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).

We put science to work.™

Savannah River National Laboratory™

OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

A U.S. DEPARTMENT OF ENERGY NATIONAL LABORATORY • SAVANNAH RIVER SITE • AIKEN, SC

Modeling Ion Exchange Performance of Crystalline Silicotitanate to Support SRS Tank 10H Closure (U)

T. Hang
D. J. McCabe
L. L. Hamm
J. L. Wohlwend

July 2017

SRNL-STI-2017-00336, Revision 0

SRNL.DOE.GOV

DISCLAIMER

Printed in the United States of America

Prepared for
U.S. Department of Energy

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

Retention: *Permanent*

Modeling Ion Exchange of Crystalline Silicotitanate to Support SRS Tank 10H Closure (U)

T. Hang
D. J. McCabe
L. L. Hamm
J. L. Wohlwend

July 2017

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

Savannah River National Laboratory™
OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

REVIEWS AND APPROVALS

AUTHORS:

____

T. Hang, Environmental Modeling Date

____

D. J. McCabe, Hanford Mission Programs Date

____

L. L. Hamm, Threat Assessments Date

____

J. L. Wohlwend, Environmental Modeling Date

TECHNICAL REVIEW:

____

S. E. Aleman, Threat Assessments, Reviewed per E7 2.60 Date

APPROVAL:

____

D. A. Crowley, Manager Date
Environmental Modeling

____

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

____

K. M. Kostelnik, Director, Environmental Restoration Technology Date

____

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

EXECUTIVE SUMMARY

The objective of this work is to calculate the maximum loading expected on the Tank Closure Cesium Removal (TCCR) columns. A key consideration in the design of the columns is the amount of ^{137}Cs that loads onto the Crystalline Silicotitanate (CST) and the heat generated by the loaded column during storage. Savannah River National Laboratory (SRNL) has utilized ZAM, a computer program developed by the research group of Professor Rayford G. Anthony of Texas A&M University, to predict the cesium loading on the CST as a function of Tank 10 compositional projections. The ZAM model output will be used as information to determine if the loading limit that is eventually established for the column (by the thermal model) is achievable based on the liquid phase compositional data. Future runs of the ZAM model may be required, based on actual Tank 10 data.

The study investigated cesium loading for different cases of Tank 10H waste compositions:

1. Dilution of Tank 10H core samples to generate the TCCR feeds at Na^+ concentrations (M) of 7.5, 7, 6, 5, 4, and 3.
2. Tank 10H nominal case and variations (Cases 1 – 10): Waste compositions for these cases were based on information provided by Savannah River Remediation (SRR) as an estimate of the composition of the Tank 10H liquid, and adjusted by SRNL to vary key parameters of potassium, sodium, and hydroxide concentrations. Cases 1 – 9 contain lower initial cesium (4.95E-6 M), while Case 10 represents salt solutions of higher cesium concentration (1.97E-5 M).
3. Tank 10H Variable Depth Sample (VDS) collected in March 2017 following a water addition to the tank, and allowing the saltcake to dissolve for a few weeks.

<u>Modeling Approach</u>

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

<u>Results Summary</u>

General results of the ZAM model predictions are:

- Dilution of salt solutions with water decreases Na^+ concentrations and increases the cesium loading primarily due to the decreased ionic strength.
- The ZAM results of all cases for projected compositions of the Tank 10H salt solutions show maximum cesium loading less than 130 Ci/L on the CST.
- The effects of key ions (Na^+, OH^-, K^+, and Cs^+) on cesium loading within the concentration range of interest are correlated as follows:
    - Na^+: Higher sodium concentrations have a strong influence on lowering the cesium loading.
    - OH^-: Higher hydroxide concentrations have a weak influence on increasing the cesium loading.
    - K^-: Higher potassium concentrations have a medium influence on lowering the cesium loading.
    - Cs^+: Higher initial cesium concentrations have the largest impact on increasing the cesium loading due to a better concentration driving force for absorption.

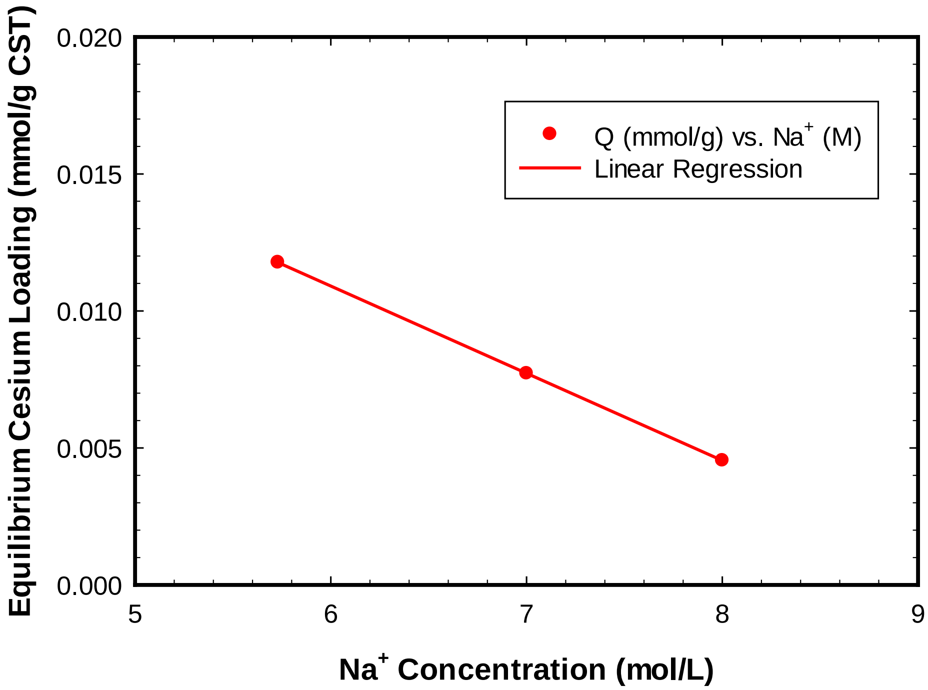


Figure E-1. Na^{+} Effect on Cesium Loading

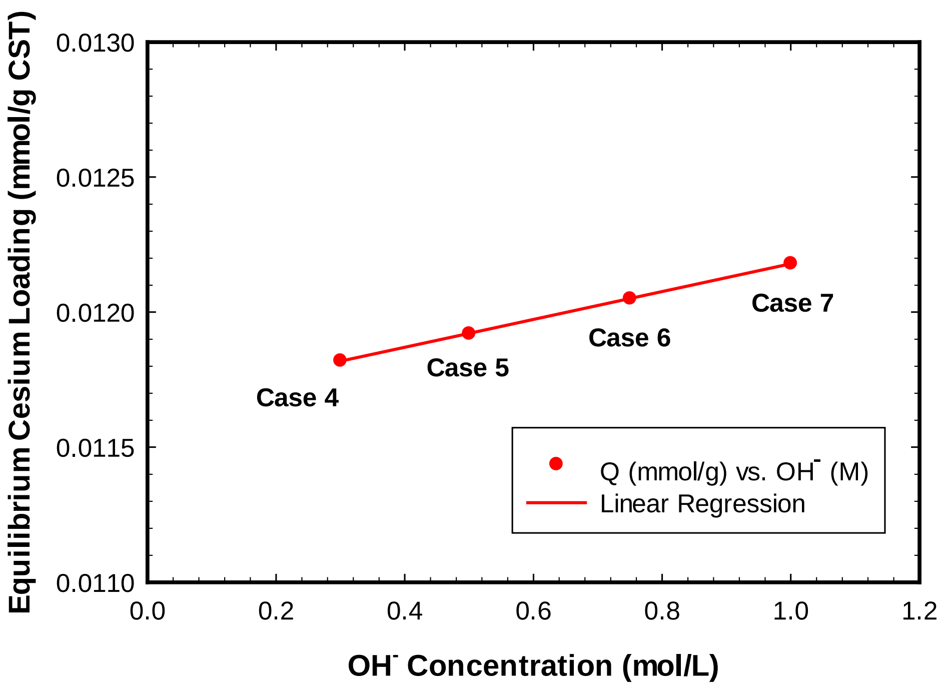


Figure E-2. OH^{-} Effect on Cesium Loading

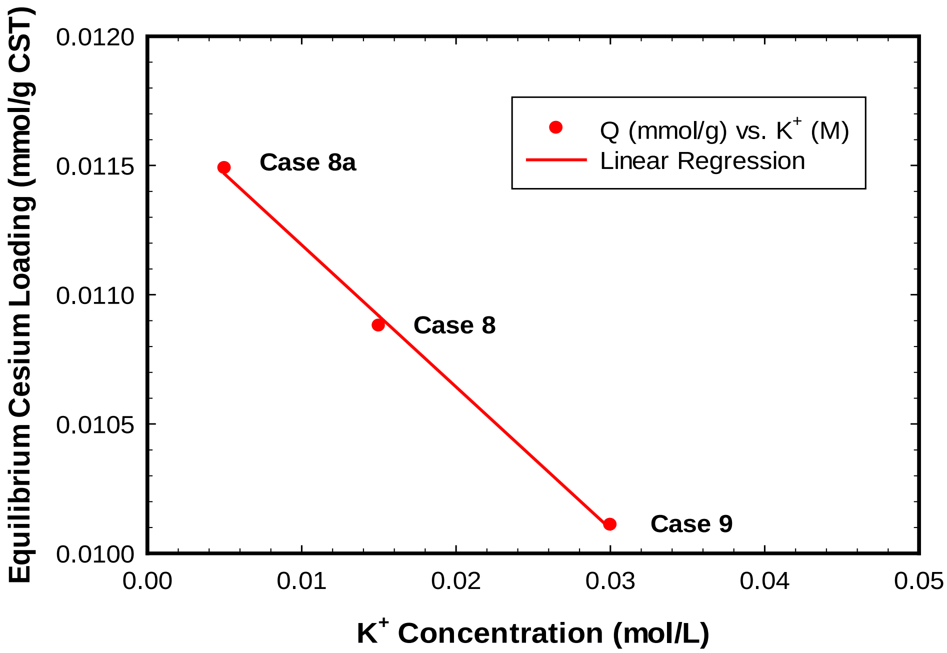


Figure E-3. K^+ Effect on Cesium Loading

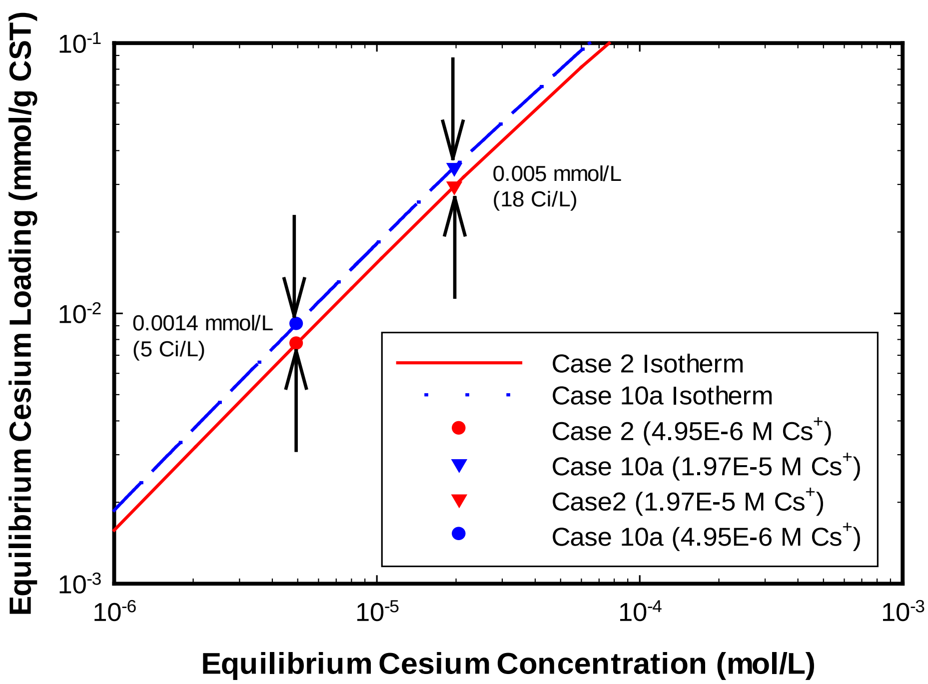


Figure E-4. Cs^+ Effect on Cesium Loading (Case 2 vs. Case 10a)

- The ZAM result for Tank 10H composition from the Variable Depth Sample (VDS) projects a loading of 0.055 $mmol_{Cs}/g_{CST}$ (7.44 mg_{Cs}/g_{CST} or 198 Ci/L_{Bed}), which is comparatively higher than the other projected compositions due to the low Na^+ concentration (i.e., 3.22 M).

The calculations in this report did not include any uncertainty (i.e., Tank 10 concentration range) in the aqueous phase composition. It is advisable to perform these for future work, depending on the intended use of the data. Both the ZAM and OLI models are currently maintained at QA Level D.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

CST	Crystalline Silicotitanate
HLW	High-Level Waste
LCS	Low Curie Salt
SRNL	Savannah River National Laboratory
SRR	Savannah River Remediation
SRS	Savannah River Site
TAMU	Texas A&M University
TCCR	Tank Closure Cesium Removal
VDS	Variable Depth Sample

1.0 Introduction

1.1 Background

Nuclear materials production at the Savannah River Site (SRS) has generated High Level Waste (HLW) contained in underground storage tanks. One isotope in the tank waste that is highly soluble in the aqueous phase is ^{137}Cs. Savannah River Remediation (SRR) is investigating use of an ion exchange process to remove the Cs. The ion exchange media being investigated is Crystalline Silicotitanate (CST). This material, developed at Texas A&M University (TAMU) and Sandia National Laboratory, as a fine particulate or "powder" form (Dosch et al., 1993). The material is now commercially available as IONSIV®[1] R9120 in the original powder form (previously known as IONSIV® IE-910) or as an engineered bead (previously known as IONSIV® IE-911).

In the current application, the Tank Closure Cesium Removal (TCCR) process will remove cesium from aqueous tank waste using an at-tank facility. The current implementation being designed will withdraw the aqueous feed from tanks scheduled for closure. In this case, water will be added to the saltcake in Tank 10H to dissolve it. The dissolved salt solution waste will be pumped out of Tank 10H, through a filter and ion exchange columns, and then stored in another nearby tank (Tank 11 in Figure 1) prior to final disposal via Tank 50H in Saltstone. Cesium will be removed by ion exchange using engineered IONSIV® R9120. The TCCR process will have two columns online in a lead-lag configuration in order to optimize media usage and achieve the target decontamination. Once the lead column is saturated with cesium, it will be removed from service, the lag column will rotate into the lead position, and a new column will be placed into the lag position. The process to remove cesium from Tank 10H is illustrated in Figure 1 (reproduced and modified from Figure 1 in X-SOW-H-00002 (Caldwell, 2017)).

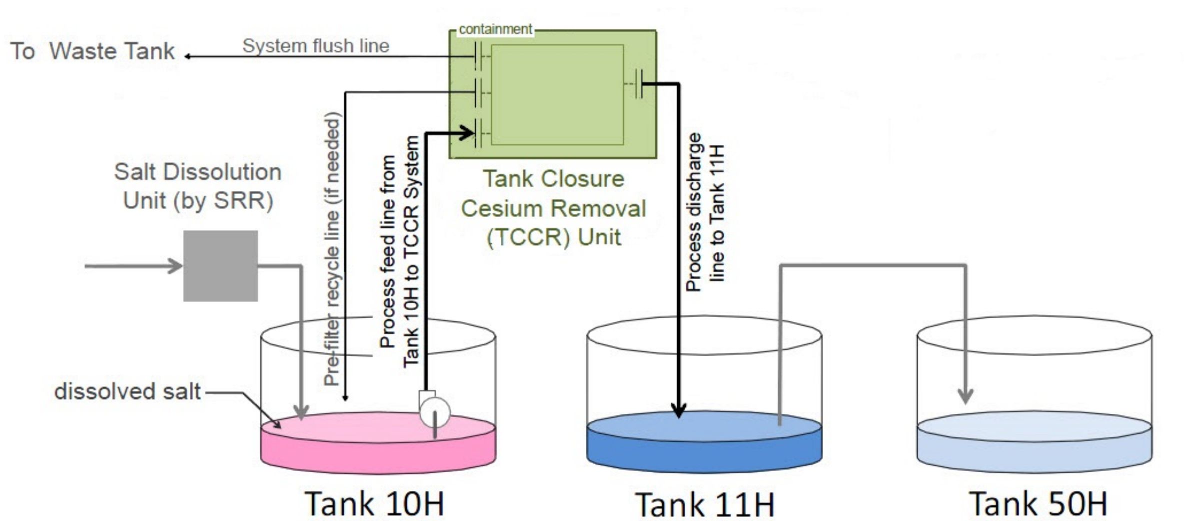


Figure 1. Cesium Removal from Tank 10H

A computer model was developed by the Texas A&M inventors of CST to allow calculation of the absorption of cesium on the media (Zheng et al, 1995; Zheng et al., 1996). That model, known as ZAM, calculates the equilibrium condition for a liquid in contact with the CST. Such equilibrium is dependent upon a number of factors, including temperature, ionic strength, and concentrations of cesium, potassium, sodium, hydroxide, rubidium, and strontium. For this task, it is important to understand that the CST and

[1] IONSIV is a trademark of UOP, LLC., Mt. Laurel, New Jersey, USA

the aqueous stream reach an equilibrium condition, not a saturation of the CST. The *total* cesium capacity of CST is much higher than usually encountered in SRS tank waste, but that total capacity cannot be reached because the loading under any condition is thermodynamically limited by the equilibrium, which depends on the composition of the aqueous stream. The current task calculates the maximum loading of cesium onto the CST, given an infinite amount of liquid feed. The maximum loading then is species/composition dependent, not volume dependent. The model accounts for the two types of exchange sites that exist on the CST solid, and the composition of the aqueous phase. The model has been used previously to predict loading on CST for both SRS and Hanford tank waste applications (Aleman et al., 2003; Hamm et al., 2001; Smith 2011).

Because the original CST was a very fine particulate solid, it was converted to an engineered bead form so that it could be used in flow-through columns with moderate pressures. The bead consists of the CST powder and a binder material. The binder material essentially dilutes the CST powder, which would be expected to cause a reduced absorption of cesium per unit weight of the material. Because the ZAM model was developed for the powdered form of CST, it is expected that there would be an "offset" of the absorption performance for the engineered bead. To determine the magnitude of this offset, SRNL used the ZAM model and compared it to measured results in prior experimental work with radioactive tank waste samples. It is also worth noting that there are three isotopes of cesium in the SRS tank waste, ^{133}Cs, ^{135}Cs, and ^{137}Cs. The CST removes all isotopes equally. The primary isotope of concern is the ^{137}Cs because it has high specific activity. Although rubidium and strontium are known to impact cesium loading, information on the soluble concentration of these species in this waste is not currently available, so they were not included in the modeling. Assuming that these species are not present is conservative, i.e., ZAM would overestimate the cesium loading because these competitors are ignored.

1.2 Task Objective

The task objective is to utilize ZAM to calculate the maximum loading expected on the TCCR columns. A key consideration in the design of the columns is the amount of ^{137}Cs that loads onto the CST and the heat generated by the loaded column during no-flow conditions and storage. SRNL has used ZAM to predict the cesium loading on the CST as a function of Tank 10 compositional projections. The ZAM model output will be used as information to determine if the loading limit that is eventually established for the column (by the thermal model) is achievable based on the compositional data.

2.0 Model Formulations

2.1 Modeling Approach

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

2.2 ZAM Description

ZAM is an equilibrium multicomponent ion exchange model developed using several experimental and structure studies characterizing the ion exchange properties of hydrous crystalline silicotitanate in its powdered form (labeled as CST or IONSIV IE-910). It predicts the ion exchange equilibria of cesium and other cations in complex electrolytic solutions by solving the liquid-solid equilibrium and material balance equations for the cesium-CST system. The model includes the competitive ion exchange at CST exchange sites between multiple homovalent cations: Na^+, Cs^+, H^+, Rb^+, K^+, and $SrOH^+$. The ZAM model was utilized to generate cesium isotherm points for each waste composition of interest at a given temperature.

Because the solid phase can be considered ideal by using a suitable solid phase representation (Multiple Interactive Ion Exchange Site Model or the supersite approach), the equilibrium constants of the model reactions are the rational selectivities. Bromley's model (Bromley, 1973) for calculating the activity coefficients of aqueous electrolytic solutions is used to account for liquid phase non-ideality.

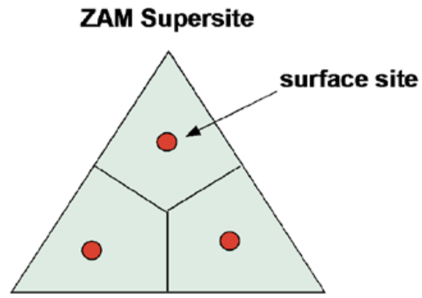
$$\log \gamma_{\pm} = \frac{-A_{\gamma}\left|z_{+}z_{-}\right| I^{1/2}}{1+\rho I^{1/2}} + \frac{\left(0.06+0.6B\left|z_{+}z_{-}\right|\right)I}{\left(1+\frac{1.5}{\left|z_{+}z_{-}\right|}I\right)^{2}} + BI \qquad (1)$$

$\gamma_{\pm}$ is the mean molal activity coefficient, and I is the ionic strength (mol/kg). At 25 ^{o}C, the Debye-Hückel constant A_{γ} is equal to 0.511 $kg^{1/2}mol^{-1/2}$ and ρ is equal to 1. Bromley tabulated values of the interaction coefficient B (Bromley, 1973).

