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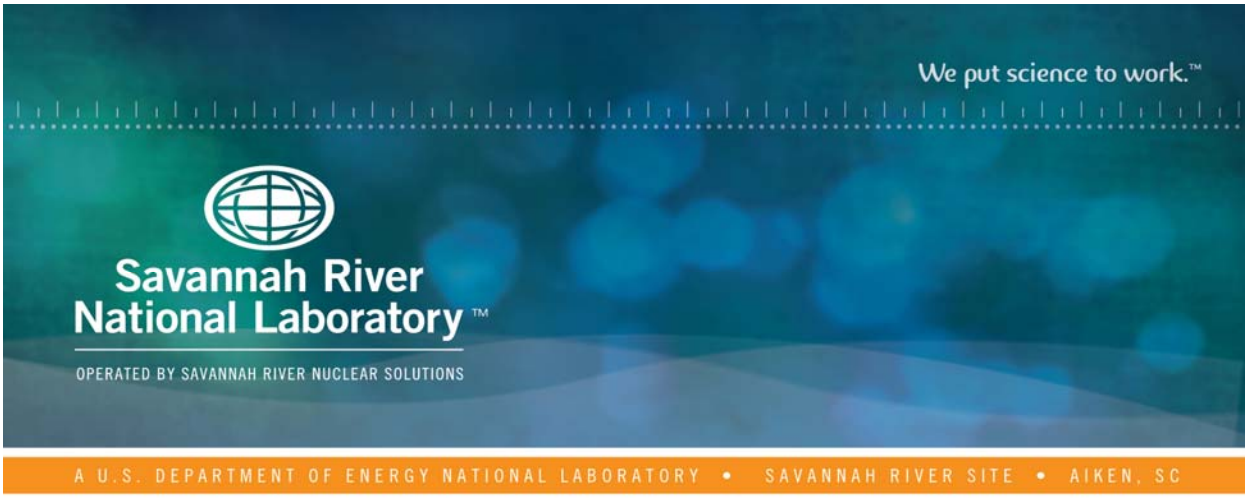

Crystalline Silicotitanate Ion Exchange Column Sizing and Sensitivity Study in Support of the Hanford Test Bed Initiative

L. Larry Hamm
Daniel J. McCabe

October 2018
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EXECUTIVE SUMMARY

The Environmental Management Office of the Department of Energy (DOE) is spearheading a Test Bed Initiative[a] (TBI) to treat and dispose 2,000 gallons of tank waste from Hanford. One step in the process is to remove radioactive ^{137}Cs from the waste using Crystalline Silicotitanate[b] (CST) ion exchange media. This report describes the modeling performed to provide an estimate of the volume of a bed of CST required to meet the design requirements. Sensitivity studies were also performed to help provide project guidance. This modeling effort assumed 2100 gallons of waste to be processed (i.e., entire 2000 gallon campaign plus a 100 gallon margin).

The Savannah River National Laboratory (SRNL) has extensive experience in the testing and modeling of ion exchange columns using CST for the explicit removal of ^{137}Cs from highly caustic feed solutions. This analysis effort uses SRNL's modeling methodology for CST based on extensive testing for Savannah River Site (SRS), Hanford Site, and other DOE Complex-wide applications. This methodology has been used to assess primarily waste streams with typically lower potassium concentrations than that expected for the TBI waste stream and with CST manufactured into a smaller bead size than planned for use in TBI. However, while applying the existing model methodology to recent CST testing of Hanford simulant and actual tank waste, it was found capable of adequately predicting measured Cs breakthrough performance at high potassium and with larger bead size media. As the results provided in this report indicate, a reliable calculational scheme has been achieved that can provide design guidance on the sizing and expected performance for the upcoming TBI ion exchange column.

For the TBI system, *design estimates* and *best estimates*, under nominal operating constraints, are provided for a range of possible CST bed volumes. The *design estimates* are conservative projections of column loading performance that attempt to account for several unknowns, while the *best estimates* are the closest fit of the parameters based on available performance test data, ignoring the potential impact of the unknowns. Although most historical testing was performed using smaller particle size beads of CST, this modeling effort assumes a larger mean particle size that is implicitly handled within the calculational scheme. The nominal conditions for modeling are: (1) a mean particle diameter of 573 microns; (2) a liquid feed flowrate of 1.0 gallon per minute (gpm); (3) a decontamination factor of 1000; (4) a very small (near zero) composited effluent volume; (5) no impact associated with the presence of Sr^{+2} within the feed solution; and (6) a composition of tank waste listed in the Functions and Requirements document.[c] The results from these various cases are listed in Table ES-1 where nominal conditions prevail unless explicitly listed otherwise. Additionally, Cs breakthrough performance calculations were made to assess the impact of:

- varying the method of compositing the decontaminated effluent stream;
- targeting a decontamination factor of 400;
- the presence of soluble strontium (Sr^{+2}) in the tank waste feed; and
- the use of a smaller diameter distribution of CST beads.

Note that Sr in the form of $SrOH^{+}$ is a strong competitor with Cs^{+} for CST exchange sites and the amount of Sr in this form within the TBI feed is currently unknown. The analyses presented in this report, where specified, assumes the estimated concentration of Sr and that all of it is available in this chemical form, which should represent a conservative projection.

[a] https://www.energy.gov/sites/prod/files/2018/08/f55/FINAL-Hanford-Test-Bed-Initiative-Fact-Sheet-8.28.18.pdf
[b] Crystalline Silicotitanate (CST) was developed by researchers at Texas A&M University along with Sandia National Laboratory; and is currently produced as an engineered inorganic bead by Honeywell UOP, LLC, Des Plaines, IL, USA. The engineered material is identified as "IONSIV™ IE-9120-B."
[c] WRPS-1801574 Rev. 4/TOC-WP-18-2290, Rev-1

At the nominal conditions listed above, a 27-gallon bed size is recommended. This is not the maximum *design estimate* size shown in Table ES-1, but is the *best estimate* plus some level of operational margin to accommodate for typical variances that occur in these sorts of unit operations (e.g., flowrate variations, non-uniform bed packing allowances, media capacity variance, feed composition changes, etc.). The strontium concentration has potential to have a significant impact on column performance as indicated in Table ES-1, but the concentration of Sr in the feed composition used in the modeling was from an inventory projection. It is recommended that the actual measured soluble Sr value, when available, should ultimately be used to gauge the expected actual impact.

Table ES-1. TBI column sizing summary under nominal conditions except where specified.

Sr Present	DF (-)	Composite Volume * (gal)	Best Est (gal)	Design Est (gal)
No	1000	<<1	20.8	27.1
		300	20.1	26.3
		2100	18.4	23.4
	400	<<1	19.2	24.9
		300	18.4	24.0
		2100	16.5	21.3
Yes	1000	<<1	25.7	33.2
		300	24.9	32.1
		2100	22.5	29.2
	400	<<1	23.7	30.5
		300	22.9	29.5
		2100	20.5	25.7

* Three options for effluent compositing were evaluated: none (<<1), collection in seven totes of 300 gallons each, and total compositing of 2100 gallons (entire campaign plus 100 gallon margin).

Since a 27-gallon column bed size is not viable due to other design constraints, modeling was also performed to examine the potential options available for use of a 20-gallon bed. A bed smaller than 27 gallons can be used if one of the following three options is selected: (1) use of a smaller bead size material; (2) use of a lower flow rate; or (3) larger composite size of the decontaminated effluent. Sensitivity calculations focusing in on these options are shown in Tables ES-2 and ES-3.

Table ES-2. Maximum feed flowrate requirements to maintain stated decontamination factors for a 20 gallon TBI column

Sr Present	DF (-)	Composite Volume (gal)	Best Est (gpm)	Design Est (gpm)
No	1000	<<1	0.91	0.53
		300	0.98	0.58
		2100	>1.10	0.70
	400	<<1	1.09	0.64
		300	>1.10	0.68
		2100	>1.10	0.88
Yes	1000	<<1	0.57	<.50
		300	0.62	<.50
		2100	0.74	<.50
	400	<<1	0.68	<.50
		300	0.73	<.50
		2100	0.94	0.57

Table ES-3. Achievable decontamination factors for a 20 gallon TBI column for two available particle size distributions at 1 gallon per minute.

Sr Present	Mean Particle Size (microns)	Composite Volume (gal)	Best Est (DF)	Design Est (DF)
No	573	<<1	618	66
		300	908	85
		2100	2,219	251
	408	<<1	79,460	1,384
		300	150,724	2,110
		2100	372,099	6,958
Yes	573	<<1	84	19
		300	112	23
		2100	325	67
	408	<<1	2,001	146
		300	3,321	201
		2100	11,335	688

The results shown in Tables ES-2 and ES-3 are one-off sensitivity studies where all parameter settings remain at their nominal values except the one stated parameter that is being considered (i.e., flow rate or particle size).

As Table ES-2 indicates, by decreasing the feed flow rate to about 0.5 gpm, either decontamination factor (1000 or 400) can be achieved. Table ES-3 indicates that by choosing the batch with the smaller 408 micron mean bead diameter, the decontamination factor of 1000 can be achieved for the *design estimate* calculation, even at 1 gpm. If the Sr is present at the projected concentrations, the DF of 400 can still be achieved with the smaller bead size material.

Overall then, the modeling provides projections of the performance of the columns as a function of bed size, bead size, flow rate, and composition. This information can be used along with other project needs and information to arrive at the optimum design and operating strategy.

Details supporting these findings are provided in the main body of this report with additional supporting information given in the appendices. Testing using a full height column and a simulant formulation that mimics the expected chemical composition of the feed would confirm these projections.

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LIST OF ABBREVIATIONS

Avg	Average
BE	Best Estimate
BV	Bed Volume
CST	Crystalline Silicotitanate
DE	Design Estimate
DF	Decontamination Factor
DOE	Department of Energy
gpm	Gallons per minute
hr	hour
Kd	Distribution coefficient
LW	Liquid Waste
M	Molar
mmole	millimole
PNNL	Pacific Northwest National Laboratory
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
TBI	Test Bed Initiative

1.0 Introduction

This report describes the calculations performed to provide an estimate of the CST bed volume required to meet or exceed the TBI design requirements as outlined in the Functions and Requirements report (WRPS-1801574 Rev. 4/TOC-WP-18-2290, Rev-1) and additional communications. The calculations presented within this report have been technically reviewed. Given that various design constraints were being investigated as options at the time of producing these results, a series of sensitivity runs were also made to help provide project guidance. For example, the major design aspects considered in the limited sensitivity studies were (the original nominal setting for each of these parameters is provided in parentheses to the right):

- Column sizes from 16 to 35 gal (20 gal bed in a 12 inch internal diameter column – implies a Length/Diameter of 3.4)
- Mean particle sizes from 408 to 573 microns (573 microns)
- Feed flowrate from 0.5 to 1.1 gpm (1.0 gpm)
- Three effluent compositing schemes of: (1) no compositing implying an instantaneous breakthrough projection; (2) collection in seven 300-gallon totes; and (3) collection in one homogeneous 2100-gallon batch.)
- Decontamination factors from 400 to 1000 (factor of 1000 reduction in feed Cs concentration)

The results shown in this report are presented in a manner in which a range of DF values within and beyond the 400 and 1000 values can be extracted. For the case of seven 300-gallon totes, the last tote will always be the most restrictive, so the results indicate the DF associated with a composite of the last 300 gallons.

SRNL typically performs "design" analyses employing what we believe to be a modestly conservative methodology. We generally perform such analyses using this methodology as establish by Hamm et al. (2002). This methodology uses the ZAM model to generate an algebraic isotherm, followed by using the isotherm in the VERSE-LC model to calculate a breakthrough profile. For *design estimate* analyses the following two key parameters for CST were set to:

- Isotherm dilution factor → $\eta_{df} = 68\%$ (historically based: mean of experimental data minus one standard deviation)
- Cs^+ particle pore tortuosity factor → $\tau = 10$ (historically bounding in conservative direction)

The isotherm dilution factor is needed because the original isotherm model, known as "ZAM," was based on the powdered form of CST, and the dilution factor is needed to account for the binder used in forming the engineered bead form of CST. The tortuosity is the adjustment in the free stream diffusion of Cs^+ inside the restrictive space inside a bead of the CST binder material. The higher the tortuosity factor, i.e., the more tortuous the path inside the bead, the earlier the predicted column breakthrough because of slower diffusion inside the bead that leads to slower absorption. Therefore, the above parameter settings should yield earlier than expected Cs exit breakthrough behavior.

Calculations presented in this report that were based on the above two parameter settings are referred to as "*design estimates.*" These settings were established by assessments made using available (i.e., prior to 2002) CST batch contact tests data, kinetics data, and column breakthrough data. This testing was performed across the DOE complex and at Texas A&M University by Dr. Raymond Anthony and his research staff. Once data for a specific batch of CST becomes available, a re-analysis can be done to the design to better predict expected performance (i.e., referred to here as our "*best estimate"*). For the TBI CST column sizing effort, this document contains the results of the above two steps (i.e., the *design estimate* analyses and then the follow-up *best estimate* analyses) and the methodology employed in this report is the best available.

The above two parameters were revised, based on recent Pacific Northwest National Laboratory (PNNL) data where a recently manufactured batch of UOP CST media (IONSIV™ R9140-B received in 2018) was used for testing. The new CST batch specific information employed was the batch contact tests and column breakthrough tests performed by Fiskum et al. (2018) for a simple simulant and by Rovira et al. (2018) for actual AP-107 tank waste. There are some results from this testing that are not consistent with historical observations (discussed later in this report), but, given the urgency in arriving at an acceptable column size *best estimate*, we employed these test results to establish more batch-specific parameter values:

- Isotherm dilution factor → $\eta_{df} = 52\%$ (at the bottom range of historical batches)
- Cs^+ tortuosity factor → $\tau = 4$ (typically observed in many historical batches)

All of the data provided in Fiskum et al. (2018) were incorporated/considered into the analyses effort to arrive at the values shown above. The data provided by Rovira et al. (2018) was only employed in a confirmatory manner as a separate check on the alignment of the projections with the testing. In addition, Fiskum et al. (2018) measured the gamma distribution in one of their lead/lag configurations. Model runs employing the *best estimate* parameter settings produced Cs loading profiles consistent with their measurements.

