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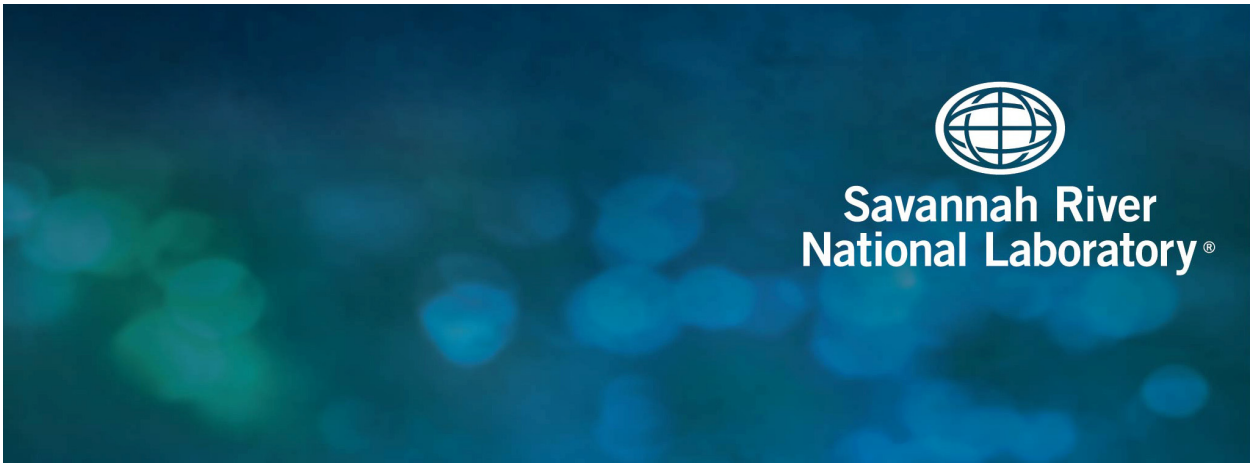

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Crystalline Silicotitanate (CST) Ion Exchange Media Performance Evaluations to Support TSCR DSA IX Media Equilibrium Contacts

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September 2021

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EXECUTIVE SUMMARY

The primary objective of this work is to calculate the maximum loading expected on the Hanford Tank Side Cesium Removal (TSCR) ion exchange 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. Per request of Washington River Protection Solutions (WRPS), 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 for a variety of waste compositions expected to be processed by TSCR.

The study evaluated cesium loadings for the following waste compositions:

1. Seventeen DFLAW campaign batches to cover projected supernate composition ranges within which TSCR may be expected to operate within the first ten years.
2. Hanford tank AP-105 and AP-107 waste solutions that will be processed by the TSCR system.

Modeling Approach

- The OLI Studio™ software (Version 10) from OLI Systems, Inc., was used to calculate charge balanced feed compositions and to estimate feed solution densities.
- Cesium loading on CST in the TSCR ion exchange columns was predicted using ZAM.

Results Summary

General results of the ZAM model predictions are:

1. Seventeen DFLAW Campaign Batches: The cesium loadings were calculated at 56 °F (13 °C) for the powder form of CST. The results provided in Table E-1 indicate that several cesium loadings exceed the established limit of 0.1 moles Cs per kg of CST. These calculations do not adjust for the correction factor that is caused by the binder used in engineered CST form that dilutes the media mass, since the ZAM model is based on the powder form of CST without binder.

Table E-1. DFLAW Campaign Batches - Maximum Cesium Loading at 13 °C

Batch #	Max. Cs Loading [CST Powder] (mol/kg)
1	0.126
2	0.102
3	0.127
4	0.126
5	0.104
6	0.100
7	0.113
8	0.102
9	0.073
10	0.093
11	0.100
12	0.100
13	0.101
14	0.102
15	0.094

Batch #	Max. Cs Loading [CST Powder] (mol/kg)
16	0.042
17	0.021

2. AP-105 and AP-107 Waste Solutions: The maximum cesium loadings on CST for the reported waste compositions evaluated at different temperatures do not exceed the limit. Correction factors, η_{CF}, were obtained by adjustment of the ZAM isotherms to match the batch contact test data at 13 °C and 21 °C. The correction factor, η_{CF}, is the necessary adjustment of the ZAM-generated calculations to account for the dilution of the powder form of CST by the binder used to produce the bead form. Results indicate very little to no dilution by the binder, and the adjusted loading is shown in the column on the right in Table E-2. Equilibrium desorption liquid-phase concentrations at temperatures as high as 90 °C and with phase ratios of less than 5 were estimated for TSCR columns while offline during operations (see Table E-3). The correction factors at high temperatures are assumed to be the same as those at 21 °C.

Table E-2. Maximum Cesium Loading on CST for Hanford Tank AP-105 and AP-107 Wastes

Feed	T (°C)	Max. Cs Loading [CST Powder] (mol/kg)	η_{CF}	Max. Cs Loading [CST Bead] (mol/kg)
AP-105	13	0.0844	0.811	0.0684
AP-105	21	0.074	0.851	0.063
AP-107	13	0.084	1.0	0.084
AP-107	17	0.079	1.0	0.079
AP-107	21	0.073	1.0	0.073

Table E-3. CST Cesium Loading and Elevated Temperature Desorption and Equilibrium Liquid Phase Cesium Concentration for Hanford Tank AP-105 and AP-107 Wastes Under Low Phase Ratio Column Conditions

Waste	Condition	η_{CF}	Liquid Phase Cs^+ (M)	Solid Phase mmol Cs^+/g_{CST}
AP-105	21 °C Loading	0.851	5.66E-05	6.30E-02
	80 °C Desorption	0.851	1.83E-04	6.30E-02
	90 °C Desorption	0.851	2.21E-04	6.30E-02
AP-107	21 °C Loading	1.0	5.73E-05	7.37E-02
	80 °C Desorption	1.0	1.87E-04	7.37E-02
	90 °C Desorption	1.0	2.26E-04	7.37E-02

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

CST	Crystalline Silicotitanate
DFLAW	Direct Feed Low Activity Waste
DSA	Documented Safety Analysis
IX	Ion Exchange
PNNL	Pacific Northwest National Laboratory
SRNL	Savannah River National Laboratory
TAMU	Texas A&M University
TSCR	Tank Side Cesium Removal
WRPS	Washington River Protection Solutions
WTP	Waste Treatment and Immobilization Plant

1.0 Introduction

1.1 Background

The Hanford site has approximately 56 million gallons of radioactive waste stored in 177 underground storage tanks. The Hanford Waste Treatment and Immobilization Plant (WTP) is being built to treat the waste in the tank farms. Waste from the tanks will be treated in the Direct Feed Low Activity Waste (DFLAW) process. The DFLAW process uses ion exchange (IX) columns containing Crystalline Silicotitanate (CST) in the Tank Side Cesium Removal (TSCR) system. The maximum loading of ^{137}Cs on the column is limited due to criteria in the safety basis. Calculations and testing are needed to examine the maximum possible loading to ensure safe operations. Washington River Protection Solutions (WRPS) has requested Savannah River National Laboratory (SRNL) conduct calculations and modeling activities to support the TSCR process (Dorsey, 2020).

SRNL has previously used calculations and computer modeling to determine the maximum loading of cesium on the CST (Hang et al., 2017). Computer modeling is based on the program developed by the Texas A&M University (TAMU) inventors of CST to predict the adsorption of cesium on the media (Zheng et al., 1997). That model, known as ZAM (named after its developers Zheng, Anthony, and Miller), calculates the equilibrium condition (cesium distribution between solid and liquid phases) for a liquid in contact with the CST. The model accounts for the temperature, the density, the composition of the aqueous phase, and the two types of exchange sites that exist on the CST solid. ZAM has been used previously to predict loading on CST for both SRS and Hanford tank waste applications (Hamm et al., 2002; Hang, 2018; Hang, 2019). SRNL typically also uses the OLI Studio computer program by OLI Systems, Inc. (OLI, 2020) to calculate the density of the aqueous solution, which is a required input to ZAM.

The originally produced CST was in the powdered form of very fine particulates. Therefore, the CST mass must be mathematically converted to an engineered porous bead form to conduct ZAM loading calculations to predict performance in flow-through columns. CST is commercially available as IONSIV™ R9120-B or IONSIV™ R9140-B. The media beads consist of the CST powder and a binder material. The binder material essentially dilutes the CST powder, which would be expected to cause a reduction in cesium adsorption 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 adsorption 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 generally there are four isotopes of cesium in the tank waste, ^{133}Cs, ^{134}Cs, ^{135}Cs, and ^{137}Cs. The CST removes all isotopes equally. The primary isotope of concern is the ^{137}Cs due to its high specific (radiolytic) activity. Although strontium is known to compete with cesium loading, the soluble strontium concentration in tank waste is typically insignificant, and therefore its effect is negligible.

1.2 Task Objective

The task objective is to perform calculations and computer modeling as described in the Statement of Work (WRPS, 2020) by the WRPS Mission Integration and Chief Technology Office. SRNL will calculate the maximum cesium loading on CST for the seventeen predicted DFLAW campaign compositions provided in WRPS-2001428 (Anderson, 2020). The CST loading and unloading of cesium in AP-105 and AP-107 waste solutions will also be determined at different temperature conditions of interest.

1.3 Technical Reviews and Quality Assurance

Requirements for performing reviews of technical reports and the extent of review are established in manual E7 2.60.

The reviewers of this report include W. D. King and J. L. Wohlwend. King provides an overall review. Wohlwend design-checks the ZAM predictions.

The ZAM model is maintained as Class D software and is not qualified to be used directly for Safety Significant or Safety Class calculations (Hang and McCabe, 2021).

2.0 Model Formulations

2.1 Modeling Approach

- The OLI Studio™ software (Version 10) from OLI Systems, Inc., was used to calculate charge balanced feed compositions and to estimate feed solution densities (OLI Systems, 2020).
- 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 was described in detail in a previous ion exchange study at SRNL (Hamm et al., 2002). 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 competing 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.

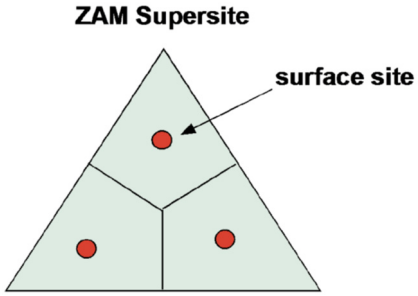
$$\log \gamma_{\pm} = \frac{-A_{\gamma}|z_{+}z_{-}|I^{1/2}}{1+\rho I^{1/2}} + \frac{\left(0.06+0.6B|z_{+}z_{-}|\right)I}{\left(1+\frac{1.5}{|z_{+}z_{-}|}I\right)^{2}} + BI \quad (1)$$

$\gamma_{\pm}$ is the mean molal activity coefficient, and I is the ionic strength (mol/kg). At 25 °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) involving three neighboring surface sites as shown below:



The CST media may exist in two forms: Na form and H form (Zheng et al., 1996). The sodium form is Na_3X, and the hydrogen form is H_2NaX (Zheng et al., 1997; Nyman et al., 2001). Ion exchange in the H-form CST results in an increase of H^+ in the liquid phase, making the solution more acidic. Note that the as-received CST media provided by UOP is in the H form (Nyman et al., 2001). To prevent potential precipitation of alumina-containing wastes as sodium aluminosilicate resulting from decreases in pH within the CST bed which could lead to fouling and interstitial space filling as well as some drop in cesium K_d, the H form must be converted to the Na form by pretreatment with caustic.