Bromley's model is an empirical approach to determine activity coefficients for aqueous electrolyte solutions whose concentrations are above the range of validity of the Debye–Hückel equation. To apply Bromley's model in complex solutions, the single electrolyte parameter for CsOH at high ionic strength and NO_2^- and $Al(OH)_4^-$ were estimated using experimental data (Zheng et al., 1997). Care must be taken when ionic strengths are above 6 molal as Bromley determined parameters for ions up to an ionic strength of only ~6 molal. However, Zheng and co-workers have produced experimentally consistent results at ionic strengths exceeding 6 molal.

The equilibrium cesium isotherm modeling is based on multiple assumptions. It is assumed that the rate of diffusion within the pore fluid and mass transfer across the liquid film at the outer boundaries of the particles are the rate limiting steps when compared to the rate of ion exchange, therefore local equilibrium exists among the pore fluid and its neighboring surface sites. Additionally, the cesium total ionic capacity is assumed to be independent of total ionic strength or solution composition.

Experimental data indicates that a thermodynamically ideal solid phase can be achieved when the CST material is viewed on a supersite basis. Surface non-idealities on the solid phase CST material are handled by a supersite approach (Zheng et al., 1997). The supersite approach involves three neighboring surface sites as shown below:



When viewing the ion exchange process between sodium and cesium we have the following three possible mass-action relationships to consider:

$$[Na_3^+]_S + [Cs^+]_l \xleftrightarrow{K_{eq,1}} [Na_2^+Cs^+]_S + [Na^+]_l \tag{2}$$

$$[H^+Na_2^+]_S + [Cs^+]_l \xleftrightarrow{K_{eq,2}} [H^+Na^+Cs^+]_S + [Na^+]_l \tag{3}$$

$$[H_2^+Na^+]_S + [Cs^+]_l \xleftrightarrow{K_{eq,2}} [H_2^+Cs^+]_S + [Na^+]_l \tag{4}$$

Equations (2), (3), and (4) represent the removal of a Na^+ cation at a surface site with a Cs^+ cation. The three possible cases reflect the three possible states that the supersite might be in prior to the ion exchange (note that a supersite cannot hold more than one Cs^+ cation at any point in time). The temperature dependence of the thermodynamic equilibrium constants, K_{eq}, for each of the above mass-action equations can be approximated by:

$$\ln\left[\frac{K_{eq}(T_2)}{K_{eq}(T_1)}\right] = -\frac{\Delta H^o}{R}\left[\frac{1}{T_2} - \frac{1}{T_1}\right] \tag{5}$$

where T is the temperature (K). The heats of ion exchange, ΔH°, under high alkaline conditions have been estimated to be:

Rection 1: $\Delta H^\circ = -2.18\text{x}10^4$ J/gmole

Reaction 2: $\Delta H^\circ = 1.46\text{x}10^4$ J/gmole

Reaction 3: ΔH° = (not recorded)

During the loading phase, the CST material will be in its Na-form with only a trace amount of H^+ present. Therefore, Equation (2) will be the dominant ion exchange reaction taking place. Under these conditions the overall ion exchange process will be exothermic implying that higher column temperatures yields lower cesium loadings consistent with currently available batch contact data.

The overall ion exchange reactions involving Cs^+ are as follows:

$$[Na^+]_S + [Cs^+]_l \xleftrightarrow{K_{13}} [Cs^+]_S + [Na^+]_l \qquad (K_{13} \sim 26{,}000) \tag{6}$$

$$[K^+]_S + [Cs^+]_l \xleftrightarrow{K_{12}} [Cs^+]_S + [K^+]_l \qquad (K_{12} \sim 1{,}400) \qquad (7)$$

$$[SrOH^+]_S + [Cs^+]_l \xleftrightarrow{K_{14}} [Cs^+]_S + [SrOH^+]_l \qquad (K_{14} \sim 1) \qquad (8)$$

where the selectivity coefficients (K_{12}, K_{13}, K_{14}) listed reflect approximate estimates and provide insight into the selectivity of CST for cesium.

Mass-action relationships similar to those above are also written for each of the potential competitors (Na^+, Cs^+, H^+, Rb^+, K^+, and $SrOH^+$). Also, species material balance equations are written relating the amount of each species within the liquid and solid phases in the initial state to amounts in the final ("equilibrium") state. To obtain these material balances, the mass of CST and mass of liquid (i.e., volume of liquid and its density) must also be specified. Solution of this set of nonlinear algebraic equations is achieved using a modified ("rate-limited") Newton- Raphson technique.

Two versions of ZAM have been used within SRNL (i.e., Version 4 and Version 5). Both versions model the effect of temperature on the system (Na^+, Cs^+, H^+, Rb^+, and K^+) when considering a basic solution of pH > 12. The newer version (Version 5) contains the following code improvements:

- Updates to aqueous phase strontium reaction (Sr^+, OH^-, and $SrOH^+$) in basic solutions of pH > 12 has been added;
- Improvements were made in estimating the effect of K^+ on cesium distribution coefficients; and
- Bromley's parameters for NO_2 and $Al(OH)_4$ have been updated.

The actual impact as a result of these updates was found to be small if Sr complexes were not included. For many of the batch feed concentrations Version 5 had difficulty in converging. Because the final results from both versions were very similar, Version 4 was used in this report.

The solid-liquid equilibrium model solves the various mass-action equations involving ion exchange in conjunction with the appropriate material balance equations. At a specified operating temperature (K) and solution density (g/L or kg/m^3) ZAM performs a simulated batch contact ("K_d") test where the quantity of the following variables at their initial state must be specified:

- Initial composition of aqueous solution (gmole/L);
- Amount of aqueous solution present (L);
- Amount of CST material present (g); and
- Initial form of CST (0 for sodium or 1 for hydrogen).

Upon solving the simulated contact test, ZAM outputs the following final ("at equilibrium") state values for four of the competing cations (Cs^+, Rb^+, $SrOH^+$, and K^+; note Na^+ and H^+ loading numbers are not provided):

- Final CST loading of cation (Q, mmole/g_{CST});
- Final aqueous phase concentration of cation (gmole/L); and
- K_d value of cation (ml/g_{CST}).

Note that the CST loading value is simply the product of the K_d value times the final concentration for each competitor. Also provided in the output is the solution pH and ionic strength values.

ZAM is written in FORTRAN 90 using the Microsoft Developer's Workbench®. For applications performed at SRNL, PC-based versions running under MS-DOS are used. The ZAM executable files for both Versions 4 and 5 available at SRS can only run on a 16-bit Windows platform. Hence, for Windows 7 and later versions, Windows Virtual PC and Windows XP Mode (downloadable from Microsoft web page) are required to simulate the 16-bit Windows XP in order to execute ZAM.

A description of the current ZAM program as well as the governing equations is provided by Zheng et al. (1997). Supporting information and earlier modeling efforts are provided by Zheng et al. (1995) and Zheng et al. (1996). A complete user guide to ZAM was not provided by TAMU; however, model details as well as verification and validation assessments are given in a previous SRNL report (Hamm et al., 2001). Updates on the ZAM input file structure description are given in Appendix A.

2.3 Reproduction of 2003 ZAM Data for LCS Average Waste Solution

Prior to using ZAM for predicting the loading of cesium on CST it is essential to verify that ZAM can produce data on the current Windows® 7 comparable to those previously obtained on Windows XP®. The ZAM model data for a Low Curie Salt (LCS) average waste solution at 30°C (Aleman and Hamm, 2003) were selected for comparison. Figure 2 shows an excellent agreement of the current cesium isotherm and the 2003 ZAM model data. Additionally, the equilibrium cesium loading at the cesium feed concentrations of 0.012 mM, 0.02 mM, and 0.026 mM was also computed and plotted along with the isotherm in Figure 2. The ZAM model input and output data to generate the isotherm for LCS average waste solution at 30°C are shown in Appendix B.

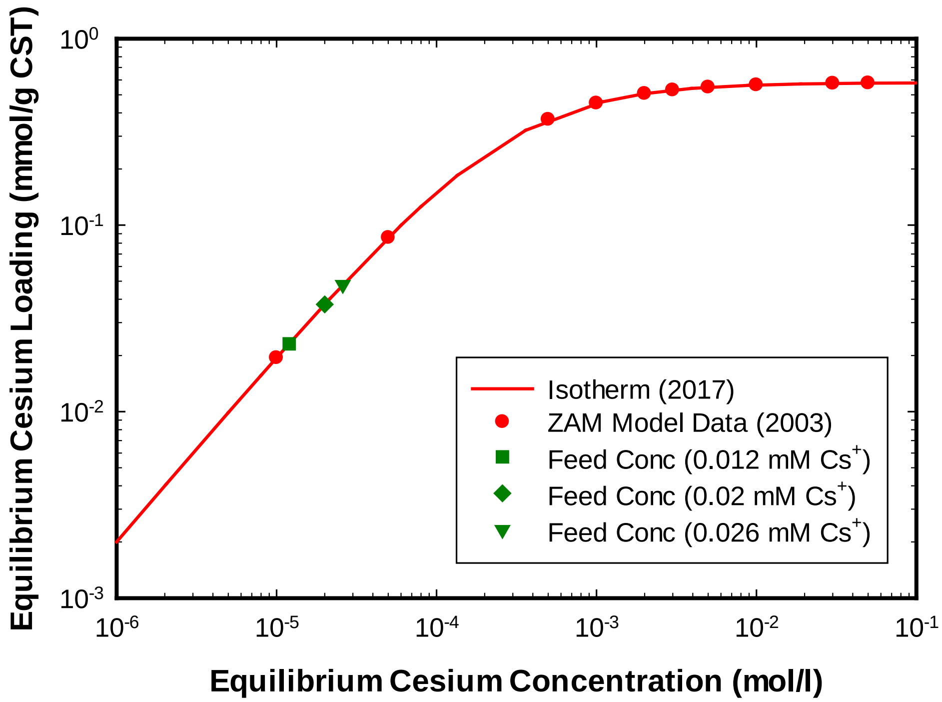


Figure 2. Cesium Isotherm for LCS Average Waste Solution at 30 °C

2.4 ZAM Validation

Data from Walker's cesium loading tests (Walker, 1999) were used to validate the ZAM program. A summary of the test data for Tank 30 and Tank 33 is given below in Table 1 and Table 2, respectively. Note that IE-911 (engineered form) containing approximately 20% inert binder (hence, only 80% CST available for Cesium removal) was used in the loading tests (Beasley et al., 2001). The ZAM data are based on IE-910 (powdered form). To examine whether the dilution by the binder needs to be included, a comparison was done using test data and ZAM results with and without an 80% dilution factor representing the lower capacity of IE-911. The ZAM results compared to the IE-911 loading test data are presented for Tank 30 and Tank 33 in Figure 3 and Figure 4, respectively. The results show the dilution impact by the binder, because the isotherm for the Tank samples is shifted to the right of the ZAM isotherm prediction at the lower cesium loadings and approaches the ZAM values at high cesium loadings. Overall, the Tank data are close to 80% dilution ZAM values, thus confirming the use of inert binder. Because the higher loading would provide more conservative outcomes (i.e., higher cesium loading and higher thermal loading), ZAM with no dilution will be used in this report to predict equilibrium cesium loading on CST for Tank 10H waste solutions.

Table 1. Cesium Loading Test Data for Tank 30

Density (g/mL)	1.242	1.242	1.242	1.242	1.242
Bottle #	19	17	5	23	25
Initial Cs (mg/L)	348.83	176.93	48.1	48.1	3.74
CST (g)	0.0859	0.0856	0.0861	0.4293	0.4285
Solution (g)	12.39	12.06	12.11	12.1	12.181
Final Cs (mg/L)	23.99	15.99	2.81	0.56	0.0412
Q (mg/g_{CST})	37.72	18.26	5.13	1.08	0.0847

Table 2. Cesium Loading Test Data for Tank 33

Density (g/mL)	1.145	1.145	1.145	1.145	1.145
Bottle #	19	17	5	23	25
Initial Cs (mg/L)	282.26	125.18	6.8	6.8	0.352
CST (g)	0.0859	0.0857	0.0857	0.4283	0.4296
Solution (g)	12.47	12.1	12.27	12.16	12.043
Final Cs (mg/L)	10.11	4.25	0.24	0.036	0.0088
Q (mg/g_{CST})	34.50	14.92	0.75	0.1677	0.0084

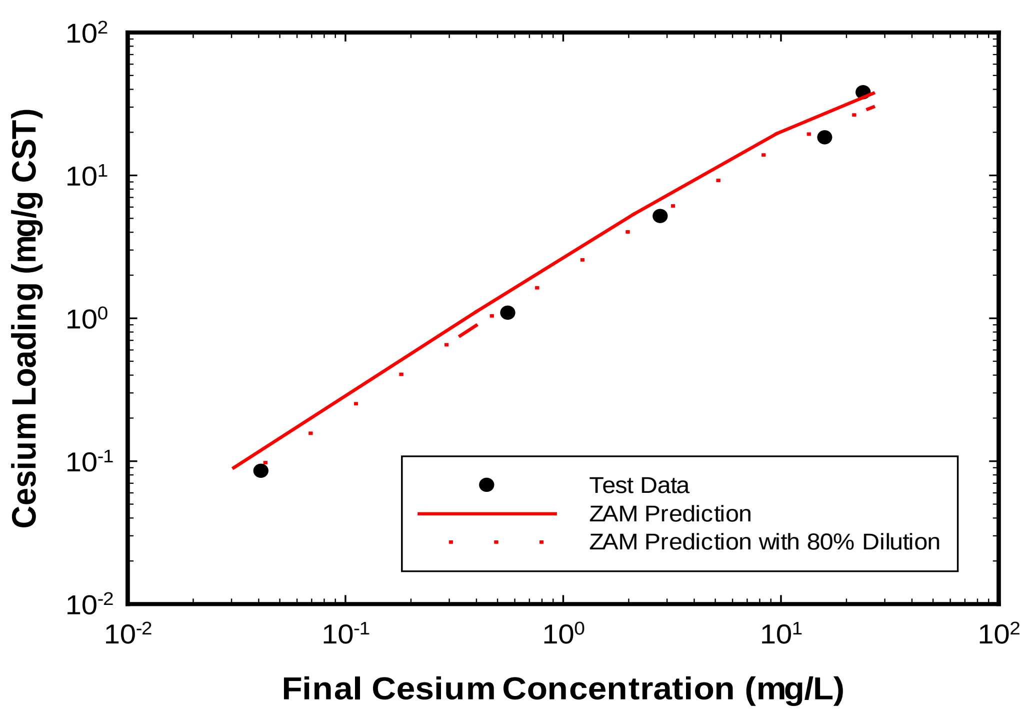


Figure 3. Comparison of ZAM and Tank 30 Cesium Loading Test Data

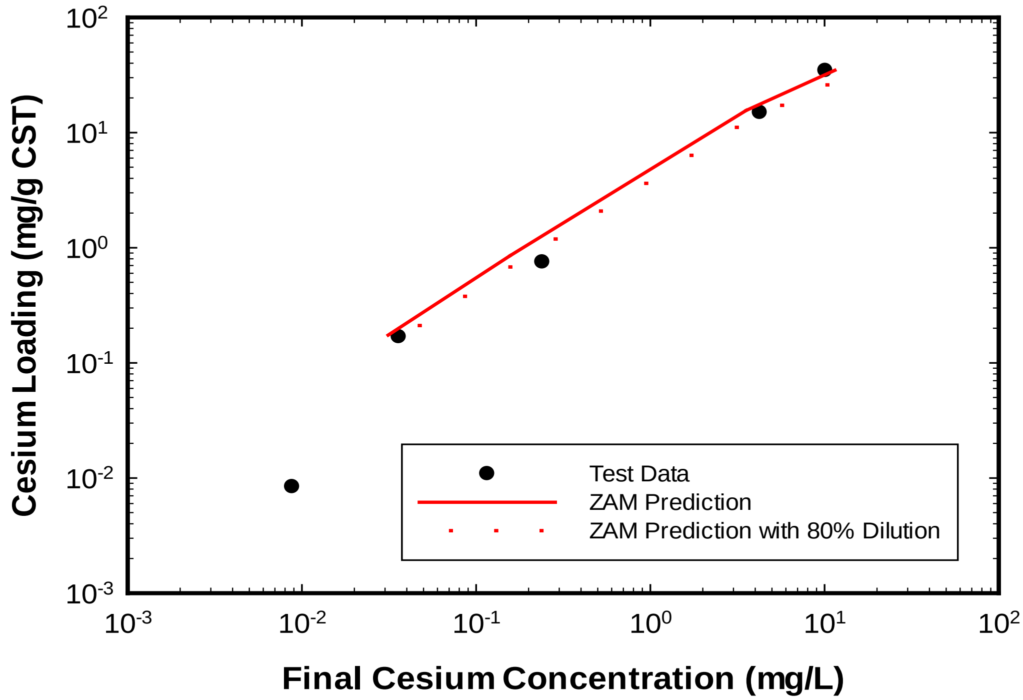


Figure 4. Comparison of ZAM and Tank 33 Cesium Loading Test Data

2.5 Prediction of Cesium Loading

The objective of this study was to predict the maximum (i.e., equilibrium) cesium loading on CST in the TCCR system to process Tank 10H waste solutions. There are two different ways to estimate cesium loading: (1) Use of an isotherm, or (2) Variation of ZAM phase ratio.

2.5.1 Use of an Isotherm

An isotherm provides the equilibrium relation between the concentration of cesium loaded on the CST surface to the concentration of cesium in the solution. The isotherm covers a wide range of liquid-phase cesium concentrations. ZAM can generate equilibrium cesium loading data at a given temperature. Generally, an excellent fit for the ZAM data would be achieved by use of the Langmuir isotherm model.

2.5.2 Variation of ZAM Phase Ratio

In a typical ion exchange column operation, the cesium concentration wave gradually moves with time from the column inlet to the column outlet until saturation is achieved. The outlet cesium concentration is approaching the feed cesium concentration, until cesium is no longer absorbed onto CST. Figure 5 illustrates the movement of cesium frontal concentration waves along the column at two different times with $t_2 > t_1$. In Figure 5, C_o is the feed cesium concentration, C is the liquid-phase cesium concentration within the column, L is the column length, and z is the location along the column axis. A phase ratio ϕ is defined as the ratio of total liquid volume (mL) processed to the mass of CST resin (g_{CST}). When the CST bed reaches saturation (i.e., $C/C_o \rightarrow 1$ at $z/L = 1$), a substantial liquid volume has passed through the column, resulting in a large phase ratio (usually >> 10^3).

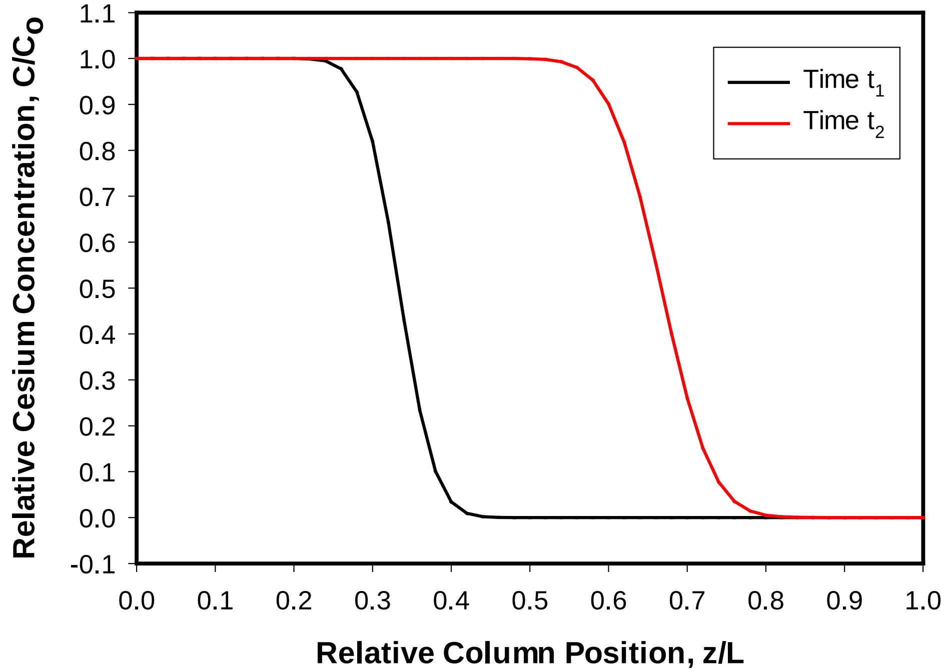


Figure 5. Movement of Cesium Frontal Concentration Waves along an Ion Exchange Column

To simulate the saturation of cesium loading on a CST bed in the ion exchange column, ZAM calculations are performed at increasing phase ratios until the calculated equilibrium liquid cesium concentration approximates the specified feed cesium concentration. The corresponding loaded cesium concentration represents the maximum (equilibrium) cesium loading at the feed cesium concentration.

Figure 6 shows the comparison of two approaches for estimation of equilibrium cesium loading. At a sufficiently large phase ratio, ZAM delivers a cesium loading value that is practically identical to that obtained from an isotherm. In this report, the approach of using ZAM with varying phase ratios was followed to predict cesium loading, unless otherwise stated.