To accomplish the column sizing and sensitivity studies mentioned above, several computational tasks were performed and are discussed in subsequent sections of this report. More detailed information on these steps is provided in the Appendices. Briefly, these computational steps are:

1. Assessment of recent batch specific testing by PNNL (Fiskum, 2018; Rovira, 2018):
   - 5.6 M Na simple simulant isotherm creation (ZAM model based)
   - Red, Blue, and Green lead/lag column breakthrough performance (VERSE-LC model based)
   - Confirmation of isotherm based on column breakthrough to exhaustion
   - Establishing *best estimate* parameter settings
   - Confirming Cs loading profiles with measured gamma profiles
   - Confirming *best estimate* settings with data from the test with actual AP-107 tank waste
2. Creation of isotherms for the projected TBI feed composition (ZAM model based)
3. TBI column sizing under nominal conditions:
   - Column *best estimate* performance varying effluent composite size (VERSE-LC model based)
   - Column *design estimate* performance varying effluent composite size (VERSE-LC model based)
   - Reviewing predicted Cs loading profiles
4. Feed flowrate impact on 20-gallon column performance:
   - Column *best estimate* performance varying effluent composite size (VERSE-LC model based)
   - Column *design estimate* performance varying effluent composite size (VERSE-LC model based)
5. Mean particle size impact on 20-gallon column performance:
   - Column *best estimate* performance varying effluent composite size (VERSE-LC model based)
   - Column *design estimate* performance varying effluent composite size (VERSE-LC model based)

Many of the key ZAM and VERSE-LC input and output files are also provided in the Appendices.

Prior to discussing the detailed computational steps, a review of the isotherm aspects of most importance for our CST analysis efforts will be presented.

2.0 Isotherms

Key features associated with the isotherms employed in the VERSE-LC column runs are discussed in Appendix A. As discussed in Hamm et al. (2002) a simple effective Cs isotherm can be used in VERSE-LC simulations since the majority of constituents within the feed pass through the CST bed un-retarded. However, Sr^{+2} (i.e., actual competitor being in the form of $SrOH^{+}$) is the one exception that exists for the feed solutions being considered here and will be discussed in this report. The three feed solutions considered in this report are provided in Table 2-1 where charge balancing was performed by manipulating the concentration of the chloride ion (Cl^{-}). For all of the anions considered, Cl^{-} is considered to be the spectator ion of choice for charge balancing because of its minimal impact on ionic strength. To create ZAM based Cs isotherms varying amounts of CsCl is added to the baseline compositions shown in Table 2-1.

For comparison purposes, also provided in Table 2-1 is the SRS Average simulant that has been used historically for generic testing of ion exchange materials by SRNL. Recent batch contact testing by King et al. (2018) employed this simulant to test UOP CST material (IONSIV R9120-B) provided to SRS in 2017. The Cs^{+} concentrations provided in Table 2-1 represent the total Cs feed concentrations employed in the column testing and VERSE-LC modeling as discussed later in this report.

The ZAM model accounts for cation competition between H^{+}, Na^{+}, K^{+}, Cs^{+}, Rb^{+}, and $SrOH^{+}$ (i.e., for all of these analyses, Rb^{+} is assumed not present). The effects from anions are accounted for in the liquid-phase activity coefficients, while nonidealities associated with the solid-phase are addressed directly within ZAM through its multi-site triad model.

Table 2-1. Feed compositions considered for ZAM isotherm creations.

Feed Solution	TBI	PNNL Simple Simulant	PNNL AP-107 Actual	SRS Average Simulant
Cations	**[M]**	**[M]**	**[M]**	**[M]**
Na+	6.0462	5.5700	5.4807	5.60
K+	0.1440	0.1220	0.1000	0.015
Sr++	8.1945E-06	0.0	3.7777E-06	0.0
Rb+	0.0	0.0	0.0	0.0
Cs+	5.06E-05	5.97E-05	6.39E-05	1.00E-04
Anions	**[M]**	**[M]**	**[M]**	**[M]**
OH-	1.1289	1.4100	0.9900	1.91
NO3-	1.9515	1.7800	1.7095	2.14
NO2-	1.2368	1.0200	1.1433	0.52
F-	0.0208	0.0000	0.0000	0.032
Cl-	0.0781	0.1179	0.0197	0.025
Al(OH)4-	0.5152	0.1660	0.3651	0.31
CO3--	0.5332	0.4680	0.6358	0.16
SO4--	0.0403	0.0660	0.0159	0.15
PO4---	0.0373	0.0434	0.0165	0.01

Table 2-2 provides additional information pertinent to the creation of ZAM-based isotherms for each of these solutions. Property estimates are based on calculations using the Environmental Simulation Program by OLI Systems, Inc., and are also provided in Table 2-2. OLI property predictions have historically been shown to be reasonably accurate and reliable. From the ZAM-based results Langmuir isotherms are generated where the predicted beta-factors are listed in Table 2-2 solutions with and without Sr^{+2} being present.

Table 2-2. OLI predicted properties at feed conditions and other key parameter settings employed in assessing batch contact data.

Feed Solution	TBI	PNNL Simple Simulant	PNNL AP-107 Actual	SRS Average Simulant
temperature (C)	22	24	27	23.2
density (g/ml)	1.244	1.227	1.222	1.230
absolute viscosity (cP)	2.695	2.391	2.147	2.562
ZAM Generated Beta-Factor [M]	without Sr: 3.6000E-04 with Sr: 5.4720E-04	without Sr: 3.1154E-04	with Sr: 3.7377E-04	without Sr: 2.3550E-04
Dilution Factor (-)	68% Design 52% BE*	68% Design 52% BE*	68% Design 52% BE*	68% Design 68% BE*
Molecular Diffusivity (cm^2/min)	6.05E-04	6.61E-04	8.10E-04	5.49E-04

*BE is "*best estimate*"

The PNNL column testing was performed at slightly different temperatures and the OLI property predictions at their feed conditions are provided in Table 2-3, along with other parameter settings employed.

Table 2-3. OLI predicted properties at feed conditions and other key parameter settings employed at column feed conditions.

Feed Solution	TBI	PNNL Simple Simulant	PNNL AP-107 Actual
temperature (C)	22	20	25
ZAM Generated Beta-Factor [M]	without Sr: 3.6000E-04 with Sr: 5.4720E-04	without Sr: 2.8982E-04	with Sr: 3.6327E-04
density (g/ml)	1.244	1.230	1.223
absolute viscosity (cP)	2.695	2.667	2.260
Molecular Diffusivity (cm^2/min)	6.05E-04	5.94E-04	7.46E-04
Tortousity Factor (-)	10 Design 4 BE*	10 Design 4 BE*	10 Design 4 BE*

*BE is "*best estimate*"

For analyzing column performance using the VERSE-LC model, a Cs pore diffusivity value must be provided. This value can be estimated using the effective Cs molecular diffusivity and a batch specific particle pore tortuosity factor. The tortuosity factors employed are also provided in Table 2-3.

2.1 The Isotherm Model

Appendix A describes how under high caustic conditions, and at a fixed temperature and solution composition, the ZAM modeling results can be represented by a single (Cs "effective") binary Langmuir isotherm. The binary Langmuir isotherm, as provided by Eq. (A-7), takes the form:

$$Q_{Cs} = \frac{Q_T c_{Cs}}{c_{Cs} + \beta} \quad (1)$$

where

- c_{Cs} - local Cs liquid-phase ionic concentration, [M].
- Q_{Cs} - local Cs ionic solid-phase concentration, (mmol/g_{CST} in its powdered-form).
- β - factor that accounts for the cation competition and anion effects, [M].
- Q_T - the total Cs^+ ion exchange capacity, (mmol/g_{CST} in its powdered-form).

Equation (1) provides the equilibrium Cs loading on a per gram of dry CST material in its powdered-form. For column applications the CST in its powdered-form is converted over to its engineered-form with an inorganic binder. The total Cs loading on a per gram of dry CST media in its engineered-form becomes:

$$\hat{Q}_{Cs} = \frac{\eta_{df} Q_T c_{Cs}}{c_{Cs} + \beta} \quad (2)$$

where

- $\hat{Q}_{Cs}$ - local Cs ionic solid-phase concentration, (mmol/g_{CST} in an engineered-form).
- η_{df} - dilution factor accounting for presence of inert binder material, (-).

It is assumed that the addition of an inert binder material does not alter the CST's ionic selectivities, and therefore the beta-factor is independent of the dilution factor. See Appendix C for further details on the dilution factor.

When employed in VERSE-LC column analyses this isotherm must be expressed on a per bed volume basis. This is accomplished by multiplying Eq. (2) by the dry bulk bed density. Appendix B discusses the wet versus dry media F-Factor for CST. Appendix D provides information on the available wet and dry measured bulk bed densities. For VERSE-LC modeling the Cs binary isotherm takes the form:

$$\overline{Q}_{Cs} = \frac{\rho_b \eta_{df} Q_T c_{Cs}}{c_{Cs} + \beta} \quad (3)$$

where

- $\overline{Q}_{Cs}$ - local Cs ionic solid-phase concentration, (mmol/ml_{bed}).
- ρ_b - CST dry bulk bed density, (g_{CST}/ml_{bed}).

Details on the various parameters contained within Eq. (3) are discussed in Appendices A, B, C, and D.

3.0 Assessment of recent batch specific testing by PNNL

Using a recent batch of CST produced by UOP, (i.e., IONSIV™ R9140-B[a]), batch contact and column breakthrough performance testing was performed at PNNL by Fiskum et al. (2018) for a 5.6 M Na simple simulant and by Rovira et al. (2018) for actual AP-107 tank waste. This specific batch (R9140-B) was provided in the sodium form with an indicated mesh size of -20/+40, but was then sieved by PNNL to -25/+60 mesh. The particle distribution measurements yielded an average particle diameter of 573 microns. Although these are larger beads, the testing indicates that the media tortuosity factor is not significantly different from values observed in the smaller beads used historically. However, even with similar tortuosity factors the overall column kinetics becomes slower because of the increased bead size (i.e., longer average distance that the Cs ions need to traverse inside a bead to reach an ion exchange site).

[a] R9140-B is the caustic-washed sodium form of engineered CST beads

The primary objective for assessing the simple simulant test data (Fiskum et al., 2018) was to establish batch-specific parameter settings for: (1) the engineered-form dilution factor and (2) the Cs^+ particle pore tortuosity factor for this larger material. As the results provided below indicate, satisfactory values for these parameters were achieved and should provide acceptable *best estimate* analysis capability for this specific batch of CST material. Details of this assessment are provided in Appendix E.

A follow up confirmatory modeling assessment was performed using the actual AP-107 tank waste test data (Rovira et al., 2018). Here the parameter settings established in the simple simulant assessment were employed to predict column performance behavior. Details of this confirmatory assessment are provided in Appendix F. These batch specific confirmatory results indicated that our existing ZAM/VERSE methodology (Hamm et al., 2002) can be safely employed for sizing the TBI CST bed.

3.1 Comparison of Batch Contact Tests

Recent batch contact testing has been performed at SRNL by King et al. (2018) and at PNNL by Fiskum et al. (2018) and Rovira et al. (2018). Table 2-1 contains the solution compositions employed by these three sets of investigators and the average temperatures that these tests were performed at. The SRNL tests used an engineered-form batch (IONSIV™ R9120-B) received in 2017 with an average particle size of 550 microns diameter. These tests were performed using a standard simulant (i.e., SRS Avg Simulant) to confirm that the more recent CST material was performing consistently with historical CST material. In February 2018 PNNL received the most recent CST batch (IONSIV™ R9140-B) with an average particle size of 573 microns and performed batch contact testing using a 5.6 M Na simple simulant (Fiskum et al., 2018) and an actual tank waste (Rovira et al., 2018).

ZAM generated Langmuir isotherms were created for all three of these cases:

- SRS Avg Simulant (King et al., 2018) – the 2017 CST batch with average particle size of 550 microns and tested at 23.2°C. Equilibrium test mixed for more than 72 hours to ensure reaching equilibrium conditions, per standard protocol. Calculation assumed no Sr was present.
- PNNL 5.6 M Na Simple Simulant (Fiskum et al., 2018) – the 2018 CST batch with average particle size of 573 microns and tested at ~24°C. Equilibrium test measured Cs uptake at 24 and 48 hours to verify it had reached equilibrium conditions. Calculation assume no Sr was present.
- PNNL Actual AP-107 tank waste (Rovira et al., 2018) – the 2018 CST batch with average particle size of 573 microns and tested at ~27°C. Equilibrium test measured Cs uptake at ~50 and 91 hours to verify it had reached equilibrium conditions. Sr concentration was measured and calculations assumed that all of it was available for competing with Cs^+ exchange sites.

The resulting Langmuir isotherms are plotted in Figure 3-1 for all three cases as well as the batch contact data taken (and their duplicates). When looking at the solution compositions provided in Table 2-1 and focusing in on the cations potentially able to compete for Cs^+ exchange sites and temperatures applied, one would expect the three isotherms would stack up as listed in the bullets above (i.e., SRS Avg Simulant highest and actual tank waste the lowest). The only portion of these isotherms relevant to the follow-on VERSE-LC analyses is Cs concentrations below the column feed composition values (i.e., as Table 2-1 indicates lower than 1.0×10^{-4} [M]).

The slope of the isotherms at the lower range of Cs concentrations is dictated by the CST materials selectivity values (i.e., composited into the beta-factors). At the upper range of Cs concentrations, the CST materials total ionic capacity for Cs^+ and its dilution factor dominate. As shown in Figure 3-1 the 2017 batch of CST material tested by SRNL has a dilution factor of ~68% that is consistent with some of the previous batches. However, for the 2018 CST material tested by PNNL, a dilution factor of ~52% is seen. This 52% value is lower than the lowest previous value observed of 59% (see Hamm et al., 2002).

As can be seen in Figure 3-1 the batch contact data at the upper range of Cs^+ concentrations exhibit behavior that suggest that the 2018 batch has higher Cs capacities; however, since only the lower range is of importance for this study no further investigations were considered, and the 52% dilution factor was used.

The lower apparent capacity of the 2018 batch could be due to several factors. Although historical protocol has demonstrated that CST typically requires 72+ hours to achieve equilibrium, the PNNL testing appears to have reached equilibrium in ~24 hours, but that observation is inconsistent with historical work and would not be expected with larger bead size material. Further, as mentioned above, the simulant used in PNNL testing contained insoluble solids. It is unknown if these solids could have blinded pores in the CST and thus contributed to the discrepancy. Other possible explanations could be the presence of Sr in the simulant, which is sometimes found in laboratory chemicals as an impurity. This would tend to explain why the loading was lower at low concentrations of Cs, but higher at high concentrations of Cs, since the concentration of Sr in the simulant would have been constant so its effect would have been minimized at the higher Cs concentration. Lastly, the caustic washed CST would have higher weight per ion exchange site because some hydronium ions are replaced by sodium ions. Although the difference should be very small, and the calculations should account for it, perhaps there is an unmeasured discrepancy in the assumptions or bases used for the correction or the F-factor. It is unlikely that the apparent capacity is due to manufacturing issues because the batch of CST received by SRNL in 2017 had also recently been manufactured, and the results from testing that batch were consistent with historical information, and, the total Cs capacity of the 2017 batch matches the historical data. Additional testing and computer modeling would be needed to resolve these discrepancies.