When viewing the ion exchange process between sodium and cesium we have the following three possible mass-action relationships to consider for the different CST ionic forms believed to adsorb cesium ions in tank waste solutions:

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

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

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

Equations (2), (3), and (4) represent the removal of a Na^+ cation at a surface site with exchange for a Cs^+ cation. The three possible cases reflect the three possible states that the supersite might be in prior to the ion exchange (note it is believed that a supersite cannot hold more than one Cs^+ cation at any point in time and the trihydrogen form is not considered to contribute significantly under the conditions of interest). 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, $\Delta H°$, under high alkaline conditions have been estimated to be:

Reaction 1: $\Delta H^\circ = -2.18 \times 10^4$ J/gmole
Reaction 2: $\Delta H^\circ = 1.46 \times 10^4$ J/gmole
Reaction 3: ΔH° = (not recorded)

During the cesium loading phase with Hanford tank waste, 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 yield lower cesium loadings consistent with currently available batch contact data.

The overall ion exchange reactions involving Cs^+ under tank waste conditions are as follows:

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

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

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

where the selectivity coefficients (K_{12}, K_{13}, K_{14}) listed reflect approximate estimates and provide insight into the selectivity of CST for cesium. Potassium and strontium monohydroxide monocations are primary competitors with cesium ions for CST exchange sites, though soluble strontium concentrations are typically sufficiently low that Equation 8 does not impact cesium loading. Competition with sodium ions as represented by Equation (6) is relevant in tank waste solutions because the molar ratio of sodium to cesium ions is very high.

Mass-action relationships similar to those above can also be written for other potential competitors (Rb^+ and other alkaline earth monohydroxide species) but, of these species, only rubidium is considered by ZAM. 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 have 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 of these updates was found to be small if Sr complexes were not included. For many of the batch feed concentrations ZAM Version 5 had difficulty in converging. Because of this issue and the fact that the 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 were calculated (Cs^+, Rb^+, $SrOH^+$, and K^+; note Na^+ and H^+ loading numbers are not provided in this report):

- 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 ZAM output is the calculated solution pH and ionic strength values. ZAM inputs and outputs for each calculation are provided in the Appendix B.

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., 2002).

2.3 Prediction of Cesium Loading

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

2.3.1 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 could be achieved by use of the Langmuir isotherm model.

2.3.2 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 on the solid phase. In this scenario, the column outlet cesium concentration of the waste liquid approaches the feed cesium concentration, until cesium is no longer adsorbed onto CST. Figure 1 illustrates the movement of cesium frontal concentration waves along the column at two different times with $t_2 > t_1$. In Figure 1, 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 $>> 10^3$).

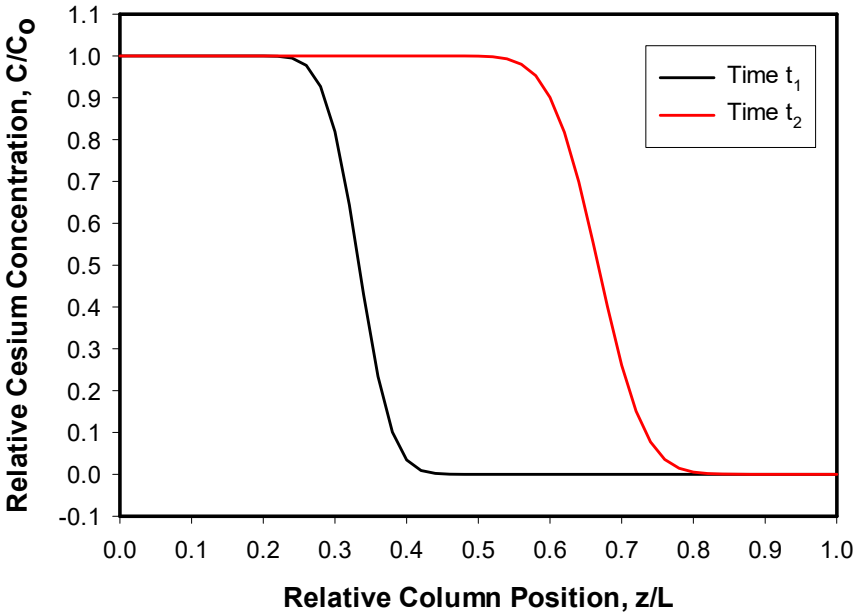


Figure 1. Movement of Cesium Frontal Concentration Waves along an Ion Exchange Column

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 2 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.

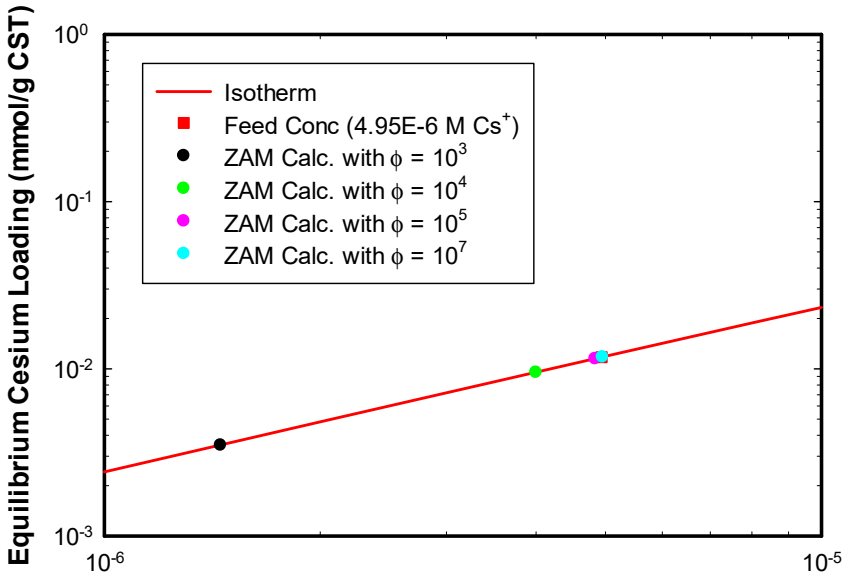


Figure 2. An Example of Cesium Loading for a specific Tank Waste @ 30 °C at Various Phase Ratios

3.0 Waste Compositions and Properties

In this report, the following TSCR feeds at varying temperatures were considered:

1. DFLAW campaign batches: Supernate composition and temperature ranges within which TSCR may be expected to operate within the first ten years were predicted using TOPSIM modeling (Anderson, 2020). The operating temperatures are expected to range from 57 °F to 95 °F. The seventeen DFLAW campaign batches covering a range of composition variation are shown in Table 1.
2. AP-105 and AP107 waste solutions: AP-105 and AP-107 tank wastes will be processed by the TSCR system. The current compositions for AP-105 and AP-107 are provided in Table 2 and Table 3, respectively.

As a requirement to run the ZAM model, the waste solution must be charge balanced. Balancing the charges for the waste solution is carried out as follows:

a. If the anion charge is less than the cation charge, Cl^- was added to the composition until change balance is achieved.
b. If the anion charge is larger than the cation charge, NO_3^- was adjusted until charge balance is achieved.
c. ZAM indicates that KNO_3 precipitation occurs in Batch 9. Therefore, both K and NO_3 were decreased precipitation.

In Table 1, adjusted concentrations for charge balance are highlighted in red. Concentrations adjusted to prevent precipitation are highlighted in blue.

Table 1. 17 DFLAW Campaign Batches

DFLAW Campaign #	1	2	3	4	5	6	7	8	9
137-Cs Liquid (M)	1.26E-05	1.03E-05	1.24E-05	1.20E-05	9.76E-06	8.46E-06	8.21E-06	7.57E-06	7.43E-06
Al(OH)4-Liquid (M)	0.12	0.15	0.12	0.12	0.13	0.16	0.17	0.16	0.19
C2O4-2 Liquid (M)	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Cl- Liquid (M)	0.2	0.07	0.09	0.09	0.09	0.09	0.39	0.4	0.04
CO3-2 Liquid (M)	0.57	0.4	0.48	0.49	0.48	0.44	0.58	0.59	0.59
CrO4-2 Liquid (M)	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Cs+ Liquid (M)	6.73E-05	5.60E-05	6.84E-05	6.71E-05	5.53E-05	4.85E-05	4.75E-05	4.44E-05	4.39E-05
F- Liquid (M)	0.03	0.01	0.01	0.01	0.01	0.01	0.04	0.03	0.07
K+ Liquid (M)	0.08	0.12	0.09	0.09	0.11	0.1	0.05	0.08	0.41
Na+ Liquid (M)	5.83	5.55	5.52	5.52	5.52	5.51	5.89	5.61	5.53
NO2- Liquid (M)	1.19	1.22	1.12	1.11	1.12	1.18	0.98	0.96	0.93
NO3- Liquid (M)	1.96	1.86	1.99	1.98	1.88	1.62	1.47	1.31	1.57
OH- Liquid (M)	1.05	1.43	1.12	1.12	1.26	1.49	1.51	1.4	1.76
PO4-3 Liquid (M)	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.03	0.02
SO4-2 Liquid (M)	0.06	0.03	0.05	0.05	0.04	0.04	0.06	0.06	0.05
TOC Liquid (M)	0.15	0.23	0.16	0.16	0.17	0.14	0.11	0.11	0.13
OLI Density (g/ml) at 56 °F	1.2668	1.2552	1.2558	1.2558	1.2550	1.2507	1.2605	1.2495	1.2648

Table 1. 17 DFLAW Campaign Batches (Cont'd)

DFLAW Campaign #	10	11	12	13	14	15	16	17
137-Cs Liquid (M)	9.32E-06	7.89E-06	8.89E-06	8.12E-06	7.67E-06	6.34E-06	2.75E-06	1.37E-06
Al(OH)4-Liquid (M)	0.14	0.12	0.14	0.14	0.14	0.13	0.07	0.05
C2O4-2 Liquid (M)	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Cl- Liquid (M)	0.07	0.19	0.13	0.08	0.16	0.36	0.31	0.11
CO3-2 Liquid (M)	0.59	0.62	0.52	0.52	0.52	0.48	0.24	0.18
CrO4-2 Liquid (M)	0.01	0.01	0.01	0.01	0.01	0.01	0	0
Cs+ Liquid (M)	5.59E-05	4.74E-05	5.46E-05	4.99E-05	4.79E-05	3.98E-05	1.75E-05	8.84E-06
F- Liquid (M)	0.04	0.02	0.03	0.02	0.02	0.01	0.01	0.01
K+ Liquid (M)	0.25	0.11	0.15	0.11	0.09	0.06	0.02	0.01
Na+ Liquid (M)	5.5	5.5	5.51	5.51	5.51	5.5	5.5	5.5
NO2- Liquid (M)	1.05	1.09	1.11	1.13	1.13	0.99	0.99	1.01
NO3- Liquid (M)	1.77	1.53	1.69	1.67	1.61	1.68	2.78	3.29
OH- Liquid (M)	1.32	1.15	1.34	1.34	1.3	1.17	0.66	0.48
PO4-3 Liquid (M)	0.02	0.03	0.02	0.02	0.02	0.04	0.04	0.04
SO4-2 Liquid (M)	0.04	0.07	0.04	0.05	0.05	0.05	0.04	0.03
TOC Liquid (M)	0.14	0.13	0.14	0.14	0.14	0.13	0.06	0.03
OLI Density (g/ml) at 56 °F	1.2598	1.2518	1.2545	1.2528	1.2511	1.2479	1.2576	1.2634