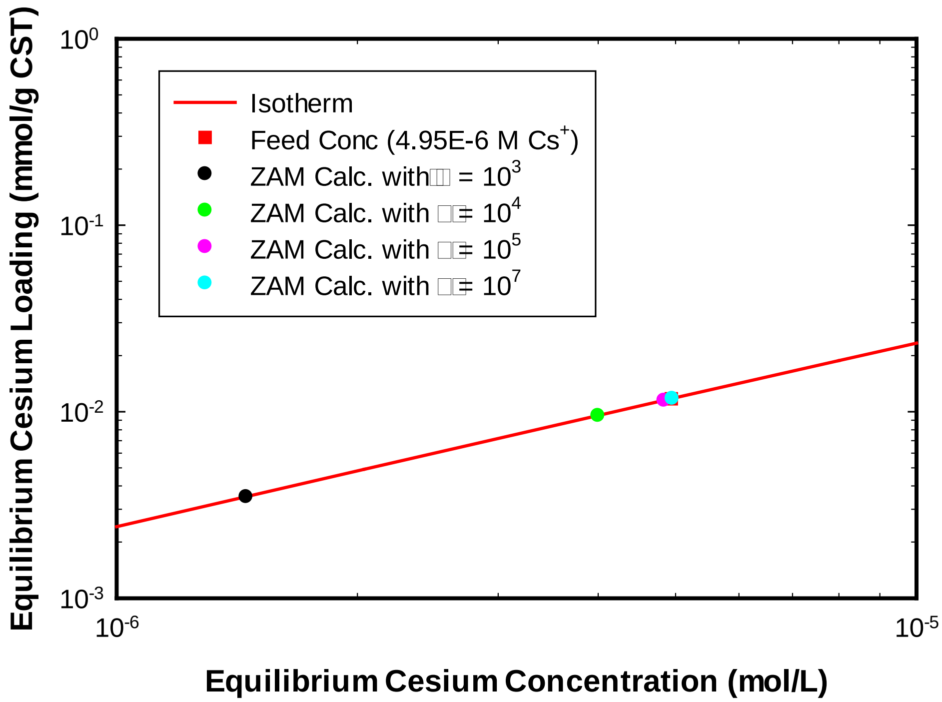


Figure 6. Cesium Loading for Tank 10 Nominal Concentrations @ 30 °C

3.0 Waste Compositions and Properties

In this study, the TCCR feeds at varying compositions from Tank 10H were considered:

1. Tank 10H saltcake core samples: Based on analysis of Tank 10H saltcake core samples, by dilution with water, the TCCR feeds were generated for Na^+ concentrations (M) of 7.5, 7, 6, 5, 4, and 3. The feed compositions at 7.5 M Na^+ shown in Table 3 are based on sample #HTF-610 (Martino et al., 2004), calculated for soluble species based on a salt:water ratio of 19 moles of salt solids and 29.8 moles of water using OLI Analyzer Studio v. 9.1, and diluted to the target [Na^+]. The 19 moles of salt is the amount of solids in approximately 1 L of sample #HTF-610 wet saltcake, and mixed with a minimal amount of water (0.536 L) to end up with roughly equal volume of solids and liquid (0.67 L). With this set of feed data the effect of dilution on cesium loading was studied.

2. Tank 10H nominal case and variations: In 2013 the top several inches of Tank 10H saltcake were dissolved. The liquid solution was subsequently transferred to another tank and analyzed. Table 4 lists the compositions for the nominal case and its variations covering the possible range of key ions in Tank 10H as saltcake dissolves.

3. Special cases of higher cesium concentration: In these cases, the effect of a higher cesium concentration (i.e., 1.97E-5 M compared with 4.95E-6 M in the nominal case) on cesium loading was investigated. Table 5 provides a summary of the special cases.

4. Tank 10H Variable Depth Sample (VDS): Waste compositions for Cases 1 – 10 given in Table 4 and Table 5 were based on information provided by SRR as an estimate of the composition of the Tank 10H liquid, and adjusted by SRNL to vary key parameters of potassium, sodium, and hydroxide concentrations. An actual composition was also used (see Table 6), which was obtained from an analysis of a variable depth sample recently collected from Tank 10H (Reboul, 2017). The VDS sample was collected in March 2017 following a water addition to the tank, and allowing the saltcake to dissolve for a few weeks. Note that total Cs concentration was derived from the measured ^{137}Cs. Although the analyzed molar ratio of ^{137}Cs to total Cs is 0.21 in the VDS composition, the ratio of 0.3 was used for comparison with other cases.

In all cases a molar ratio of ^{137}Cs to total Cs was 0.30. This was based on a rough estimate from the Tank 10H core sample analysis. The specific activity of ^{137}Cs used for calculations was 87 Ci/g, but the curie loading due to ^{135}Cs was ignored, because its specific activity is so low (1.15E-3 Ci/g) (DOE, 1997).

Table 3. Diluted Tank 10H Salt Solution at 25 °C and 7.5 M Na^+

Cations	**(M)**	**Anions**	**(M)**
Na^+	7.5	OH^-	1.04
Cs^+	8.48E-05	NO_3^-	3.70
H^+	9.63E-15	NO_2^-	0.52
Rb^+		$Al(OH)_4^-$	0.06
K^+	1.3E-02	SO_4^{2-}	0.098
$SrOH^+$		CO_3^{2-}	0.782
Sr^{2+}		PO_4^{3-}	0.023
		F^-	0.0073
		Cl^-	0.0709
		$COOH^-$	0.284
		$C_2O_4^{2-}$	1.75E-04
Density[(a)] (g/mL)	1.343		

[(a)] Density is calculated by Walker's correlation for the average salt solutions: $\rho = 1.009 + 0.04454\,[Na^+]$ (Walker and Georgeton, 1989)

Table 4. Nominal Case and Variations of Tank 10H Salt Solutions at 30 °C

Tank 10H Salt Solutions			Nominal	Vary Na	Vary Na	Vary OH	Vary OH	Vary OH	Vary OH	Vary K	Vary K	Vary K
	Min (M)	Max (M)	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8a	Case 8	Case 9
Na^+	5.73	8	5.73	7	8 [b]	5.73	5.73	5.73	5.73	5.73	5.73	5.73
Cs^+	4.95E-06		4.95E-06	4.95E-06	4.95E-06	4.95E-06	4.95E-06	4.95E-06	4.95E-06	4.95E-06	4.95E-06	4.95E-06
K^+	0	0.03	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.005	0.015	0.03
$NO3^-$	2.25	3.877	2.25	2.877	3.877	2.25	2.25	2.25	2.25	2.25	2.25	2.25
$NO2^-$	0.105		0.105	0.105	0.105	0.105	0.105	0.105	0.105	0.105	0.105	0.105
OH^-	0.2007	1	0.2007	0.2007	0.2007	0.3	0.5	0.75	1	0.2007	0.2007	0.2007
CO_3^{2-}	0.686		0.686	0.686	0.686	0.686	0.686	0.686	0.686	0.686	0.686	0.686
SO_4^{2-}	0.116	1.223	0.902	1.223	1.223	0.852	0.752	0.627	0.502	0.9037	0.909	0.916
Cs-137 Ci/L			0.018	0.018	0.018	0.018	0.018	0.018	0.018	0.018	0.018	0.018
Density[a] (g/mL)			1.264	1.310	1.330	1.263	1.260	1.257	1.2545	1.264	1.265	1.266

[a] Densities are calculated by OLI
[b] Na^+ concentration may be outside the ZAM prediction range

Table 5. Special Cases of High Cesium Concentration at 30 °C

	Case 10a	Case 10b	Case 10c	Case 10d	Case 10e
Density[(a)] (g/mL)	1.327	1.327	1.324	1.289	1.282
	(M)	(M)	(M)	(M)	(M)
Na^+	7.7 [(b)]	7.7 [(b)]	7.7 [(b)]	6.54	6.54
Cs^+	1.97E-05	1.97E-05	1.97E-05	1.97E-05	1.97E-05
K^+	3.30E-03	0.00E+00	3.30E-03	3.30E-03	3.30E-03
OH^-	0.356	0.356	1.0	0.356	1.0
NO_3^-	2.48	2.48	2.48	2.48	2.48
NO_2^-	0.179	0.179	0.179	0.179	0.179
CO_3^{2-}	1.17	1.17	1.17	0.688	0.524
SO_4^{2-} [(b)]	1.01736	1.01571	0.69536	0.919	0.759
PO_4^{3-}	4.32E-02	4.32E-02	4.32E-02	4.32E-02	4.32E-02
Cl^-	2.31E-02	2.31E-02	2.31E-02	2.31E-02	2.31E-02
F^-	4.31E-02	4.31E-02	4.31E-02	4.31E-02	4.31E-02
$C_2O_4^{2-}$	1.33E-02	1.33E-02	1.33E-02	1.33E-02	1.33E-02
CHO_2^-	9.12E-02	9.12E-02	9.12E-02	9.12E-02	9.12E-02
Cs-137	5.91E-06	5.91E-06	5.91E-06	5.91E-06	5.91E-06

[(a)] Densities are calculated by OLI
[(b)] Na^+ concentration may be outside the ZAM prediction range

Table 6. VDS Tank 10H Composition at 30 °C

Cations	**(M)**	**Anions**	**(M)**
Na^+	3.22	OH^-	0.184
Cs^+ [(a)]	1.09E-05	NO_3^- [(b)]	1.052
H^+	5.43E-14	NO_2^-	0.128
Rb^+		$Al(OH)_4^-$	0.063
K^+	3.32E-03	SO_4^{2-}	0.381
$SrOH^+$		CO_3^{2-}	0.506
Sr^{2+}		PO_4^{3-}	0
		F^-	0
		Cl^-	0.004
		$COOH^-$	0
		$C_2O_4^{2-}$	9.20E-03
Density[(c)] (g/mL)	1.155		

(Reference: Reboul, 2017)
[(a)] Total Cs is derived from measured ^{137}Cs and molar Cs ratio of 0.3
[(b)] NO_3^- is adjusted for charge balance
[(c)] Density is calculated by OLI

3.1 Quality Assurance

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

4.0 Results and Discussion

The calculated results of waste compositions specified in Section 3.0 are presented and discussed in this section. Relevant ZAM data (input, output) and isotherms are provided in Appendix D.

4.1 Dilution of Saltcake Samples

Table 7 summarizes the ZAM results for the calculated composition that would be expected during dilution of Tank 10H saltcake core samples HTF-610. Cesium loading on CST was calculated for diluted salt solutions of Na^+ concentrations varying from 3 M to 7.5 M. For comparison, a loading of cesium to yield 100 Ci/L is given in Table 7. The ZAM model also calculated pH and the total ionic strength (mol/kg) of the solutions as listed in Table 8. Table 8 shows a very large increase in the ionic strength with increasing Na^+ concentrations. Zheng et al. (1996) observed that the cesium loading decreases with increasing Na^+ concentrations primarily due to the increased ionic strength. Table 7 confirms the increasing cesium loading in more diluted salt solutions. Note that the following estimates are relevant to the conversion of $mmol_{Cs}/g_{CST}$ to mg_{Cs}/g_{CST} and Ci/L_{Bed}:

- ^{137}Cs/Total Cs = 0.3
- $(M_{Cs})_{avg}$ = 134.1 g/gmol
- 11926.67 $Ci/mol_{^{137}Cs}$
- CST bed density = 1 g/mL

Table 7. Dilution Effect on Cesium Loading at 25 °C for HTF-610 Sample

Na^+ (mol/L)	Q ($mmol_{Cs}/g_{CST}$)	Q (mg_{Cs}/g_{CST})	Q (Ci/L_{Bed})	$C_f = C_o$ ($mmol_{Cs}/L$)
7.5	0.0905	12.14	329.21	0.0848
7	0.0964	12.93	350.67	0.0791
6	0.1080	14.49	392.86	0.0678
5	0.1200	16.10	436.52	0.0565
4	0.1330	17.84	483.81	0.0452
3	0.1450	19.45	527.46	0.0339
Cs Loading yielding 100 Ci/L	0.0275	3.69	100	

C_o: Initial cesium concentration

C_f: Equilibrium cesium concentration

Table 8. pH and Total Ionic Strength of Diluted Salt Solutions at 25 °C

Na^+ (mol/L)	pH	Total Ionic Strength (mol/kg)
7.5	14.9	11.1
7	14.8	10.2
6	14.6	8.5
5	14.3	6.8
4	14.1	5.3
3	13.9	3.8

4.2 Projected Tank 10H Salt Solution Cases

The ZAM results of all cases for Tank 10H salt solution SRR-projected compositions are provided in Table 9. These compositions were based on prior dissolution of Tank 10H waste which was then mathematically adjusted to vary the key components. The ZAM calculations indicate cesium loading on the CST resin at concentrations below the safety threshold of 170 Ci/L. The effects of key ions (i.e., Na^+, OH^-, K^+, and Cs^+) on cesium loading are discussed in the following sections.

Table 9. Results of SRR-Projected Tank 10H Salt Solution Cases

Cases	Q			$C_f = C_o$
	($mmol_{Cs}/g_{CST}$)	(mg_{Cs}/g_{CST})	(Ci/L_{Bed})	($mmol_{Cs}/L$)
1	0.0118	1.58	42.11	0.00495
2	0.0077	1.04	27.62	0.00495
3	0.0045	0.61	16.25	0.00495
4	0.0118	1.59	42.29	0.00495
5	0.0119	1.60	42.65	0.00495
6	0.0120	1.62	43.11	0.00495
7	0.0122	1.63	43.58	0.00495
8a	0.0115	1.54	41.11	0.00495
8	0.0109	1.46	38.93	0.00495
9	0.0101	1.36	36.17	0.00495
10a	0.0347	4.65	124.01	0.0197
10b	0.0352	4.72	125.98	0.0197
10c	0.0357	4.79	127.73	0.0197
10d	0.0360	4.83	128.77	0.0197
10e	0.0353	4.74	126.45	0.0197

C_o: Initial cesium concentration

C_f: Equilibrium cesium concentration

4.2.1 Effect of Na^+

In Cases 1, 2, and 3, the impact of Na^+ on cesium loading was investigated by Na^+ variation with a fixed concentration of Cs^+. As discussed in Section 4.1, the cesium loading decreases with increasing Na^+ concentrations primarily due to the increased ionic strength. The correlation in Figure 7 shows a linear effect within the concentration range of interest. The ratio of change was computed to be -2.1. Note that the 8 M Na^+ condition exceeds the range of legitimate Bromley coefficients, which were confirmed to produce good predictions for solutions up to 7 M Na^+ (Zheng et al., 1997).

Linear regression: $Q = -3.1848E-3*[Na^+]+0.03$ ($R^2 = 1$)

Ratio of change: $\frac{\Delta Q\%_{avg}}{\Delta Na^+\%} = -2.1$

$\Delta Q\%_{avg}$: Avg. % change of mmol/g

$\Delta Na^+\%$: % change of mol/L

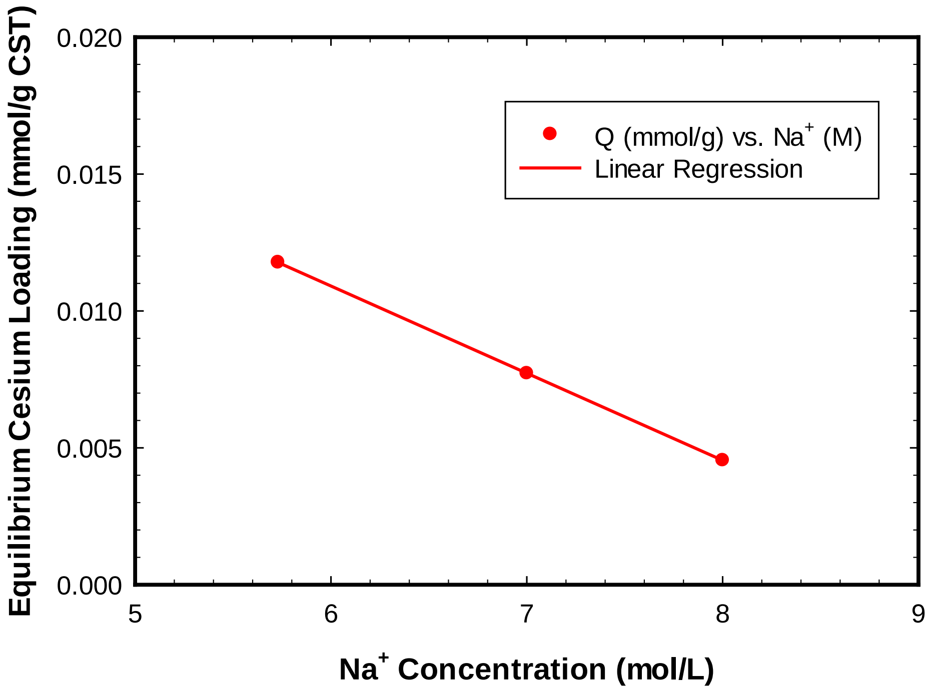


Figure 7. Na^+ Effect on Cesium Loading

4.2.2 Effect of OH^-

Similarly, in Cases 4 - 7, the impact of OH^- on cesium loading was investigated by OH^- variation with a fixed concentration of Cs^+. The anion used to allow the variation was sulfate, so there is a complication of the larger impact of a divalent ion versus a monovalent ion on the ionic strength. This would mean that the lower ionic strength caused by lower sulfate would increase the cesium loading; which convolutes interpretation of the results as being strictly due to hydroxide variability. As shown below, cesium loading increases with increasing OH^- and decreasing sulfate concentrations. The correlation in Figure 8 shows a linear effect within the concentration range of interest. The ratio of change was computed to be 0.02. These results must not be used for other compositions because of the complications caused by the impact of sulfate on ionic strength.

Linear regression: $Q = 5.1512E - 4 * [OH^-] + 0.0117$ (R^2 = 0.9999)

Ratio of change: $\dfrac{\Delta Q\%_{avg}}{\Delta OH^- \%} = 0.02$

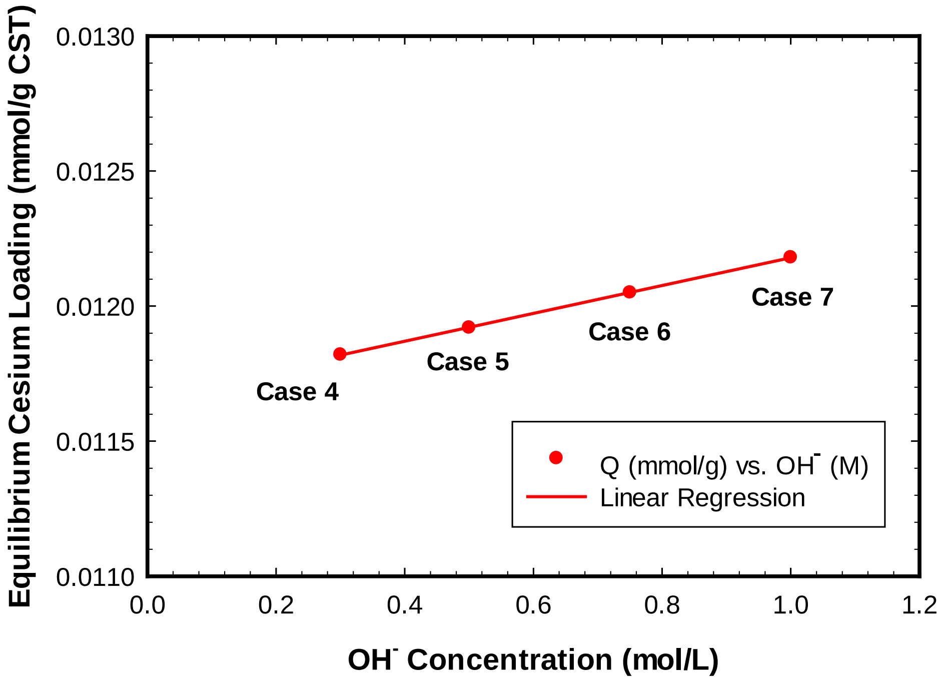


Figure 8. OH^- Effect on Cesium Loading

4.2.3 Effect of K^+

In Cases 8, 8a, and 9, the impact of K^+ on cesium loading was investigated by K^+ variation with a fixed concentration of Cs^+. In this case, the sulfate ion concentration was adjusted to achieve a charge-balanced composition, leaving the Na^+ and Cs^+ concentrations constant. As discussed in Section 4.1, cesium loading decreases with increasing K^+ concentrations primarily due to the increased competition for binding sites. The correlation in Figure 9 shows a linear effect within the concentration range of interest. The ratio of change was computed to be -0.0265.

Linear regression: $Q = -0.0549 * [K^+] + 0.0117$ ($R^2 = 0.9977$)

Ratio of change: $$\frac{\Delta Q\%_{avg}}{\Delta K^+\%} = -0.0265$$

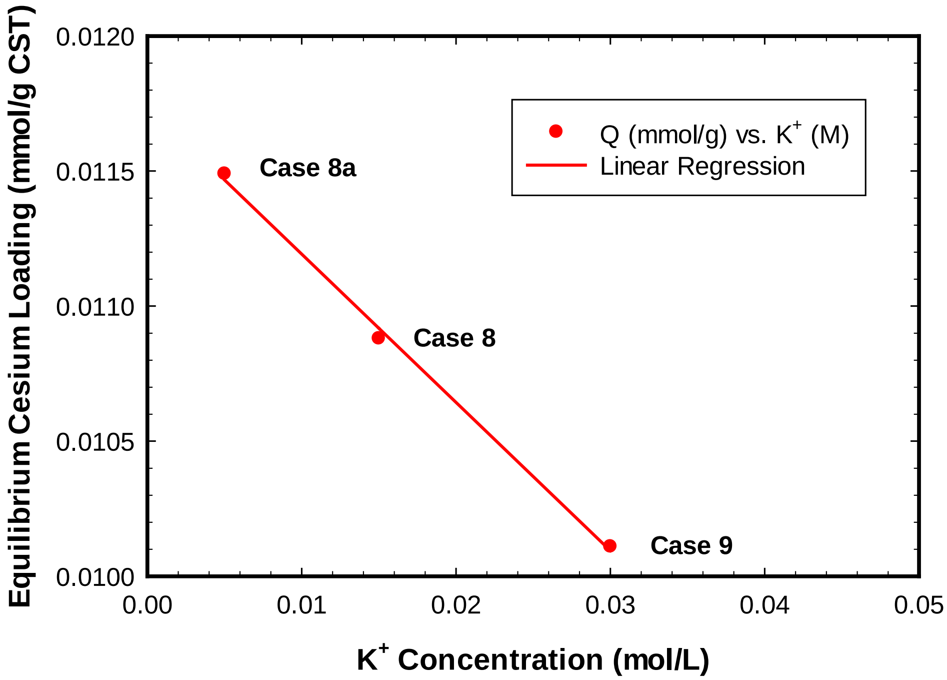


Figure 9. K^+ Effect on Cesium Loading

4.2.4 Effect of Cs^+

Table 9 indicates that a 4x increase in initial cesium concentrations results in a 4.5x increase in cesium loading. In general, higher cesium concentrations would yield larger cesium loading due to a better concentration driving force for absorption. Figure 10 shows the isotherms for Case 2 and Case 10a waste solutions, and confirms the computed effect of initial cesium on loading.