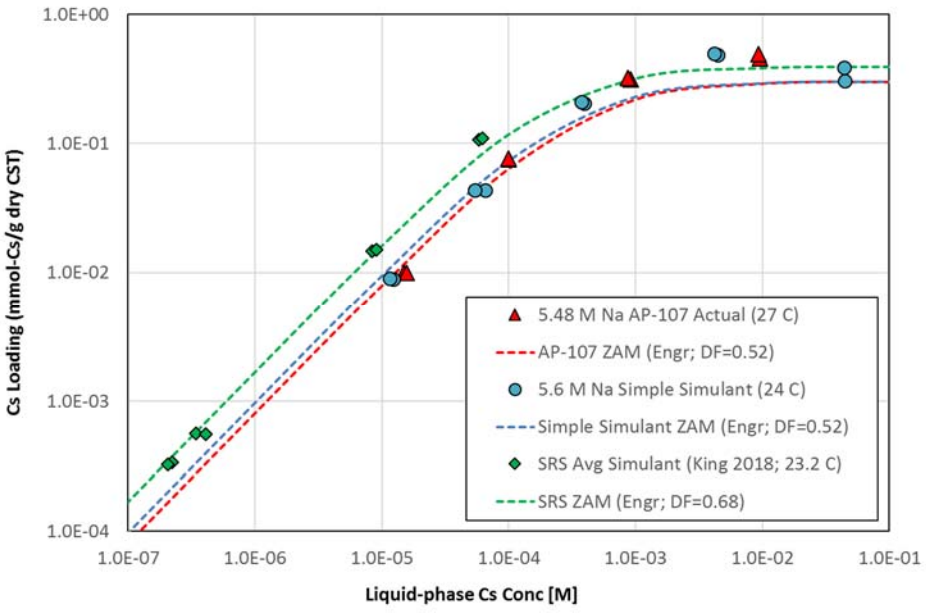

Figure 3-1 ZAM generated Langmuir fits to recent SRNL and PNNL batch contact test results (engineered-form only).

Updated ZAM generated isotherms were created at the average temperatures that the column testing was performed. These isotherms are discussed in Appendix E for the 5.6 M Na simple simulant study and Appendix F for the actual AP-107 tank waste study.

3.2 Assessment of PNNL Simple Simulant Column Tests

Fiskum et al. (2018) recently performed both batch contact and lead/lag column studies using the most recent CST batch (i.e., IONSIV™ R9140-B) where a 5.6 M Na simple simulant was used. This was the first

available column performance data indicating how this new, larger CST media behaves. Below, the column breakthrough data are reviewed where the SRNL ZAM/VERSE methodology is employed. The details associated with the creation of Cs isotherms for use in VERSE-LC column runs are provided in Appendix E, along with the details associated with the VERSE-LC column runs.

Fiskum et al. (2018) ran two equally sized ~10 ml columns in series at an average temperature of ~20°C. Identical lead/lag column configurations were employed where the only parameter value changing was the feed flowrate given as:

Red columns – 1.19 BV/hr = 0.195 ml/min
Blue columns – 1.99 BV/hr = 0.326 ml/min
Green columns – 4.56 BV/hr = 0.747 ml/min

VERSE-LC runs were made for each column configuration (i.e., Red, Blue, and Green) where all parameters were at nominal settings based on our current methodology. Two different tortuosity factor settings were considered: (1) our *design estimate* value of "10" for computing conservative breakthrough estimates and (2) our *best estimate* value based on a limited parameter search effort using only the Red lead column Cs breakthrough data. The best overall value observed was chosen (i.e., value was determine looking only at the Red column data):

- $\tau = 10$ (-) (for *design estimate* purposes)
- $\tau = 4$ (-) (for *best estimate* purposes)

A comparison between the Red lead column data (1.19 BV/hr case) and VERSE-LC runs at both the *design* and *best estimate* settings is provided in Figure 3-1.

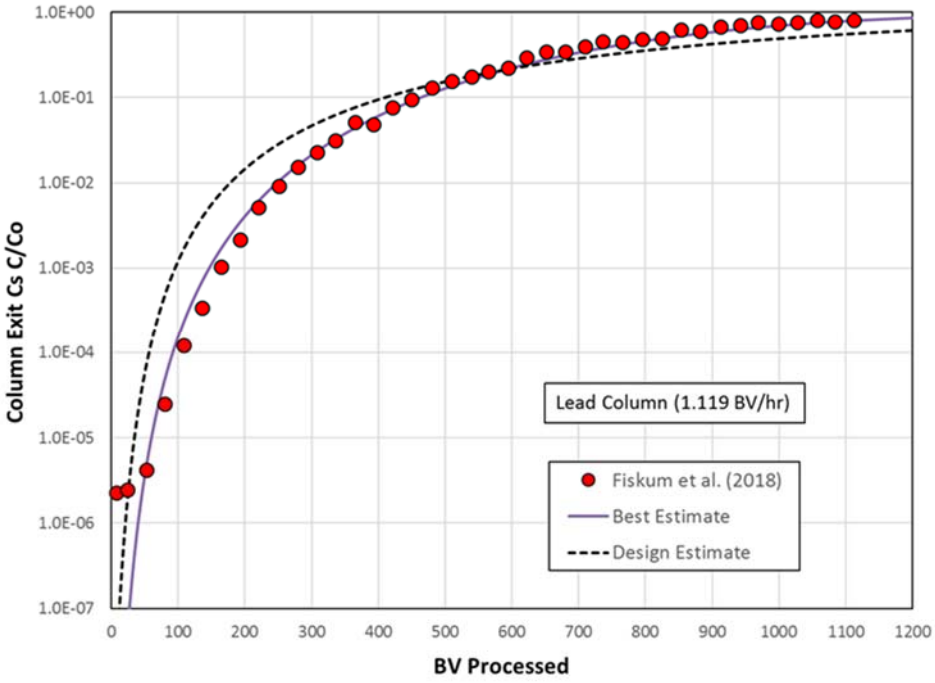

Figure 3-1 VERSE-LC predicted breakthrough for red lead column using *design* and *Best estimate* settings (1.19 BV/hr; semi-log scale plot).

As expected, the VERSE-LC *design estimate* results show an earlier than measured Cs breakthrough curve. As such, column sizing employing the *design estimate* parameter settings will result in a conservative bed volume estimate. However, this is not overly conservative because several unknowns cannot be resolved, such as non-ideal bed packing, varying particle size, strontium concentration, actual operating temperature,

actual waste composition vs. projected composition, etc. The *best estimate* results are in good agreement with the data as expected since some degree of parameter adjustment was made in obtaining the tortuosity factor value of 4 (i.e., all other parameters remained fixed). As shown in Hamm et al. (2002) a tortuosity factor of 4 is within the historical range of values observed.

Using the same set of *best estimate* parameter settings, all three column cases (i.e., lead and lag Red, Blue, and Green cases) were run using VERSE-LC (i.e., basically the only variable changing was an increasing feed flowrate). An overall comparison is made in Figure 3-2 of the Cs breakthrough curves for both the lead and lag columns versus the data.

Column exit breakthrough data represent a composite of all of the ion-exchange aspects of importance. It's an interplay between equilibrium and kinetics aspects. The ability to capture flowrate changes (i.e., here almost a factor of 4 increase) strongly indicates that the VERS-LC model is adequately handling column kinetic aspects (e.g., the pore diffusion and particle surface film mass transfer aspects).

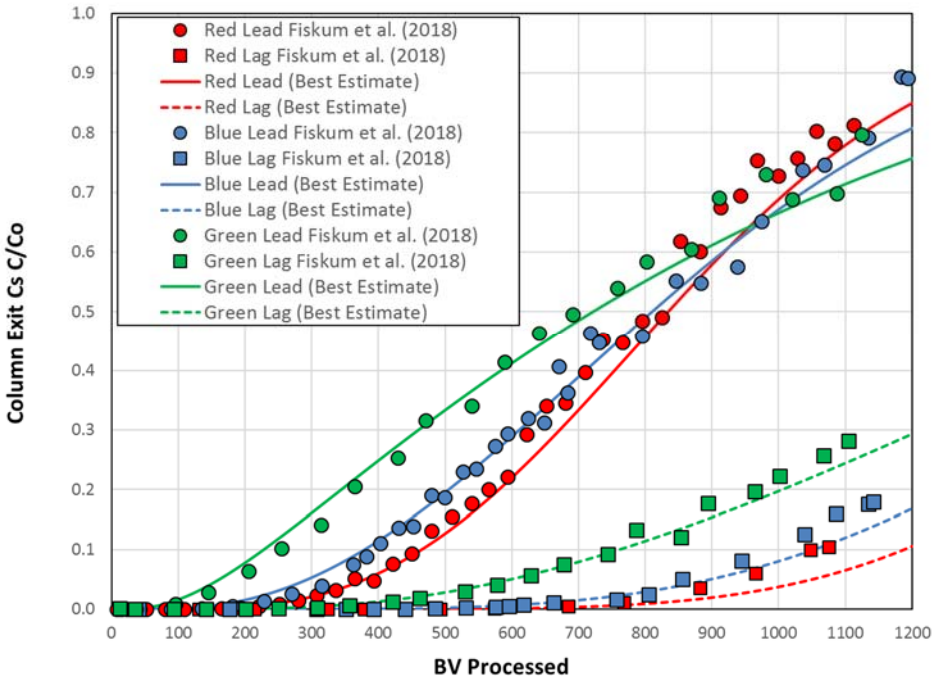

Figure 3-2 VERSE-LC predicted breakthrough for red-blue-green lead/lag column using *best estimate* settings (1.19, 1.99, and 4.56 BV/hr; linear scale plot).

As the lead and lag Cs breakthrough comparisons indicate, the VERSE-LC *best estimate* results are in fairly good agreement for all three feed flowrates. These results provide some overall degree of confidence in the data sets provided by Fiskum et al. (2018) and the ZAM/VERSE methodology established by Hamm et al. (2002). Example input and output files for ZAM and VERSE-LC are provided in Appendices G and H, respectively.

However, it should be noted that the test report indicated that insoluble solids collected on the CST media during the test, as reported by PNNL as a colored layer on the top portion of the material. The simulant had not been filtered, and the solids appeared to be iron hydroxide. How these solids impacted either the Distribution Coefficient (K_d) measurements or the column experiments cannot be known without further testing. Presumably, the solids could have blinded pores on the CST and therefore could have decreased the rate of absorption of Cs. This effect, if it occurred, would have decreased the loading profile, and not have caused an *improvement* to either the K_d or the column performance, so using the test results to project performance would be conservative.

It is also interesting to note that the isotherm that was applied did not include any impact from strontium, but did include the lower dilution factor (52%) because that was the measured value from the equilibrium testing for that batch. As mentioned above, although no strontium had been intentionally added to the simulant, strontium is often present in trace amounts in simulants due to its presence as a contaminant in laboratory chemicals. Since 1 mg/L of strontium would be enough to cause an impact on Cs absorption, even the trace contaminants in lab chemicals can have an effect and could have contributed to the lower dilution factor. This may have had an effect on the breakthrough profiles, but additional testing and modeling would be needed to resolve.

3.3 Assessment of PNNL Actual AP-107 Tank Waste Tests

To assess the accuracy of the projections based on the simulant data, we performed a confirmatory assessment on the data sets provided by Rovira et al. (2018) where actual AP-107 tank waste was employed along with the same new CST batch (i.e., IONSIV™ R9140-B). The details associated with the creation of Cs isotherms for use in VERSE-LC column runs are provided in Appendix F, along with the details associated with the VERSE-LC column runs.

Rovira et al. (2018) ran two equally sized columns in series within shielded cells at ~25°C. Only the initial feed flowrate of 2.2 BV/hr was considered in these analyses. During these tests, one carousel action was taken at about 500 BVs into the testing where the lead column was removed from the system, the lag column was transferred to the lead position, and fresh lag column was installed. Since we are only interested in breakthrough performance of a fresh lead column, data collected after that event were not considered here.

VERSE-LC runs were made for the initial column configuration (i.e., fresh lead and lag columns operating at 2.2 BV/hr) where all parameters were at nominal settings based on our current methodology and the batch specific parameter settings established during the simple simulant assessments were used. Both *design* and *best estimate* runs were made. VERSE-LC runs were extended out to ~1000 BVs (i.e., about 500 BVs beyond when an actual carousel action was taken). VERSE-LC predicted Cs breakthrough curves are compared to the data in Figure 3-3.

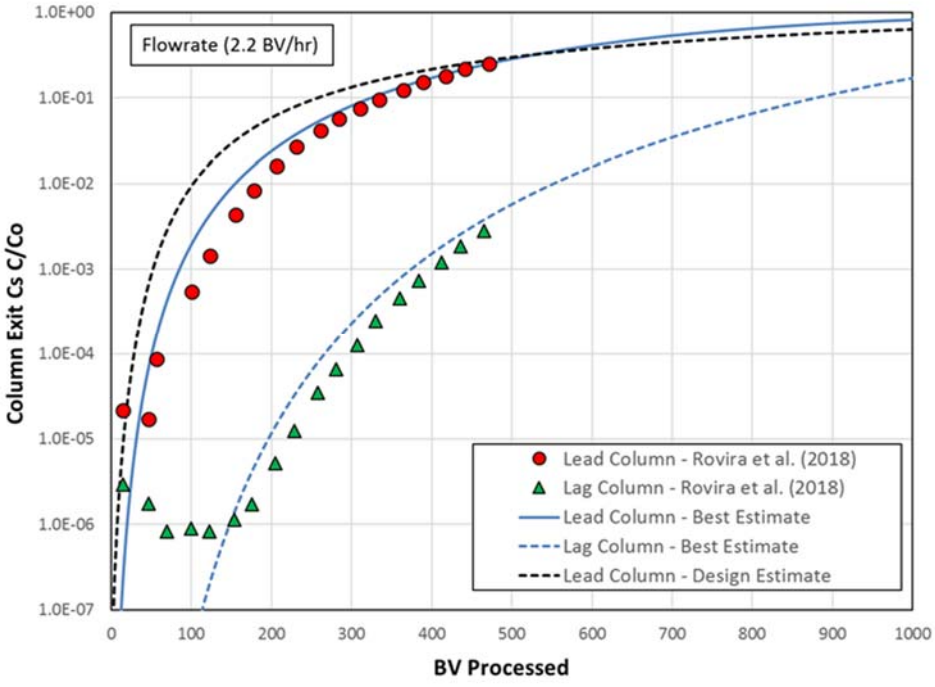

Figure 3-3 VERSE-LC predicted breakthrough for lead/lag column using *design* and *best estimate* settings (semi-log scale plot).

As observed for the simple simulant VERSE-LC runs: (1) the *design estimate* breakthrough is conservative with respect to the data and (2) the *best estimate* results are fairly consistent (but slightly conservative) with respect to the data. Example input and output files for ZAM and VERSE-LC are provided in Appendices G and H, respectively.