Table 2. Diluted AP-105 Composition

Ions	Concentration [a] (M)
Na^+	5.92
Cs^+	5.66E-05
K^+	0.102
OH^-	1.24
$NO3^-$	1.89
$NO2^-$	1.38
$Al(OH)_4^-$ [b]	0.526
Cl^- [c]	0.90542
F^-	0
SO_4^{-2}	0.0244
$C_2O_4^{-2}$	0.00284
PO_4^{-3}	0.00872
Measured Density (g/ml)	1.285
OLI Density (g/ml) @ 80 °C	1.253
OLI Density (g/ml) @ 90 °C	1.250

[a]: Fiskum et al., 2021b
[b]: May precipitate as $Al(OH)_3$ (Gibbsite)
[c]: Added for charge balance

Table 3. AP-107 Composition

Ions	Concentration [a] (M)
Na^+	5.795
Cs^+	5.728E-05
K^+	0.096
OH^-	0.89
$NO3^-$	2.064
$NO2^-$	1.293
$Al(OH)_4^-$ [b]	0.373
Cl^- [c]	1.0728
F^-	0.01858
SO_4^{-2}	0.0455
$C_2O_4^{-2}$	0.0052
PO_4^{-3}	0.02585
Measured Density (g/ml)	1.266
OLI Density (g/ml) @ 80 °C	1.247
OLI Density (g/ml) @ 90 °C	1.244

[a]: Fiskum et al., 2019
[b]: May precipitate as $Al(OH)_3$ (Gibbsite)
[c]: Added for charge balance

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 B.

4.1 Seventeen DFLAW Campaign Batches

Variation of compositions for the supernate feeds to be processed by TSCR is captured by the 17 DFLAW campaign batches shown in Table 1. The maximum cesium loading on CST for each of these 17 batches is calculated using the variation of ZAM phase ratio discussed under Section 2.3.2 above. The loading limit on CST in a TSCR column has been established at 0.1 moles Cs per kg CST bed (Fiskum et al., 2021a).

Since the ZAM model is based on the CST powder, the maximum cesium loading calculated by ZAM must be converted to the cesium loading on CST bed that is consisting of the CST powder and a binder material by use of a dilution/correction factor η_{CF}. Based on historical SRS and Hanford waste data, a correction/dilution factor of 0.68 is usually applied to cesium loading on the engineered CST form (Hamm et al., 2002). This value was calculated as a conservative estimate of the break-through profile when modeling column processing, not as a conservative estimate of the loading, and was determined from other batches of the media. A conservative estimate of the loading would use a factor of 1.0, or one derived from testing with the actual tank waste and that batch of media. Since the recent test data indicates a much higher correction factor with specific simulant compositions (see section below), no correction factor is applied in Table 4. The conversion is typically done as follows:

$$Q_{Cs,eng} = \eta_{CF} Q_{Cs,pow}$$

$Q_{Cs,pow}$: Max. cesium loading calculated by ZAM (powdered CST)
$Q_{Cs,eng}$: Max. cesium loading on CST bed (engineered CST)
η_{CF}: Correction/dilution factor

The cesium loading results for the 17 batches at 56 °F (13 °C) are given in Table 4. The results indicate that several cesium loadings (9 of 17) exceed the established limit and several other batches (3 of 17) equal the limit.

Table 4. Maximum Cesium Loading at 13 °C

Batch #	Max. Cs Loading [CST Powder] (mol/kg)
1	0.126
2	0.102
3	0.127
4	0.126
5	0.104
6	0.100
7	0.113
8	0.102
9	0.073
10	0.093
11	0.100
12	0.100
13	0.101

Batch #	Max. Cs Loading [CST Powder] (mol/kg)
14	0.102
15	0.094
16	0.042
17	0.021

4.2 AP-105 and AP-107 Tank Waste Solutions

4.2.1 Adsorption Isotherms

Adsorption isotherms for the feed solutions were determined by use of the Freundlich/Langmuir model to fit the equilibrium data generated by ZAM.

The Freundlich/Langmuir isotherm can be expressed as:

$$Q = \frac{\eta_{CF} C_T C_p}{\beta + C_p}$$

Q: Cesium loading on CST ($mmol_{Cs}/g_{CST,dry\text{-}eng}$)
C_p: Liquid-phase cesium concentration ($mmol_{Cs}/mL$)
C_T: Total ion-exchange capacity of CST (0.58 $mmol_{Cs}/g_{CST,dry\text{-}powder}$)
β: Isotherm parameter
η_{CF}: Correction/dilution factor ($g_{CST,dry\text{-}powder}/g_{CST,dry\text{-}eng}$)

The resulting isotherm parameters for both AP-105 and AP-107 are given in Table 5. To determine the correction factor η_{CF}, the ZAM isotherms were adjusted to match the experimental test data. The measured batch contact test data for AP-105 and AP-107 at different temperatures were provided by Pacific Northwest National Laboratory (PNNL) in an Excel spreadsheet (Peterson, 2021) as reproduced in Appendix A. Correction factors η_{CF} are given in Table 5. Isotherm adjustment is graphically displayed in Figure 3 to Figure 6 for AP-105 and AP-107 at 13 °C and 21 °C. Figure 7 shows a parity plot of cesium loadings between modeled and test data. Overall, the agreement is much better at loading concentrations lower than the loading limit of 0.1 mol/kg_{CST}.

Table 5. Isotherm Parameters

Feed	T (°C)	η_{CF}	C_T ($mmol_{Cs}/g_{CST,dry\text{-}powder}$)	β
AP-105	13	0.811	0.58	3.3216E-04
AP-105	21	0.851	0.58	3.8649E-04
AP-107	13	1	0.58	3.3732E-04
AP-107	17	1	0.58	3.6423E-04
AP-107	21	1	0.58	3.9348E-04
AP-107	80	1	0.58	1.2848E-03
AP-107	90	1	0.58	1.5549E-03