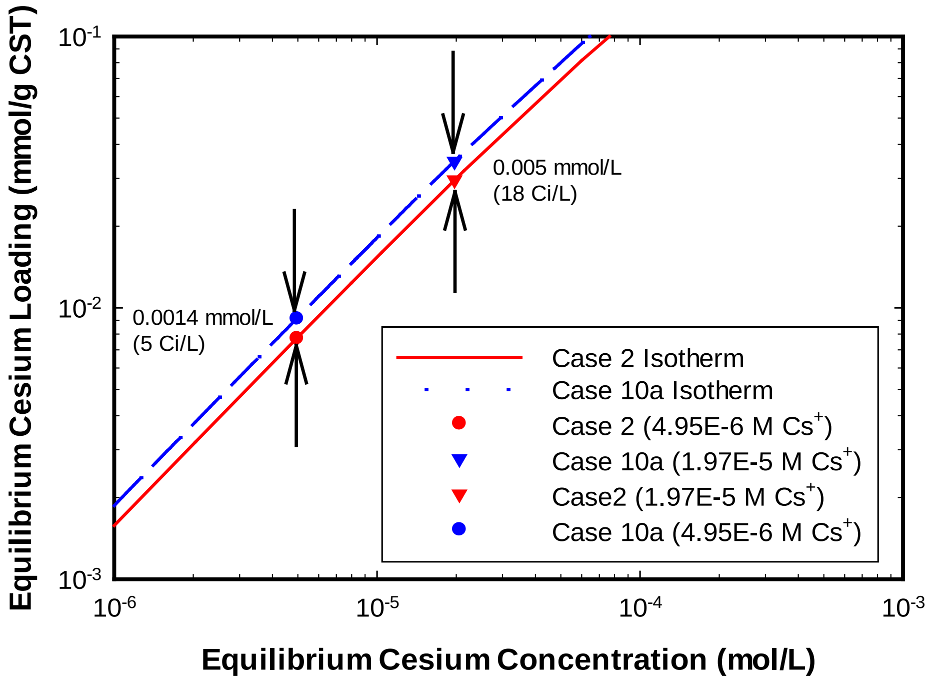


Figure 10. Cs^+ Effect on Cesium Loading (Case 2 vs. Case 10a)

4.3 Tank 10H VDS Composition

The ZAM calculation indicates cesium loading on the CST resin at a concentration of 0.055 $mmol_{Cs}/g_{CST}$ (7.44 mg_{Cs}/g_{CST} or 198.4 Ci/L_{Bed}) that is above the safety threshold of 170 Ci/L_{Bed}. This result is consistent with the findings in Section 4.1, i.e., cesium loading increases with decreasing Na^+ concentrations.

5.0 Conclusions

Tank 10H salt solutions of varying compositions to be processed in the TCCR system were examined. General results of the ZAM model predictions are:

- Dilution of salt solutions with water decreases Na^+ concentrations and increases the cesium loading primarily due to the decreased ionic strength.
- The ZAM results of all cases for SRR-projected Tank 10H salt solution compositions show maximum cesium loading less than 130 Ci/L. Results using compositions of salt solution based on a core sample from Tank 10H indicate much higher cesium loadings, of ~300 Ci/L to 500 Ci/L.
- The effects of key ions (Na^+, OH^-, K^+, and Cs^+) on cesium loading within the concentration range of interest are correlated as shown below. These correlations cannot be extrapolated to other conditions or compositions because they are applicable to only a very specific set of compositions.
  - Na^+: $Q = -3.1848E-3*[Na^+] + 0.03$
  - OH^-: $Q = 5.1512E-4*[OH^-] + 0.0117$
  - K^-: $Q = -0.0549*[K^+] + 0.0117$
  - Cs^+: Higher initial cesium concentrations would yield larger cesium loading due to better concentration driving force for absorption.
- For Tank 10H VDS composition, because of the low Na^+ concentration (i.e., 3.22 M) a cesium loading of 0.055 $mmol_{Cs}/g_{CST}$ (7.44 mg_{Cs}/g_{CST} or 198.4 Ci/L_{Bed}), which is higher than other cases evaluated because of the low Na+ concentratioin; which can also be viewed as a higher Cs:Na mole ratio.

These calculations did not include any uncertainty in the aqueous phase composition. It is advisable to perform these for future work, depending on the intended use of the data. Both the ZAM and OLI models are currently maintained at QA Level D.

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.

Beasley, M. H., A. D. Coleman, B. H. Croy, S. D. Fink, R. A. Jacobs, and D. D. Walker, 2001. “IONSIV® IE-911 Performance in Savannah River Site Radioactive Waste,” WSRC-TR-2000-00526, Rev. 0, April.

Bromley, L. A., 1973. “Thermodynamic Properties of Strong Electrolytes in Aqueous Solutions,” AIChE J., **19**(2), 313-320 (1973).

Caldwell, T. B., 2017. “Tank Closure Cesium Removal (TCCR) System,” X-SOW-H-00002, Rev. 4.

DOE/RW-0006, Rev. 13, Integrated Data Base Report – 1996: U.S. Spent Nuclear Fuel and Radioactive Waste Inventories, Projections, and Characteristics, U.S. Department of Energy, December, 1997

Dosch, R. G., N. E. Brown, H. P. Stephens, and R. G. Anthony, 1993. "Treatment of Liquid Nuclear Wastes with Advanced Forms of Titanate Ion Exchangers," '93 Waste Management Symposia, Tucson, AZ, 1993.

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.

Martino, C. J., Nichols, R. L., McCabe, D. J., Millings M. R., 2004. “Tank 10H Saltcake Core Sample Analysis,” WSRC-TR-2004-00164, April 19.

OLI Systems, Inc., 2014. “A Guide to Using OLI Studio Including Studio ScaleChem – Version 9.2” (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.

Smith, F. G., 2011. “Modeling CST Ion-Exchange for Cesium Removal from SCIX Batches 1 – 4,” SRNL-STI-2011-00181, Rev. 0, April.

Walker, D. D., 1999. Laboratory Notebook, WSRC-NB-99-204, pp. 84-85.

Walker, D. D., and G. K. Georgeton, 1989. “Viscosity and Density of Simulated Salt Solutions,” WSRC-RP-89-1088, October.

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. Updated ZAM Input File Structure Description

[This Appendix is reproduced from part of Appendix F of a previous report (Hamm et al., 2001) with some updates for clarification. The updates are written in red italics.]

The standard input file is named "CSTIEXV.in" and contains all the necessary input to perform a single simulated Kd test. This file contains the information required prior to ion-exchange and the program then calculates the equilibrium based on this initial information. Briefly, you need to specify the choice of activity coefficient model, temperature, the title, the liquid molar density, the number of cations, the number of anions, cation concentrations, anion concentrations, amount of liquid, amount of solid, the initial solid form parameter, and the calculation adjustment parameter. The liquid phase concentrations must be charged balanced (i.e., ZAM assumes the solution to be charged balance to within a small tolerance). If the solution charge miss-balance exceed the tolerance an error message is printed and ZAM execution is terminated. Charge balancing should be performed using a species having a small overall impact like chlorine.

The following is a line-by-line description of the input needs for "CSTIEXV.in":

Line 1) **Choice of activity model and temperature:** Option 1 is the only activity model currently available and presents Bromley's model. Temperature is input in K units. The temperature dependent parameter within the ZAM model are based on experimental data taken within the range 298.15 K to 317.15 K. The temperature effect in neutral to acidic solutions (pH<12) is not included, and the effect of temperature for strontium is not addressed.

Line 2) **Title:** The title inputted is printed out as a header in the output file and must be less than 33 characters long.

Line 3) **Number of Cations:** An integer whose number must exceed 6. A minimum of 7 cations is required because Na^+, Cs^+, H^+, Rb^+, K^+, and $SrOH^+$ are competing cations for CST exchange sites and Sr^{2+} is in equilibrium with $SrOH^+$ in the aqueous phase.

Line 4) **Number of Anions:** An integer whose number must exceed 1. A minimum of 2 anions is required because OH^- and $NO3^-$ are assumed to be always considered within the aqueous phase solution model formulation.

Line 5) **Solution Density (g/L or kg/m3):** The aqueous phase density is required to convert molar ion concentrations (gmole/L) into molal units (gmole/kgwater). Bromley's activity coefficient model is based on molal units.

Line 6) **Cation Code IDs:** These are integer ID numbers specifying which cations are being considered (see Table A-1). The first 7 cations (minimum number required) must be Na^+, Cs^+, H^+, Rb^+, K^+, $SrOH^+$, and Sr^{2+} in this order (i.e., 3, 6, 1,1, 5, 4, 40, 13). Additional cations can be added to the list starting in the 8th position and beyond in any given order. Even under conditions where some of the first 7 cations do not exist within the aqueous phase, they must still be given with zero concentrations inputted.

Line 7) **Anion Code IDs:** These are integer ID numbers specifying which anions are being considered (see Table A-1). The first 2 anions (minimum number required) must be OH- and NO3- in this order (i.e., 13, 9). Additional anions can be added to the list starting in the 3rd position and beyond in any given order. Even under conditions where some of the first 2 anions do not exist within the aqueous phase, they must still be given with zero concentrations inputted.

Line 8) **Formula Weight:** If you have chosen an ion not explicitly listed in Table A-1, then its molecular weight (g/gmole) must be supplied. If you have only requested ions contained within Table A-1, this line can be skipped. Three unlisted cations and three unlisted anions are optional. For cations the possible code IDs are 37, 38, and 39 (see Table A-1). For anions the possible code IDs are 24, 25, and 26 (see Table A-1). *Molecular weights must be specified on separate lines (i.e., one molecular weight per line).*

Line 9) **Cation Concentrations (M):** Here the concentrations should be listed in the same order as the cation code IDs are listed. Zero concentrations can be used. However the concentration of H+ must be greater than zero. For example, if the solution is basic use $[H^+][OH^-]=1x10^{-14}$ to estimate the H^+ concentration. The ZAM program will internally correct the H^+ concentration. If the solution is neutral use $1x10^{-7}$. For strontium considerations, input zero concentration for $SrOH^+$ (cation #40) and the actual concentration of total strontium as Sr^{2+} (cation #13). The program will calculate the liquid-phase equilibrium between $SrOH^+$ and Sr^{2+} based on available free OH^-.

Line 10) **Anion Concentrations (M):** Here the concentrations should be listed in the same order as the anion code IDs are listed. Zero concentrations can be used. However the concentration of OH^- must be greater than zero. For example, if the solution is acidic use $[H^+][OH^-]=1x10^{-14}$ to estimate the OH^- concentration. The ZAM program will internally correct the OH^- concentration. If the solution is neutral use $1x10^{-7}$.

Line 11) **Liquid Volume (L) and Solid Mass (g):** Enter the amount of volume of aqueous phase solution being placed in contact with CST. Enter the amount of mass of CST being considered. The phase ratio is the ratio of these two quantities.

Line 12) **Initial form of solid:** There are two initial forms for the CST material (its Na-form or its H-form). Here it is assumed that all exchange sites are initially occupied by either Na^+ (option 0) or by H^+ (option 1).

Line 13) **Calculational Adjustment Parameter:** Real number ranging from 0.0 to 1.0. This is an under-relaxation iteration parameter used to assist in convergence of the non-linear equation solver. The larger the number the faster (less under-relaxed) convergence is generally achieved (however, the larger the risk of divergence). The best overall value is around 0.7. The program has more difficulty in converging under near neutral conditions. Note that concentration ranges covering 5 to 10 orders in magnitude are typically being computed and the system of equations can become very stiff. This set of equilibrium and material balance equations are a very non-linear set of algebraic equations that can be difficult to solve for most standard solvers. Generally, low values of this adjustment parameter helps convergence but can greatly extend the overall runtime.

Table A-1. Ionic species available within the ZAM CST ion-exchange equilibrium model.

ID	Cations	Anions
1	H^+	F^-
2	Li^+	Cl^-
3	Na^+	Br^-
4	K^+	I^-
5	Rb^+	ClO_3^-
6	Cs^+	ClO_4^-
7	NH_4^+	BrO_3^-
8	Tl^+	IO_3^-
9	Ag^+	NO_3^-
10	Be^{2+}	$H_2PO_4^-$
11	Mg^{2+}	$H_2AsO_4^-$
12	Ca^{2+}	CNS^-
13	Sr^{2+}	OH^-
14	Ba^{2+}	CrO_4^{2-}
15	Mn^{2+}	SO_4^{2-}
16	Fe^{2+}	$S_2O_3^{2-}$
17	Co^{2+}	HPO_4^{2-}
18	Ni^{2+}	$HAsO_4^{2-}$
19	Cu^{2+}	CO_3^{2-}
20	Zn^{2+}	PO_4^{3-}

ID	Cations	Anions
21	Cd^{2+}	AsO_4^{3-}
22	Pb^{2+}	$Fe(CN)_6^{3-}$
23	UO_2^{2+}	$Mo(CN)_8^{3-}$
24	Cr^{3+}	User defined [a]
25	Al^{3+}	User defined
26	Sc^{3+}	User defined
27	Y^{3+}	NO_2^-
28	La^{3+}	$Al(OH)_4^-$
29	Ce^{3+}	na [b]
30	Pr^{3+}	na
31	Nd^{3+}	na
32	Sm^{3+}	na
33	Eu^{3+}	na
34	Ga^{3+}	na
35	Co^{3+}	na
36	Th^{4+}	na
37	User defined [a]	na
38	User defined	na
39	User defined	na
40	$SrOH^+$	na

[a] Array locations in storage that are available for user to specify additional species. *(Cation IDs: 37 (1^+ valence), 38 (2^+ valence), 39 (3^+ valence); Anion ID: 24 (1^- valence), 25 (2^- valence), 26 (3^- valence))*

[b] Array locations in storage that are currently unused.

ZAM is written in FORTRAN 90 using the Microsoft Developer's Workbench. For applications performed at SRNL, PC-based versions running under MS-DOS are used. The ZAM executable files for both Versions 4 and 5 available at SRS can only run on a 16-bit Windows platform. Hence, for Windows 7 and later versions, Windows Virtual PC and Windows XP Mode (downloadable from Microsoft web page) are required to simulate the 16-bit Windows XP in order to execute ZAM.

A ZAM input file example for Case 10a of a Tank 10H solution containing high cesium concentration and two additional anions (i.e., $COOH^-$, and $C_2O_4^{2-}$) that are not listed in Table A-1 is shown below.

```
1, 303.15                                                                   Activity Coeff. Model, Temperature
Tank 10 Case 10a @ 30C                                                      Title
7, 11                                                                       Number of Cations & Anions
1326.93                                                                     Density(kg/m3)
 3, 6,  1,  5,  4, 40, 13                                                   Names of Cations
13, 9, 27, 28, 15, 19, 20, 1, 2, 24, 25                                     Names of Anions (Add COOH-, C2O4--)
45.018                                                                      COOH- MW
88.02                                                                       C2O4-2 MW
7.7, 1.97E-05, 2.81E-14, 0, 0.00330, 0, 0                                   Concentrations of Cations
0.3560, 2.48, 0.179, 0, 1.01736, 1.17, 0.0432, 0.0431, 2.31E-02, 9.12E-02, 1.33E-02  Concentrations of Anions
1, 0.0001                                                                   Liquid (L), Solid (g)
0                                                                           Initial Solid Form (Na+ (0); H- (1))
1                                                                           Calculation Adjustment
```

The corresponding ZAM output file is obtained as follows. Note that $COOH^-$ and $C_2O_4^{2-}$ appear as “Other-” and “Other--”, respectively.

```
   Solution:  Tank 10 Case 10a @ 30C
  ***********************INPUT************************

    Density=  .1327E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....        22.9898         1.        .7700E+01
  Cs+.....       132.9054         1.        .1970E-04
  H+......         1.0079         1.        .2810E-13
  Rb+.....        85.4678         1.        .0000E+00
  K+......        39.0983         1.        .3300E-02
  SrOH+...       105.0000         1.        .0000E+00
  Sr++....        87.6200         2.        .0000E+00
  OH-.....        17.0073        -1.        .3560E+00
  NO3-....        62.0049        -1.        .2480E+01
  NO2-....        46.0000        -1.        .1790E+00
  Al(OH)4-        95.0000        -1.        .0000E+00
  SO4--...        96.0636        -2.        .1017E+01
  CO3--...        60.0092        -2.        .1170E+01
  PO4---..        94.9712        -3.        .4320E-01
  F-......        18.9984        -1.        .4310E-01
  Cl-.....        35.4527        -1.        .2310E-01
  Other-..        45.0180        -1.        .9120E-01
  Other--.        88.0200        -2.        .1330E-01

  Liquid(L)= .1000E+01   Solid(g)= .1000E-03

   Material: Na Form


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

   Ionic Strength=          14.632406205448290 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .3466E-01      .1970E-01      .1760E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .1679E-01      .3300E+01      .5088E+01
```

Appendix B. Isotherm for LCS Average Waste Solution

To generate the isotherm data, a series of ZAM calculations were performed in which the cesium concentrations were varied from $1x10^{-9}$ to 0.1 mol/L. Cl^- was adjusted accordingly to maintain the charge balance. The ZAM input and output data are shown below in this Appendix.

The Freundlich/Langmuir form was selected to represent an isotherm for LCS average waste solution:

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

Q:	Equilibrium Cs loading (mmol/g_{CST})
C_{Cs}:	Equilibrium Cs concentration in the solution (mol/L)
C_T:	0.58 (mmol/g_{CST})
β:	2.8857E-04

The Freundlich/Langmuir parameters, C_T and β, were obtained by fitting the isotherm to ZAM data.