The original ZAM/VERSE methodology developed by Hamm et al. (2018) appears to be acceptable here for reliably estimating the ion-exchange performance of the planned TBI. Both sizing analyses as well as sensitivity studies are discussed in the next several sections.

Although the sample of AP-107 was filtered, a substantial portion of it was filtered with 5 micron filters and there was no measurement of the filtrate turbidity as reported in Geeting et. al, (2018). Although unlikely, it is possible that, similar to the simulant testing, these filters may have allowed insoluble solids to be present in the feed to the CST column. More testing would be needed to resolve if there was an impact.

4.0 Creation of TBI isotherms (ZAM based)

ZAM-based Langmuir isotherms at 22°C were created for the TBI feed solution listed in Table 2-1. To see the impact Sr^{+2} has on isotherms, ZAM runs were generated with and without Sr^{+2} being present. As Table 2-1 indicates the Cs-to-Sr molar ratio in the feed is 6.18. We are conservatively assuming that this Sr^{+2} does not complex with other constituents within the feed and is completely available to form $SrOH^{+}$ and then becomes a competitor for exchange sites with Cs^{+}, K^{+}, and Na^{+}. SRNL has two versions of ZAM (i.e., versions 4.0 and 5.0). As discussed in Hamm et al. (2002) updates were made to version 4.0 in version 5.0 to better handle the $SrOH^{+}$ mass action equation. Model runs were made based on the TBI feed composition to assess the impact of using either ZAM version. The differences in isotherm predictions were consistently within a very small range and so version 4.0 was primarily employed, since it converges more easily. CST has a higher selectivity for $SrOH^{+}$ than for Cs^{+} and a higher total $SrOH^{+}$ exchange capacity. For example, given the composition provided in Table 2-1 for the TBI feed at 22°C, ZAM predicts the following K_d values:

- K → K_d = 3.95 ml/g_{CST}
- Cs → K_d = 1,041 ml/g_{CST}
- Sr → K_d = 25,640 ml/g_{CST}

The ZAM generated isotherms for CST in its powdered-form are shown in Figure 4-1.

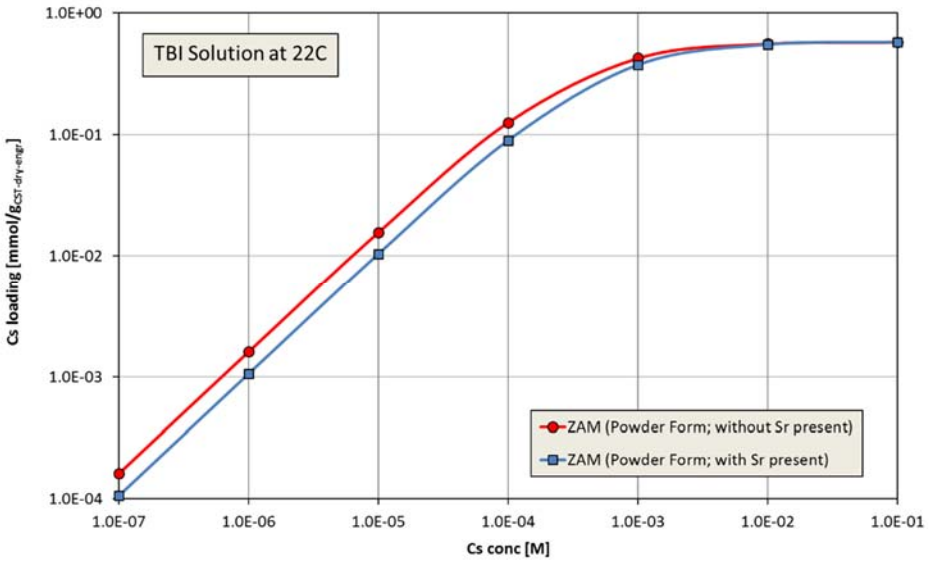

Figure 4-1 ZAM generated Langmuir fits to TBI waste at 22°C with and without Sr^{++} present (powdered-form only).

At Cs concentrations below about $1x10^{-5}$ M, the Sr competition for sites can result in reduced Cs loadings of about 34%. Thus, accounting for the presence of Sr within the TBI column sizing effort is important. Historically, accounting for Sr was not important because CST was primarily developed for application at SRS, and the SRS flowsheet included a Sr-removal step prior to the CST columns. The ZAM generated beta-factors for these two isotherms are:

$\beta = 3.6000x10^{-4}$ [M] (value without Sr present)

$\beta = 5.4720x10^{-4}$ [M] (value with Sr present at $8.19x10^{-6}$ M)

and as expected an increased value is observed when this competitor is present. The actual amount of Sr contained within the TBI feed is uncertain, as well as how much of that Sr is available to form $SrOH^+$. As such the above ~50% increase in value of the beta-factor should be considered conservative. Hanford tank waste is known to contain organic complexants. If soluble Sr is bound to an organic complexant, it is unlikely that it would form the $SrOH^+$ species and therefore is unlikely to compete with Cs^+ for the CST binding sites. However, this would need to be confirmed experimentally.

As before, isotherms based on the engineered-form are required as VERSE-LC input. The beta-factor is temperature and composition dependent, but is unaffected by the form (i.e., either powdered or engineered). For the TBI column sizing effort the following dilution factor settings are considered:

$\eta_{df} = 68\%$ (*design estimate* analyses)

$\eta_{df} = 52\%$ (*best estimate* analyses)

There are four different TBI isotherms that were considered based on the combinations of with/without Sr being present and *design/best estimate* cases. These four TBI isotherms are plotted in Figure 4-2.

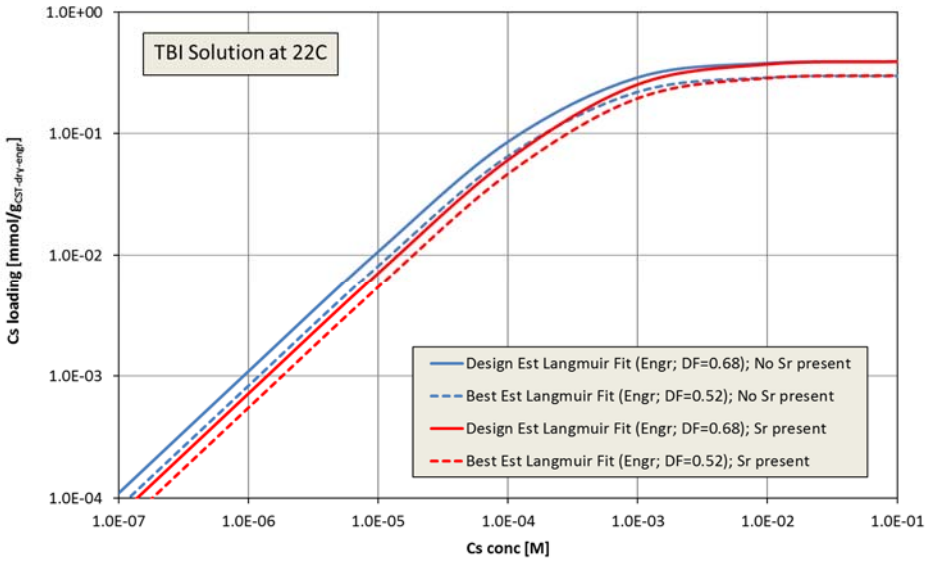

Figure 4-2 ZAM generated Langmuir fits to TBI waste at 22°C with and without Sr^{++} present (*design* and *best estimate* isotherms; engineered-form only).

All four of these TBI isotherms were employed in performing a series of VERSE-LC column sizing analyses.

5.0 TBI column sizing under nominal conditions

Four separate sets of VERSE-LC runs were made to examine nominal and varying conditions. For each set, a series of VERSE-LC column runs were made where the height of the CST bed was varied while all other input settings remained fixed. The ID of the column was fixed at 12 inches while the bed height varied yielding bed volumes ranging from 16 gallons up to 37 gallons. The wide range of bed volumes considered was the result of wanting to address: (1) a range of decontamination factors (DFs of 400 and 1000); (2) different potential effluent criterion (composite volume sizes); (3) effect that the presence of Sr has on Cs loading performance; and (4) *design* versus *best estimate* analyses. Different waste effluent composite volume sizes were considered:

- Instantaneous exit Cs concentration (very small sample size; no compositing).
- 300 gal exit bucket average Cs concentration (the last of seven 300 gallon totes processed; most restrictive).
- 2100 gal exit bucket average Cs concentration (the entire process campaign composite, plus margin).

The instantaneous exit criterion is equivalent to measuring the Cs content in the last few milliliters of effluent at the end of the column run. Note that all of the above runs were made at a nominal flowrate of 1.0 gpm, temperature of 22°C, column ID of 1 ft, mean particle size of 573 microns, and 2100 gal of waste processed (i.e., nominal conditions). The results of all of these various VERSE-LC runs are plotted in Figure 5-1 for the case of no Sr being present and Figure 5-2 for the case of Sr being present (and free to become a competitor, i.e., not complexed).

In the various figures to follow, the VERSE-LC computed total Cs liquid-phase concentration exiting the CST bed is normalized to its feed condition. These plotted results can be related to an exit decontamination factor by:

$$DF = \frac{1}{\left(\frac{c_{Cs,e}}{c_{Cs,o}} \right)} \tag{4}$$

where

- DF - Decontamination factor at column exit, (-).
- $c_{Cs,e}$ - Cs liquid-phase concentration exiting the bed, [M].
- $c_{Cs,o}$ - Cs liquid-phase concentration within the feed, [M].

The presence of Sr^{+2} within the feed is being handled in an approximate manner in these VERSE-LC runs. Technically, a multi-component transport analyses should be performed; however, we have chosen to keep the effective binary approach. Follow up multi-component analyses could be considered but is outside the scope of this specific column sizing effort.

Table 5-1. Summary of TBI column sizes considered and their key features.

Column Identifer =	(units)	16 gal	18 gal	20 gal	21 gal	25 gal	27 gal	30 gal	35 gal
Bed ID =	ft	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	inches	12.0	12.0	12.0	12.0	12.0	12.0	12.0	12.0
	cm	30.48	30.48	30.48	30.48	30.48	30.48	30.48	30.48
Length =	ft	2.73	3.06	3.4	3.6	4.2	4.6	5.1	6.0
	inches	32.760	36.720	40.800	43.200	50.400	55.200	61.200	72.000
	cm	83.21	93.27	103.63	109.73	128.02	140.21	155.45	182.88
L/D =	(-)	2.7	3.1	3.4	3.6	4.2	4.6	5.1	6.0
Bed Area =	ft2	0.7854	0.7854	0.7854	0.7854	0.7854	0.7854	0.7854	0.7854
	in2	113.0973	113.0973	113.0973	113.0973	113.0973	113.0973	113.0973	113.0973
	cm2	729.6588	729.6588	729.6588	729.6588	729.6588	729.6588	729.6588	729.6588
Bed Volume =	ft3	2.1441	2.4033	2.6704	2.8274	3.2987	3.6128	4.0055	4.7124
	gal	16.039	17.978	19.976	21.151	24.676	27.026	29.963	35.251
	in3	3705.07	4152.93	4614.37	4885.80	5700.11	6242.97	6921.56	8143.01
	cm3	60715.2	68054.4	75616.0	80064.0	93408.0	102304.0	113424.0	133440.0
Flowrate =	gpm	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
	ml/min	3785.41	3785.41	3785.41	3785.41	3785.41	3785.41	3785.41	3785.41
Superficial flow velocity =	cm/hr	311.275	311.275	311.275	311.275	311.275	311.275	311.275	311.275
Particle Diameter =	microns	573	573	573	573	573	573	573	573
Particle Radius =	microns	286.5	286.5	286.5	286.5	286.5	286.5	286.5	286.5
Bed Void =	(-)	0.548	0.548	0.548	0.548	0.548	0.548	0.548	0.548
Particle Void =	(-)	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24
Total Void =	(-)	0.65648	0.65648	0.65648	0.65648	0.65648	0.65648	0.65648	0.65648
CSTR Volume Fraction to Bed =	(-)	25%	25%	25%	25%	25%	25%	25%	25%
CSTR-Volume	ml	15178.8	17013.6	18904.0	20016.0	23352.0	25576.0	28356.0	33360.0

In Table 5-1, the 27-gallon bed is highlighted since it was SRNL's originally recommended size. The 20-gallon bed is also highlighted since it was indicated that it was the largest size practical with the other facility constraints and sensitivity studies were performed about this bed size.

DFs of 1000 and 400 are shown in both figures as horizontal solid and dashed lines, respectively. The dashed curves represent the *design estimate* results while the solid curves represent the *best estimate* results.

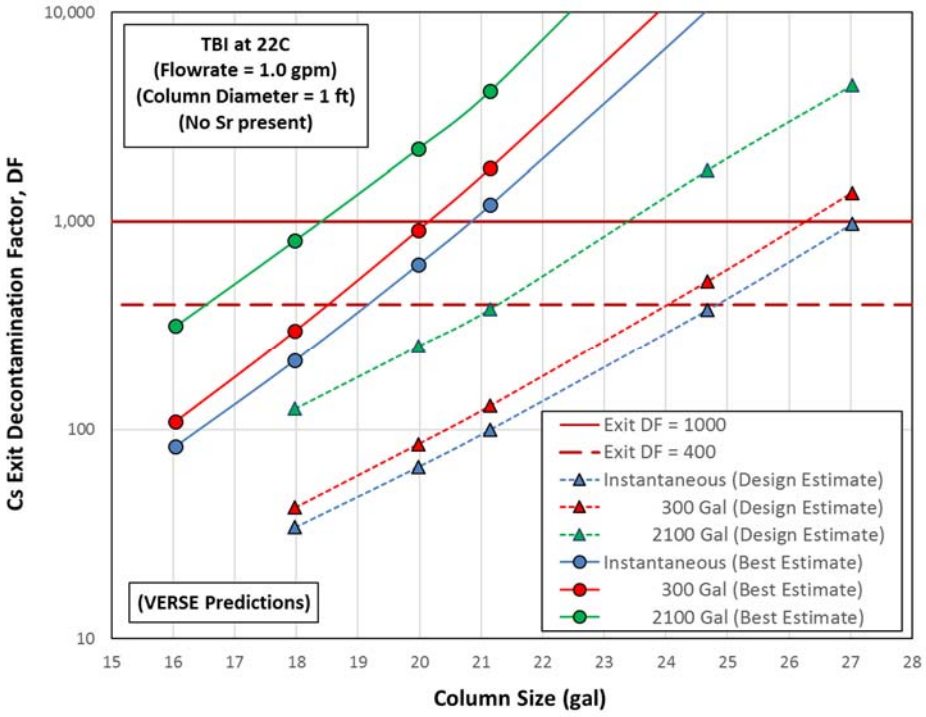

Figure 5-1 VERSE-LC predicted TBI column performance under nominal conditions (no Sr present in the feed).