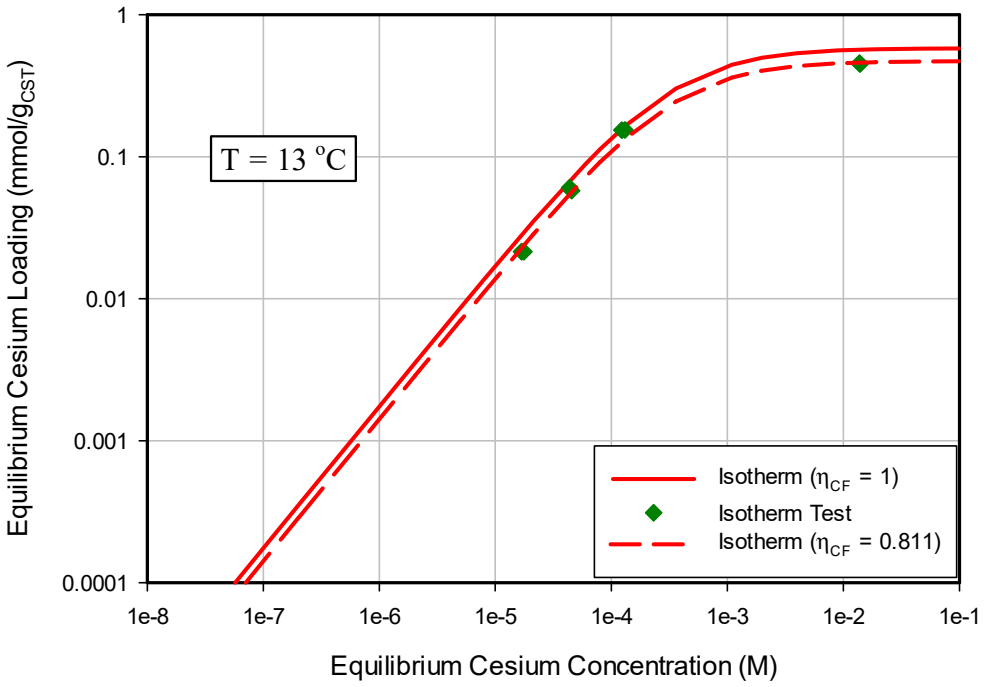


Figure 3. Calculated AP-105 Waste Isotherms and Measured Test Data at 13 °C

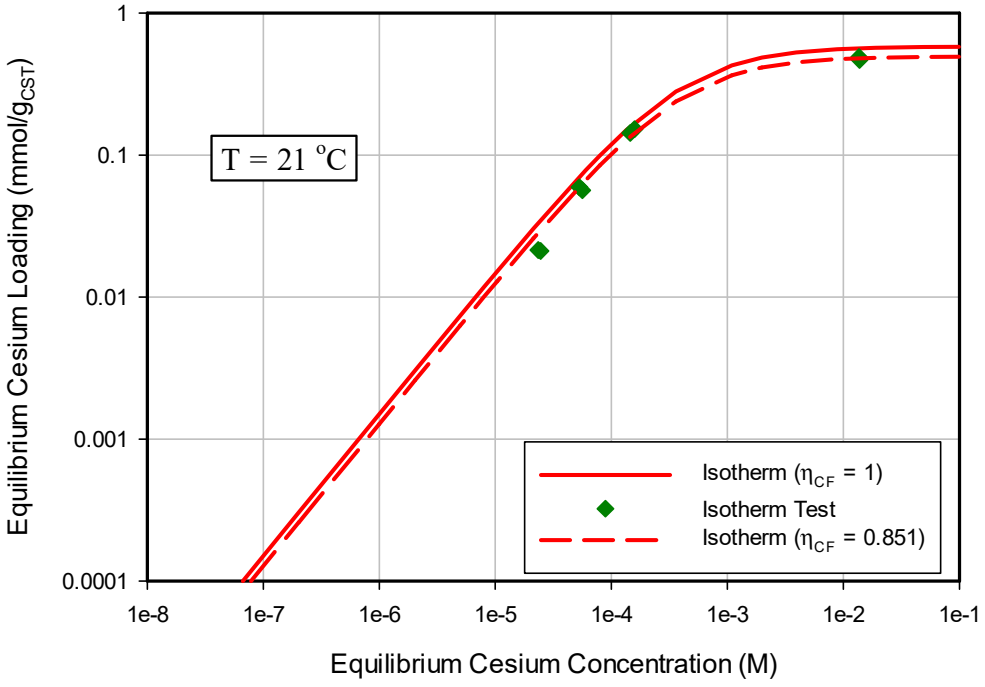


Figure 4. Calculated AP-105 Waste Isotherms and Measured Test Data at 21 °C

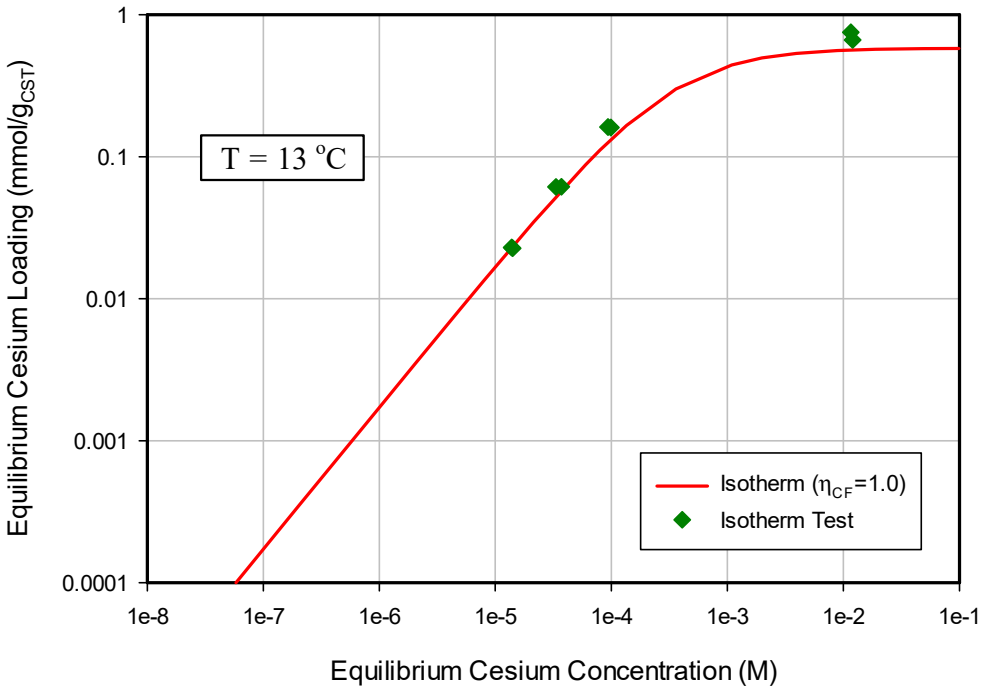


Figure 5. Calculated AP-107 Waste Isotherm and Measured Test Data at 13 °C

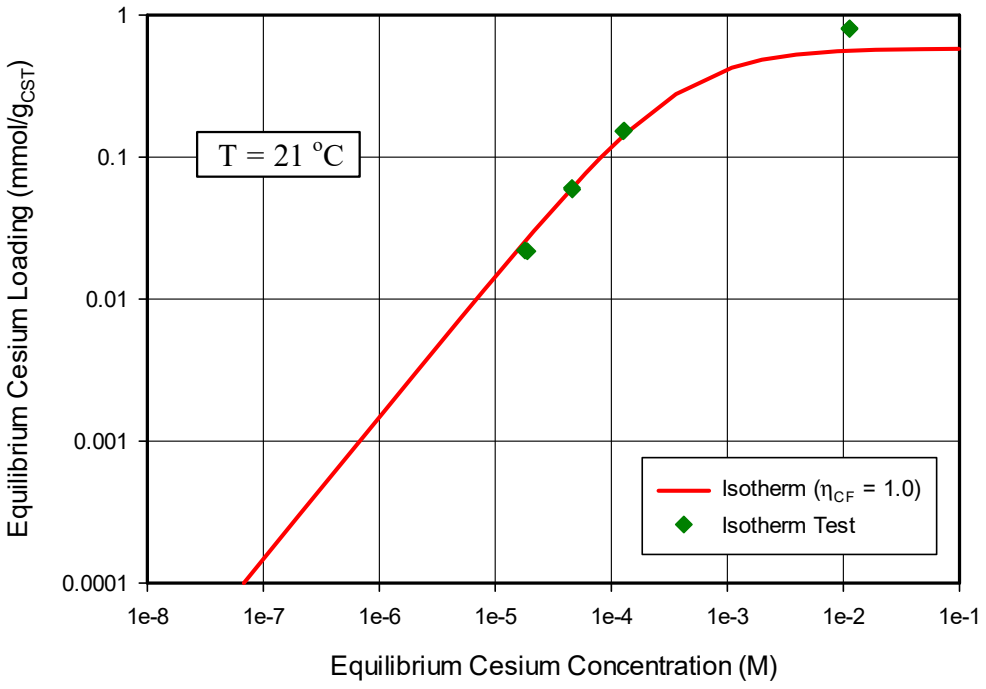


Figure 6. Calculated AP-107 Waste Isotherms and Measured Test Data at 21 °C

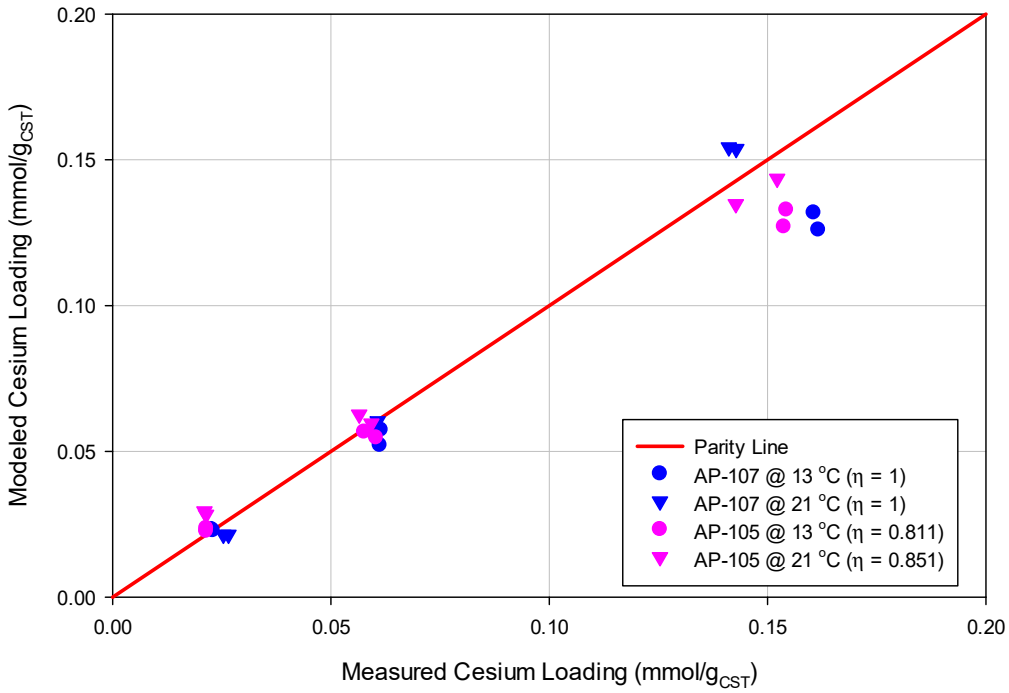


Figure 7. Parity Plot – Modeled Cesium Loadings vs. Cesium Loading Test Data

4.2.2 Maximum Cesium Loading

Similar to the 17 DFLAW campaign batches, the maximum cesium loading on CST for AP-105 and AP-107 is also computed using the variation of ZAM phase ratio. These results given in Table 6 clearly state that the maximum cesium loadings are below the established limit. The table shows the ZAM calculated loading (CST powder), the correction factor calculated from the PNNL data, and the maximum Cs loading calculated based on the correction-factor adjusted ZAM loading. Since the AP-107 correction value was 1.0, i.e., the measured values vs. ZAM calculations were the same, there is no difference between the calculated loading values.

Table 6. ZAM-calculated Maximum Cesium Loading for AP-105 and AP-107

Feed	T (°C)	Max. Cs Loading [CST Powder] (mol/kg)	η_{CF}	Max. Cs Loading [CST Engineered] (mol/kg)
AP-105	13	0.0844	0.811	0.0684
AP-105	21	0.074	0.851	0.063
AP-107	13	0.084	1.0	0.084
AP-107	17	0.079	1.0	0.079
AP-107	21	0.074	1.0	0.074

4.2.3 Cesium Loading and Unloading

During TSCR operation outages, the columns may be offline for a period of time while still filled with feed. Due to the cesium adsorbed on the CST media, the columns will gradually warm to higher temperatures than when fluid is flowing. Therefore some cesium will be unloaded (desorbed) from the CST back into

the liquid phase. This section estimates the liquid-phase cesium concentrations at equilibrium after desorption.

Assuming a low liquid:solid phase ratio of less than 5 in the columns, it has been shown previously (King et al., 2018) that the decrease in the solid-phase cesium concentrations be negligible (< 1%). Therefore, in this study, the equilibrium cesium loading at high temperatures is assumed the same as the loading at 21 °C. This assumption is conservative because it delivers somewhat higher equilibrium liquid-phase cesium concentrations. ZAM predictions of cesium equilibrium desorption at 80 °C and 90 °C are provided for both AP-105 and AP-107 compositions in Figure 8 and Figure 9, respectively. As shown in each figure, cesium desorption occurs moving from left to right along the magenta operating line indicated until reaching the 80 °C and 90 °C isotherms. Cesium loading and unloading concentrations for AP-105 and AP-107 compositions at temperatures of interest are summarized in Table 7. All data represent as the engineered bead form of CST after adjustment for the correction factor calculated for the two compositions tested. As shown in Table 7, the cesium concentrations in the liquid phase increased by 3.2 to 3.3 at 80 °C relative to the concentrations at 21 °C for the two waste compositions. The cesium concentrations in the liquid phase increased by 3.9 at 90 °C relative to the concentrations at 21 °C for the two waste compositions.

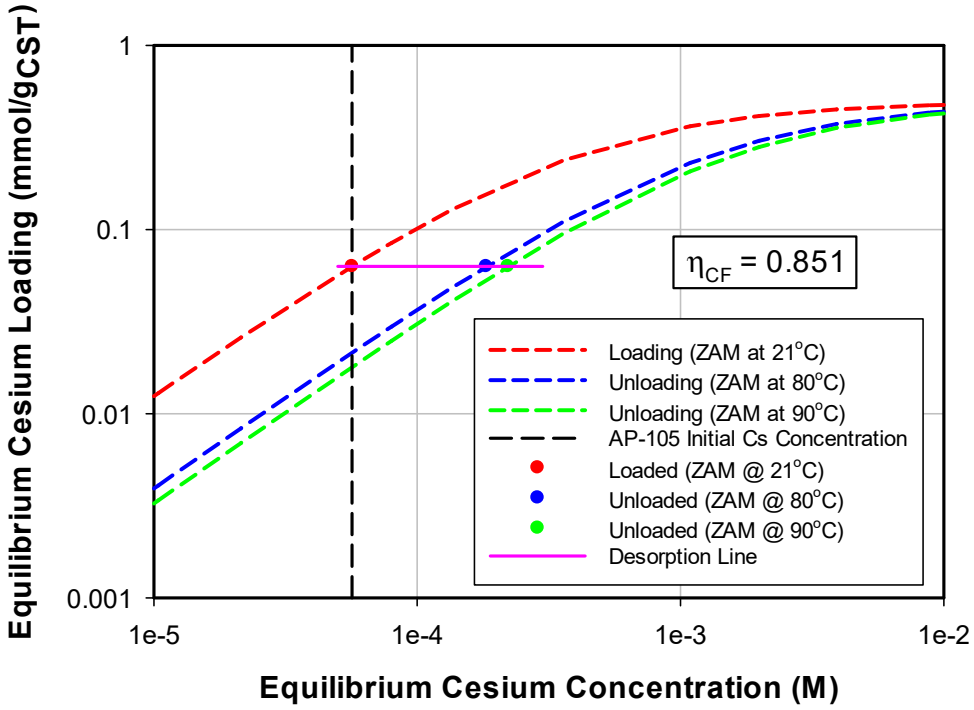


Figure 8. ZAM Model Predictions of Cesium Equilibrium Sorption at 21 °C and Equilibrium Desorption at 80 °C and 90 °C for AP-105