ZAM Inputs

C_{Cs+} = 1E-9 M

```
1, 303.15                                                          Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                             Title
7, 9                                                               Number of Cations & Anions
1265                                                               Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                         Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                  Names of Anions
6.0, 1E-9, 6.02E-15, 0, 0.006, 0, 0                                Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-9            Concentrations of Anions
1, 0.001                                                           Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 1E-8 M

```
1, 303.15                                                          Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                             Title
7, 9                                                               Number of Cations & Anions
1265                                                               Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                         Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                  Names of Anions
6.0, 1E-8, 6.02E-15, 0, 0.006, 0, 0                                Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-8            Concentrations of Anions
1, 0.001                                                           Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 1E-7 M

```
1, 303.15                                                          Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                             Title
7, 9                                                               Number of Cations & Anions
1265                                                               Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                         Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                  Names of Anions (Add COOH-, C2O4--)
6.0, 1E-7, 6.02E-15, 0, 0.006, 0, 0                                Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-7            Concentrations of Anions
1, 0.001                                                           Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 1E-6 M

```
1, 303.15                                                          Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                             Title
7, 9                                                               Number of Cations & Anions
1265                                                               Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                         Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                  Names of Anions
6.0, 1E-6, 6.02E-15, 0, 0.006, 0, 0                                Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-6            Concentrations of Anions
1, 0.001                                                           Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 1E-5 M

```
1, 303.15                                                          Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                             Title
7, 9                                                               Number of Cations & Anions
1265                                                               Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                         Names of Cations
```

```
13,  9, 27,  28, 15, 19, 20, 1, 2                         Names of Anions
6.0, 1E-5, 6.02E-15, 0, 0.006, 0, 0                       Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-5   Concentrations of Anions
1, 0.001                                                  Liquid (L), Solid (g)
0                                                         Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 5E-5 M

```
1, 303.15                                                 Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                    Title
7, 9                                                      Number of Cations & Anions
1265                                                      Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                         Names of Anions
6.0, 5E-5, 6.02E-15, 0, 0.006, 0, 0                       Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 5E-5   Concentrations of Anions
1, 0.001                                                  Liquid (L), Solid (g)
0                                                         Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 1E-4 M

```
1, 303.15                                                 Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                    Title
7, 9                                                      Number of Cations & Anions
1265                                                      Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                         Names of Anions
6.0, 1E-4, 6.02E-15, 0, 0.006, 0, 0                       Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-4   Concentrations of Anions
1, 0.001                                                  Liquid (L), Solid (g)
0                                                         Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 5E-4 M

```
1, 303.15                                                 Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                    Title
7, 9                                                      Number of Cations & Anions
1265                                                      Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                         Names of Anions
6.0, 5E-4, 6.02E-15, 0, 0.006, 0, 0                       Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 5E-4   Concentrations of Anions
1, 0.001                                                  Liquid (L), Solid (g)
0                                                         Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 1E-3 M

```
1, 303.15                                                 Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                    Title
7, 9                                                      Number of Cations & Anions
1265                                                      Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                         Names of Anions
6.0, 1E-3, 6.02E-15, 0, 0.006, 0, 0                       Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-3   Concentrations of Anions
1, 0.001                                                  Liquid (L), Solid (g)
0                                                         Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 2E-3 M

```
1, 303.15                                                       Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                          Title
7, 9                                                            Number of Cations & Anions
1265                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                      Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                               Names of Anions
6.0, 2E-3, 6.02E-15, 0, 0.006, 0, 0                             Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 2E-3         Concentrations of Anions
1, 0.001                                                        Liquid (L), Solid (g)
0                                                               Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 3E-3 M

```
1, 303.15                                                       Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                          Title
7, 9                                                            Number of Cations & Anions
1265                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                      Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                               Names of Anions
6.0, 3E-3, 6.02E-15, 0, 0.006, 0, 0                             Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 3E-3         Concentrations of Anions
1, 0.001                                                        Liquid (L), Solid (g)
0                                                               Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 5E-3 M

```
1, 303.15                                                       Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                          Title
7, 9                                                            Number of Cations & Anions
1265                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                      Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                               Names of Anions
6.0, 5E-3, 6.02E-15, 0, 0.006, 0, 0                             Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 5E-3         Concentrations of Anions
1, 0.001                                                        Liquid (L), Solid (g)
0                                                               Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 1E-2 M

```
1, 303.15                                                       Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                          Title
7, 9                                                            Number of Cations & Anions
1265                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                      Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                               Names of Anions
6.0, 1E-2, 6.02E-15, 0, 0.006, 0, 0                             Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-2         Concentrations of Anions
1, 0.001                                                        Liquid (L), Solid (g)
0                                                               Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 2E-2 M

```
1, 303.15                                                       Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                          Title
7, 9                                                            Number of Cations & Anions
1265                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                      Names of Cations
```

```
13,  9, 27,  28, 15, 19, 20, 1, 2                          Names of Anions
6.0, 2E-2, 6.02E-15, 0, 0.006, 0, 0                        Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 2E-2    Concentrations of Anions
1, 0.001                                                   Liquid (L), Solid (g)
0                                                          Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 5E-2 M

```
1, 303.15                                                  Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                     Title
7, 9                                                       Number of Cations & Anions
1265                                                       Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                 Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                          Names of Anions
6.0, 5E-2, 6.02E-15, 0, 0.006, 0, 0                        Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 5E-2    Concentrations of Anions
1, 0.001                                                   Liquid (L), Solid (g)
0                                                          Initial Solid Form (Na+ (0); H- (1))
1
```

C_{Cs+} = 1E-1 M

```
1, 303.15                                                  Activity Coeff. Model, Temperature
LCS Avg Isotherm @ 30C                                     Title
7, 9                                                       Number of Cations & Anions
1265                                                       Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                 Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                          Names of Anions
6.0, 1E-1, 6.02E-15, 0, 0.006, 0, 0                        Concentrations of Cations
1.66, 2.3, 0.71, 0.37, 0.1620, 0.12, 0.132, 0.006, 1E-1    Concentrations of Anions
1, 0.001                                                   Liquid (L), Solid (g)
0                                                          Initial Solid Form (Na+ (0); H- (1))
1
```

<u>ZAM Outputs</u>

C_{Cs+} = 1E-9 M

```
Solution:  LCS Avg Isotherm @ 30C
  **********************INPUT***********************

    Density=  .1265E+04 kg/m3

                  Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898          1.        .6000E+01
  Cs+.....        132.9054          1.        .1000E-08
  H+......          1.0079          1.        .6020E-14
  Rb+.....         85.4678          1.        .0000E+00
  K+......         39.0983          1.        .6000E-02
  SrOH+...        105.0000          1.        .0000E+00
  Sr++....         87.6200          2.        .0000E+00
  OH-.....         17.0073         -1.        .1660E+01
  NO3-....         62.0049         -1.        .2300E+01
  NO2-....         46.0000         -1.        .7100E+00
  Al(OH)4-         95.0000         -1.        .3700E+00
  SO4--...         96.0636         -2.        .1620E+00
  CO3--...         60.0092         -2.        .1200E+00
  PO4---..         94.9712         -3.        .1320E+00
  F-......         18.9984         -1.        .6000E-02
  Cl-.....         35.4527         -1.        .1000E-08

   Material: Na Form


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

   Ionic Strength=           .825E+01 mol/kg
   Equilibrium pH=          14.6

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs         .201E-05        .998E-06       .201E+04
  Rb         .000E+00        .000E+00       .000E+00
  SrOH       .000E+00        .000E+00       .000E+00
  K          .327E-01        .600E+01       .546E+01
```

C_{Cs+} = 1E-8 M

```
   Solution:  LCS Avg Isotherm @ 30C
  **********************INPUT***********************

    Density=  .1265E+04 kg/m3

                  Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898          1.        .6000E+01
  Cs+.....        132.9054          1.        .1000E-07
  H+......          1.0079          1.        .6020E-14
  Rb+.....         85.4678          1.        .0000E+00
  K+......         39.0983          1.        .6000E-02
  SrOH+...        105.0000          1.        .0000E+00
  Sr++....         87.6200          2.        .0000E+00
  OH-.....         17.0073         -1.        .1660E+01
  NO3-....         62.0049         -1.        .2300E+01
  NO2-....         46.0000         -1.        .7100E+00
  Al(OH)4-         95.0000         -1.        .3700E+00
  SO4--...         96.0636         -2.        .1620E+00
  CO3--...         60.0092         -2.        .1200E+00
  PO4---..         94.9712         -3.        .1320E+00
  F-......         18.9984         -1.        .6000E-02
  Cl-.....         35.4527         -1.        .1000E-07

   Material: Na Form


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

   Ionic Strength=           .825E+01 mol/kg
   Equilibrium pH=          14.6
```

```
        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .201E-04       .998E-05       .201E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .327E-01       .600E+01       .546E+01
```

C_{Cs+} = 1E-7 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.        .6000E+01
Cs+.....       132.9054          1.        .1000E-06
H+......         1.0079          1.        .6020E-14
Rb+.....        85.4678          1.        .0000E+00
K+......        39.0983          1.        .6000E-02
SrOH+...       105.0000          1.        .0000E+00
Sr++....        87.6200          2.        .0000E+00
OH-.....        17.0073         -1.        .1660E+01
NO3-....        62.0049         -1.        .2300E+01
NO2-....        46.0000         -1.        .7100E+00
Al(OH)4-        95.0000         -1.        .3700E+00
SO4--...        96.0636         -2.        .1620E+00
CO3--...        60.0092         -2.        .1200E+00
PO4---..        94.9712         -3.        .1320E+00
F-......        18.9984         -1.        .6000E-02
Cl-.....        35.4527         -1.        .1000E-06

 Material: Na Form


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

 Ionic Strength=           .825E+01 mol/kg
 Equilibrium pH=          14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .201E-03       .998E-04       .201E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .327E-01       .600E+01       .546E+01
```

C_{Cs+} = 1E-6 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.        .6000E+01
Cs+.....       132.9054          1.        .1000E-05
H+......         1.0079          1.        .6020E-14
Rb+.....        85.4678          1.        .0000E+00
K+......        39.0983          1.        .6000E-02
SrOH+...       105.0000          1.        .0000E+00
Sr++....        87.6200          2.        .0000E+00
OH-.....        17.0073         -1.        .1660E+01
NO3-....        62.0049         -1.        .2300E+01
NO2-....        46.0000         -1.        .7100E+00
Al(OH)4-        95.0000         -1.        .3700E+00
SO4--...        96.0636         -2.        .1620E+00
CO3--...        60.0092         -2.        .1200E+00
PO4---..        94.9712         -3.        .1320E+00
F-......        18.9984         -1.        .6000E-02
Cl-.....        35.4527         -1.        .1000E-05

 Material: Na Form


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

```
 Ionic Strength=           .825E+01 mol/kg
 Equilibrium pH=          14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .200E-02       .998E-03       .201E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .327E-01       .600E+01       .545E+01
```

C_{Cs+} = 1E-5 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT************************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.        .6000E+01
Cs+.....       132.9054          1.        .1000E-04
H+......         1.0079          1.        .6020E-14
Rb+.....        85.4678          1.        .0000E+00
K+......        39.0983          1.        .6000E-02
SrOH+...       105.0000          1.        .0000E+00
Sr++....        87.6200          2.        .0000E+00
OH-.....        17.0073         -1.        .1660E+01
NO3-....        62.0049         -1.        .2300E+01
NO2-....        46.0000         -1.        .7100E+00
Al(OH)4-        95.0000         -1.        .3700E+00
SO4--...        96.0636         -2.        .1620E+00
CO3--...        60.0092         -2.        .1200E+00
PO4---..        94.9712         -3.        .1320E+00
F-......        18.9984         -1.        .6000E-02
Cl-.....        35.4527         -1.        .1000E-04

 Material: Na Form



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

 Ionic Strength=           .825E+01 mol/kg
 Equilibrium pH=          14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .194E-01       .998E-02       .195E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .322E-01       .600E+01       .536E+01
```

C_{Cs+} = 5E-5 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT************************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.        .6000E+01
Cs+.....       132.9054          1.        .5000E-04
H+......         1.0079          1.        .6020E-14
Rb+.....        85.4678          1.        .0000E+00
K+......        39.0983          1.        .6000E-02
SrOH+...       105.0000          1.        .0000E+00
Sr++....        87.6200          2.        .0000E+00
OH-.....        17.0073         -1.        .1660E+01
NO3-....        62.0049         -1.        .2300E+01
NO2-....        46.0000         -1.        .7100E+00
Al(OH)4-        95.0000         -1.        .3700E+00
SO4--...        96.0636         -2.        .1620E+00
CO3--...        60.0092         -2.        .1200E+00
PO4---..        94.9712         -3.        .1320E+00
F-......        18.9984         -1.        .6000E-02
Cl-.....        35.4527         -1.        .5000E-04

 Material: Na Form
```

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

 Ionic Strength=           .825E+01 mol/kg
 Equilibrium pH=          14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .856E-01       .499E-01       .172E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .301E-01       .600E+01       .502E+01
```

C_{Cs+} = 1E-4 M

```
 Solution:  LCS Avg Isotherm @ 30C
**********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.        .6000E+01
Cs+.....       132.9054          1.        .1000E-03
H+......         1.0079          1.        .6020E-14
Rb+.....        85.4678          1.        .0000E+00
K+......        39.0983          1.        .6000E-02
SrOH+...       105.0000          1.        .0000E+00
Sr++....        87.6200          2.        .0000E+00
OH-.....        17.0073         -1.        .1660E+01
NO3-....        62.0049         -1.        .2300E+01
NO2-....        46.0000         -1.        .7100E+00
Al(OH)4-        95.0000         -1.        .3700E+00
SO4--...        96.0636         -2.        .1620E+00
CO3--...        60.0092         -2.        .1200E+00
PO4---..        94.9712         -3.        .1320E+00
F-......        18.9984         -1.        .6000E-02
Cl-.....        35.4527         -1.        .1000E-03

 Material: Na Form


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

 Ionic Strength=           .825E+01 mol/kg
 Equilibrium pH=          14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .149E+00       .999E-01       .149E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .282E-01       .600E+01       .470E+01
```

C_{Cs+} = 5E-4 M

```
 Solution:  LCS Avg Isotherm @ 30C
**********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.        .6000E+01
Cs+.....       132.9054          1.        .5000E-03
H+......         1.0079          1.        .6020E-14
Rb+.....        85.4678          1.        .0000E+00
K+......        39.0983          1.        .6000E-02
SrOH+...       105.0000          1.        .0000E+00
Sr++....        87.6200          2.        .0000E+00
OH-.....        17.0073         -1.        .1660E+01
NO3-....        62.0049         -1.        .2300E+01
NO2-....        46.0000         -1.        .7100E+00
Al(OH)4-        95.0000         -1.        .3700E+00
SO4--...        96.0636         -2.        .1620E+00
CO3--...        60.0092         -2.        .1200E+00
PO4---..        94.9712         -3.        .1320E+00
F-......        18.9984         -1.        .6000E-02
```

```
Cl-.....        35.4527        -1.       .5000E-03

 Material: Na Form



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

 Ionic Strength=           .825E+01 mol/kg
 Equilibrium pH=          14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .368E+00       .500E+00       .736E+03
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .216E-01       .600E+01       .359E+01
```

C_{Cs+} = 1E-3 M

```
 Solution:  LCS Avg Isotherm @ 30C
**********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .6000E+01
Cs+.....       132.9054          1.       .1000E-02
H+......         1.0079          1.       .6020E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .6000E-02
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1660E+01
NO3-....        62.0049         -1.       .2300E+01
NO2-....        46.0000         -1.       .7100E+00
Al(OH)4-        95.0000         -1.       .3700E+00
SO4--...        96.0636         -2.       .1620E+00
CO3--...        60.0092         -2.       .1200E+00
PO4---..        94.9712         -3.       .1320E+00
F-......        18.9984         -1.       .6000E-02
Cl-.....        35.4527         -1.       .1000E-02

 Material: Na Form



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

 Ionic Strength=           .825E+01 mol/kg
 Equilibrium pH=          14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .450E+00       .100E+01       .450E+03
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .191E-01       .600E+01       .318E+01
```

C_{Cs+} = 2E-3 M

```
 Solution:  LCS Avg Isotherm @ 30C
**********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .6000E+01
Cs+.....       132.9054          1.       .2000E-02
H+......         1.0079          1.       .6020E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .6000E-02
SrOH+...       105.0000          1.       .0000E+00
Sr++....        87.6200          2.       .0000E+00
OH-.....        17.0073         -1.       .1660E+01
NO3-....        62.0049         -1.       .2300E+01
NO2-....        46.0000         -1.       .7100E+00
Al(OH)4-        95.0000         -1.       .3700E+00
```

```
SO4--...        96.0636         -2.        .1620E+00
CO3--...        60.0092         -2.        .1200E+00
PO4---..        94.9712         -3.        .1320E+00
F-......        18.9984         -1.        .6000E-02
Cl-.....        35.4527         -1.        .2000E-02

 Material: Na Form


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

 Ionic Strength=           .825E+01 mol/kg
 Equilibrium pH=          14.6

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .507E+00       .200E+01       .254E+03
Rb        .000E+00       .000E+00       .000E+00
SrOH      .000E+00       .000E+00       .000E+00
K         .173E-01       .600E+01       .289E+01
```

C_{Cs+} = 3E-3 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.        .6000E+01
Cs+.....       132.9054          1.        .3000E-02
H+......         1.0079          1.        .6020E-14
Rb+.....        85.4678          1.        .0000E+00
K+......        39.0983          1.        .6000E-02
SrOH+...       105.0000          1.        .0000E+00
Sr++....        87.6200          2.        .0000E+00
OH-.....        17.0073         -1.        .1660E+01
NO3-....        62.0049         -1.        .2300E+01
NO2-....        46.0000         -1.        .7100E+00
Al(OH)4-        95.0000         -1.        .3700E+00
SO4--...        96.0636         -2.        .1620E+00
CO3--...        60.0092         -2.        .1200E+00
PO4---..        94.9712         -3.        .1320E+00
F-......        18.9984         -1.        .6000E-02
Cl-.....        35.4527         -1.        .3000E-02

 Material: Na Form


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

 Ionic Strength=           .826E+01 mol/kg
 Equilibrium pH=          14.6

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .529E+00       .300E+01       .176E+03
Rb        .000E+00       .000E+00       .000E+00
SrOH      .000E+00       .000E+00       .000E+00
K         .166E-01       .600E+01       .277E+01
```

C_{Cs+} = 5E-3 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.        .6000E+01
Cs+.....       132.9054          1.        .5000E-02
H+......         1.0079          1.        .6020E-14
Rb+.....        85.4678          1.        .0000E+00
```

```
K+......         39.0983          1.        .6000E-02
SrOH+...        105.0000          1.        .0000E+00
Sr++....         87.6200          2.        .0000E+00
OH-.....         17.0073         -1.        .1660E+01
NO3-....         62.0049         -1.        .2300E+01
NO2-....         46.0000         -1.        .7100E+00
Al(OH)4-         95.0000         -1.        .3700E+00
SO4--...         96.0636         -2.        .1620E+00
CO3--...         60.0092         -2.        .1200E+00
PO4---..         94.9712         -3.        .1320E+00
F-......         18.9984         -1.        .6000E-02
Cl-.....         35.4527         -1.        .5000E-02

 Material: Na Form


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

 Ionic Strength=           .826E+01 mol/kg
 Equilibrium pH=          14.6

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .548E+00       .500E+01       .110E+03
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .161E-01       .600E+01       .268E+01
```

C_{Cs+} = 1E-2 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT***********************

  Density=  .1265E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.        .6000E+01
Cs+.....        132.9054          1.        .1000E-01
H+......          1.0079          1.        .6020E-14
Rb+.....         85.4678          1.        .0000E+00
K+......         39.0983          1.        .6000E-02
SrOH+...        105.0000          1.        .0000E+00
Sr++....         87.6200          2.        .0000E+00
OH-.....         17.0073         -1.        .1660E+01
NO3-....         62.0049         -1.        .2300E+01
NO2-....         46.0000         -1.        .7100E+00
Al(OH)4-         95.0000         -1.        .3700E+00
SO4--...         96.0636         -2.        .1620E+00
CO3--...         60.0092         -2.        .1200E+00
PO4---..         94.9712         -3.        .1320E+00
F-......         18.9984         -1.        .6000E-02
Cl-.....         35.4527         -1.        .1000E-01

 Material: Na Form


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

 Ionic Strength=           .828E+01 mol/kg
 Equilibrium pH=          14.6

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .564E+00       .100E+02       .564E+02
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .156E-01       .600E+01       .260E+01
```

C_{Cs+} = 2E-2 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT***********************

  Density=  .1265E+04 kg/m3

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

```
Na+.....       22.9898        1.       .6000E+01
Cs+.....      132.9054        1.       .2000E-01
H+......        1.0079        1.       .6020E-14
Rb+.....       85.4678        1.       .0000E+00
K+......       39.0983        1.       .6000E-02
SrOH+...      105.0000        1.       .0000E+00
Sr++....       87.6200        2.       .0000E+00
OH-.....       17.0073       -1.       .1660E+01
NO3-....       62.0049       -1.       .2300E+01
NO2-....       46.0000       -1.       .7100E+00
Al(OH)4-       95.0000       -1.       .3700E+00
SO4--...       96.0636       -2.       .1620E+00
CO3--...       60.0092       -2.       .1200E+00
PO4---..       94.9712       -3.       .1320E+00
F-......       18.9984       -1.       .6000E-02
Cl-.....       35.4527       -1.       .2000E-01

 Material: Na Form


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

 Ionic Strength=          .830E+01 mol/kg
 Equilibrium pH=         14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .572E+00        .200E+02       .286E+02
Rb         .000E+00        .000E+00       .000E+00
SrOH       .000E+00        .000E+00       .000E+00
K          .153E-01        .600E+01       .255E+01
```

C_{Cs+} = 5E-2 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT***********************

  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....       22.9898        1.       .6000E+01
Cs+.....      132.9054        1.       .5000E-01
H+......        1.0079        1.       .6020E-14
Rb+.....       85.4678        1.       .0000E+00
K+......       39.0983        1.       .6000E-02
SrOH+...      105.0000        1.       .0000E+00
Sr++....       87.6200        2.       .0000E+00
OH-.....       17.0073       -1.       .1660E+01
NO3-....       62.0049       -1.       .2300E+01
NO2-....       46.0000       -1.       .7100E+00
Al(OH)4-       95.0000       -1.       .3700E+00
SO4--...       96.0636       -2.       .1620E+00
CO3--...       60.0092       -2.       .1200E+00
PO4---..       94.9712       -3.       .1320E+00
F-......       18.9984       -1.       .6000E-02
Cl-.....       35.4527       -1.       .5000E-01

 Material: Na Form


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

 Ionic Strength=          .839E+01 mol/kg
 Equilibrium pH=         14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .577E+00        .500E+02       .115E+02
Rb         .000E+00        .000E+00       .000E+00
SrOH       .000E+00        .000E+00       .000E+00
K          .151E-01        .600E+01       .251E+01
```

C_{Cs+} = 1E-1 M

```
 Solution:  LCS Avg Isotherm @ 30C
***********************INPUT***********************
```

```
  Density=  .1265E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .6000E+01
Cs+.....        132.9054          1.       .1000E+00
H+......          1.0079          1.       .6020E-14
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .6000E-02
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1660E+01
NO3-....         62.0049         -1.       .2300E+01
NO2-....         46.0000         -1.       .7100E+00
Al(OH)4-         95.0000         -1.       .3700E+00
SO4--...         96.0636         -2.       .1620E+00
CO3--...         60.0092         -2.       .1200E+00
PO4---..         94.9712         -3.       .1320E+00
F-......         18.9984         -1.       .6000E-02
Cl-.....         35.4527         -1.       .1000E+00

 Material: Na Form


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

 Ionic Strength=           .854E+01 mol/kg
 Equilibrium pH=          14.6

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .578E+00       .100E+03       .578E+01
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .149E-01       .600E+01       .248E+01
```

Appendix C. ZAM Validation using Tank 30 and Tank 33 Test Data

The ZAM model was validated using data from Walker's cesium loading tests (Walker, 1999). This Appendix provides the ZAM input and output for each test condition.

