163259756939361 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2412E+00	.6569E-01	.3672E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 4a (3% Dilution)

## ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 4a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1190.89	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
3.8835, 6.5049E-05, 4.4984E-14, 0, 0, 0, 0	Concentrations of Cations
0.2223, 1.2524, 0.1544, 0.0761, 0.4592, 0.61885, 6.5049E-05, 0.0111	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 4a Maximum Loading @ 20C			
*****INPUT*****			
Density= .1191E+04 kg/m3			
	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3884E+01
Cs+....	132.9054	1.	.6505E-04
H+....	1.0079	1.	.4498E-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.	.2223E+00
NO3-....	62.0049	-1.	.1252E+01
NO2-....	46.0000	-1.	.1544E+00
Al(OH)4-	95.0000	-1.	.7610E-01
SO4--...	96.0636	-2.	.4592E+00
CO3--...	60.0092	-2.	.6189E+00
Cl-....	35.4527	-1.	.6505E-04
Other--.	88.0200	-2.	.1110E-01
Liquid(L)= .1000E+01 Solid(g)= .1000E-05			
Material: Na Form			
*****OUTPUT*****			
Ionic Strength= 6.095911159295398 mol/kg			
	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2415E+00	.6505E-01	.3712E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 5a (4% Dilution)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 5a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1189.23	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
3.8462, 6.4423E-05, 4.5413E-14, 0, 0, 0, 0	Concentrations of Cations
0.2202, 1.2404, 0.1529, 0.0754, 0.4548, 0.61285, 6.4423E-05, 0.0110	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

Solution: Case 5a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1189E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3846E+01
Cs+....	132.9054	1.	.6442E-04
H+....	1.0079	1.	.4541E-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.	.2202E+00
NO3-....	62.0049	-1.	.1240E+01
NO2-....	46.0000	-1.	.1529E+00
Al(OH)4-	95.0000	-1.	.7540E-01
SO4--...	96.0636	-2.	.4548E+00
CO3--...	60.0092	-2.	.6129E+00
Cl-....	35.4527	-1.	.6442E-04
Other--.	88.0200	-2.	.1100E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.030081320695456 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2418E+00	.6442E-01	.3753E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 6a (5% Dilution)

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 6a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1187.6	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
3.8095, 6.3810E-05, 4.5851E-14, 0, 0, 0, 0	Concentrations of Cations
0.2181, 1.2286, 0.1514, 0.07467, 0.4505, 0.606965, 6.3810E-05, 0.0109	Concentrations of Anions
1, 0.0000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

Solution: Case 6a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1188E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3810E+01
Cs+....	132.9054	1.	.6381E-04
H+....	1.0079	1.	.4585E-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.	.2181E+00
NO3-....	62.0049	-1.	.1229E+01
NO2-....	46.0000	-1.	.1514E+00
Al(OH)4-	95.0000	-1.	.7467E-01
SO4--...	96.0636	-2.	.4505E+00
CO3--...	60.0092	-2.	.6070E+00
Cl-....	35.4527	-1.	.6381E-04
Other--.	88.0200	-2.	.1090E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 5.965514051516402 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2420E+00	.6381E-01	.3793E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 7a (10% Dilution)

ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 7a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1179.89	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
3.6364, 6.0909E-05, 4.8031E-14, 0, 0, 0, 0	Concentrations of Cations
0.2082, 1.1727, 0.1445, 0.0713, 0.4300, 0.579450, 6.0909E-05, 0.0104	Concentrations of Anions
1, 0.0000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 7a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1180E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3636E+01
Cs+....	132.9054	1.	.6091E-04
H+....	1.0079	1.	.4803E-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.	.2082E+00
NO3-....	62.0049	-1.	.1173E+01
NO2-....	46.0000	-1.	.1445E+00
Al(OH)4-	95.0000	-1.	.7130E-01
SO4--...	96.0636	-2.	.4300E+00
CO3--...	60.0092	-2.	.5795E+00
Cl-....	35.4527	-1.	.6091E-04
Other--.	88.0200	-2.	.1040E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 5.663088941242205 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2433E+00	.6091E-01	.3995E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 8a (15% Dilution)

ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 8a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1172.83	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
3.4783, 5.8261E-05, 5.0226E-14, 0, 0, 0, 0	Concentrations of Cations
0.1991, 1.1217, 0.1383, 0.0682, 0.4113, 0.5543, 5.8261E-05, 0.0099	Concentrations of Anions
1, 0.0000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 8a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1173E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.3478E+01
Cs+.....	132.9054	1.	.5826E-04
H+.....	1.0079	1.	.5023E-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.	.1991E+00
NO3-....	62.0049	-1.	.1122E+01
NO2-....	46.0000	-1.	.1383E+00
Al(OH)4-	95.0000	-1.	.6820E-01
SO4-....	96.0636	-2.	.4113E+00
CO3-....	60.0092	-2.	.5543E+00
Cl-.....	35.4527	-1.	.5826E-04
Other--.	88.0200	-2.	.9900E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 5.389824278487013 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2445E+00	.5826E-01	.4197E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 9a (20% Dilution)

ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 9a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1166.29	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
3.3333, 5.5833E-05, 5.2411E-14, 0, 0, 0, 0	Concentrations of Cations
0.1908, 1.0750, 0.1325, 0.0653, 0.3942, 0.53115, 5.5833E-05, 0.0095	Concentrations of Anions
1, 0.0000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 9a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1166E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.3333E+01
Cs+....	132.9054	1.	.5583E-04
H+....	1.0079	1.	.5241E-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.	.1908E+00
NO3-....	62.0049	-1.	.1075E+01
NO2-....	46.0000	-1.	.1325E+00
Al(OH)4-	95.0000	-1.	.6530E-01
SO4-....	96.0636	-2.	.3942E+00
CO3-....	60.0092	-2.	.5312E+00
Cl-....	35.4527	-1.	.5583E-04
Other--.	88.0200	-2.	.9500E-02

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 5.141992849011238 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2456E+00	.5583E-01	.4399E+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 1a

- Case 1a at 20°C

### ZAM input

1, 293.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 20C	Title
7, 8	Number of Cations & Anions
1196.07	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 C204--)
88.02	C204-2 MW
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

### ZAM output

Solution: Case 1a Maximum Loading @ 20C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1196E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4--...	96.0636	-2.	.4730E+00
CO3--...	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.302380125585418 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2406E+00	.6700E-01	.3591E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00



- Case 1a at 21 °C

## ZAM input

1, 294.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 21C	Title
7, 8	Number of Cations & Anions
1195.68	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 21C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1196E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.4000E+01
Cs+....	132.9054	1.	.6700E-04
H+....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.305106347788279 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2363E+00	.6700E-01	.3527E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 22 °C

## ZAM input

1, 295.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 22C	Title
7, 8	Number of Cations & Anions
1195.3	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 22C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1195E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.307766070700395 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2321E+00	.6700E-01	.3464E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 23 °C

## ZAM input

1, 296.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 23C	Title
7, 8	Number of Cations & Anions
1194.93	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 23C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1195E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.310357452331911 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2279E+00	.6700E-01	.3402E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 24 °C

## ZAM input

1, 297.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 24C	Title
7, 8	Number of Cations & Anions
1194.57	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 24C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1195E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.312881993423198 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2238E+00	.6700E-01	.3340E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 25 °C

## ZAM input

1, 298.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 25C	Title
7, 8	Number of Cations & Anions
1194.22	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 25C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1194E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.315337439322955 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2197E+00	.6700E-01	.3280E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 26 °C

## ZAM input

1, 299.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 26C	Title
7, 8	Number of Cations & Anions
1193.88	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 26C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1194E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.317724045034465 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2157E+00	.6700E-01	.3220E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 27 °C

## ZAM input

1, 300.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 27C	Title
7, 8	Number of Cations & Anions
1193.55	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 27C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1194E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.320042490169476 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2118E+00	.6700E-01	.3161E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 28 °C

## ZAM input

1, 301.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 28C	Title
7, 8	Number of Cations & Anions
1193.22	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 28C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1193E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.322363476062121 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2079E+00	.6700E-01	.3103E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00



- Case 1a at 29 °C

## ZAM input

1, 302.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 29C	Title
7, 8	Number of Cations & Anions
1192.9	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 29C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1193E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.324614842260107 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2041E+00	.6700E-01	.3046E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 1a at 30 °C

ZAM input

1, 303.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 30C	Title
7, 8	Number of Cations & Anions
1192.59	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 1a Maximum Loading @ 30C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1193E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.326797697701903 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.2003E+00	.6700E-01	.2990E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 1a at 31 °C

ZAM input

1, 304.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 31C	Title
7, 8	Number of Cations & Anions
1192.28	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 1a Maximum Loading @ 31C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1192E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.328981640296136 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1966E+00	.6700E-01	.2934E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 32 °C

## ZAM input

1, 305.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 32C	Title
7, 8	Number of Cations & Anions
1191.93	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 32C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1192E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+....	22.9898	1.	.4000E+01
Cs+....	132.9054	1.	.6700E-04
H+....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.331449628786745 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1929E+00	.6700E-01	.2880E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 1a at 33 °C

ZAM input

1, 306.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 33C	Title
7, 8	Number of Cations & Anions
1191.58	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 1a Maximum Loading @ 33C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1192E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.333920384393737 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1893E+00	.6700E-01	.2826E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 1a at 34 °C

ZAM input

1, 307.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 34C	Title
7, 8	Number of Cations & Anions
1191.24	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 1a Maximum Loading @ 34C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1191E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.336321058662369 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1858E+00	.6700E-01	.2773E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 1a at 35 °C

ZAM input

1, 308.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 35C	Title
7, 8	Number of Cations & Anions
1190.89	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 1a Maximum Loading @ 35C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1191E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.338794775607798 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1823E+00	.6700E-01	.2721E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 1a at 36 °C