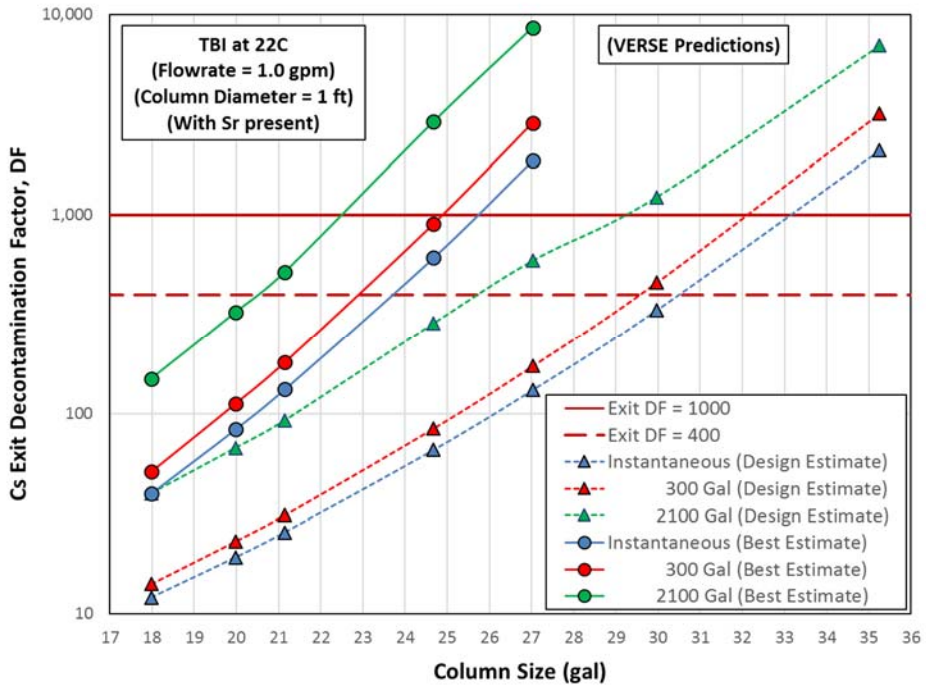

Figure 5-2 VERSE-LC predicted TBI column performance under nominal conditions (with Sr present in the feed).

The results presented graphically in Figures 5-1 and 5-2 can be used to determine a TBI column size for a broad range of DF values and composite volume sizes by way of interpolation. For the specific DFs and

composite volume sizes highlighted above, the corresponding TBI column volumes are tabulated in Table 5-2. Table 5-2 provides estimated (both *design* and *best estimate* values) TBI column volumes for the cases where:

- Sr being present or not;
- DF values of 1000 and 400; and
- Composite volume sizes of no compositing, seven 300-gallon totes, and 2100 gallon sizes.

Table 5-2. TBI column sizing summary.

Sr Present	DF (-)	Composite Volume (gal)	Best Est (gal)	Design Est (gal)
No	1000	<<1	20.8	27.1
		300	20.1	26.3
		2100	18.4	23.4
	400	<<1	19.2	24.9
		300	18.4	24.0
		2100	16.5	21.3
Yes	1000	<<1	25.7	33.2
		300	24.9	32.1
		2100	22.5	29.2
	400	<<1	23.7	30.5
		300	22.9	29.5
		2100	20.5	25.7

SRNL's original design recommendation of the column was 27 gallons assuming an instantaneous criterion as shown in Table 5-2 where a DF of 1000 was assumed and the initial assumption that Sr was not present in the TBI feed. Under these same assumptions the *best estimate* results indicate a column size of ~21 gallon.

Traditionally, we would not recommend sizing a column based on *best estimate* results. *Best estimate* results are viewed as our best ability at predicting the columns actual performance. Under these conditions no margin for errors (either computational, experimental, or operational in nature) has been allowed for. Various column fabrication or operational aspects, as well as batch variability, formation of bubbles, channeling, temperature, flow rate, and composition, can result in poorer than expected performance.

Experience indicates that the VERSE-LC predicted impact of Sr in the feed is an upper bound estimate of its impact on Cs breakthrough. Therefore, we recommend our original 27-gallon bed volume since it exceeds the 25.7 gallon *best estimate* value when Sr is accounted for, assuming the nominal conditions of 1 gpm, larger bead size CST, and instantaneous DF of 1000. Varying these nominal conditions can result in accommodating a smaller bed size.

After the loading of the Cs on the CST is complete, the bed will exhibit a high radiation dose. The radiation dose will be unevenly distributed because the top of the column will be more fully loaded with Cs than the lower portion. To provide insight into the Cs loading distribution once the TBI campaign has processed the full 2100 gallons of waste, a total Cs loading profile in the column was generated for the 20 gallon and 27 gallon cases. VERSE-LC model predictions under *best estimate* settings were generated and are shown in Figure 5-3. Also shown in Figure 5-3 is the *best estimate* saturated Cs loading associated with the feed concentration of 5.06×10^{-5} [M] (i.e., a loading value of 3.72×10^{-2} mmol/g_{CST}). Under *design estimate* settings, the peak values of these loading values would increase by ~31% (i.e., 68%/52% = 1.31). Loading values are beneath the saturated value due to the mass transfer limited aspects of CST.

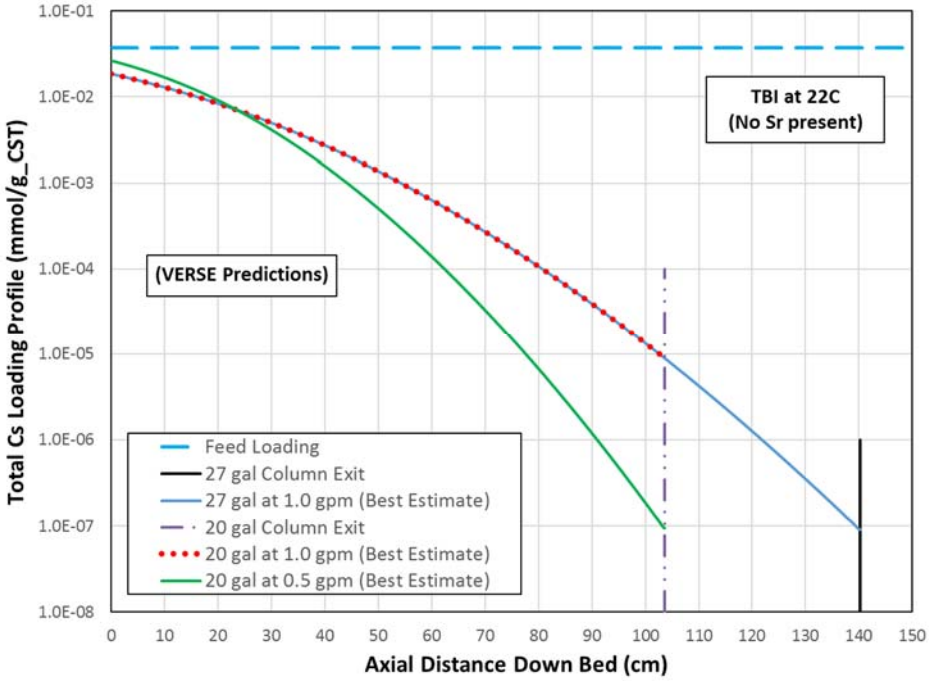

Figure 5-3 VERSE-LC predicted TBI column total Cs loading profiles under nominal conditions (no Sr present in the feed).

At the same liquid feed flowrate (i.e., 1.0 gpm) the Cs loading profile for the 20 versus 27 gallon beds will be completely overlapped as shown. The downstream impacts of a longer column have very little upstream effects. By lowering the liquid feed flowrate from 1.0 to 0.5 gpm (and doubling the processing time required to maintain a 2100 gallon feed processed constraint) results in better kinetics. Better kinetics means that a closer approach to local equilibrium conditions results. As Figure 5-3 indicates, a significantly non-uniform Cs loading profile will exist in the columns regardless of column size or feed flowrate.

Fiskum et al. (2018) made gamma measurements to estimate the ^{137}Cs loading profiles down their lead/lag column configuration at the end of their loading period. VERSE-LC comparisons to that data are provided in Appendix E and exhibit fairly consistent results in the predicted versus measured profiles.

6.0 Feed flowrate impact on 20 gallon column performance

The impact of using a 20 gallon column was calculated using a nominal TBI feed flowrate set to 1.0 gpm. To assess the potential impact of varying this flowrate, a series of VERSE-LC runs were performed. All VERSE-LC inputs were kept the same and flowrate was varied from a flowrate of 0.5 gpm up to 1.1 gpm. This sensitivity study was performed for a bed size of 20 gallons. Both with and without Sr being present within the feed were considered. Graphically, the results from the VERSE-LC model runs are shown in Figures 6-1 and 6-2.

By way of an example, for a 20 gallon bed Figure 6-1 indicates that the feed flowrate would need to be less than 0.9 gpm not to exceed a DF=1000 for an instantaneous exit criterion (i.e., in the *best estimate* sense).

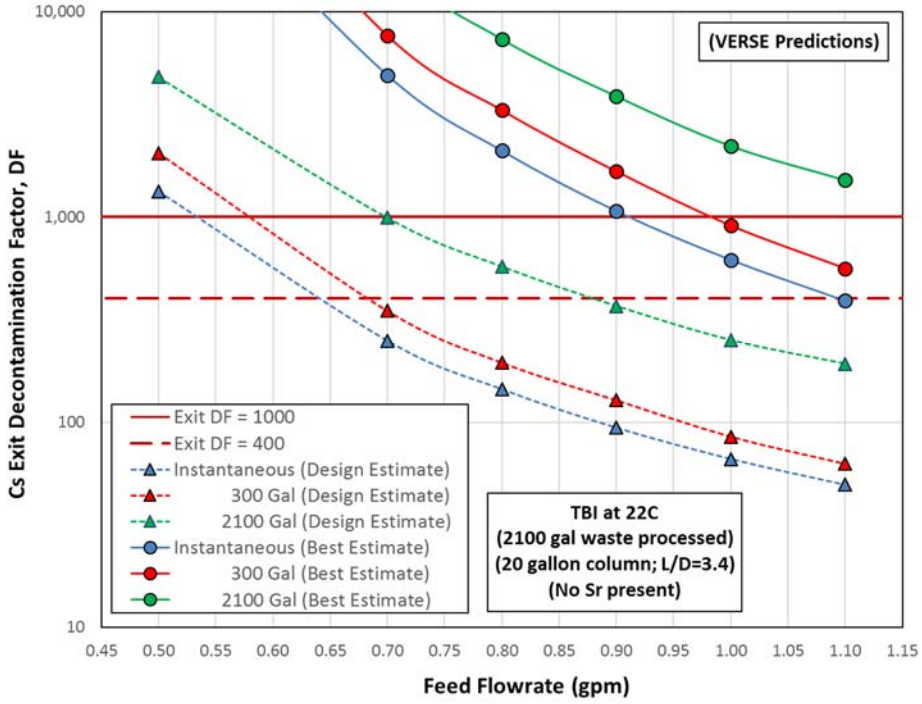

Figure 6-1 VERSE-LC predicted TBI column performance for various feed flowrates (no Sr present in the feed).

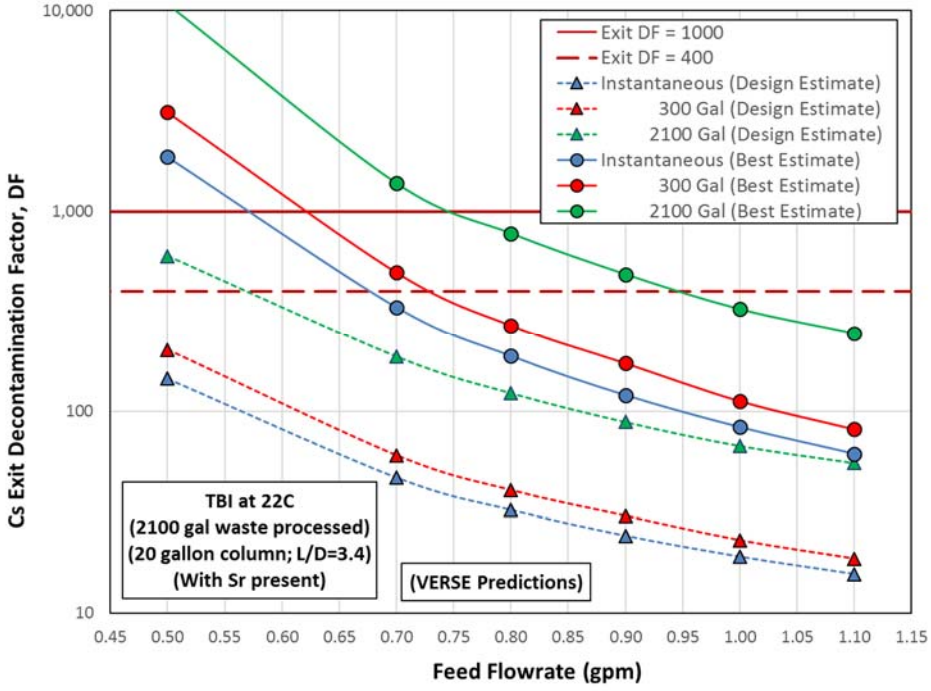

Figure 6-2 VERSE-LC predicted TBI column performance for various feed flowrates (with Sr present in the feed).

The results graphically shown in Figures 6-1 and 6-2 are also provided in Table 6-1. For a few cases, the required flowrate was outside the range of cases run (i.e., either >1.1 gpm or <0.5 gpm) as labeled. As

Table 6-1 indicates, under the "no Sr present" assumption, the 20 gallon column could be viable for four out of the six cases listed when considering *best estimate* predictions (i.e., gpm values greater than 1.0); however, the *best estimate* scenario does not account for any margins to accommodate operational uncertainties as well as the impact of Sr^{+2} being present in the feed. When considering Sr^{+2} being present, all of the *best estimate* cases required a flowrate reduction.

Table 6-1. 20 Gallon TBI column maximum feed flowrate requirements to maintain stated decontamination factors.

Sr Present	DF (-)	Composite Volume (gal)	Best Est (gpm)	Design Est (gpm)
No	1000	<<1	0.91	0.53
		300	0.98	0.58
		2100	>1.10	0.70
	400	<<1	1.09	0.64
		300	>1.10	0.68
		2100	>1.10	0.88
Yes	1000	<<1	0.57	<.50
		300	0.62	<.50
		2100	0.74	<.50
	400	<<1	0.68	<.50
		300	0.73	<.50
		2100	0.94	0.57

7.0 Mass transfer lengths for 20 gallon bed

A column with a 20-gallon bed, whose inner dimeter is 12 inches, results in a bed length of 103.63 cm. Mass transfer lengths (or zones) are velocity dependent and at a feed flowrate of 1.0 gpm a linear velocity of 9.467 cm/min is reached. This is a reasonably high linear velocity that should result in a fairly long mass transfer zone.