Tank 30 Bottle #5 Test

ZAM Input

```
1, 298.15                                                           Activity Coeff. Model, Temperature
Tank 30H Bottle # 5                                                 Title
7, 9                                                                Number of Cations & Anions
1242                                                                Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                          Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                   Names of Anions
5.6, 0.000358472, 3.89e-15, 0, 2.80E-02, 0, 0                       Concentrations of Cations
2.5697, 1.4900, 0.57, 0.36, 0.022, 0.29, 0.0049, 0, 0               Concentrations of Anions
0.01, 0.0861                                                        Liquid (L), Solid (g)
0                                                                   Initial Solid Form (Na+ (0); H- (1))
0.7                                                                 Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 30H Bottle # 5
  **********************INPUT***********************

    Density=  .1242E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .5600E+01
  Cs+.....        132.9054         1.        .3585E-03
  H+......          1.0079         1.        .3890E-14
  Rb+.....         85.4678         1.        .0000E+00
  K+......         39.0983         1.        .2800E-01
  SrOH+...        105.0000         1.        .0000E+00
  Sr++....         87.6200         2.        .0000E+00
  OH-.....         17.0073        -1.        .2570E+01
  NO3-....         62.0049        -1.        .1490E+01
  NO2-....         46.0000        -1.        .5700E+00
  Al(OH)4-         95.0000        -1.        .3600E+00
  SO4--...         96.0636        -2.        .2200E-01
  CO3--...         60.0092        -2.        .2900E+00
  PO4---..         94.9712        -3.        .4900E-02
  F-......         18.9984        -1.        .0000E+00
  Cl-.....         35.4527        -1.        .0000E+00

   Material: Na Form



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

   Ionic Strength=           .687E+01 mol/kg
   Equilibrium pH=          14.8

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs         .398E-01       .157E-01       .254E+04
  Rb         .000E+00       .000E+00       .000E+00
  SrOH       .000E+00       .000E+00       .000E+00
  K          .188E+00       .264E+02       .711E+01
```

Tank 30 Bottle #17 Test

ZAM Input

```
1, 298.15                                                           Activity Coeff. Model, Temperature
Tank 30H Bottle # 17                                                Title
7, 9                                                                Number of Cations & Anions
1242                                                                Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                          Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                   Names of Anions
```

```
5.6, 0.001318597, 3.89e-15, 0, 2.80E-02, 0, 0                      Concentrations of Cations
2.5697, 1.4909, 0.57, 0.36, 0.022, 0.29, 0.0049, 0, 0              Concentrations of Anions
0.01, 0.0856                                                        Liquid (L), Solid (g)
0                                                                   Initial Solid Form (Na+ (0); H- (1))
0.7                                                                 Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 30H Bottle # 17
  ***********************INPUT************************

    Density=  .1242E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....        22.9898          1.        .5600E+01
  Cs+.....       132.9054          1.        .1319E-02
  H+......         1.0079          1.        .3890E-14
  Rb+.....        85.4678          1.        .0000E+00
  K+......        39.0983          1.        .2800E-01
  SrOH+...       105.0000          1.        .0000E+00
  Sr++....        87.6200          2.        .0000E+00
  OH-.....        17.0073         -1.        .2570E+01
  NO3-....        62.0049         -1.        .1491E+01
  NO2-....        46.0000         -1.        .5700E+00
  Al(OH)4-        95.0000         -1.        .3600E+00
  SO4--...        96.0636         -2.        .2200E-01
  CO3--...        60.0092         -2.        .2900E+00
  PO4---..        94.9712         -3.        .4900E-02
  F-......        18.9984         -1.        .0000E+00
  Cl-.....        35.4527         -1.        .0000E+00

   Material: Na Form



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

   Ionic Strength=           .687E+01 mol/kg
   Equilibrium pH=          14.8

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .146E+00       .714E-01       .204E+04
  Rb        .000E+00       .000E+00       .000E+00
  SrOH      .000E+00       .000E+00       .000E+00
  K         .171E+00       .265E+02       .644E+01
```

Tank 30 Bottle #19 Test

ZAM Input

```
1, 298.15                                                           Activity Coeff. Model, Temperature
Tank 30H Bottle # 19                                                Title
7, 9                                                                Number of Cations & Anions
1242                                                                Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                          Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                   Names of Anions
5.6, 0.002599706, 3.89e-15, 0, 0.028, 0, 0                          Concentrations of Cations
2.5697, 1.4922, 0.57, 0.36, 0.022, 0.29, 0.0049, 0, 0              Concentrations of Anions
0.01, 0.0859                                                        Liquid (L), Solid (g)
0                                                                   Initial Solid Form (Na+ (0); H- (1))
0.7                                                                 Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 30H Bottle # 19
  ***********************INPUT************************

    Density=  .1242E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....        22.9898          1.        .5600E+01
  Cs+.....       132.9054          1.        .2600E-02
  H+......         1.0079          1.        .3890E-14
  Rb+.....        85.4678          1.        .0000E+00
```

```
 K+......         39.0983          1.       .2800E-01
 SrOH+...        105.0000          1.       .0000E+00
 Sr++....         87.6200          2.       .0000E+00
 OH-.....         17.0073         -1.       .2570E+01
 NO3-....         62.0049         -1.       .1492E+01
 NO2-....         46.0000         -1.       .5700E+00
 Al(OH)4-         95.0000         -1.       .3600E+00
 SO4--...         96.0636         -2.       .2200E-01
 CO3--...         60.0092         -2.       .2900E+00
 PO4---..         94.9712         -3.       .4900E-02
 F-......         18.9984         -1.       .0000E+00
 Cl-.....         35.4527         -1.       .0000E+00

  Material: Na Form


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

  Ionic Strength=           .687E+01 mol/kg
  Equilibrium pH=          14.8

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs        .280E+00       .198E+00       .141E+04
 Rb        .000E+00       .000E+00       .000E+00
 SrOH      .000E+00       .000E+00       .000E+00
 K         .150E+00       .267E+02       .561E+01
```

Tank 30 Bottle #23 Test

ZAM Input

1, 298.15	Activity Coeff. Model, Temperature
Tank 30H Bottle # 23	Title
7, 9	Number of Cations & Anions
1242	Density(kg/m3)
3, 6, 1, 5, 4, 40, 13	Names of Cations
13, 9, 27, 28, 15, 19, 20, 1, 2	Names of Anions
5.6, 0.000358472, 3.89e-15, 0, 2.80E-02, 0, 0	Concentrations of Cations
2.5697, 1.4900, 0.57, 0.36, 0.022, 0.29, 0.0049, 0, 0	Concentrations of Anions
0.01, 0.4293	Liquid (L), Solid (g)
0	Initial Solid Form (Na+ (0); H- (1))
0.7	Calculation Adjustment

ZAM Output

```
  Solution:  Tank 30H Bottle # 23
 ***********************INPUT************************

   Density=  .1242E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898          1.       .5600E+01
 Cs+.....        132.9054          1.       .3585E-03
 H+......          1.0079          1.       .3890E-14
 Rb+.....         85.4678          1.       .0000E+00
 K+......         39.0983          1.       .2800E-01
 SrOH+...        105.0000          1.       .0000E+00
 Sr++....         87.6200          2.       .0000E+00
 OH-.....         17.0073         -1.       .2570E+01
 NO3-....         62.0049         -1.       .1490E+01
 NO2-....         46.0000         -1.       .5700E+00
 Al(OH)4-         95.0000         -1.       .3600E+00
 SO4--...         96.0636         -2.       .2200E-01
 CO3--...         60.0092         -2.       .2900E+00
 PO4---..         94.9712         -3.       .4900E-02
 F-......         18.9984         -1.       .0000E+00
 Cl-.....         35.4527         -1.       .0000E+00

  Material: Na Form


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

  Ionic Strength=           .686E+01 mol/kg
```

```
  Equilibrium pH=          14.8

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs         .828E-02       .297E-02       .278E+04
 Rb         .000E+00       .000E+00       .000E+00
 SrOH       .000E+00       .000E+00       .000E+00
 K          .161E+00       .211E+02       .761E+01
```

Tank 30 Bottle #25 Test

ZAM Input

```
1, 298.15                                                             Activity Coeff. Model, Temperature
Tank 30H Bottle # 25                                                  Title
7, 9                                                                  Number of Cations & Anions
1242                                                                  Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                            Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                     Names of Anions
5.6, 2.78729E-05, 3.89e-15, 0, 2.80E-02, 0, 0                         Concentrations of Cations
2.5697, 1.4896, 0.57, 0.36, 0.022, 0.29, 0.0049, 0, 0                 Concentrations of Anions
0.01, 0.4285                                                          Liquid (L), Solid (g)
0                                                                     Initial Solid Form (Na+ (0); H- (1))
0.7                                                                   Calculation Adjustment
```

ZAM Output

```
  Solution:  Tank 30H Bottle # 25
 ***********************INPUT************************

   Density=  .1242E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....        22.9898         1.       .5600E+01
 Cs+.....       132.9054         1.       .2787E-04
 H+......         1.0079         1.       .3890E-14
 Rb+.....        85.4678         1.       .0000E+00
 K+......        39.0983         1.       .2800E-01
 SrOH+...       105.0000         1.       .0000E+00
 Sr++....        87.6200         2.       .0000E+00
 OH-.....        17.0073        -1.       .2570E+01
 NO3-....        62.0049        -1.       .1490E+01
 NO2-....        46.0000        -1.       .5700E+00
 Al(OH)4-        95.0000        -1.       .3600E+00
 SO4--...        96.0636        -2.       .2200E-01
 CO3--...        60.0092        -2.       .2900E+00
 PO4---..        94.9712        -3.       .4900E-02
 F-......        18.9984        -1.       .0000E+00
 Cl-.....        35.4527        -1.       .0000E+00

  Material: Na Form


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

  Ionic Strength=           .686E+01 mol/kg
  Equilibrium pH=          14.8

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs         .645E-03       .229E-03       .282E+04
 Rb         .000E+00       .000E+00       .000E+00
 SrOH       .000E+00       .000E+00       .000E+00
 K          .161E+00       .211E+02       .766E+01
```

Tank 33 Bottle #5 Test

ZAM Input

```
1, 298.15                                                             Activity Coeff. Model, Temperature
Tank 33 Bottle # 5                                                    Title
7, 9                                                                  Number of Cations & Anions
1145                                                                  Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                            Names of Cations
```

```
13,  9, 27,  28, 15, 19, 20, 1, 2                                     Names of Anions
3.58, 5.11151E-05, 6.62E-15, 0, 0.0034, 0, 0                          Concentrations of Cations
1.51005, 1.3101, 0, 0.024, 0.035, 0.332, 0.0018, 0, 0                 Concentrations of Anions
0.011, 0.0857                                                         Liquid (L), Solid (g)
0                                                                     Initial Solid Form (Na+ (0); H- (1))
0.7                                                                   Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 33 Bottle # 5
  **********************INPUT***********************

    Density=  .1145E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .3580E+01
  Cs+.....        132.9054         1.        .5112E-04
  H+......          1.0079         1.        .6620E-14
  Rb+.....         85.4678         1.        .0000E+00
  K+......         39.0983         1.        .3400E-02
  SrOH+...        105.0000         1.        .0000E+00
  Sr++....         87.6200         2.        .0000E+00
  OH-.....         17.0073        -1.        .1510E+01
  NO3-....         62.0049        -1.        .1310E+01
  NO2-....         46.0000        -1.        .0000E+00
  Al(OH)4-         95.0000        -1.        .2400E-01
  SO4--...         96.0636        -2.        .3500E-01
  CO3--...         60.0092        -2.        .3320E+00
  PO4---..         94.9712        -3.        .1800E-02
  F-......         18.9984        -1.        .0000E+00
  Cl-.....         35.4527        -1.        .0000E+00

   Material: Na Form



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

   Ionic Strength=           .448E+01 mol/kg
   Equilibrium pH=          14.3

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs         .641E-02       .118E-02       .544E+04
  Rb         .000E+00       .000E+00       .000E+00
  SrOH       .000E+00       .000E+00       .000E+00
  K          .436E-01       .306E+01       .143E+02
```

Tank 33 Bottle #17 Test

ZAM Input

```
1, 298.15                                                             Activity Coeff. Model, Temperature
Tank 33 Bottle # 17                                                   Title
7, 9                                                                  Number of Cations & Anions
1145                                                                  Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                            Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                     Names of Anions
3.58, 9.40969E-04, 6.62E-15, 0, 0.0034, 0, 0                          Concentrations of Cations
1.51005, 1.3109, 0, 0.024, 0.035, 0.332, 0.0018, 0, 0                 Concentrations of Anions
0.011, 0.0857                                                         Liquid (L), Solid (g)
0                                                                     Initial Solid Form (Na+ (0); H- (1))
0.7                                                                   Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 33 Bottle # 17
  **********************INPUT***********************

    Density=  .1145E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .3580E+01
  Cs+.....        132.9054         1.        .9410E-03
  H+......          1.0079         1.        .6620E-14
```

```
Rb+.....        85.4678         1.       .0000E+00
K+......        39.0983         1.       .3400E-02
SrOH+...       105.0000         1.       .0000E+00
Sr++....        87.6200         2.       .0000E+00
OH-.....        17.0073        -1.       .1510E+01
NO3-....        62.0049        -1.       .1311E+01
NO2-....        46.0000        -1.       .0000E+00
Al(OH)4-        95.0000        -1.       .2400E-01
SO4--...        96.0636        -2.       .3500E-01
CO3--...        60.0092        -2.       .3320E+00
PO4---..        94.9712        -3.       .1800E-02
F-......        18.9984        -1.       .0000E+00
Cl-.....        35.4527        -1.       .0000E+00

 Material: Na Form


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

 Ionic Strength=           .448E+01 mol/kg
 Equilibrium pH=          14.3

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .117E+00       .267E-01       .439E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .394E-01       .309E+01       .127E+02
```

Tank 33 Bottle #19 Test

ZAM Input

```
1, 298.15                                           Activity Coeff. Model, Temperature
Tank 33 Bottle # 19                                 Title
7, 9                                                Number of Cations & Anions
1145                                                Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                          Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                   Names of Anions
3.58, 2.12173E-03, 6.62E-15, 0, 0.0034, 0, 0        Concentrations of Cations
1.51005, 1.3121, 0, 0.024, 0.035, 0.332, 0.0018, 0, 0   Concentrations of Anions
0.011, 0.0859                                       Liquid (L), Solid (g)
0                                                   Initial Solid Form (Na+ (0); H- (1))
0.7                                                 Calculation Adjustment
```

ZAM Output

```
 Solution:  Tank 33 Bottle # 19
***********************INPUT************************

  Density=  .1145E+04 kg/m3

            Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898         1.       .3580E+01
Cs+.....       132.9054         1.       .2122E-02
H+......         1.0079         1.       .6620E-14
Rb+.....        85.4678         1.       .0000E+00
K+......        39.0983         1.       .3400E-02
SrOH+...       105.0000         1.       .0000E+00
Sr++....        87.6200         2.       .0000E+00
OH-.....        17.0073        -1.       .1510E+01
NO3-....        62.0049        -1.       .1312E+01
NO2-....        46.0000        -1.       .0000E+00
Al(OH)4-        95.0000        -1.       .2400E-01
SO4--...        96.0636        -2.       .3500E-01
CO3--...        60.0092        -2.       .3320E+00
PO4---..        94.9712        -3.       .1800E-02
F-......        18.9984        -1.       .0000E+00
Cl-.....        35.4527        -1.       .0000E+00

 Material: Na Form


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

```
 Ionic Strength=           .449E+01 mol/kg
 Equilibrium pH=          14.3

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .261E+00       .862E-01       .302E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .338E-01       .314E+01       .108E+02
```

Tank 33 Bottle #23 Test

ZAM Input

```
1, 298.15                                                        Activity Coeff. Model, Temperature
Tank 33 Bottle # 23                                              Title
7, 9                                                             Number of Cations & Anions
1145                                                             Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                       Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                Names of Anions
3.58, 5.11151E-05, 6.62E-15, 0, 0.0034, 0, 0                     Concentrations of Cations
1.51005, 1.3101, 0, 0.024, 0.035, 0.332, 0.0018, 0, 0            Concentrations of Anions
0.011, 0.4283                                                    Liquid (L), Solid (g)
0                                                                Initial Solid Form (Na+ (0); H- (1))
0.7                                                              Calculation Adjustment
```

ZAM Output

```
 Solution:  Tank 33 Bottle # 23
***********************INPUT************************

  Density=  .1145E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898         1.        .3580E+01
Cs+.....       132.9054         1.        .5112E-04
H+......         1.0079         1.        .6620E-14
Rb+.....        85.4678         1.        .0000E+00
K+......        39.0983         1.        .3400E-02
SrOH+...       105.0000         1.        .0000E+00
Sr++....        87.6200         2.        .0000E+00
OH-.....        17.0073        -1.        .1510E+01
NO3-....        62.0049        -1.        .1310E+01
NO2-....        46.0000        -1.        .0000E+00
Al(OH)4-        95.0000        -1.        .2400E-01
SO4--...        96.0636        -2.        .3500E-01
CO3--...        60.0092        -2.        .3320E+00
PO4---..        94.9712        -3.        .1800E-02
F-......        18.9984        -1.        .0000E+00
Cl-.....        35.4527        -1.        .0000E+00

 Material: Na Form



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

 Ionic Strength=           .447E+01 mol/kg
 Equilibrium pH=          14.3

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .131E-02       .235E-03       .557E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .316E-01       .217E+01       .145E+02
```

Tank 33 Bottle #25 Test

ZAM Input

```
1, 298.15                                                        Activity Coeff. Model, Temperature
Tank 33 Bottle # 25                                              Title
7, 9                                                             Number of Cations & Anions
1145                                                             Density(kg/m3)
```

```
 3,  6,  1,  5,  4, 40, 13                                       Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                Names of Anions
3.58, 2.64596E-06, 6.62E-15, 0, 0.0034, 0, 0                     Concentrations of Cations
1.51005, 1.3100, 0, 0.024, 0.035, 0.332, 0.0018, 0, 0            Concentrations of Anions
0.011, 0.4296                                                    Liquid (L), Solid (g)
0                                                                Initial Solid Form (Na+ (0); H- (1))
0.7                                                              Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 33 Bottle # 25
  ***********************INPUT************************

    Density=  .1145E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .3580E+01
  Cs+.....        132.9054         1.        .2646E-05
  H+......          1.0079         1.        .6620E-14
  Rb+.....         85.4678         1.        .0000E+00
  K+......         39.0983         1.        .3400E-02
  SrOH+...        105.0000         1.        .0000E+00
  Sr++....         87.6200         2.        .0000E+00
  OH-.....         17.0073        -1.        .1510E+01
  NO3-....         62.0049        -1.        .1310E+01
  NO2-....         46.0000        -1.        .0000E+00
  Al(OH)4-         95.0000        -1.        .2400E-01
  SO4--...         96.0636        -2.        .3500E-01
  CO3--...         60.0092        -2.        .3320E+00
  PO4---..         94.9712        -3.        .1800E-02
  F-......         18.9984        -1.        .0000E+00
  Cl-.....         35.4527        -1.        .0000E+00

   Material: Na Form



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

   Ionic Strength=           .447E+01 mol/kg
   Equilibrium pH=          14.3

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs         .674E-04       .121E-04       .558E+04
  Rb         .000E+00       .000E+00       .000E+00
  SrOH       .000E+00       .000E+00       .000E+00
  K          .316E-01       .217E+01       .146E+02
```

Appendix D. ZAM Calculations

1) Dilution of Saltcake Samples

- 3 M Na^+ Dilution

ZAM Input

```
1, 298.15                                                          Activity Coeff. Model, Temperature
Tank 10 Na+ 3M                                                     Title
7, 11                                                              Number of Cations & Anions
1143                                                               Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                         Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                          Names of Anions (Add COOH-, C2O4--)
45.022                                                             Molar mass (COOH-)
88.01946                                                           Molar mass (C2O4--)
3.0002, 3.39044E-05, 2.41E-14, 0, 5.20151E-03, 0, 0                Concentrations of Cations
0.4155, 1.4816, 0.2081, 0.0242, 0.0393, 0.3128, 0.0090, 0.0029, 0.0284, 0.1135, 7.01263E-05    Concentrations of Anions
1, 0.0008                                                          Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
0.01                                                               Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Na+ 3M
 **********************INPUT***********************

    Density=  .1143E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898          1.        .3000E+01
 Cs+.....        132.9054          1.        .3390E-04
 H+......          1.0079          1.        .2410E-13
 Rb+.....         85.4678          1.        .0000E+00
 K+......         39.0983          1.        .5202E-02
 SrOH+...        105.0000          1.        .0000E+00
 Sr++....         87.6200          2.        .0000E+00
 OH-.....         17.0073         -1.        .4155E+00
 NO3-....         62.0049         -1.        .1482E+01
 NO2-....         46.0000         -1.        .2081E+00
 Al(OH)4-         95.0000         -1.        .2420E-01
 SO4--...         96.0636         -2.        .3930E-01
 CO3--...         60.0092         -2.        .3128E+00
 PO4---..         94.9712         -3.        .9000E-02
 F-......         18.9984         -1.        .2900E-02
 Cl-.....         35.4527         -1.        .2840E-01
 Other-..         45.0220         -1.        .1135E+00
 Other--.         88.0195         -2.        .7013E-04

  Material: Na Form


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

  Ionic Strength=           .385E+01 mol/kg
  Equilibrium pH=          13.9

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs         .145E+00       .338E-01       .429E+04
 Rb         .000E+00       .000E+00       .000E+00
 SrOH       .000E+00       .000E+00       .000E+00
 K          .629E-01       .520E+01       .121E+02
```

- 4 M Na^+ Dilution

ZAM Input

```
1, 298.15                                                          Activity Coeff. Model, Temperature
Tank 10 Na+ 4M                                                     Title
```