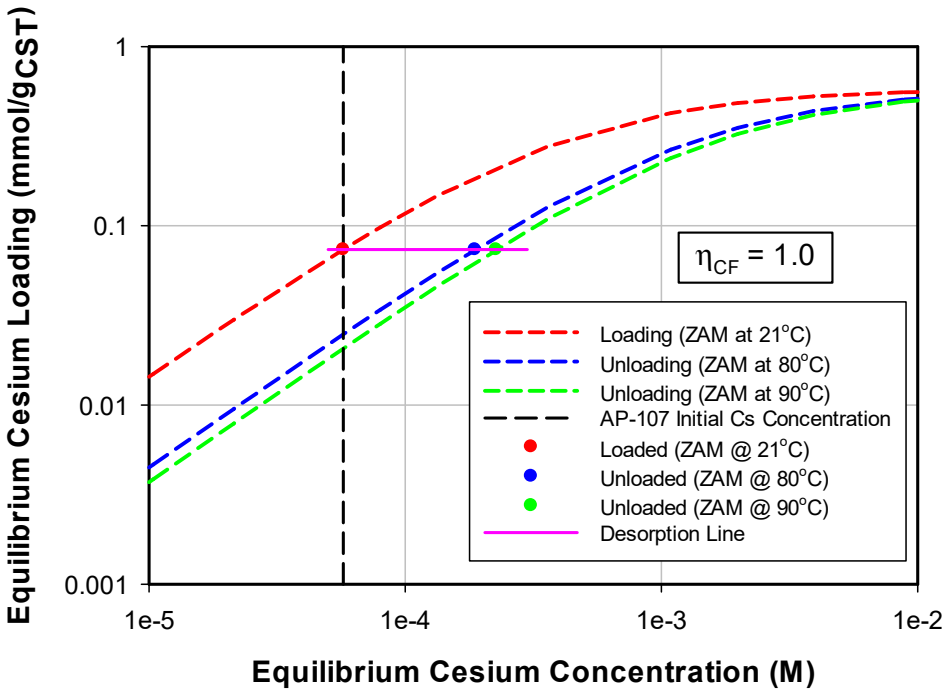


Figure 9. ZAM Model Predictions of Cesium Equilibrium Sorption at 21 °C and Equilibrium Desorption at 80 °C and 90 °C for AP-107

Table 7. Cesium Loading/Desorption for AP-105 and AP-107 Compositions on Bead Form of CST

Waste	Condition	η_{CF}	Liquid Phase Cs^+ (M)	Solid Phase mmol Cs^+/g_{CST}	Liquid Concentration Increase Relative to 21 °C
AP-105	21 °C Loading	0.851	5.66E-05	6.30E-02	---
	80 °C Desorption	0.851	1.83E-04	6.30E-02	3.2
	90 °C Desorption	0.851	2.21E-04	6.30E-02	3.9
AP-107	21 °C Loading	1.0	5.73E-05	7.37E-02	---
	80 °C Desorption	1.0	1.87E-04	7.37E-02	3.3
	90 °C Desorption	1.0	2.26E-04	7.37E-02	3.9

5.0 Conclusions

The ZAM model was used to predict the maximum cesium loading and the adsorption and desorption isotherms at different temperatures for a variety of waste solutions to be processed by the TSCR system. General evaluation results of the ZAM model predictions are:

1. Seventeen DFLAW Campaign Batches: The cesium loadings were calculated at 56 °F. The results indicate that several cesium loadings are projected to exceed the established limit of 0.1 moles Cs per kg CST bed.
2. AP-105 and AP-107 Waste Solutions: The maximum cesium loadings evaluated at different temperatures do not exceed the limit. Correction factors were obtained by adjustment of the ZAM isotherms to match the experimental batch contact data. Equilibrium desorption liquid-phase concentrations at temperatures as high as 90 °C were estimated for TSCR columns while offline during operations. The liquid phase cesium concentrations in the cesium loaded columns are expected increase by a factor of nearly 4 when the temperature is increased to 90 °C.

6.0 References

Anderson, K. A., 2020. "Anticipated Composition and Temperature Ranges for the first 10 years of TSCR Operation," Interoffice Memorandum WRPS-2001428 to L. H. Cree, dated 23 April 2020.

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

Dorsey, A. M., 2020. "Request for Proposal 340320 - TSCR DSA IX MEDIA BATCH CONTACTS (MAX CURRIE LOADING)," Email to Jacqueline Brigido (SRNL) dated 29 July 2020.

Fiskum, S. K., E. L. Campbell, J. L. George, R. A. Peterson, and T. T. Trang-Le, 2021a. "Maximum Cs-137 Curie Loading onto Crystalline Silicotitanate for the Documented Safety Analysis of the Tank Side Cesium Removal Platform," RPT-DSA-001, Rev. 0 (PNNL-30976, Rev. 0), March 2021.

Fiskum, S. K., A. M. Rovira, H. A. Colburn, A. M. Carney, and R. A. Peterson, 2019. "Cesium Ion Exchange Testing Using a Three-Column System with Crystalline Silicotitanate and Hanford Tank Waste 241-AP-107," RPT-DFTP-013, Rev. 0 (PNNL-28958, Rev. 0), August 2019.

Fiskum, S. K., A. M. Westesen, A. M. Carney, T. T. Trang-Le, and R.A. Peterson, 2021b. "Ion Exchange Processing of AP-105 Hanford Tank Waste through Crystalline Silicotitanate in a Staged 2- then 3-Column System," RPT-DFTP-025, Rev. 0 (PNNL-30712, Rev. 0), January 2021.

Hamm, L. L., T. Hang, D. J. McCabe, and W. D. King, 2002. "Preliminary Ion Exchange Modeling for Removal of Cesium from Hanford Waste Using Hydrous Crystalline Silicotitanate Material," WSRC-TR-2001-00400, July 2002.

Hang, T., and D. J. McCabe, 2021. "Software Quality Assurance Plan for the ZAM Software to Support Ion-Exchange (IX) Projects using Crystalline Silicotitanate (CST) Media," Q-SQP-A-00019, Revision 0, February 2021.

Hang, T., D. J. McCabe, L. L. Hamm, and J. L. Wohlwend, 2017. "Modeling Ion Exchange Performance of Crystalline Silicotitanate to Support SRS Tank 10H Closure," SRNL-STI-2017-00336, Rev. 0, July 2017.

Hang, T., 2018. "Sensitivity ZAM Modeling Study of Tank 10H VDS Waste Sample," SRNL-STI-2018-00215, Rev. 0, June 2018.

Hang, T., 2019. "Modeling Crystalline Silicotitanate Performance to Support TCCR Batch 1 and Batch 1A Operations," SRNL-STI-2019-00147, Rev. 0, May 2019.

King, W. D., L. L. Hamm, C. J. Coleman, F. F. Fondeur, and S. H. Reboul, 2018. "Crystalline Silicotitanate (CST) Ion Exchange Media Performance Evaluations in SRS Average Supernate Simulant and Tank 10H Waste Solution to Support TCCR," SRNL-STI-2018-00277, Revision 0, June 2018.

Nyman, M., T. M. Nenoff, and T. J. Headley, 2001. "Characterization of UOP IONSIV IE-911," Sandia Report SAND2001-0999, June 2001.

OLI Systems, Inc., 2020. *"*Introduction to OLI Studio - Version 10*"* (www.olisystems.com).

Peterson, R. A., 2021. "RE: Isotherms for AP-105 and AP-107," Email to T. Hang, dated 2 March 2021.

WRPS, 2020. "SRNL Support to TSCR DSA IX Media Equilibrium Contacts (Max Currie Loading)," Statement of Work, Requisition #: 340320 (BMA#: 55220), Revision 0, 28 July 2020.

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. PNNL Batch Contact Test Data

(Reference: Peterson, R. A., 2021. "RE: Isotherms for AP-105 and AP-107," Email to T. Hang, dated 2 March 2021)

Feed	Temp	Cs in Solution (M)	Cs on CST (mmole/g)
AP-107	13 °C	1.38488E-05	0.022957192
		3.70426E-05	0.061456865
		9.92452E-05	0.16053782
		0.012008374	0.663654868
		1.40866E-05	0.022663559
		3.33203E-05	0.061176815
		9.3656E-05	0.161615398
		0.011596449	0.751046884
AP-107	21 °C	1.88869E-05	0.021709155
		4.60097E-05	0.058955982
		0.000128596	0.153803733
		0.011279337	0.807403143
		1.80188E-05	0.021977132
		4.57805E-05	0.060633036
		0.000126567	0.151944782
		0.011299187	0.79647095
AP-105	13 °C	1.76172E-05	0.021447258
		4.37086E-05	0.060344481
		0.000122916	0.15370469
		0.013864059	0.448375286
		1.68167E-05	0.021425132
		4.54981E-05	0.057625507
		0.000130716	0.154282744
		0.013815262	0.45642528
	21 °C	2.4534E-05	0.021060589
		5.30635E-05	0.059281955
		0.000158547	0.152205862
		0.013650007	0.48925504
		2.3507E-05	0.021412679
		5.6174E-05	0.056470151
		0.000145349	0.14276406
		0.013802155	0.467345742
Baseline Simulant	13 °C	1.58503E-05	0.024598064
		3.84969E-05	0.063043524
		0.000105437	0.164248813
		0.013475424	0.546464515

Feed	Temp	Cs in Solution (M)	Cs on CST (mmole/g)
	21 °C	1.87815E-05	0.023768502
		5.06165E-05	0.06135432
		0.000135032	0.160509163
		0.01323116	0.587722719
Simple Simulant	13 °C	1.61277E-05	0.023019763
		4.5203E-05	0.057668224
		0.000120116	0.158509906
		0.013855989	0.488918577
	21 °C	2.4349E-05	0.021582614
		5.79951E-05	0.053773897
		0.000138182	0.145136366
		0.012266044	0.829160018

Appendix B. ZAM Calculations

Maximum Cesium Loading

- DFLAW Batch 1

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 1 MaxLoading@56F                                                       Title
9, 11                                                                        Number of Cations & Anions
1266.83                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.83, 6.730E-05, 9.5238E-15, 0, 0.08, 0, 0, 0, 0                            Concentrations of Cations
1.05, 1.96, 1.19, 0.12, 0.06, 0.57, 0.03, 0.200067, 0.01, 0.01, 0.02         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 1 MaxLoading@56F
**********INPUT**********

  Density=  .1267E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5830E+01
Cs+.....       132.9054          1.       .6730E-04
H+......         1.0079          1.       .9524E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .8000E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1050E+01
NO3-....        62.0049         -1.       .1960E+01
NO2-....        46.0000         -1.       .1190E+01
Al(OH)4-        95.0000         -1.       .1200E+00
SO4--...        96.0636         -2.       .6000E-01
CO3--...        60.0092         -2.       .5700E+00
F-......        18.9984         -1.       .3000E-01
Cl-.....        35.4527         -1.       .2001E+00
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           8.091125116615517 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1259E+00      .6730E-01      .1871E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3991E+00      .8000E+02      .4989E+01
```

- DFLAW Batch 2

ZAM Input