A look at the mass transfer zone (or length) can be seen when plotting up the VERSE-LC liquid-phase total Cs concentration profile. For the 20-gallon bed case where we assume no Sr present and under *best estimate* settings, a series of liquid-phase Cs concentration profiles are shown in Figure 7-1. Its exit is shown as the black dashed vertical line in Figure 7-1. Given the nominal feed flowrate of 1.0 gpm, profiles are shown at four different points in time:

- 500 minutes (500 gallon processed = 25 BVs)
- 1000 minutes (1000 gallon processed = 50 BVs)
- 1500 minutes (1500 gallon processed = 75 BVs)
- 2100 minutes (2100 gallon processed = 105 BVs)

The mass transfer lengths for this bed under these flowing conditions greatly exceeds the length of the bed.

As Figure 5-1 indicates, at these conditions/settings a 20-gallon bed based on *design estimate* analyses will have a DF less than 400 regardless of composite volume size. Based on *best estimate* analyses, the achievable DF values for each of the three possible composite volume sizes are:

- DF = 618 for small sample (i.e., instantaneous)
- DF = 908 for 300-gallon composite volume size
- DF = 2200 for 2100 gallon composite volume size

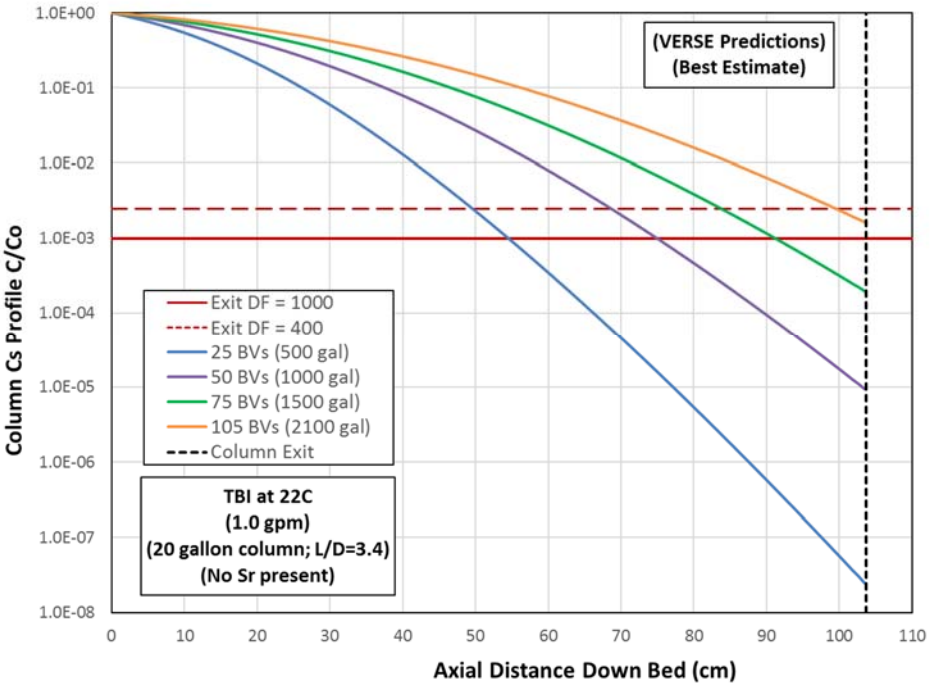

Figure 7-1 Best estimate VERSE-LC predicted TBI total Cs liquid-phase concentration profiles under nominal conditions (20 gal bed without Sr present in the feed).

8.0 Mean particle size impact on 20 gallon column performance

Historically, CST particles have been mass transfer limited primarily due to pore diffusion limitations. As such, it is expected that particle size distribution should have a large impact on Cs breakthrough performance. VERSE-LC only addresses a mean particle size and the nominal value employed for the earlier TBI results was 573 microns in diameter. SRS has on hand an earlier batch of CST whose mean particle diameter is 408 microns. However, no batch specific test data are available on this older CST material. A sensitivity study was performed by varying just the mean particle size while holding all other parameter settings fixed.

This mean particle size sensitivity study also included an intermediate mean particle diameter of 490 microns. This sensitivity study only varies the mean particle diameter size. The changing of particle size distribution within a batch or the use of another batch would most likely alter the dilution factor and/or the tortuosity factor; however, in this sensitivity study these parameters remained fixed.

All VERSE-LC inputs were kept constant, and mean particle diameter was varied from 408 microns up to 573 microns. This sensitivity study was performed for a bed size of 20 gallons, while both with and without Sr being present within the feed were considered. Graphically, the results from the VERSE-LC model runs are shown in Figures 8-1 and 8-2.

As expected, mean particle size has a large impact on the resulting DF achievable with a fixed bed volume. When looking at the *best estimate* results presented in Figures 8-1 and 8-2, a factor of 100 reduction is achieved in DF when going from the larger 573 micron diameter (new batch) back down to the 408 micron diameter (older batch) (i.e., and assuming the other parameter settings fixed).

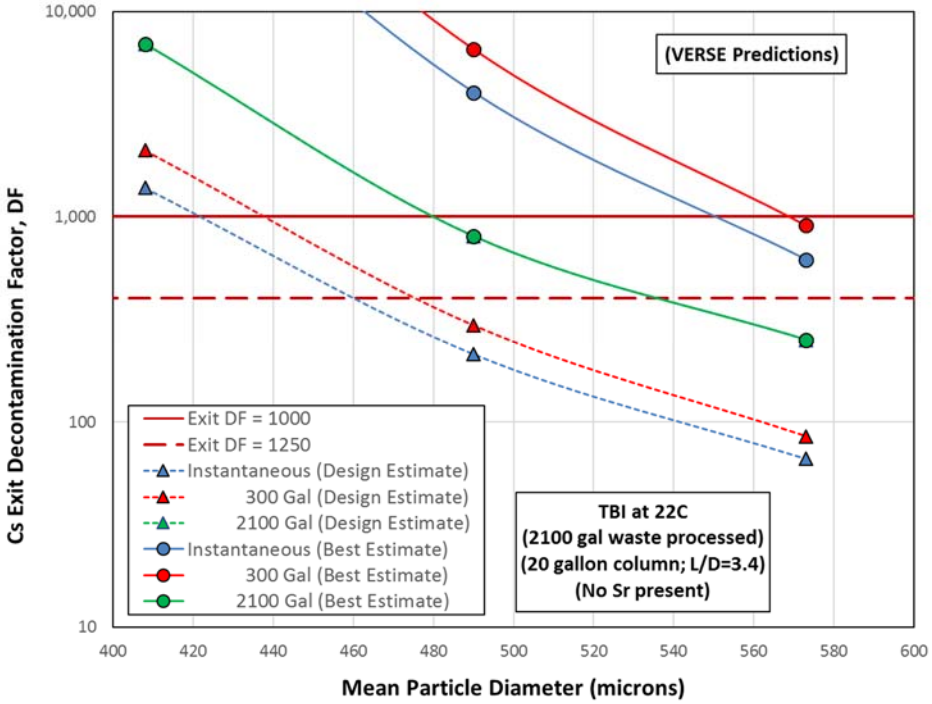

Figure 8-1 VERSE-LC predicted TBI column performance for various mean particle sizes (no Sr present in the feed).

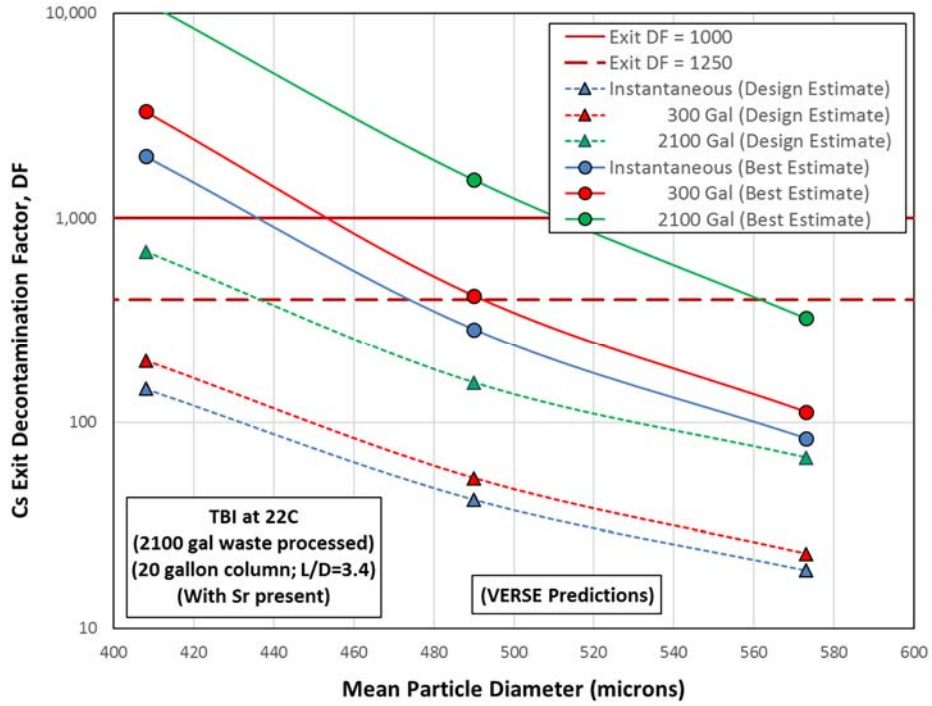

Figure 8-2 VERSE-LC predicted TBI column performance for various mean particle sizes (with Sr present in the feed).

The results graphically shown in Figures 8-1 and 8-2 are also partially provided in Table 8-1. Table 8-1 focuses only on the two currently available particle size distributions (i.e., the new 573 micron batch and the older 408 micron batch). As Table 8-1 indicates, under the case of no Sr being assumed present, the older batch with a mean particle size distribution (i.e., 408 microns) yields decontamination factor margins for all combinations of composite sizes, *best estimate*, and *design estimate* options. Note that the 408 micron results do not include any potential dilution or tortuosity factor changes. When Sr is assumed to be present at the levels provided, *best estimate* DF values are acceptable.

Table 8-1. Achievable decontamination factors for a 20 Gallon TBI column for two available particle size distributions.

Sr Present	Mean Particle Size (microns)	Composite Volume (gal)	Best Est (DF)	Design Est (DF)
No	573	<<1	618	66
		300	908	85
		2100	2,219	251
	408	<<1	79,460	1,384
		300	150,724	2,110
		2100	372,099	6,958
Yes	573	<<1	84	19
		300	112	23
		2100	325	67
	408	<<1	2,001	146
		300	3,321	201
		2100	11,335	688

As can be seen from the various TBI results provided (i.e., Table 5-2 for nominal conditions, Table 6-1 for flowrate effects, and Table 8-1 for particle size effects) "options exist" for establishing an acceptable column size when certain constraints and operating conditions are imposed.

9.0 Conclusions

The Environmental Management Office of the DOE is pursuing TBI to treat and dispose 2,000 gallons of tank waste from Hanford. One step in the process is to remove radioactive ^{137}Cs from the waste using CST ion exchange media. Modeling has been performed to provide an estimate of the volume of a bed of CST required to meet the design requirements. Sensitivity studies were also performed to help provide project guidance. This analysis effort uses SRNL's modeling methodology for CST based on extensive testing results.

At the nominal conditions, a 27-gallon bed size is recommended. This is not the maximum calculated *design estimate* size, but is the *best estimate* plus some level of operational margin to accommodate for typical variances that occur in these sorts of unit operations (e.g., flowrate variations, non-uniform bed packing allowances, media capacity variance, feed composition changes, etc.). The strontium concentration has potential to have a significant impact on column performance, but the concentration of Sr in the feed composition used in the modeling was from a projection and is not reliable.

Since a 27-gallon column bed size is not viable due to other design constraints, modeling was also performed to examine the potential options available for use of a 20-gallon bed. A bed smaller than 27 gallons can be used if one of the following three options is/are selected: (1) use of a smaller bead size material; (2) use of a lower flow rate; or (3) larger composite size of the decontaminated effluent.

Overall, the modeling provides projections of the performance of the columns as a function of bed size, bead size, flow rate, and composition. This information can then be used along with other project needs and information to arrive at the optimum design and operating strategy.

10.0 Recommendations and Future Work

The modeling was performed using parameters based largely on testing with significantly different chemical compositions of the waste, and with smaller bead size CST. Testing using a full height column and a simulant formulation that mimics the expected chemical composition of the feed is recommended to confirm the modeling projections, coupled with further refinement of the model parameters. Testing is also recommended to confirm the equilibrium conditions (distribution coefficients) at higher potassium concentrations.

Because most historical testing did not include Sr (the SRS flowsheet had a Sr-removal step), there is minimal information on its impact. The ZAM computer model indicates it has a substantial impact, even at low concentrations. Furthermore, the Sr in some Hanford wastes is complexed by organic ligands. It is assumed that this complex would prohibit the absorption of Sr by the CST, but confirmatory testing would be needed to confirm. Once the actual measured Sr concentration in the TBI feed is known, it is recommended that the actual measured value should ultimately be used to calculate the expected impact.

There are discrepancies in the results of testing performed by PNNL versus the historical information. The most significant is the apparent reduced Cs^+ ionic capacity versus what is typically due to the binder, i.e., a dilution factor of 52% vs. the on average value that's greater than 68%. It is unlikely that the lower apparent capacity is due to manufacturing issues because the batch of CST received by SRNL in 2017 had also recently been manufactured, and the results from testing that batch were consistent with historical information, and the total Cs capacity of the 2018 batch of CST matches the historical data. The discrepancy is significant, and testing and modeling are recommended to provide resolution.

The impact of insoluble solids in the feed to the ion exchange column is unknown. Historical work had always filtered the feed to ~0.5 microns. The use of larger pore filters will permit some solids to pass to the ion exchange bed, where they are very likely to be absorbed by the CST. How quickly these solids decrease the loading curve, and thereby decrease the decontamination factor, is unknown

During this study it was identified that SRNL and PNNL used differing protocols in defining their "wet" and "dry" mass reference states and in determining batch-specific F-Factors. It is highly recommended that standardized protocols be established and followed in future CST testing efforts.

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12.0 Appendix A (Isotherm Aspects of Interest)

Key features associated with the isotherms employed in the VERSE-LC column runs are discussed below. As discussed in Hamm et al. (2002) a simple effective Cs isotherm can be used in VERSE-LC simulations since the majority of constituents within the feed pass through the CST bed un-retarded. However, Sr^{+2} (i.e., actual competitor being in the form of $SrOH^{+}$) is the one exception that exists for the feed solutions being considered here and will be discussed in this report. For any analyte of interest tight charge balancing is required within the input to ZAM and typically SRNL balances based on Cl^{-} when considering CST media. For all of the anions considered, Cl^{-} is considered to be the spectator of choice for charge balancing. To create ZAM based Cs isotherms varying amounts of CsCl are added to the baseline compositions.