```
7, 11                                                                     Number of Cations & Anions
1187                                                                      Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                                Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                                 Names of Anions (Add COOH-, C2O4--)
45.022                                                                    Molar mass (COOH-)
88.01946                                                                  Molar mass (C2O4--)
4.0, 4.52037E-05, 1.81E-14, 0, 6.93501E-03, 0, 0                          Concentrations of Cations
0.5540, 1.9754, 0.2774, 0.0323, 0.0524, 0.4170, 0.0120, 0.0039, 0.0378, 0.1513, 9.34972E-05   Concentrations of Anions
1, 0.0008                                                                 Liquid (L), Solid (g)
0                                                                         Initial Solid Form (Na+ (0); H- (1))
0.01                                                                      Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Na+ 4M
  ***********************INPUT************************

    Density=  .1187E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .4000E+01
  Cs+.....        132.9054         1.        .4520E-04
  H+......          1.0079         1.        .1810E-13
  Rb+.....         85.4678         1.        .0000E+00
  K+......         39.0983         1.        .6935E-02
  SrOH+...        105.0000         1.        .0000E+00
  Sr++....         87.6200         2.        .0000E+00
  OH-.....         17.0073        -1.        .5540E+00
  NO3-....         62.0049        -1.        .1975E+01
  NO2-....         46.0000        -1.        .2774E+00
  Al(OH)4-         95.0000        -1.        .3230E-01
  SO4--...         96.0636        -2.        .5240E-01
  CO3--...         60.0092        -2.        .4170E+00
  PO4---..         94.9712        -3.        .1200E-01
  F-......         18.9984        -1.        .3900E-02
  Cl-.....         35.4527        -1.        .3780E-01
  Other-..         45.0220        -1.        .1513E+00
  Other--.         88.0195        -2.        .9350E-04

   Material: Na Form



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

   Ionic Strength=           .529E+01 mol/kg
   Equilibrium pH=          14.1

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .133E+00       .451E-01       .294E+04
  Rb        .000E+00       .000E+00       .000E+00
  SrOH      .000E+00       .000E+00       .000E+00
  K         .592E-01       .693E+01       .854E+01
```

- 5 M Na^+ Dilution

ZAM Input

```
1, 298.15                                                                 Activity Coeff. Model, Temperature
Tank 10 Na+ 5M                                                            Title
7, 11                                                                     Number of Cations & Anions
1232                                                                      Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                                Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                                 Names of Anions (Add COOH-, C2O4--)
45.022                                                                    Molar mass (COOH-)
88.01946                                                                  Molar mass (C2O4--)
5.0, 5.65057E-05, 1.44E-14, 0, 8.66894E-03, 0, 0                          Concentrations of Cations
0.6925, 2.4693, 0.3468, 0.0404, 0.0655, 0.5212, 0.0150, 0.0048, 0.0473, 0.1891, 1.16874E-04   Concentrations of Anions
1, 0.001                                                                  Liquid (L), Solid (g)
0                                                                         Initial Solid Form (Na+ (0); H- (1))
0.01                                                                      Calculation Adjustment
```

ZAM Output

```
 Solution:  Tank 10 Na+ 5M
**********************INPUT************************

   Density=  .1232E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898         1.        .5000E+01
 Cs+.....        132.9054         1.        .5651E-04
 H+......          1.0079         1.        .1440E-13
 Rb+.....         85.4678         1.        .0000E+00
 K+......         39.0983         1.        .8669E-02
 SrOH+...        105.0000         1.        .0000E+00
 Sr++....         87.6200         2.        .0000E+00
 OH-.....         17.0073        -1.        .6925E+00
 NO3-....         62.0049        -1.        .2469E+01
 NO2-....         46.0000        -1.        .3468E+00
 Al(OH)4-         95.0000        -1.        .4040E-01
 SO4--...         96.0636        -2.        .6550E-01
 CO3--...         60.0092        -2.        .5212E+00
 PO4---..         94.9712        -3.        .1500E-01
 F-......         18.9984        -1.        .4800E-02
 Cl-.....         35.4527        -1.        .4730E-01
 Other-..         45.0220        -1.        .1891E+00
 Other--.         88.0195        -2.        .1169E-03

  Material: Na Form


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

  Ionic Strength=           .682E+01 mol/kg
  Equilibrium pH=          14.3

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs         .120E+00       .564E-01       .214E+04
 Rb         .000E+00       .000E+00       .000E+00
 SrOH       .000E+00       .000E+00       .000E+00
 K          .554E-01       .867E+01       .639E+01
```

- 6 M Na^+ Dilution

ZAM Input

```
1, 298.15                                                            Activity Coeff. Model, Temperature
Tank 10 Na+ 6M                                                       Title
7, 11                                                                Number of Cations & Anions
1276                                                                 Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                           Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                            Names of Anions (Add COOH-, C2O4--)
45.022                                                               Molar mass (COOH-)
88.01946                                                             Molar mass (C2O4--)
6.0, 6.781E-05, 1.20E-14, 0, 1.04030E-02, 0, 0                       Concentrations of Cations
0.8310, 2.9632, 0.4161, 0.0485, 0.0786, 0.6255, 0.0180, 0.0058, 0.0567, 0.2270, 1.40252E-04    Concentrations of Anions
1, 0.001                                                             Liquid (L), Solid (g)
0                                                                    Initial Solid Form (Na+ (0); H- (1))
0.01                                                                 Calculation Adjustment
```

ZAM Output

```
 Solution:  Tank 10 Na+ 6M
**********************INPUT************************

   Density=  .1276E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898         1.        .6000E+01
 Cs+.....        132.9054         1.        .6781E-04
 H+......          1.0079         1.        .1200E-13
 Rb+.....         85.4678         1.        .0000E+00
 K+......         39.0983         1.        .1040E-01
 SrOH+...        105.0000         1.        .0000E+00
 Sr++....         87.6200         2.        .0000E+00
 OH-.....         17.0073        -1.        .8310E+00
 NO3-....         62.0049        -1.        .2963E+01
 NO2-....         46.0000        -1.        .4161E+00
```

```
Al(OH)4-         95.0000         -1.       .4850E-01
SO4--...         96.0636         -2.       .7860E-01
CO3--...         60.0092         -2.       .6255E+00
PO4---..         94.9712         -3.       .1800E-01
F-......         18.9984         -1.       .5800E-02
Cl-.....         35.4527         -1.       .5670E-01
Other-..         45.0220         -1.       .2270E+00
Other--.         88.0195         -2.       .1403E-03

 Material: Na Form


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

 Ionic Strength=           .846E+01 mol/kg
 Equilibrium pH=          14.6

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .108E+00       .677E-01       .160E+04
Rb        .000E+00       .000E+00       .000E+00
SrOH      .000E+00       .000E+00       .000E+00
K         .516E-01       .104E+02       .496E+01
```

- 7 M Na^+ Dilution

ZAM Input

```
1, 298.15                                                                       Activity Coeff. Model, Temperature
Tank 10 Na+ 7M                                                                  Title
7, 11                                                                           Number of Cations & Anions
1321                                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                                      Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                                       Names of Anions (Add COOH-, C2O4--)
45.022                                                                          Molar mass (COOH-)
88.01946                                                                        Molar mass (C2O4--)
7.0, 7.91053E-05, 1.03E-14, 0, 1.21361E-02, 0, 0                                Concentrations of Cations
0.9695, 3.4569, 0.4854, 0.0566, 0.0917, 0.7297, 0.0210, 0.0068, 0.0662, 0.2648, 1.63618E-04       Concentrations of Anions
1, 0.0001                                                                       Liquid (L), Solid (g)
0                                                                               Initial Solid Form (Na+ (0); H- (1))
0.01                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Tank 10 Na+ 7M
***********************INPUT************************

  Density=  .1321E+04 kg/m3

            Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .7000E+01
Cs+.....        132.9054          1.       .7911E-04
H+......          1.0079          1.       .1030E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .1214E-01
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .9695E+00
NO3-....         62.0049         -1.       .3457E+01
NO2-....         46.0000         -1.       .4854E+00
Al(OH)4-         95.0000         -1.       .5660E-01
SO4--...         96.0636         -2.       .9170E-01
CO3--...         60.0092         -2.       .7297E+00
PO4---..         94.9712         -3.       .2100E-01
F-......         18.9984         -1.       .6800E-02
Cl-.....         35.4527         -1.       .6620E-01
Other-..         45.0220         -1.       .2648E+00
Other--.         88.0195         -2.       .1636E-03

 Material: Na Form


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

```
 Ionic Strength=           .102E+02 mol/kg
 Equilibrium pH=          14.8

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .964E-01       .791E-01       .122E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .477E-01       .121E+02       .393E+01
```

- 7.5 M Na^+ Dilution

ZAM Input

```
1, 298.15                                                       Activity Coeff. Model, Temperature
Tank 10 Na+ 7.5M                                                Title
7, 11                                                           Number of Cations & Anions
1343                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                      Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                       Names of Anions (Add COOH-, C2O4--)
45.022                                                          Molar mass (COOH-)
88.01946                                                        Molar mass (C2O4--)
7.5, 8.47572E-05, 9.63E-15, 0, 1.30032E-02, 0, 0                Concentrations of Cations
1.0387, 3.7039, 0.5201, 0.0606, 0.0982, 0.7819, 0.0225, 0.0073, 0.0709, 0.2837, 1.75308E-04    Concentrations of Anions
1, 0.0001                                                       Liquid (L), Solid (g)
0                                                               Initial Solid Form (Na+ (0); H- (1))
0.01                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Tank 10 Na+ 7.5M
***********************INPUT************************

  Density=  .1343E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898         1.       .7500E+01
Cs+.....        132.9054         1.       .8476E-04
H+......          1.0079         1.       .9630E-14
Rb+.....         85.4678         1.       .0000E+00
K+......         39.0983         1.       .1300E-01
SrOH+...        105.0000         1.       .0000E+00
Sr++....         87.6200         2.       .0000E+00
OH-.....         17.0073        -1.       .1039E+01
NO3-....         62.0049        -1.       .3704E+01
NO2-....         46.0000        -1.       .5201E+00
Al(OH)4-         95.0000        -1.       .6060E-01
SO4--...         96.0636        -2.       .9820E-01
CO3--...         60.0092        -2.       .7819E+00
PO4---..         94.9712        -3.       .2250E-01
F-......         18.9984        -1.       .7300E-02
Cl-.....         35.4527        -1.       .7090E-01
Other-..         45.0220        -1.       .2837E+00
Other--.         88.0195        -2.       .1753E-03

 Material: Na Form


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

 Ionic Strength=           .111E+02 mol/kg
 Equilibrium pH=          14.9

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs         .905E-01       .847E-01       .107E+04
Rb         .000E+00       .000E+00       .000E+00
SrOH       .000E+00       .000E+00       .000E+00
K          .457E-01       .130E+02       .352E+01
```

2) Projected Tank 10H Salt Solution Cases

- Case 1

ZAM Input

```
1, 303.15                                                        Activity Coeff. Model, Temperature
Tank 10 Case 1 feed @ 30C                                        Title
7, 9                                                             Number of Cations & Anions
1264                                                             Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                       Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                Names of Anions
5.73, 4.95E-06, 4.98E-14, 0, 0.001, 0, 0                         Concentrations of Cations
0.2007, 2.25, 0.1050, 0, 0.9017, 0.6860, 0, 0, 0                 Concentrations of Anions
1, 0.00005                                                       Liquid (L), Solid (g)
0                                                                Initial Solid Form (Na+ (0); H- (1))
1                                                                Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 1 feed @ 30C
  ***********************INPUT************************

    Density=  .1264E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .5730E+01
  Cs+.....        132.9054         1.        .4950E-05
  H+......          1.0079         1.        .4980E-13
  Rb+.....         85.4678         1.        .0000E+00
  K+......         39.0983         1.        .1000E-02
  SrOH+...        105.0000         1.        .0000E+00
  Sr++....         87.6200         2.        .0000E+00
  OH-.....         17.0073        -1.        .2007E+00
  NO3-....         62.0049        -1.        .2250E+01
  NO2-....         46.0000        -1.        .1050E+00
  Al(OH)4-         95.0000        -1.        .0000E+00
  SO4--...         96.0636        -2.        .9017E+00
  CO3--...         60.0092        -2.        .6860E+00
  PO4---..         94.9712        -3.        .0000E+00
  F-......         18.9984        -1.        .0000E+00
  Cl-.....         35.4527        -1.        .0000E+00

  Liquid(L)= .1000E+01   Solid(g)= .5000E-04

   Material: Na Form


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

   Ionic Strength=           9.777867231847836 mol/kg

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs       .1177E-01      .4949E-02      .2378E+04
  Rb       .0000E+00      .0000E+00      .0000E+00
  Sr       .0000E+00      .0000E+00      .0000E+00
  K        .6425E-02      .1000E+01      .6425E+01
```

Freunlich/Langmuir Isotherm

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

C_T: 0.5799 (mmol/g_{CST})

β: 2.3895E-04

- Case 2

ZAM Input

```
1, 303.15                                         Activity Coeff. Model, Temperature
Tank 10 Case 2 feed @ 30C                         Title
7, 9                                              Number of Cations & Anions
1310                                              Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                        Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                 Names of Anions
7, 4.95E-06, 4.98E-14, 0, 0.001, 0, 0             Concentrations of Cations
0.2007, 2.8770, 0.1050, 0, 1.2232, 0.6860, 0, 0, 0  Concentrations of Anions
1, 0.00001                                        Liquid (L), Solid (g)
0                                                 Initial Solid Form (Na+ (0); H- (1))
1                                                 Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 2 feed @ 30C
  **********************INPUT***********************

    Density=  .1310E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .7000E+01
  Cs+.....        132.9054         1.        .4950E-05
  H+......          1.0079         1.        .4980E-13
  Rb+.....         85.4678         1.        .0000E+00
  K+......         39.0983         1.        .1000E-02
  SrOH+...        105.0000         1.        .0000E+00
  Sr++....         87.6200         2.        .0000E+00
  OH-.....         17.0073        -1.        .2007E+00
  NO3-....         62.0049        -1.        .2877E+01
  NO2-....         46.0000        -1.        .1050E+00
  Al(OH)4-         95.0000        -1.        .0000E+00
  SO4--...         96.0636        -2.        .1223E+01
  CO3--...         60.0092        -2.        .6860E+00
  PO4---..         94.9712        -3.        .0000E+00
  F-......         18.9984        -1.        .0000E+00
  Cl-.....         35.4527        -1.        .0000E+00

  Liquid(L)= .1000E+01   Solid(g)= .1000E-04

   Material: Na Form


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

   Ionic Strength=          12.790519430245010 mol/kg

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs       .7720E-02      .4950E-02      .1560E+04
  Rb       .0000E+00      .0000E+00      .0000E+00
  Sr       .0000E+00      .0000E+00      .0000E+00
  K        .4613E-02      .1000E+01      .4613E+01
```

Freunlich/Langmuir Isotherm

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

C_T: 0.5799 (mmol/g_{CST})

β: 3.6687E-04

- Case 3

ZAM Input

```
1, 303.15                                         Activity Coeff. Model, Temperature
Tank 10 Case 3 feed @ 30C                         Title
```

```
7, 9                                                           Number of Cations & Anions
1330                                                           Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                     Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                              Names of Anions
8, 4.95E-06, 4.98E-14, 0, 0.001, 0, 0                          Concentrations of Cations
0.2007, 3.8770, 0.1050, 0, 1.2232, 0.6860, 0, 0, 0             Concentrations of Anions
1, 0.00001                                                     Liquid (L), Solid (g)
0                                                              Initial Solid Form (Na+ (0); H- (1))
1                                                              Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 3 feed @ 30C
  **********************INPUT***********************

    Density=  .1330E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .8000E+01
  Cs+.....        132.9054         1.        .4950E-05
  H+......          1.0079         1.        .4980E-13
  Rb+.....         85.4678         1.        .0000E+00
  K+......         39.0983         1.        .1000E-02
  SrOH+...        105.0000         1.        .0000E+00
  Sr++....         87.6200         2.        .0000E+00
  OH-.....         17.0073        -1.        .2007E+00
  NO3-....         62.0049        -1.        .3877E+01
  NO2-....         46.0000        -1.        .1050E+00
  Al(OH)4-         95.0000        -1.        .0000E+00
  SO4--...         96.0636        -2.        .1223E+01
  CO3--...         60.0092        -2.        .6860E+00
  PO4---..         94.9712        -3.        .0000E+00
  F-......         18.9984        -1.        .0000E+00
  Cl-.....         35.4527        -1.        .0000E+00

  Liquid(L)= .1000E+01   Solid(g)= .1000E-04

   Material: Na Form



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

   Ionic Strength=          15.383481936137480 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .4541E-02      .4950E-02      .9173E+03
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .3032E-02      .1000E+01      .3032E+01
```

- Case 4

ZAM Input

```
1, 303.15                                                      Activity Coeff. Model, Temperature
Tank 10 Case 4 feed @ 30C                                      Title
7, 9                                                           Number of Cations & Anions
1263                                                           Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                     Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                              Names of Anions
5.73, 4.95E-06, 3.33E-14, 0, 0.001, 0, 0                       Concentrations of Cations
0.3, 2.25, 0.1050, 0, 0.8520, 0.6860, 0, 0, 0                  Concentrations of Anions
1, 0.00001                                                     Liquid (L), Solid (g)
0                                                              Initial Solid Form (Na+ (0); H- (1))
1                                                              Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 4 feed @ 30C
  **********************INPUT***********************

    Density=  .1263E+04 kg/m3
```

```
               Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898         1.        .5730E+01
 Cs+.....        132.9054         1.        .4950E-05
 H+......          1.0079         1.        .3330E-13
 Rb+.....         85.4678         1.        .0000E+00
 K+......         39.0983         1.        .1000E-02
 SrOH+...        105.0000         1.        .0000E+00
 Sr++....         87.6200         2.        .0000E+00
 OH-.....         17.0073        -1.        .3000E+00
 NO3-....         62.0049        -1.        .2250E+01
 NO2-....         46.0000        -1.        .1050E+00
 Al(OH)4-         95.0000        -1.        .0000E+00
 SO4--...         96.0636        -2.        .8520E+00
 CO3--...         60.0092        -2.        .6860E+00
 PO4---..         94.9712        -3.        .0000E+00
 F-......         18.9984        -1.        .0000E+00
 Cl-.....         35.4527        -1.        .0000E+00

 Liquid(L)= .1000E+01   Solid(g)= .1000E-04

  Material: Na Form


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

  Ionic Strength=           9.653931443218855 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs       .1182E-01      .4950E-02      .2388E+04
 Rb       .0000E+00      .0000E+00      .0000E+00
 Sr       .0000E+00      .0000E+00      .0000E+00
 K        .6465E-02      .1000E+01      .6465E+01
```

- Case 5

ZAM Input

```
1, 303.15                                      Activity Coeff. Model, Temperature
Tank 10 Case 5 feed @ 30C                      Title
7, 9                                           Number of Cations & Anions
1260                                           Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                     Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2              Names of Anions
5.73, 4.95E-06, 2.00E-14, 0, 0.001, 0, 0       Concentrations of Cations
0.5, 2.25, 0.1050, 0, 0.7520, 0.6860, 0, 0, 0  Concentrations of Anions
1, 0.00001                                     Liquid (L), Solid (g)
0                                              Initial Solid Form (Na+ (0); H- (1))
1                                              Calculation Adjustment
```

ZAM Output

```
  Solution:  Tank 10 Case 5 feed @ 30C
 **********************INPUT***********************

   Density=  .1260E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....         22.9898         1.        .5730E+01
 Cs+.....        132.9054         1.        .4950E-05
 H+......          1.0079         1.        .2000E-13
 Rb+.....         85.4678         1.        .0000E+00
 K+......         39.0983         1.        .1000E-02
 SrOH+...        105.0000         1.        .0000E+00
 Sr++....         87.6200         2.        .0000E+00
 OH-.....         17.0073        -1.        .5000E+00
 NO3-....         62.0049        -1.        .2250E+01
 NO2-....         46.0000        -1.        .1050E+00
 Al(OH)4-         95.0000        -1.        .0000E+00
 SO4--...         96.0636        -2.        .7520E+00
 CO3--...         60.0092        -2.        .6860E+00
 PO4---..         94.9712        -3.        .0000E+00
 F-......         18.9984        -1.        .0000E+00
 Cl-.....         35.4527        -1.        .0000E+00

 Liquid(L)= .1000E+01   Solid(g)= .1000E-04
```

```
  Material: Na Form


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

  Ionic Strength=           9.418285820749157 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs       .1192E-01      .4950E-02      .2408E+04
 Rb       .0000E+00      .0000E+00      .0000E+00
 Sr       .0000E+00      .0000E+00      .0000E+00
 K        .6546E-02      .1000E+01      .6546E+01
```

- Case 6

ZAM Input

```
1, 303.15                                                       Activity Coeff. Model, Temperature
Tank 10 Case 6 feed @ 30C                                       Title
7, 9                                                            Number of Cations & Anions
1257                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                      Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                               Names of Anions
5.73, 4.95E-06, 1.33E-14, 0, 0.001, 0, 0                        Concentrations of Cations
0.75, 2.25, 0.1050, 0, 0.6270, 0.6860, 0, 0, 0                  Concentrations of Anions
1, 0.00001                                                      Liquid (L), Solid (g)
0                                                               Initial Solid Form (Na+ (0); H- (1))
1                                                               Calculation Adjustment
```