```
1, 286.48                                                                  Activity Coeff. Model, Temperature
Batch 2 MaxLoading@56F                                                     Title
9, 11                                                                      Number of Cations & Anions
1255.18                                                                    Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                        Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                 Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2,
                                                                                   CO3-2, F-, Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                      C2O4-- MW
5.55, 5.6E-05, 6.9930E-15, 0, 0.12, 0, 0, 0, 0                             Concentrations of Cations
1.43, 1.86, 1.22, 0.15, 0.03, 0.4, 0.01, 0.070056, 0.01, 0.01, 0.01        Concentrations of Anions
1, 0.000001                                                                Liquid (L), Solid (g)
0                                                                          Initial Solid Form (Na+ (0); H- (1))
1                                                                          Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 2 MaxLoading@56F
**********INPUT**********

  Density=  .1255E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5550E+01
Cs+.....       132.9054          1.       .5600E-04
H+......         1.0079          1.       .6993E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1200E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1430E+01
NO3-....        62.0049         -1.       .1860E+01
NO2-....        46.0000         -1.       .1220E+01
Al(OH)4-        95.0000         -1.       .1500E+00
SO4--...        96.0636         -2.       .3000E-01
CO3--...        60.0092         -2.       .4000E+00
F-......        18.9984         -1.       .1000E-01
Cl-.....        35.4527         -1.       .7006E-01
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .1000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.319587718762507 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1017E+00      .5600E-01      .1815E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .5190E+00      .1200E+03      .4325E+01
```

- DFLAW Batch 3

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 3 MaxLoading@56F                                                       Title
9, 11                                                                        Number of Cations & Anions
1255.83                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.52, 6.84E-05, 8.9286E-15, 0, 0.09, 0, 0, 0, 0                              Concentrations of Cations
1.12, 1.990068, 1.12, 0.12, 0.05, 0.48, 0.01, 0.09, 0.01, 0.01, 0.02         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
  Solution:  Batch 3 MaxLoading@56F
**********INPUT**********

   Density=  .1256E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .5520E+01
Cs+.....        132.9054          1.       .6840E-04
H+......          1.0079          1.       .8929E-14
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .9000E-01
Sr++....         87.6200          2.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Ca++....         40.0780          2.       .0000E+00
Pb++....        207.2000          2.       .0000E+00
OH-.....         17.0073         -1.       .1120E+01
NO3-....         62.0049         -1.       .1990E+01
NO2-....         46.0000         -1.       .1120E+01
Al(OH)4-         95.0000         -1.       .1200E+00
SO4--...         96.0636         -2.       .5000E-01
CO3--...         60.0092         -2.       .4800E+00
F-......         18.9984         -1.       .1000E-01
Cl-.....         35.4527         -1.       .9000E-01
CrO4--..        115.9937         -2.       .1000E-01
Other--.         88.0200         -2.       .1000E-01
PO4---..         94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.496570478579506 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .1272E+00      .6840E-01      .1859E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .4383E+00      .9000E+02      .4869E+01
```

- DFLAW Batch 4

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 4 MaxLoading@56F                                                       Title
9, 11                                                                        Number of Cations & Anions
1255.79                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.52, 6.71E-05, 8.9286E-15, 0, 0.09, 0, 0, 0, 0                              Concentrations of Cations
1.12, 1.980067, 1.11, 0.12, 0.05, 0.49, 0.01, 0.09, 0.01, 0.01, 0.02         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 4 MaxLoading@56F
**********INPUT**********

  Density=  .1256E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5520E+01
Cs+.....       132.9054          1.       .6710E-04
H+......         1.0079          1.       .8929E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .9000E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1120E+01
NO3-....        62.0049         -1.       .1980E+01
NO2-....        46.0000         -1.       .1110E+01
Al(OH)4-        95.0000         -1.       .1200E+00
SO4--...        96.0636         -2.       .5000E-01
CO3--...        60.0092         -2.       .4900E+00
F-......        18.9984         -1.       .1000E-01
Cl-.....        35.4527         -1.       .9000E-01
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.511493476440324 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .1257E+00      .6710E-01      .1873E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .4401E+00      .9000E+02      .4890E+01
```

- DFLAW Batch 5

ZAM Input

```
1, 286.48                                                                  Activity Coeff. Model, Temperature
Batch 5 MaxLoading@56F                                                     Title
9, 11                                                                      Number of Cations & Anions
1255.05                                                                    Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                        Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                 Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                      C2O4-- MW
5.52, 5.53E-05, 7.9365E-15, 0, 0.11, 0, 0, 0, 0                            Concentrations of Cations
1.26, 1.880055, 1.12, 0.13, 0.04, 0.48, 0.01, 0.09, 0.01, 0.01, 0.02       Concentrations of Anions
1, 0.000001                                                                Liquid (L), Solid (g)
0                                                                          Initial Solid Form (Na+ (0); H- (1))
1                                                                          Calculation Adjustment
```

ZAM Output

```
  Solution:  Batch 5 MaxLoading@56F
**********INPUT**********

   Density=  .1255E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .5520E+01
Cs+.....        132.9054          1.       .5530E-04
H+......          1.0079          1.       .7936E-14
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .1100E+00
Sr++....         87.6200          2.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Ca++....         40.0780          2.       .0000E+00
Pb++....        207.2000          2.       .0000E+00
OH-.....         17.0073         -1.       .1260E+01
NO3-....         62.0049         -1.       .1880E+01
NO2-....         46.0000         -1.       .1120E+01
Al(OH)4-         95.0000         -1.       .1300E+00
SO4--...         96.0636         -2.       .4000E-01
CO3--...         60.0092         -2.       .4800E+00
F-......         18.9984         -1.       .1000E-01
Cl-.....         35.4527         -1.       .9000E-01
CrO4--..        115.9937         -2.       .1000E-01
Other--.         88.0200         -2.       .1000E-01
PO4---..         94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.475977771148533 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .1044E+00      .5530E-01      .1888E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .5023E+00      .1100E+03      .4567E+01
```

- DFLAW Batch 6

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 6 MaxLoading@56F                                                       Title
9, 11                                                                        Number of Cations & Anions
1250.73                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.51, 4.85E-05, 6.7114E-15, 0, 0.1, 0, 0, 0, 0                               Concentrations of Cations
1.49, 1.620049, 1.18, 0.16, 0.04, 0.44, 0.01, 0.09, 0.01, 0.01, 0.02         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 6 MaxLoading@56F
**********INPUT**********

  Density=  .1251E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5510E+01
Cs+.....       132.9054          1.       .4850E-04
H+......         1.0079          1.       .6711E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1000E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1490E+01
NO3-....        62.0049         -1.       .1620E+01
NO2-....        46.0000         -1.       .1180E+01
Al(OH)4-        95.0000         -1.       .1600E+00
SO4--...        96.0636         -2.       .4000E-01
CO3--...        60.0092         -2.       .4400E+00
F-......        18.9984         -1.       .1000E-01
Cl-.....        35.4527         -1.       .9000E-01
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.333934458345263 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .9979E-01      .4850E-01      .2058E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .4949E+00      .1000E+03      .4949E+01
```

- DFLAW Batch 7

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 7 MaxLoading@56F                                                       Title
9, 11                                                                        Number of Cations & Anions
1260.48                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.89, 4.75E-05, 6.6225E-15, 0, 0.05, 0, 0, 0, 0                              Concentrations of Cations
1.51, 1.47, 0.98, 0.17, 0.06, 0.58, 0.04, 0.390048, 0.01, 0.01, 0.02         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 7 MaxLoading@56F
**********INPUT**********

  Density=  .1260E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5890E+01
Cs+.....       132.9054          1.       .4750E-04
H+......         1.0079          1.       .6623E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .5000E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1510E+01
NO3-....        62.0049         -1.       .1470E+01
NO2-....        46.0000         -1.       .9800E+00
Al(OH)4-        95.0000         -1.       .1700E+00
SO4--...        96.0636         -2.       .6000E-01
CO3--...        60.0092         -2.       .5800E+00
F-......        18.9984         -1.       .4000E-01
Cl-.....        35.4527         -1.       .3900E+00
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           8.020210709035263 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1134E+00      .4750E-01      .2387E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3314E+00      .5000E+02      .6629E+01
```

- DFLAW Batch 8

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 8 MaxLoading@56F                                                       Title
9, 11                                                                        Number of Cations & Anions
1249.49                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.61, 4.44E-05, 7.1429E-15, 0, 0.08, 0, 0, 0, 0                              Concentrations of Cations
1.4, 1.31, 0.96, 0.16, 0.06, 0.59, 0.03, 0.400044, 0.01, 0.01, 0.03          Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 8 MaxLoading@56F
**********INPUT**********

  Density=  .1249E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5610E+01
Cs+.....       132.9054          1.       .4440E-04
H+......         1.0079          1.       .7143E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .8000E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1400E+01
NO3-....        62.0049         -1.       .1310E+01
NO2-....        46.0000         -1.       .9600E+00
Al(OH)4-        95.0000         -1.       .1600E+00
SO4--...        96.0636         -2.       .6000E-01
CO3--...        60.0092         -2.       .5900E+00
F-......        18.9984         -1.       .3000E-01
Cl-.....        35.4527         -1.       .4000E+00
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .3000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.746485401708123 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1024E+00      .4440E-01      .2307E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .4594E+00      .8000E+02      .5743E+01
```

- DFLAW Batch 9

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 9a MaxLoading@56F                                                      Title
9, 11                                                                        Number of Cations & Anions
1266.94                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.53, 4.39E-05, 5.6818E-15, 0, 0.41, 0, 0, 0, 0                              Concentrations of Cations
1.76, 1.57, 0.93, 0.19, 0.05, 0.59, 0.07, 0.040044, 0.01, 0.01, 0.02         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
  Solution:  Batch 9a MaxLoading@56F
**********INPUT**********

   Density=  .1267E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .5530E+01
Cs+.....        132.9054          1.       .4390E-04
H+......          1.0079          1.       .5682E-14
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .4100E+00
Sr++....         87.6200          2.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Ca++....         40.0780          2.       .0000E+00
Pb++....        207.2000          2.       .0000E+00
OH-.....         17.0073         -1.       .1760E+01
NO3-....         62.0049         -1.       .1570E+01
NO2-....         46.0000         -1.       .9300E+00
Al(OH)4-         95.0000         -1.       .1900E+00
SO4--...         96.0636         -2.       .5000E-01
CO3--...         60.0092         -2.       .5900E+00
F-......         18.9984         -1.       .7000E-01
Cl-.....         35.4527         -1.       .4004E-01
CrO4--..        115.9937         -2.       .1000E-01
Other--.         88.0200         -2.       .1000E-01
PO4---..         94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.994521146178503 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .7344E-01      .4390E-01      .1673E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .8641E+00      .4100E+03      .2108E+01
```

- DFLAW Batch 10

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 10 MaxLoading@56F                                                      Title
9, 11                                                                        Number of Cations & Anions
1259.82                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                                  C2O4-- MW
5.5, 5.59E-05, 7.5758E-15, 0, 0.25, 0, 0, 0, 0                               Concentrations of Cations
1.32, 1.77, 1.05, 0.14, 0.04, 0.59, 0.04, 0.070056, 0.01, 0.01, 0.02         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 10 MaxLoading@56F
**********INPUT**********

  Density=  .1260E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5500E+01
Cs+.....       132.9054          1.       .5590E-04
H+......         1.0079          1.       .7576E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .2500E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1320E+01
NO3-....        62.0049         -1.       .1770E+01
NO2-....        46.0000         -1.       .1050E+01
Al(OH)4-        95.0000         -1.       .1400E+00
SO4--...        96.0636         -2.       .4000E-01
CO3--...        60.0092         -2.       .5900E+00
F-......        18.9984         -1.       .4000E-01
Cl-.....        35.4527         -1.       .7006E-01
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.807286612227051 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .9267E-01      .5590E-01      .1658E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .7287E+00      .2500E+03      .2915E+01
```