The ZAM model accounts for cation competition between H^{+}, Na^{+}, K^{+}, Cs^{+}, Rb^{+}, and $SrOH^{+}$. The effects from anions come in through liquid-phase activity coefficients, while nonidealities associated with the solid-phase are addressed directly within ZAM through its multi-site triad model.

The ion exchange aspects of CST media have been quantified within the ZAM model developed during the 90's at Texas A&M (see Zheng et al., 1996). The model was developed for CST media in its powered form. For column applications this powdered form is combined with an inert material (i.e., a binder) to provide structural support and hydraulic porosity. This reduces its loading capacity where a "dilution factor" (η_{df}) has been employed to account for this directly and the resulting media is referred to as being in its engineered form.

We consider ZAM in either its powdered or engineered forms to be functionally correct for addressing ionic selectivity. Below we show under some limiting conditions how the complex set of mass-action equations in ZAM can be quickly reduced down to a simple binary-like Langmuir isotherm model. Under the more complex conditions however, we have routinely found ZAM results to fit the Langmuir form well.

The ZAM model (Fortran based code; Zheng et al., 1996, both its 4.0 and 5.0 versions) contains a complex set of equations addressing the solid phase which when under:

1. high levels of caustic conditions (i.e., $[OH^{-}] > 0.1$ M) and
2. no other site competitors than Na^{+} and Cs^{+} (i.e., $[K^{+}]=[Rb^{+}]=[SrOH^{+}]= 0$ M)

reduces down to the following single mass-action equation:

$$Cs^{+} + \overline{Na - X - Na_2} \xleftrightarrow{K(T)} Na^{+} + \overline{Cs - X - Na_2} \tag{A-1}$$

Equation (A-1) can be expressed as:

$$K(T) = \frac{Q_{Cs} c_{Na} \gamma_{Na}}{Q_{Na} c_{Cs} \gamma_{Cs}} \tag{A-2}$$

where the equilibrium constant (K) is only temperature dependent since nonidealities are addressed (i.e., liquid-phase handled with Bromley model and solid-phase handled as ideal solution of triad sites). A Cs mass balance equation between the solid and liquid phases can be expressed as:

$$Q_{Cs} = Q^{o}_{Cs} + \phi\left(c^{o}_{Cs} - c_{Cs}\right) \tag{A-3}$$

where ϕ represents the liquid-to-solid phase ratio. Also, it is assumed that the total number of exchangeable sites is fixed:

$$Q_T = Q_{Na} + Q_{Cs} \tag{A-4}$$

Combining Eqs. (A-2) through (A-4) results is a simple isotherm model:

$$Q_{Cs} = \frac{Q_T c_{Cs}}{c_{Cs} + \frac{\alpha}{K} c_{Na}} \quad \text{(A-5)}$$

where $$\alpha = \frac{\gamma_{Na}}{\gamma_{Cs}} \quad \text{(A-6)}$$

Note that the α parameter defined by Eq. (A-6) contains all of the functional dependence associated with anion concentrations. The following three concerns exist with ZAM:

- ZAM uses the old Bromley model without liquid-phase association reactions handled;
- OLI α comparisons differ from ZAM computed values under certain compositional situations; and
- ZAM ionic strength output values are sometimes in error.

However, under most conditions the results of ZAM have fallen within the uncertainty of the data provided. In the more general case Eq. (A-5) can be expressed in the standard Langmuir form as:

$$Q_{Cs} = \frac{Q_T c_{Cs}}{c_{Cs} + \beta} \quad \text{(A-7)}$$

where

- c_{Cs} - local Cs liquid-phase ionic concentration, [M].
- Q_{Cs} - local Cs ionic solid-phase concentration, (mmol/g_{CST} in its powdered-form).
- β - factor that accounts for the cation competition and anion effects, [M].
- Q_T - the total Cs^+ ion exchange capacity, (mmol/g_{CST} in its powdered-form).

The beta-factor is dependent upon the solution temperature along with its anion and cation compositions. It reflects the selectivities of the various cation competitors present. The total Cs exchange capacity is hardwired in ZAM to be 0.58 mmol/g_{CST} media. This value corresponds to CST media in its dry powdered form under high caustic conditions. Multi-component Langmuir isotherms can also be derived but the derivations are much more complicated than the binary one provided above as an illustrative example.

When performing either batch contact or column testing or modeling, the key quantity of interest is the total number of Cs exchange sites that are present. Both a CST media's moisture content and geometric-form are important aspects that should be defined, and both are further discussed below.

13.0 Appendix B (Media F-Factor)

The amount of engineered-form CST media to be employed in a batch contact experiment is to be obtained in its Na-based reference state. This is a pre-defined state of moisture typically referred to as its "wet" state. The actual amount of engineered-form CST media being employed is computed from this wet reference state using the F-factor defined as:

$$F_{factor} = \frac{m_{engr}^{dry}}{m_{engr}^{wet}} \quad \text{(B-1)}$$

where F_{factor} F-factor for handling media moisture in its engineered-form

m_{engr}^{dry} dried media in its engineered-form (pre-determined protocol)

m_{engr}^{wet} wet media in its engineered-form (pre-determined protocol)

Consistent protocols should be employed to obtain these mass values. The moisture content of a specific batch of CST media (i.e., UOP batch IONSIV R9120-B) has been recently measured by King et al. (2018) to be ~18 wt%. For this specific batch this yields an estimated F-factor of:

$$F_{factor} \approx 1 - 0.18 = 0.82 \quad \text{(B-2)}$$

Prior to performing these moisture analyses, the as-received media was pretreated to ensure that the media was completely in its Na-form. Results indicated that this media was not completely in its Na-form. During the conversion from its H-form over to its Na-form the results confirmed that the ~4.6 mmol/g_{CST} of H-Na exchangeable sites existed (consistent with results performed by Zheng et al., 1996).

From the UOP product receipt during shipment (dated 5/26/2017) the moisture contents provided for two different lots of this material were 20.9% and 19.0%, respectively. Fairly consistent moisture contents were observed and not greatly different from the SRNL measured value.

For CST engineered-form material SRNL uses the protocol:

- **Wet-reference state** – the media is dried at 35°C until a constant weight is achieve (typically overnight).
- **Dry-reference state** – the wet-reference state media is further dried at 400°C for ~hours and reaching a constant weight (a 5°C per minute ramp is used up to 400°C).

In the recent PNNL reports (i.e., Fiskum et al., 2018, and Rovira et al., 2018) F-Factor analyses were performed on a recent batch of CST (i.e., IONSIV R9140-B received on 2/26/2018). Rovira et al. (2018) reported measured F-Factors with an average value of ~75% (i.e., 25% moisture content). PNNL protocol differs from the SRNL protocol and appears to be more consistent with earlier RF resin methods:

- **Wet-reference state** – the media is air-dried at ambient temperature overnight to a free-flowing condition.
- **Dry-reference state** – the wet-reference state media is further dried at 100°C overnight (to constant mass at 100°C).

As discussed by King et al. (2018), an additional ~7% moisture loss can be expected when media is heated beyond 100°C. However, this appears to be inconsistent when viewing PNNL's results.

The dry state of the media employed by Zheng et al. (1996) in establishing their total ionic capacities in the ZAM code is somewhat unclear. As such, care should be employed when using ZAM and when performing batch contact and column testing. The best advice at this time is to employ as much consistency as possible.

14.0 Appendix C (Media Dilution Factor)

ZAM was developed based on CST in its powdered-form and can handle it in either its Na state or H state. For column applications this powdered-form is combined with an inert material to provide structural support and hydraulic porosity. This reduces its loading capacity where a "dilution factor" (η_{df}) has been employed to account for this directly and the resulting media is referred to as being in its engineered-form. Since the media's selectivities are not impacted by the inert material, beta-factors are unaltered and therefore ZAM computed beta-factors for the powdered-form can be applied directly to its various engineered-forms. As such, the Langmuir isotherm expressed by Eq. (A-7) for CST in its powdered-form can be converted over to an engineered-form by simply multiplying by this dilution factor:

$$\hat{Q}_{Cs} = \frac{\eta_{df} Q_T c_{Cs}}{c_{Cs} + \beta} \quad \text{(C-1)}$$

where

- $\hat{Q}_{Cs}$ - local Cs ionic solid-phase concentration, (mmol/g_{CST} in an engineered-form).
- η_{df} - dilution factor accounting for presence of inert material, (-).

Note that under well-defined reference states this dilution factor should always be less than one and given the possibility that inert material could also obstruct pores it could also be smaller than the mass increase due to the addition of inert material.

In Hamm et al. (2002) media prior to 2002 were reviewed and an average dilution factor of ~73% was observed. Based on the ~5% variability observed a conservative value of:

$$\eta_{df} = 73\% - 5\% = 68\% \text{ (mean minus one standard deviation)} \quad \text{(C-2)}$$

was established for generic "design" analysis purposes. When specific batch data are available updated values can and should be considered.

15.0 Appendix D (Media Dry Bulk Bed Density)

Note that Eq. (C-1) represents the "effective" binary Cs isotherm for CST media in its engineered-form. It applies to a unit gram of CST media at its dry-reference state condition. For application in VERSE-LC for performing column analyses, this isotherm needs to be expressed in terms of CST bed volume. This is accomplished by multiplying it by the CST dry bulk bed density:

$$\overline{Q}_{Cs} = \frac{\rho_b \eta_{df} Q_T c_{Cs}}{c_{Cs} + \beta} \quad \text{(D-1)}$$

where

- $\overline{Q}_{Cs}$ - local Cs ionic solid-phase concentration, (mmol/ml_{bed}).
- ρ_b - CST dry bulk bed density, (g_{CST}/ml_{bed}).

As Eq. (D-1) indicates, consistency in units needs to be carefully considered when performing column analyses. CST dry bulk bed densities have been measured by various researchers over the years and in Hamm et al. (2002) it ranged from 0.77 to 1.13 g_{CST}/ml_{bed}.

King et al. (2018) measured a wet bulk bed density of 1.03 g_{CST}/ml_{bed} (i.e., the mass being in their wet-reference state). This gave a dry bulk bed density of:

$$\rho_b = (0.82)(1.03) = 0.8446 \ (g_{CST}/ml_{bed}) \quad \text{(D-2)}$$

Fiskum et al. (2018) measured dry bulk bed densities 0.987 and 1.02 g_{CST}/ml_{bed} (i.e., the mass being in their dry-reference state).

As the above values indicate, variations in bed densities have also been observed in the most recent CST batches (i.e., 2017 and 2018 batches).

16.0 Appendix E (Assessment of PNNL Simple Simulant Tests)

Fiskum et al. (2018) recently performed both batch contact and lead/lag column studies using the most recent CST batch (i.e., IONSIV™ R9140-B) where a 5.6 M Na simple simulant was employed. This was the first available data indicating how this new CST media behaves. For this report this data set was used to help establish key batch specific parameter values for: (1) the engineered-form dilution factor; and (2) the Cs^+ particle pore tortuosity factor.

Below both the batch contact and the column breakthrough data are reviewed where the SRNL ZAM/VERSE methodology is employed.

Batch Contact Tests

The batch contact data performed by Fiskum et al. (2018) were originally evaluated by SRNL to determine if the tests actually achieved equilibrium due to the short contacts time employed (i.e., 24 and 45 hour

agitation times). Historically and recent SRNL testing would have indicated 72 plus hours should have been required.

Two sets of batch contact tests were performed: one for 24 hours and the other for 45 hours. Contact temperatures ranged from 24°C to 25°C. Historically CST takes longer to reach a true equilibrium and given the much larger mean particle size than prior studies it should take even longer (4 plus days). Recent SRNL batch contact studies (i.e., see King et al., 2018, and Nash and Hamm, 2018) using a 2017 CST batch (IONSIV R9120-B) indicated that equilibrium is not reach until four plus days of stirring. The batch employed had a mean particle diameter of about 550 microns, somewhat consistent with the material used by PNNL (with a mean diameter of 573 microns). From prior experience these batch contact tests would not have been expected to reach equilibrium. However, when comparing the 24 hour versus the 45 hour K_d and Q values it is evident that they were close to equilibrium. This implies that the overall particle kinetics is much faster for this new media batch, or some other factor caused the material to be at an "apparent" equilibrium condition. It is noted that PNNL agitated the samples at much faster rotation speeds than normal protocol. Normally, this higher speed would have caused the CST beads to disintegrate, but the researchers reported (via private communication) that the beads remained intact. The reason that these beads appear to reach equilibrium faster than expected is not understood at this time.

The Langmuir fit provided by Fiskum et al. (2018) can be seen in their Eq. (3.2). Below, this fit is provided where the units have been changed to be consistent with our previous historical efforts as provided in Eq. (D-1):

$$\eta_{df} = 0.988 \ \text{(-)}$$

$$\beta = 6.8465\text{x}10^{-4} \ \text{[M]}$$

A plot of their isotherm fit and data are provided in Figure E-1. The high Cs data is also shown for completeness. Note that the dilution factor above is nearly one suggesting that either: (1) the addition of inert binder did not reduce the CST media's total Cs exchange capacity on a per mass basis or (2) this new media has a larger total Cs exchange capacity. The recent SRNL testing (King et al., 2018, and Nash and Hamm, 2018) indicated that a dilution factor close to 68% remains consistent with historical expectations. Recognize that the material received by SRNL was only partially converted to the sodium form but was fully converted to the sodium form and underwent the caustic washing procedure by SRNL prior to the capacity measurements, so it should have been in the same condition as the PNNL material. Note that the two high Cs data points (i.e., the far-right data in Figure E-1) represent dilution factors of 52% and 68%, respectively. Hamm et al. (2002) reviewed CST data up through 2001 to determine various batch dilution factors. See Appendix C Table C-6 in that document where the mean value of 73% was calculated and the lowest value observed was ~59%.