ZAM Output

```
  Solution:  Tank 10 Case 6 feed @ 30C
 **********************INPUT***********************

   Density=  .1257E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....        22.9898         1.       .5730E+01
 Cs+.....       132.9054         1.       .4950E-05
 H+......         1.0079         1.       .1330E-13
 Rb+.....        85.4678         1.       .0000E+00
 K+......        39.0983         1.       .1000E-02
 SrOH+...       105.0000         1.       .0000E+00
 Sr++....        87.6200         2.       .0000E+00
 OH-.....        17.0073        -1.       .7500E+00
 NO3-....        62.0049        -1.       .2250E+01
 NO2-....        46.0000        -1.       .1050E+00
 Al(OH)4-        95.0000        -1.       .0000E+00
 SO4--...        96.0636        -2.       .6270E+00
 CO3--...        60.0092        -2.       .6860E+00
 PO4---..        94.9712        -3.       .0000E+00
 F-......        18.9984        -1.       .0000E+00
 Cl-.....        35.4527        -1.       .0000E+00

 Liquid(L)= .1000E+01   Solid(g)= .1000E-04

  Material: Na Form


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

  Ionic Strength=           9.119474343449003 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs       .1205E-01      .4950E-02      .2434E+04
 Rb       .0000E+00      .0000E+00      .0000E+00
 Sr       .0000E+00      .0000E+00      .0000E+00
 K        .6647E-02      .1000E+01      .6647E+01
```

- Case 7

ZAM Input

```
1, 303.15                                                            Activity Coeff. Model, Temperature
Tank 10 Case 7 feed @ 30C                                            Title
7, 9                                                                 Number of Cations & Anions
1254.52                                                              Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                           Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                    Names of Anions
5.73, 4.95E-06, 1.00E-14, 0, 0.001, 0, 0                             Concentrations of Cations
1.0, 2.25, 0.1050, 0, 0.5020, 0.6860, 0, 0, 0                        Concentrations of Anions
1, 0.00001                                                           Liquid (L), Solid (g)
0                                                                    Initial Solid Form (Na+ (0); H- (1))
1                                                                    Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 7 feed @ 30C
  ***********************INPUT***********************

    Density=  .1255E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.        .5730E+01
  Cs+.....        132.9054         1.        .4950E-05
  H+......          1.0079         1.        .1000E-13
  Rb+.....         85.4678         1.        .0000E+00
  K+......         39.0983         1.        .1000E-02
  SrOH+...        105.0000         1.        .0000E+00
  Sr++....         87.6200         2.        .0000E+00
  OH-.....         17.0073        -1.        .1000E+01
  NO3-....         62.0049        -1.        .2250E+01
  NO2-....         46.0000        -1.        .1050E+00
  Al(OH)4-         95.0000        -1.        .0000E+00
  SO4--...         96.0636        -2.        .5020E+00
  CO3--...         60.0092        -2.        .6860E+00
  PO4---..         94.9712        -3.        .0000E+00
  F-......         18.9984        -1.        .0000E+00
  Cl-.....         35.4527        -1.        .0000E+00

  Liquid(L)= .1000E+01   Solid(g)= .1000E-04

   Material: Na Form


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

   Ionic Strength=           8.820107275447615 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .1218E-01      .4950E-02      .2461E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .6750E-02      .1000E+01      .6750E+01
```

- Case 8

ZAM Input

```
1, 303.15                                                            Activity Coeff. Model, Temperature
Tank 10 Case 8 feed @ 30C                                            Title
7, 9                                                                 Number of Cations & Anions
1265                                                                 Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                           Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                    Names of Anions
5.73, 4.95E-06, 4.98E-14, 0, 0.015, 0, 0                             Concentrations of Cations
0.2007, 2.25, 0.1050, 0, 0.9087, 0.6860, 0, 0, 0                     Concentrations of Anions
1, 0.00001                                                           Liquid (L), Solid (g)
0                                                                    Initial Solid Form (Na+ (0); H- (1))
1                                                                    Calculation Adjustment
```

ZAM Output

```
 Solution:  Tank 10 Case 8 feed @ 30C
**********************INPUT***********************

   Density=  .1265E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898         1.        .5730E+01
Cs+.....        132.9054         1.        .4950E-05
H+......          1.0079         1.        .4980E-13
Rb+.....         85.4678         1.        .0000E+00
K+......         39.0983         1.        .1500E-01
SrOH+...        105.0000         1.        .0000E+00
Sr++....         87.6200         2.        .0000E+00
OH-.....         17.0073        -1.        .2007E+00
NO3-....         62.0049        -1.        .2250E+01
NO2-....         46.0000        -1.        .1050E+00
Al(OH)4-         95.0000        -1.        .0000E+00
SO4--...         96.0636        -2.        .9087E+00
CO3--...         60.0092        -2.        .6860E+00
PO4---..         94.9712        -3.        .0000E+00
F-......         18.9984        -1.        .0000E+00
Cl-.....         35.4527        -1.        .0000E+00

Liquid(L)= .1000E+01   Solid(g)= .1000E-04

 Material: Na Form



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

 Ionic Strength=           9.811403574222789 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .1088E-01      .4950E-02      .2198E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .8859E-01      .1500E+02      .5906E+01
```

- Case 8a

ZAM Input

```
1, 303.15                                                           Activity Coeff. Model, Temperature
Tank 10 Case 8a feed @ 30C                                          Title
7, 9                                                                Number of Cations & Anions
1264                                                                Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                          Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                   Names of Anions
5.73, 4.95E-06, 4.98E-14, 0, 0.005, 0, 0                            Concentrations of Cations
0.2007, 2.25, 0.1050, 0, 0.9037, 0.6860, 0, 0, 0                    Concentrations of Anions
1, 0.00001                                                          Liquid (L), Solid (g)
0                                                                   Initial Solid Form (Na+ (0); H- (1))
1                                                                   Calculation Adjustment
```

ZAM Output

```
 Solution:  Tank 10 Case 8a feed @ 30C
**********************INPUT***********************

   Density=  .1264E+04 kg/m3

               Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898         1.        .5730E+01
Cs+.....        132.9054         1.        .4950E-05
H+......          1.0079         1.        .4980E-13
Rb+.....         85.4678         1.        .0000E+00
K+......         39.0983         1.        .5000E-02
SrOH+...        105.0000         1.        .0000E+00
Sr++....         87.6200         2.        .0000E+00
OH-.....         17.0073        -1.        .2007E+00
NO3-....         62.0049        -1.        .2250E+01
NO2-....         46.0000        -1.        .1050E+00
Al(OH)4-         95.0000        -1.        .0000E+00
SO4--...         96.0636        -2.        .9037E+00
CO3--...         60.0092        -2.        .6860E+00
```

```
  PO4---..         94.9712         -3.       .0000E+00
  F-......         18.9984         -1.       .0000E+00
  Cl-.....         35.4527         -1.       .0000E+00

  Liquid(L)= .1000E+01   Solid(g)= .1000E-04

   Material: Na Form


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

   Ionic Strength=           9.790818413420158 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .1149E-01      .4950E-02      .2322E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .3133E-01      .5000E+01      .6266E+01
```

- Case 9

ZAM Input

```
1, 303.15                                                           Activity Coeff. Model, Temperature
Tank 10 Case 9 feed @ 30C                                           Title
7, 9                                                                Number of Cations & Anions
1266                                                                Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                          Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2                                   Names of Anions
5.73, 4.95E-06, 4.98E-14, 0, 0.03, 0, 0                             Concentrations of Cations
0.2007, 2.25, 0.1050, 0, 0.9162, 0.6860, 0, 0, 0                    Concentrations of Anions
1, 0.00001                                                          Liquid (L), Solid (g)
0                                                                   Initial Solid Form (Na+ (0); H- (1))
1                                                                   Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 9 feed @ 30C
  **********************INPUT***********************

    Density=  .1266E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898          1.       .5730E+01
  Cs+.....        132.9054          1.       .4950E-05
  H+......          1.0079          1.       .4980E-13
  Rb+.....         85.4678          1.       .0000E+00
  K+......         39.0983          1.       .3000E-01
  SrOH+...        105.0000          1.       .0000E+00
  Sr++....         87.6200          2.       .0000E+00
  OH-.....         17.0073         -1.       .2007E+00
  NO3-....         62.0049         -1.       .2250E+01
  NO2-....         46.0000         -1.       .1050E+00
  Al(OH)4-         95.0000         -1.       .0000E+00
  SO4--...         96.0636         -2.       .9162E+00
  CO3--...         60.0092         -2.       .6860E+00
  PO4---..         94.9712         -3.       .0000E+00
  F-......         18.9984         -1.       .0000E+00
  Cl-.....         35.4527         -1.       .0000E+00

  Liquid(L)= .1000E+01   Solid(g)= .1000E-04

   Material: Na Form


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

   Ionic Strength=           9.848214739288716 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .1011E-01      .4950E-02      .2043E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .1633E+00      .3000E+02      .5442E+01
```

- Case 10a

ZAM Input

```
1, 303.15                                                                   Activity Coeff. Model, Temperature
Tank 10 Case 10a @ 30C                                                      Title
7, 11                                                                       Number of Cations & Anions
1326.93                                                                     Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                                  Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                                   Names of Anions (Add COOH-, C2O4--)
45.018                                                                      COOH- MW
88.02                                                                       C2O4-2 MW
7.7, 1.97E-05, 2.81E-14, 0, 0.00330, 0, 0                                   Concentrations of Cations
0.3560, 2.48, 0.179, 0, 1.01736, 1.17, 0.0432, 0.0431, 2.31E-02, 9.12E-02, 1.33E-02   Concentrations of Anions
1, 0.00001                                                                  Liquid (L), Solid (g)
0                                                                           Initial Solid Form (Na+ (0); H- (1))
1                                                                           Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 10a @ 30C
  ***********************INPUT************************

    Density=  .1327E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....        22.9898          1.       .7700E+01
  Cs+.....       132.9054          1.       .1970E-04
  H+......         1.0079          1.       .2810E-13
  Rb+.....        85.4678          1.       .0000E+00
  K+......        39.0983          1.       .3300E-02
  SrOH+...       105.0000          1.       .0000E+00
  Sr++....        87.6200          2.       .0000E+00
  OH-.....        17.0073         -1.       .3560E+00
  NO3-....        62.0049         -1.       .2480E+01
  NO2-....        46.0000         -1.       .1790E+00
  Al(OH)4-        95.0000         -1.       .0000E+00
  SO4--...        96.0636         -2.       .1017E+01
  CO3--...        60.0092         -2.       .1170E+01
  PO4---..        94.9712         -3.       .4320E-01
  F-......        18.9984         -1.       .4310E-01
  Cl-.....        35.4527         -1.       .2310E-01
  Other-..        45.0180         -1.       .9120E-01
  Other--.        88.0200         -2.       .1330E-01

  Liquid(L)= .1000E+01   Solid(g)= .1000E-04

   Material: Na Form


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

   Ionic Strength=          14.632406225948090 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .3466E-01      .1970E-01      .1760E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .1679E-01      .3300E+01      .5088E+01
```

Freunlich/Langmuir Isotherm

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

C_T: 0.5799 (mmol/g_{CST})

β: 3.099E-04

- Case 10b

ZAM Input

```
1, 303.15                                                                     Activity Coeff. Model, Temperature
Tank 10 Case 10b @ 30C                                                        Title
7, 11                                                                         Number of Cations & Anions
1326.85                                                                       Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                                    Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                                     Names of Anions (Add COOH-, C2O4--)
45.018                                                                        COOH- MW
88.02                                                                         C2O4-2 MW
7.7, 1.97E-05, 2.81E-14, 0, 0, 0, 0                                           Concentrations of Cations
0.3560, 2.48, 0.179, 0, 1.01571, 1.17, 0.0432, 0.0431, 2.31E-02, 9.12E-02, 1.33E-02  Concentrations of Anions
1, 0.00001                                                                    Liquid (L), Solid (g)
0                                                                             Initial Solid Form (Na+ (0); H- (1))
1                                                                             Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 10b @ 30C
  **********************INPUT************************

    Density=  .1327E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898          1.       .7700E+01
  Cs+.....        132.9054          1.       .1970E-04
  H+......          1.0079          1.       .2810E-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.       .3560E+00
  NO3-....         62.0049         -1.       .2480E+01
  NO2-....         46.0000         -1.       .1790E+00
  Al(OH)4-         95.0000         -1.       .0000E+00
  SO4--...         96.0636         -2.       .1016E+01
  CO3--...         60.0092         -2.       .1170E+01
  PO4---..         94.9712         -3.       .4320E-01
  F-......         18.9984         -1.       .4310E-01
  Cl-.....         35.4527         -1.       .2310E-01
  Other-..         45.0180         -1.       .9120E-01
  Other--.         88.0200         -2.       .1330E-01

  Liquid(L)= .1000E+01   Solid(g)= .1000E-04

   Material: Na Form



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

   Ionic Strength=          14.620339052824790 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .3521E-01      .1970E-01      .1787E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .0000E+00      .0000E+00      .0000E+00
```

- Case 10c

ZAM Input

```
1, 303.15                                                                     Activity Coeff. Model, Temperature
Tank 10 Case 10c @ 30C                                                        Title
7, 11                                                                         Number of Cations & Anions
1323.67                                                                       Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                                    Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                                     Names of Anions (Add COOH-, C2O4--)
45.018                                                                        COOH- MW
```

```
88.02                                                              C2O4-2 MW
7.7, 1.97E-05, 1.00E-14, 0, 3.3E-03, 0, 0                          Concentrations of Cations
1.0, 2.48, 0.179, 0, 0.69536, 1.17, 0.0432, 0.0431, 2.31E-02, 9.12E-02, 1.33E-02     Concentrations of Anions
1, 0.00001                                                         Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 10c @ 30C
  ***********************INPUT***********************

    Density=  .1324E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898         1.         .7700E+01
  Cs+.....        132.9054         1.         .1970E-04
  H+......          1.0079         1.         .1000E-13
  Rb+.....         85.4678         1.         .0000E+00
  K+......         39.0983         1.         .3300E-02
  SrOH+...        105.0000         1.         .0000E+00
  Sr++....         87.6200         2.         .0000E+00
  OH-.....         17.0073        -1.         .1000E+01
  NO3-....         62.0049        -1.         .2480E+01
  NO2-....         46.0000        -1.         .1790E+00
  Al(OH)4-         95.0000        -1.         .0000E+00
  SO4--...         96.0636        -2.         .6954E+00
  CO3--...         60.0092        -2.         .1170E+01
  PO4---..         94.9712        -3.         .4320E-01
  F-......         18.9984        -1.         .4310E-01
  Cl-.....         35.4527        -1.         .2310E-01
  Other-..         45.0180        -1.         .9120E-01
  Other--.         88.0200        -2.         .1330E-01

  Liquid(L)= .1000E+01   Solid(g)= .1000E-04

   Material: Na Form



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

   Ionic Strength=          13.604766708559860 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .3570E-01      .1970E-01      .1812E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .1749E-01      .3300E+01      .5299E+01
```

- Case 10d

ZAM Input

```
1, 303.15                                                          Activity Coeff. Model, Temperature
Tank 10 Case 10d @ 30C                                             Title
7, 11                                                              Number of Cations & Anions
1288.85                                                            Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                         Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                          Names of Anions (Add COOH-, C2O4--)
45.018                                                             COOH- MW
88.02                                                              C2O4-2 MW
6.54, 1.97E-05, 2.81E-14, 0, 3.3E-03, 0, 0                         Concentrations of Cations
0.3560, 2.48, 0.179, 0, 0.91936, 0.688, 0.0432, 0.0431, 2.31E-02, 9.12E-02, 1.33E-02  Concentrations of Anions
1, 0.00001                                                                         Liquid (L), Solid (g)
0                                                                                  Initial Solid Form (Na+
(0); H- (1))
1                                                                                  Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case 10d @ 30C
  ***********************INPUT***********************
```

```
  Density=  .1289E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....        22.9898         1.       .6540E+01
 Cs+.....       132.9054         1.       .1970E-04
 H+......         1.0079         1.       .2810E-13
 Rb+.....        85.4678         1.       .0000E+00
 K+......        39.0983         1.       .3300E-02
 SrOH+...       105.0000         1.       .0000E+00
 Sr++....        87.6200         2.       .0000E+00
 OH-.....        17.0073        -1.       .3560E+00
 NO3-....        62.0049        -1.       .2480E+01
 NO2-....        46.0000        -1.       .1790E+00
 Al(OH)4-        95.0000        -1.       .0000E+00
 SO4--...        96.0636        -2.       .9194E+00
 CO3--...        60.0092        -2.       .6880E+00
 PO4---..        94.9712        -3.       .4320E-01
 F-......        18.9984        -1.       .4310E-01
 Cl-.....        35.4527        -1.       .2310E-01
 Other-..        45.0180        -1.       .9120E-01
 Other--.        88.0200        -2.       .1330E-01

 Liquid(L)= .1000E+01   Solid(g)= .1000E-04

  Material: Na Form



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

  Ionic Strength=          11.424588693958740 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
 Cs       .3599E-01      .1970E-01      .1827E+04
 Rb       .0000E+00      .0000E+00      .0000E+00
 Sr       .0000E+00      .0000E+00      .0000E+00
 K        .1726E-01      .3300E+01      .5231E+01
```

- Case 10e

ZAM Input

```
1, 303.15                                                             Activity Coeff. Model, Temperature
Tank 10 Case 10e @ 30C                                                Title
7, 11                                                                 Number of Cations & Anions
1281.95                                                               Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                            Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                             Names of Anions (Add COOH-, C2O4--)
45.018                                                                COOH- MW
88.02                                                                 C2O4-2 MW
6.54, 1.97E-05, 1.00E-14, 0, 3.3E-03, 0, 0                            Concentrations of Cations
1.0, 2.48, 0.179, 0, 0.76136, 0.524, 0.0432, 0.0431, 2.31E-02, 9.12E-02, 1.33E-02     Concentrations of Anions
1, 0.00001                                                            Liquid (L), Solid (g)
0                                                                     Initial Solid Form (Na+ (0); H- (1))
1                                                                     Calculation Adjustment
```

ZAM Output

```
  Solution:  Tank 10 Case 10e @ 30C
 **********************INPUT***********************

  Density=  .1282E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
 Na+.....        22.9898         1.       .6540E+01
 Cs+.....       132.9054         1.       .1970E-04
 H+......         1.0079         1.       .1000E-13
 Rb+.....        85.4678         1.       .0000E+00
 K+......        39.0983         1.       .3300E-02
 SrOH+...       105.0000         1.       .0000E+00
 Sr++....        87.6200         2.       .0000E+00
 OH-.....        17.0073        -1.       .1000E+01
 NO3-....        62.0049        -1.       .2480E+01
 NO2-....        46.0000        -1.       .1790E+00
 Al(OH)4-        95.0000        -1.       .0000E+00
 SO4--...        96.0636        -2.       .7614E+00
```

```
CO3--...         60.0092         -2.       .5240E+00
PO4---..         94.9712         -3.       .4320E-01
F-......         18.9984         -1.       .4310E-01
Cl-.....         35.4527         -1.       .2310E-01
Other-..         45.0180         -1.       .9120E-01
Other--.         88.0200         -2.       .1330E-01

Liquid(L)= .1000E+01   Solid(g)= .1000E-04

 Material: Na Form



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

 Ionic Strength=          10.653105717198160 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .3534E-01      .1970E-01      .1794E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .1746E-01      .3300E+01      .5290E+01
```

3) Tank 10H VDS Case

ZAM Input

```
1, 303.15                                                              Activity Coeff. Model, Temperature
Tank 10 Case VDS @ 30C                                                 Title
7, 11                                                                  Number of Cations & Anions
1155                                                                   Density(kg/m3)
 3,  6,  1,  5,  4, 40, 13                                             Names of Cations
13,  9, 27,  28, 15, 19, 20, 1, 2, 24, 25                              Names of Anions (Add COOH-, C2O4--)
45.018                                                                 COOH- MW
88.02                                                                  C2O4-2 MW
3.22, 1.0883E-05, 5.43E-14, 0, 3.32E-03, 0, 0                          Concentrations of Cations
0.184, 1.05177, 0.128, 0.0631, 0.381, 0.506, 0, 0, 0.00406, 0, 9.20E-03       Concentrations of Anions
1, 0.000001                                                            Liquid (L), Solid (g)
0                                                                      Initial Solid Form (Na+ (0); H- (1))
1                                                                      Calculation Adjustment
```

ZAM Output

```
   Solution:  Tank 10 Case VDS @ 30C
  ***********************INPUT************************

    Density=  .1155E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....        22.9898         1.         .3220E+01
  Cs+.....       132.9054         1.         .1088E-04
  H+......         1.0079         1.         .5430E-13
  Rb+.....        85.4678         1.         .0000E+00
  K+......        39.0983         1.         .3320E-02
  SrOH+...       105.0000         1.         .0000E+00
  Sr++....        87.6200         2.         .0000E+00
  OH-.....        17.0073        -1.         .1840E+00
  NO3-....        62.0049        -1.         .1052E+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.         .5060E+00
  PO4---..        94.9712        -3.         .0000E+00
  F-......        18.9984        -1.         .0000E+00
  Cl-.....        35.4527        -1.         .4060E-02
  Other-..        45.0180        -1.         .0000E+00
  Other--.        88.0200        -2.         .9200E-02

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

   Material: Na Form



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

   Ionic Strength=           4.978596737618521 mol/kg

         Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .5546E-01      .1088E-01      .5096E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .4153E-01      .3320E+01      .1251E+02
```

Distribution:

S. E. Aleman, 735-A
D. A. Crowley, 773-42A
D. A. Dooley, 773-A
L. L. Hamm, 735-A
T. Hang, 773-42A
M. S. Hay, 773-42A
K. M. Kostelnik, 773-42A
S. Y. Lee, 703-41A
J. J. Mayer, 773-42A
D. J. McCabe, 773-42A
T. O. Oliver, 773-42A
S. H. Reboul, 773-42A
B. J. Wiedenman, 773-42A
W. R. Wilmarth, 773-42A
J. L. Wohlwend, 703-41A

P. A. Fairchild, 766-H
T. L. Fellinger, 766-H
M. T. Keefer, 766-H
J. D. Segura, 766-H

H. M. Cardona, 773-42A
Records Administration (EDWS)