- DFLAW Batch 11

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 11 MaxLoading@56F                                                      Title
9, 11                                                                        Number of Cations & Anions
1251.85                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.5, 4.74E-05, 8.6957E-15, 0, 0.11, 0, 0, 0, 0                               Concentrations of Cations
1.15, 1.53, 1.09, 0.12, 0.07, 0.62, 0.02, 0.190047, 0.01, 0.01, 0.03         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
  Solution:  Batch 11 MaxLoading@56F
**********INPUT**********

   Density=  .1252E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .5500E+01
Cs+.....        132.9054          1.       .4740E-04
H+......          1.0079          1.       .8696E-14
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .1100E+00
Sr++....         87.6200          2.       .0000E+00
SrOH+...        105.0000          1.       .0000E+00
Ca++....         40.0780          2.       .0000E+00
Pb++....        207.2000          2.       .0000E+00
OH-.....         17.0073         -1.       .1150E+01
NO3-....         62.0049         -1.       .1530E+01
NO2-....         46.0000         -1.       .1090E+01
Al(OH)4-         95.0000         -1.       .1200E+00
SO4--...         96.0636         -2.       .7000E-01
CO3--...         60.0092         -2.       .6200E+00
F-......         18.9984         -1.       .2000E-01
Cl-.....         35.4527         -1.       .1900E+00
CrO4--..        115.9937         -2.       .1000E-01
Other--.         88.0200         -2.       .1000E-01
PO4---..         94.9712         -3.       .3000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.756022276246446 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .9997E-01      .4740E-01      .2109E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .5300E+00      .1100E+03      .4818E+01
```

- DFLAW Batch 12

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 12 MaxLoading@56F                                                      Title
9, 11                                                                        Number of Cations & Anions
1254.46                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.51, 5.46E-05, 7.4627E-15, 0, 0.15, 0, 0, 0, 0                              Concentrations of Cations
1.34, 1.69, 1.11, 0.14, 0.04, 0.52, 0.03, 0.130055, 0.01, 0.01, 0.02         Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 12 MaxLoading@56F
**********INPUT**********

  Density=  .1254E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5510E+01
Cs+.....       132.9054          1.       .5460E-04
H+......         1.0079          1.       .7463E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1500E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1340E+01
NO3-....        62.0049         -1.       .1690E+01
NO2-....        46.0000         -1.       .1110E+01
Al(OH)4-        95.0000         -1.       .1400E+00
SO4--...        96.0636         -2.       .4000E-01
CO3--...        60.0092         -2.       .5200E+00
F-......        18.9984         -1.       .3000E-01
Cl-.....        35.4527         -1.       .1301E+00
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.552076549143477 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .1002E+00      .5460E-01      .1835E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .5962E+00      .1500E+03      .3975E+01
```

- DFLAW Batch 13

ZAM Input

```
1, 286.48                                                                  Activity Coeff. Model, Temperature
Batch 13 MaxLoading@56F                                                    Title
9, 11                                                                      Number of Cations & Anions
1252.85                                                                    Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                        Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                 Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                      C2O4-- MW
5.51, 4.99E-05, 7.4627E-15, 0, 0.11, 0, 0, 0, 0                            Concentrations of Cations
1.34, 1.67005, 1.13, 0.14, 0.05, 0.52, 0.02, 0.08, 0.01, 0.01, 0.02        Concentrations of Anions
1, 0.000001                                                                Liquid (L), Solid (g)
0                                                                          Initial Solid Form (Na+ (0); H- (1))
1                                                                          Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 13 MaxLoading@56F
**********INPUT**********

  Density=  .1253E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5510E+01
Cs+.....       132.9054          1.       .4990E-04
H+......         1.0079          1.       .7463E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1100E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1340E+01
NO3-....        62.0049         -1.       .1670E+01
NO2-....        46.0000         -1.       .1130E+01
Al(OH)4-        95.0000         -1.       .1400E+00
SO4--...        96.0636         -2.       .5000E-01
CO3--...        60.0092         -2.       .5200E+00
F-......        18.9984         -1.       .2000E-01
Cl-.....        35.4527         -1.       .8000E-01
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.514018892751782 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .1007E+00      .4990E-01      .2017E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .5197E+00      .1100E+03      .4725E+01
```

- DFLAW Batch 14

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 14 MaxLoading@56F                                                      Title
9, 11                                                                        Number of Cations & Anions
1252.85                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.51, 4.79E-05, 7.6923E-15, 0, 0.09, 0, 0, 0, 0                              Concentrations of Cations
1.3, 1.61, 1.13, 0.14, 0.05, 0.52, 0.02, 0.160048, 0.01, 0.01, 0.02          Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 14 MaxLoading@56F
**********INPUT**********

  Density=  .1253E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5510E+01
Cs+.....       132.9054          1.       .4790E-04
H+......         1.0079          1.       .7692E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .9000E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1300E+01
NO3-....        62.0049         -1.       .1610E+01
NO2-....        46.0000         -1.       .1130E+01
Al(OH)4-        95.0000         -1.       .1400E+00
SO4--...        96.0636         -2.       .5000E-01
CO3--...        60.0092         -2.       .5200E+00
F-......        18.9984         -1.       .2000E-01
Cl-.....        35.4527         -1.       .1600E+00
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .2000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.471178058446445 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1024E+00      .4790E-01      .2137E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .4702E+00      .9000E+02      .5224E+01
```

- DFLAW Batch 15

ZAM Input

```
1, 286.48                                                                    Activity Coeff. Model, Temperature
Batch 15 MaxLoading@56F                                                      Title
9, 11                                                                        Number of Cations & Anions
1247.95                                                                      Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.5, 3.98E-05, 8.5470E-15, 0, 0.06, 0, 0, 0, 0                               Concentrations of Cations
1.17, 1.68, 0.99, 0.13, 0.05, 0.48, 0.01, 0.36004, 0.01, 0.01, 0.04          Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 15 MaxLoading@56F
**********INPUT**********

  Density=  .1248E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5500E+01
Cs+.....       132.9054          1.       .3980E-04
H+......         1.0079          1.       .8547E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .6000E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1170E+01
NO3-....        62.0049         -1.       .1680E+01
NO2-....        46.0000         -1.       .9900E+00
Al(OH)4-        95.0000         -1.       .1300E+00
SO4--...        96.0636         -2.       .5000E-01
CO3--...        60.0092         -2.       .4800E+00
F-......        18.9984         -1.       .1000E-01
Cl-.....        35.4527         -1.       .3600E+00
CrO4--..       115.9937         -2.       .1000E-01
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .4000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.487903844783251 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs       .9355E-01      .3980E-01      .2350E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3713E+00      .6000E+02      .6189E+01
```

- DFLAW Batch 16

ZAM Input

```
1, 286.48                                                          Activity Coeff. Model, Temperature
Batch 16 MaxLoading@56F                                            Title
9, 11                                                              Number of Cations & Anions
1257.6                                                             Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                               Cations(Na+, Cs+, H+, Rb+, K+, Sr+2,
SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                         Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2,
CO3-2, F-, Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                              C2O4-- MW
5.5, 1.75E-05, 1.5152E-14, 0, 0.02, 0, 0, 0, 0                     Concentrations of Cations
0.66, 2.78, 0.99, 0.07, 0.04, 0.24, 0.01, 0.310018, 0, 0.01, 0.04  Concentrations of Anions
1, 0.000001                                                        Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 16 MaxLoading@56F
**********INPUT**********

  Density=  .1258E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5500E+01
Cs+.....       132.9054          1.       .1750E-04
H+......         1.0079          1.       .1515E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .2000E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .6600E+00
NO3-....        62.0049         -1.       .2780E+01
NO2-....        46.0000         -1.       .9900E+00
Al(OH)4-        95.0000         -1.       .7000E-01
SO4--...        96.0636         -2.       .4000E-01
CO3--...        60.0092         -2.       .2400E+00
F-......        18.9984         -1.       .1000E-01
Cl-.....        35.4527         -1.       .3100E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .4000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.158892491722497 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .4185E-01      .1750E-01      .2391E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .1375E+00      .2000E+02      .6876E+01
```

- DFLAW Batch 17

ZAM Input

```
1, 286.48                                                          Activity Coeff. Model, Temperature
Batch 17 MaxLoading@56F                                            Title
9, 11                                                              Number of Cations & Anions
1263.42                                                            Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                         Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                           Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                              C2O4-- MW
5.5, 8.84E-06, 2.0833E-14, 0, 0.01, 0, 0, 0, 0                     Concentrations of Cations
0.48, 3.29, 1.01, 0.05, 0.03, 0.18, 0.01, 0.110009, 0, 0.01, 0.04  Concentrations of Anions
1, 0.000001                                                        Liquid (L), Solid (g)
0                                                                  Initial Solid Form (Na+ (0); H- (1))
1                                                                  Calculation Adjustment
```

ZAM Output

```
 Solution:  Batch 17 MaxLoading@56F
**********INPUT**********

  Density=  .1263E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5500E+01
Cs+.....       132.9054          1.       .8840E-05
H+......         1.0079          1.       .2083E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1000E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .4800E+00
NO3-....        62.0049         -1.       .3290E+01
NO2-....        46.0000         -1.       .1010E+01
Al(OH)4-        95.0000         -1.       .5000E-01
SO4--...        96.0636         -2.       .3000E-01
CO3--...        60.0092         -2.       .1800E+00
F-......        18.9984         -1.       .1000E-01
Cl-.....        35.4527         -1.       .1100E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .1000E-01
PO4---..        94.9712         -3.       .4000E-01

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

 Material: Na Form


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

 Ionic Strength=           7.095073905589499 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .2069E-01      .8840E-02      .2340E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .6821E-01      .1000E+02      .6821E+01
```

- Hanford Tank AP-105 @ 13 °C

ZAM Input

```
1, 286.15                                                                    Activity Coeff. Model, Temperature
AP-105 MaxLoading @ 13C                                                      Title
9, 11                                                                        Number of Cations & Anions
1285.0                                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.92, 5.66E-05, 8.0645E-15, 0, 0.102, 0, 0, 0, 0                             Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 0.90542, 0, 0.00284, 0.00872          Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 MaxLoading @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .5660E-04
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9054E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

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

 Material: Na Form


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

 Ionic Strength=           7.116164945515645 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs       .8443E-01      .5660E-01      .1492E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .4080E+00      .1020E+03      .4000E+01
```

- Hanford Tank AP-105 @ 21 °C

ZAM Input

```
1, 294.15                                                                    Activity Coeff. Model, Temperature
AP-107 MaxLoading @ 21C                                                      Title
9, 11                                                                        Number of Cations & Anions
1285.0                                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.92, 5.66E-05, 8.0645E-15, 0, 0.102, 0, 0, 0, 0                             Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 0.90542, 0, 0.00284, 0.00872          Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-107 MaxLoading @ 21C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .5660E-04
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9054E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