ZAM input

1, 309.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 36C	Title
7, 8	Number of Cations & Anions
1190.55	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 1a Maximum Loading @ 36C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1191E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.341199568727936 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1789E+00	.6700E-01	.2670E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00



- Case 1a at 37 °C

## ZAM input

1, 310.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 37C	Title
7, 8	Number of Cations & Anions
1190.22	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 37C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1190E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.343535700976236 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1755E+00	.6700E-01	.2620E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

- Case 1a at 38 °C

## ZAM input

1, 311.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 38C	Title
7, 8	Number of Cations & Anions
1189.88	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

## ZAM output

Solution: Case 1a Maximum Loading @ 38C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1190E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.345944093321301 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1722E+00	.6700E-01	.2570E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 1a at 39 °C

ZAM input

1, 312.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 39C	Title
7, 8	Number of Cations & Anions
1189.55	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 1a Maximum Loading @ 39C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1190E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.348283300638929 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1689E+00	.6700E-01	.2522E+04
Rb	.0000E+00	.0000E+00	.0000E+00
Sr	.0000E+00	.0000E+00	.0000E+00
K	.0000E+00	.0000E+00	.0000E+00

• Case 1a at 40 °C

ZAM input

1, 313.15	Activity Coeff. Model, Temperature
Case 1a Maximum Loading @ 40C	Title
7, 8	Number of Cations & Anions
1189.21	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
4.0, 6.7E-05, 4.3668E-14, 0, 0, 0, 0	Concentrations of Cations
0.229, 1.29, 0.159, 0.0784, 0.473, 0.6374, 6.70E-05, 0.0114	Concentrations of Anions
1, 0.000001	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
1	Calculation Adjustment

ZAM output

Solution: Case 1a Maximum Loading @ 40C  
\*\*\*\*\*INPUT\*\*\*\*\*

Density= .1189E+04 kg/m3

	Molecular Wt.	Valance	Molarity(mol/L)
Na+.....	22.9898	1.	.4000E+01
Cs+.....	132.9054	1.	.6700E-04
H+.....	1.0079	1.	.4367E-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.	.2290E+00
NO3-....	62.0049	-1.	.1290E+01
NO2-....	46.0000	-1.	.1590E+00
Al(OH)4-	95.0000	-1.	.7840E-01
SO4-....	96.0636	-2.	.4730E+00
CO3-....	60.0092	-2.	.6374E+00
Cl-.....	35.4527	-1.	.6700E-04
Other--.	88.0200	-2.	.1140E-01

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

Material: Na Form

\*\*\*\*\*OUTPUT\*\*\*\*\*

Ionic Strength= 6.350696146017588 mol/kg

	Q (mmol/gCST)	C (mmol/L)	Kd (ml/gCST)
Cs	.1657E+00	.6700E-01	.2474E+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](mailto:sebastian.aleman@srnl.doe.gov)  
[cj.bannochie@srnl.doe.gov](mailto:cj.bannochie@srnl.doe.gov)  
[luther.hamm@srnl.doe.gov](mailto:luther.hamm@srnl.doe.gov)  
[thong.hang@srnl.doe.gov](mailto:thong.hang@srnl.doe.gov)  
[michael.hay@srnl.doe.gov](mailto:michael.hay@srnl.doe.gov)  
[william02.king@srnl.doe.gov](mailto:william02.king@srnl.doe.gov)  
[si.lee@srnl.doe.gov](mailto:si.lee@srnl.doe.gov)  
[daniel.mccabe@srnl.doe.gov](mailto:daniel.mccabe@srnl.doe.gov)  
[charles.nash@srnl.doe.gov](mailto:charles.nash@srnl.doe.gov)  
[frank.pennebaker@srnl.doe.gov](mailto:frank.pennebaker@srnl.doe.gov)  
[boyd.wiedenman@srnl.doe.gov](mailto:boyd.wiedenman@srnl.doe.gov)  
[jennifer.wohlwend@srnl.doe.gov](mailto:jennifer.wohlwend@srnl.doe.gov)

[gregory.arthur@srs.gov](mailto:gregory.arthur@srs.gov)  
[richard.edwards@srs.gov](mailto:richard.edwards@srs.gov)  
[drew.fairchild@srs.gov](mailto:drew.fairchild@srs.gov)  
[terri.fellinger@srs.gov](mailto:terri.fellinger@srs.gov)  
[alexander.luzzatti@srs.gov](mailto:alexander.luzzatti@srs.gov)  
[john.occhipinti@srs.gov](mailto:john.occhipinti@srs.gov)  
[aubrey.silker@srs.gov](mailto:aubrey.silker@srs.gov)  
[kenneth.wells@srs.gov](mailto:kenneth.wells@srs.gov)

[heather.capogreco@srnl.doe.gov](mailto:heather.capogreco@srnl.doe.gov)  
Records Administration (EDWS)