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

 Material: Na Form


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

 Ionic Strength=           7.116164945515644 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .7409E-01      .5660E-01      .1309E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3576E+00      .1020E+03      .3506E+01
```

- Hanford Tank AP-107 @ 13 °C

ZAM Input

```
1, 286.15                                                                    Activity Coeff. Model, Temperature
AP-107 MaxLoading @ 13C                                                      Title
9, 11                                                                        Number of Cations & Anions
1266.0                                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.795, 5.728E-05, 1.1236E-14, 0, 0.096, 0, 0, 0, 0                          Concentrations of Cations
0.89, 2.06435, 1.2933, 0.373, 0.04554, 0, 0.01858, 1.072797, 0, 0.0052, 0.02585  Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-107 MaxLoading @ 13C
**********INPUT**********

  Density=  .1266E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5795E+01
Cs+.....       132.9054          1.       .5728E-04
H+......         1.0079          1.       .1124E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .9600E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .8900E+00
NO3-....        62.0049         -1.       .2064E+01
NO2-....        46.0000         -1.       .1293E+01
Al(OH)4-        95.0000         -1.       .3730E+00
SO4--...        96.0636         -2.       .4554E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .1858E-01
Cl-.....        35.4527         -1.       .1073E+01
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .5200E-02
PO4---..        94.9712         -3.       .2585E-01

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

 Material: Na Form


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

 Ionic Strength=           7.196601910654217 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs       .8418E-01      .5728E-01      .1470E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3847E+00      .9600E+02      .4007E+01
```

- Hanford Tank AP-107 @ 17 °C

ZAM Input

```
1, 290.15                                                                    Activity Coeff. Model, Temperature
AP-107 MaxLoading @ 17C                                                      Title
9, 11                                                                        Number of Cations & Anions
1266.0                                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.795, 5.728E-05, 1.1236E-14, 0, 0.096, 0, 0, 0, 0                          Concentrations of Cations
0.89, 2.06435, 1.2933, 0.373, 0.04554, 0, 0.01858, 1.072797, 0, 0.0052, 0.02585  Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-107 MaxLoading @ 17C
**********INPUT**********

  Density=  .1266E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5795E+01
Cs+.....       132.9054          1.       .5728E-04
H+......         1.0079          1.       .1124E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .9600E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .8900E+00
NO3-....        62.0049         -1.       .2064E+01
NO2-....        46.0000         -1.       .1293E+01
Al(OH)4-        95.0000         -1.       .3730E+00
SO4--...        96.0636         -2.       .4554E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .1858E-01
Cl-.....        35.4527         -1.       .1073E+01
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .5200E-02
PO4---..        94.9712         -3.       .2585E-01

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

 Material: Na Form


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

 Ionic Strength=           7.196601910654215 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs       .7881E-01      .5728E-01      .1376E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3595E+00      .9600E+02      .3745E+01
```

- Hanford Tank AP-107 @ 21 °C

ZAM Input

```
1, 294.15                                                                    Activity Coeff. Model, Temperature
AP-107 MaxLoading @ 21C                                                      Title
9, 11                                                                        Number of Cations & Anions
1266.0                                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-,
                                                                                     Cl-, CrO4-2, C2O4-2, PO4-3)
88.02                                                                        C2O4-- MW
5.795, 5.728E-05, 1.1236E-14, 0, 0.096, 0, 0, 0, 0                          Concentrations of Cations
0.89, 2.06435, 1.2933, 0.373, 0.04554, 0, 0.01858, 1.072797, 0, 0.0052, 0.02585  Concentrations of Anions
1, 0.000001                                                                  Liquid (L), Solid (g)
0                                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-107 MaxLoading @ 21C
**********INPUT**********

  Density=  .1266E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5795E+01
Cs+.....       132.9054          1.       .5728E-04
H+......         1.0079          1.       .1124E-13
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .9600E-01
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .8900E+00
NO3-....        62.0049         -1.       .2064E+01
NO2-....        46.0000         -1.       .1293E+01
Al(OH)4-        95.0000         -1.       .3730E+00
SO4--...        96.0636         -2.       .4554E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .1858E-01
Cl-.....        35.4527         -1.       .1073E+01
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .5200E-02
PO4---..        94.9712         -3.       .2585E-01

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

 Material: Na Form


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

 Ionic Strength=           7.196601910654214 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs       .7370E-01      .5728E-01      .1287E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3347E+00      .9600E+02      .3486E+01
```

Adsorption/Desorption Isotherm Data

The ZAM model is used to generate the equilibrium cesium loading/unloading data at a specific temperature. The isotherm data cover a wide range of liquid-phase cesium concentrations (i.e., from 1E-9M to 1E-1M). For demonstration, isotherm data for Tank AP-105 at 13 °C are given in this Appendix.

Hanford Tank AP-105 at 13 ℃

- C_{Cs+} = 1E-9 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-09, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.05360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E-08
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9054E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.116019844913684 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1743E-05      .9983E-06      .1746E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .4322E+00      .1020E+03      .4237E+01
```

- C_{Cs+} = 1E-8 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-08, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.05360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E-07
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9054E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.116019850174299 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1743E-04      .9983E-05      .1746E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .4322E+00      .1020E+03      .4237E+01
```

- C_{Cs+} = 1E-7 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-07, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.05360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E-06
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9054E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.116019902780423 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1742E-03      .9983E-04      .1745E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .4321E+00      .1020E+03      .4236E+01
```

- C_{Cs+} = 1E-6 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-06, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.05361E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E-05
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9054E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.116021649895344 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1738E-02      .9983E-03      .1741E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .4317E+00      .1020E+03      .4232E+01
```

- C_{Cs+} = 1E-5 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-05, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.05370E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E-04
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9054E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.116044527301685 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .1692E-01      .9983E-02      .1695E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .4273E+00      .1020E+03      .4190E+01
```

- C_{Cs+} = 5E-5 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 5.0E-05, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.05410E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .5000E-04
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9054E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.116147140610574 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .7578E-01      .4992E-01      .1518E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .4105E+00      .1020E+03      .4025E+01
```

- C_{Cs+} = 1E-4 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-04, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.05460E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E-03
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9055E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.116275285765049 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .1341E+00      .9987E-01      .1342E+04
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3938E+00      .1020E+03      .3861E+01
```

- C_{Cs+} = 5E-4 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 5.0E-04, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.05860E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .5000E-03
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9059E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.117301032604240 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .3483E+00      .4997E+00      .6972E+03
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .3326E+00      .1020E+03      .3260E+01
```

- C_{Cs+} = 1E-3 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-03, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.06360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E-02
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9064E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.118584309443002 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .4353E+00      .9996E+00      .4355E+03
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .3077E+00      .1020E+03      .3017E+01
```

- C_{Cs+} = 2E-3 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 2.0E-03, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.07360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .2000E-02
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9074E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.121150629127079 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .4973E+00      .2000E+01      .2487E+03
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .2899E+00      .1020E+03      .2842E+01
```

- C_{Cs+} = 3E-3 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 3.0E-03, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.08360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .3000E-02
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9084E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.123718453423388 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .5221E+00      .2999E+01      .1741E+03
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .2828E+00      .1020E+03      .2772E+01
```

- C_{Cs+} = 5E-3 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 5.0E-03, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.10360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .5000E-02
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9104E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.128856636129060 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs        .5438E+00      .4999E+01      .1088E+03
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .2765E+00      .1020E+03      .2711E+01
```

- C_{Cs+} = 1E-2 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-02, 8.0645E-15, 0, 0.102, 0, 0, 0, 0             Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.15360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E-01
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9154E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.141720042485129 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .5613E+00      .9999E+01      .5613E+02
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .2713E+00      .1020E+03      .2659E+01
```

- C_{Cs+} = 2E-2 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 2.0E-02, 8.0645E-15, 0, 0.102, 0, 0, 0, 0             Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.25360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .2000E-01
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9254E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.167522973986551 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .5704E+00      .2000E+02      .2852E+02
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .2682E+00      .1020E+03      .2629E+01
```

- C_{Cs+} = 5E-2 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                         Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 5.0E-02, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 9.55360E-01, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .5000E-01
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .9554E+00
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.245545647171354 mol/kg

       Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs       .5761E+00      .5000E+02      .1152E+02
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .2652E+00      .1020E+03      .2600E+01
```

- C_{Cs+} = 1E-1 M:

ZAM Input

```
1, 286.15                                                    Activity Coeff. Model, Temperature
AP-105 Isotherm @ 13C                                        Title
9, 11                                                        Number of Cations (min: 7) & Anions (min: 2)
1285.0                                                       Density(kg/m3)
 3,  6,  1,   5,  4, 13, 40, 12, 22                          Cations(Na+, Cs+, H+, Rb+, K+, Sr+2, SrOH+, Ca++, Pb++)
13,  9, 27,  28, 15, 19, 1, 2, 14, 25, 20                   Anions (OH-, NO3-, NO2-, Al(OH)4-, SO4-2, CO3-2, F-, Cl-, CrO4-2,
                                                                C2O4-2, PO4-3)
88.02                                                        C2O4-- MW
5.92, 1.0E-01, 8.0645E-15, 0, 0.102, 0, 0, 0, 0              Concentrations of Cations
1.24, 1.89, 1.38, 0.526, 0.0244, 0, 0, 1.00536E+00, 0, 0.00284, 0.00872  Concentrations of Anions
1, 0.001                                                     Liquid (L), Solid (g)
0                                                            Initial Solid Form (Na+ (0); H- (1))
1                                                            Calculation Adjustment
```

ZAM Output

```
 Solution:  AP-105 Isotherm @ 13C
**********INPUT**********

  Density=  .1285E+04 kg/m3

             Molecular Wt.    Valance    Molarity(mol/L)
Na+.....        22.9898          1.       .5920E+01
Cs+.....       132.9054          1.       .1000E+00
H+......         1.0079          1.       .8065E-14
Rb+.....        85.4678          1.       .0000E+00
K+......        39.0983          1.       .1020E+00
Sr++....        87.6200          2.       .0000E+00
SrOH+...       105.0000          1.       .0000E+00
Ca++....        40.0780          2.       .0000E+00
Pb++....       207.2000          2.       .0000E+00
OH-.....        17.0073         -1.       .1240E+01
NO3-....        62.0049         -1.       .1890E+01
NO2-....        46.0000         -1.       .1380E+01
Al(OH)4-        95.0000         -1.       .5260E+00
SO4--...        96.0636         -2.       .2440E-01
CO3--...        60.0092         -2.       .0000E+00
F-......        18.9984         -1.       .0000E+00
Cl-.....        35.4527         -1.       .1005E+01
CrO4--..       115.9937         -2.       .0000E+00
Other--.        88.0200         -2.       .2840E-02
PO4---..        94.9712         -3.       .8720E-02

Liquid(L)= .1000E+01   Solid(g)= .1000E-02

 Material: Na Form


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

 Ionic Strength=           7.377668644154255 mol/kg

       Q (mmol/gCST)    C (mmol/L)     Kd (ml/gCST)
Cs       .5780E+00      .1000E+03      .5780E+01
Rb       .0000E+00      .0000E+00      .0000E+00
Sr       .0000E+00      .0000E+00      .0000E+00
K        .2624E+00      .1020E+03      .2572E+01
```

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