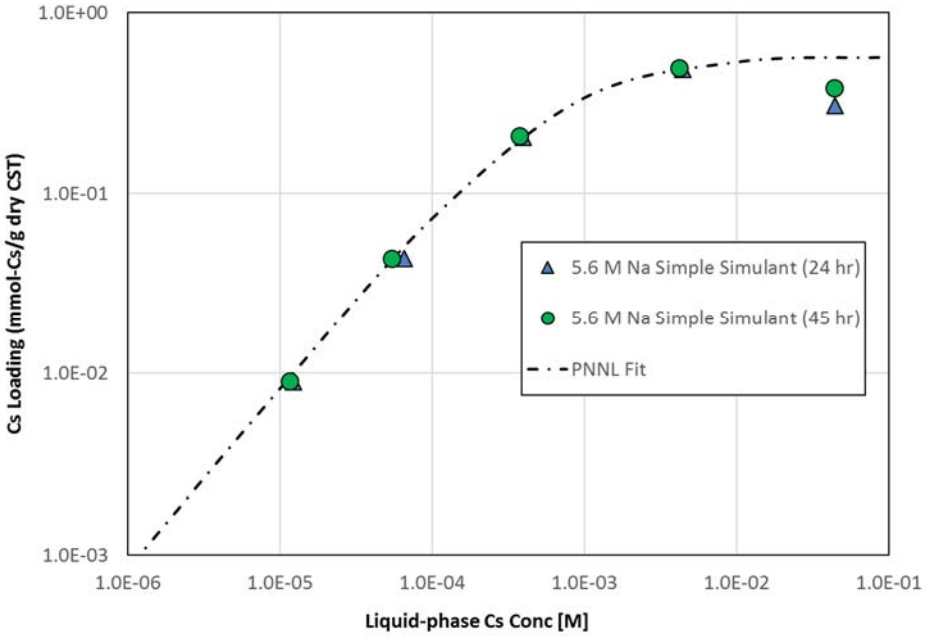

Figure E-1 Fiskum et al. (2018) Langmuir fit to the 5.6 M Na Simple Simulant at 24°C.

Also note the majority of the data shown in Figure E-1 suggests that 24 hour contact tests are sufficient to reach near-equilibrium, although, as discussed above, that is contrary to prior experience with both smaller and larger CST particles. Given the column feed compositions of interest (i.e., $<1x10^{-4}$ M) only the two data points to the far left are of practical interest for our purposes; however, the various observations noted above do bring up questions with regard to this new media batch:

- Particle kinetics appears to be faster than historical batches.
- Total Cs exchange capacity might be larger than the 0.58 mmol/g of historical batches.

For CST column predictions, it is preferable to generate isotherms using ZAM. Limited batch contact testing is performed using the batch of interest and a simulant that contains the key ions in it. Using ZAM provides us with a foundation to make temperature and composition changes without having to continue to perform batch contact testing and kinetic testing.

Following our standard methodology for creating an isotherm using ZAM, a series of numerical batch contact runs were made employing the composition listed in Table 2-1. The results from these runs were also fitted to Eq. (D-1) resulting in:

$$\beta = 3.1154x10^{-4} \text{ [M]}$$

where the dilution factor in its standard values are:

$\eta_{df} = 1.00$ (-) (for CST in its powdered-form)

$\eta_{df} = 0.68$ (-) (for CST in its engineered-form and used in *design estimates*)

This beta-factor corresponds to 24°C isotherm. Both of these ZAM predicted Langmuir isotherms are superimposed onto Figure E-1 in Figure E-2.

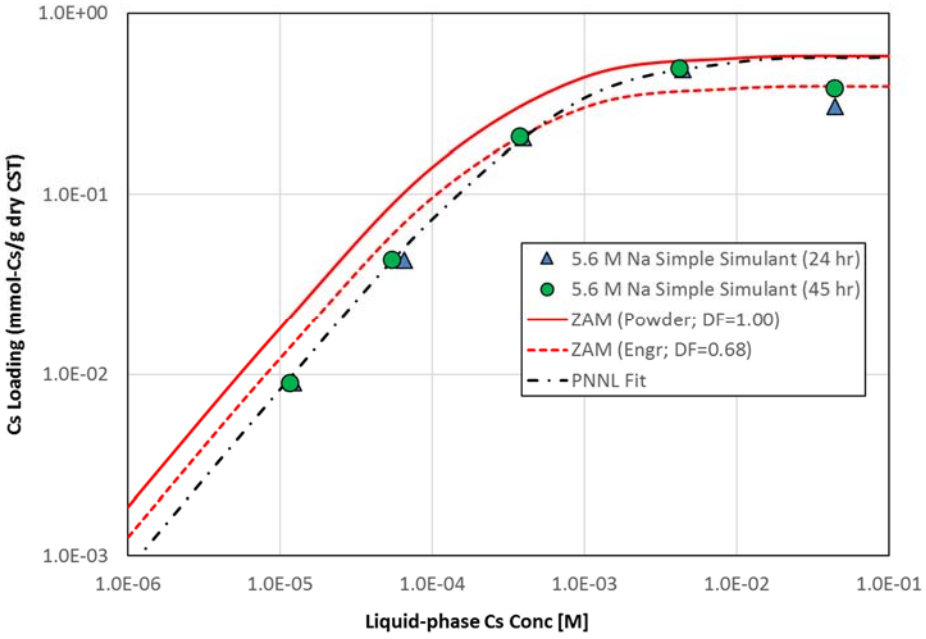

Figure E-2 ZAM generated Langmuir fits to 5.6 M Na Simple Simulant at 24°C.

The data obtained by PNNL for the samples with high initial Cs concentration falls in-line with the dilution factor of 68% (i.e., see red dashed line). However, PNNL's lower Cs concentration data falls below both ZAM predicted isotherms. No single Langmuir isotherm will fall through all of the data. By dropping off the highest Cs concentration data a single Langmuir isotherm will represent all of the remaining data as shown in Figures E-1 and E-2. Historically, a single Langmuir isotherm will fit most of the data. In Figure E-2 the Langmuir isotherm projected by PNNL (shown as a black dashed curve) was a two-parameter fit to all the data (excluding the upper set). The other two Langmuir isotherms (shown in red) are ZAM generated.

In order to generate a ZAM-based isotherm that adheres to the low concentration range data a dilution factor of 52% must be employed:

$$\eta_{df} = 0.52 \ (-) \ \text{(for this specific CST batch and used in } \textit{best estimates}\text{)}$$

This case along with the isotherm fitted by PNNL are shown in Figure E-3.

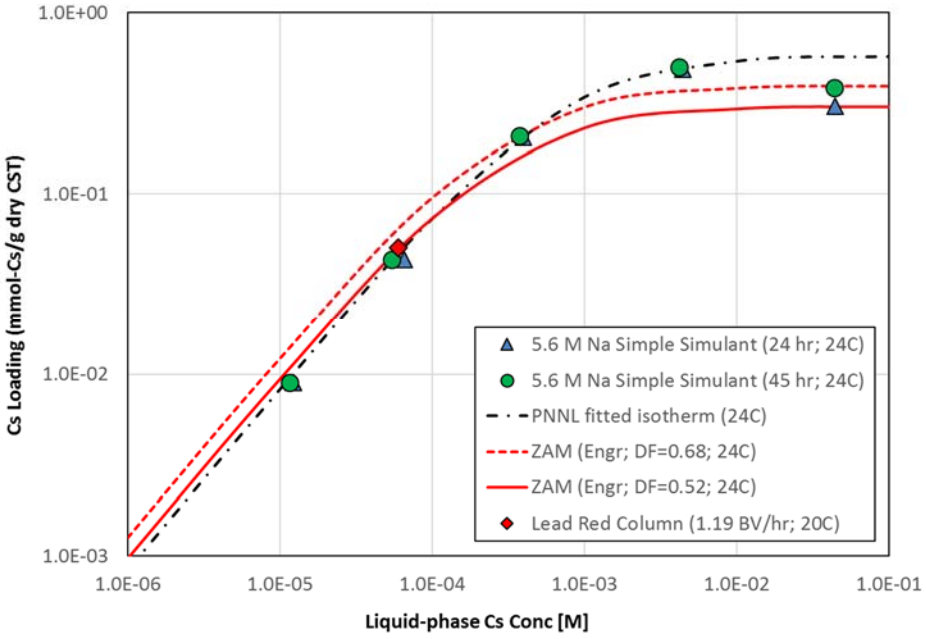

Figure E-3 ZAM generated Langmuir fits to 5.6 M Na Simple Simulant at 24°C.

As shown in Figure E-3, two ZAM generated isotherms will be employed to make VERSE column simulations. These two isotherms are based on different assumed dilution factors:

- $\eta_{df} = 0.68$ (-) (for *design estimate* purposes)
- $\eta_{df} = 0.52$ (-) (for *best estimate* purposes)

Since Fiskum et al. (2018) ran their column runs at the lower temperature range of 18°C to 22°C, a new ZAM-based isotherm was created at the average temperature of 20°C. Under high caustic conditions the dominate ion-exchange reaction is exothermic resulting in increased loadings. The results from these runs were also fitted to Eq. (D-1) resulting in:

$$\beta = 2.8982 \text{x} 10^{-4} \quad [\text{M}]$$

This beta-factor corresponds to a 20°C isotherm and was used in the following column simulations.

Fiskum et al. (2018) did run their column tests out to a sufficient number of BVs to estimate a point on the isotherm based on near exhaustion of their lead columns. Chapter 5 of Helfferich (1962) states that the most reliable method of establishing an isotherm is through column exhaustion testing. We took the Red lead column data and ran VERSE-LC for an extended number of BVs (i.e., ~2000 BVs). The parameter settings employed (i.e., our Best estimate settings) are provided in the column assessment section below. The only parameter that was adjusted for further breakthrough refinement was the dilution factor. Our Best estimate value is 52%, but to obtain as precise an extended breakthrough curve over the entire data range this value was reduced to 49% for this application only. The results are shown in Figure E-4.

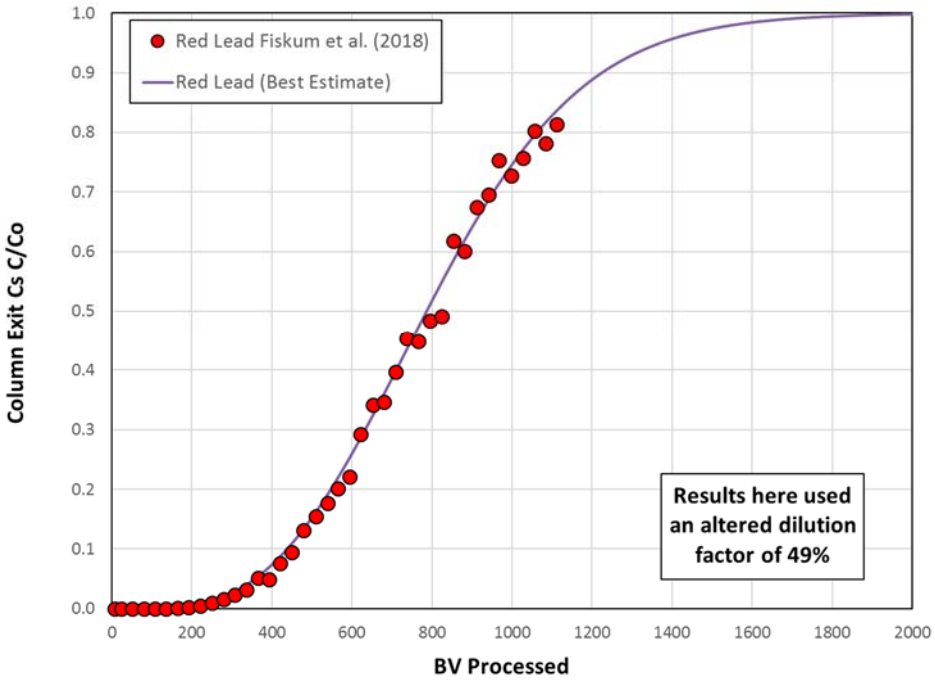

Figure E-4 Extended VERSE-LC predicted breakthrough for red lead column (1.19 BV/hr; linear scale plot).

We employed VERSE-LC here to allow us to extrapolate this lead column on out to exhaustion (i.e., about 2000 BVs). The area above the breakthrough curve represents the total amount of Cs loaded onto the CST bed (see Hamm et al., 2002, for details). With this information we now have a fairly reliable estimate of the equilibrium curve at the feed concentration and 20°C employed:

Cs feed concentration = 5.97×10^{-5} [M]
Cs column loading = 0.0507 mmol/g-CST(dry)
Column CST mass = 9.83 grams of dry CST in engr-form

In Figure E-3 a comparison was made between the batch contact data and this column-based loading number. The above loading point on the isotherm corresponds to the column operating temperature of ~20°C. The other loading points on Figure E-3 corresponds to batch contact data at about 24°C.

In Figure E-3 a comparison was made between the batch contact data and this column-based loading number. Only the isotherm at and below the feed concentration is relevant for column performance and as Figure E-3 indicates the *best estimate* isotherm is in fairly close agreement with the data.

Lead/Lag Column Tests

Fiskum et al. (2018) ran two equally sized ~10 ml columns in series. Each column had headspaces above their packed CST beds. Each column was stated to be 1.44 cm in ID. From their legend to their Eq. (4-1) the total amount of dry CST mass per column was ~9.8289 g. We assume that the dry bulk bed density is 1.0 g/ml. This results in bed lengths of 6.0352 cm each. The two columns operated at ambient conditions that ranged 18°C to 22°C. We used the average temperature of 20°C for the isotherms.

Geometrically, the Red, Blue, and Green set of columns are assumed identical where the only parameter value changing was the feed flowrate given as:

Red columns – 1.19 BV/hr = 0.195 ml/min

Blue columns – 1.99 BV/hr = 0.326 ml/min

Green columns – 4.56 BV/hr = 0.747 ml/min

VERSE-LC runs were made for each column configuration (i.e., Red, Blue, and Green) where all parameters were at nominal settings based on our current methodology.

For this 5.6 M Na simple simulant at the average temperature of 20°C (i.e., 18°C to 22°C range during operation), the OLI code (which employs significantly improved methods) computed the following property values required as input to VERSE-LC:

$D_{\infty,Cs} = 5.94x10^{-4}$ (cm^2/min) (effective Cs binary diffusivity)

$\rho_f = 1.230$ (g/ml) (liquid-phase solution density)

$\mu_f = 2.667$ (cP) (absolute viscosity of the solution)

Two different tortuosity factor settings were considered: (1) our *design estimate* value of 10 for computing conservative breakthrough estimates and (2) our *best estimate* value based on a parameter search effort to achieve the observed breakthrough data. An extensive parameter optimization was not performed here. Instead a few trial values (i.e., 5x, 4x, 3x, and 2x) were considered and the best overall value observed was chosen (i.e., value was determine looking only at the Red column data):

- $\tau = 10$ (-) (for *design estimate* purposes)
- $\tau = 4$ (-) (for *best estimate* purposes)

A more refined estimate would have resulted in a tortuosity factor slightly less than 4. Given these tortuosity factor settings, a Cs pore diffusion coefficient was computed using:

$$D_{p,Cs} = \frac{D_{\infty,Cs}}{\tau} \quad (cm^2/min) \qquad (D\text{-}3)$$

A comparison between the Red lead column data (1.19 BV/hr case) and VERSE-LC runs at both the *design* and *best estimate* settings is provided in Figure E-5.

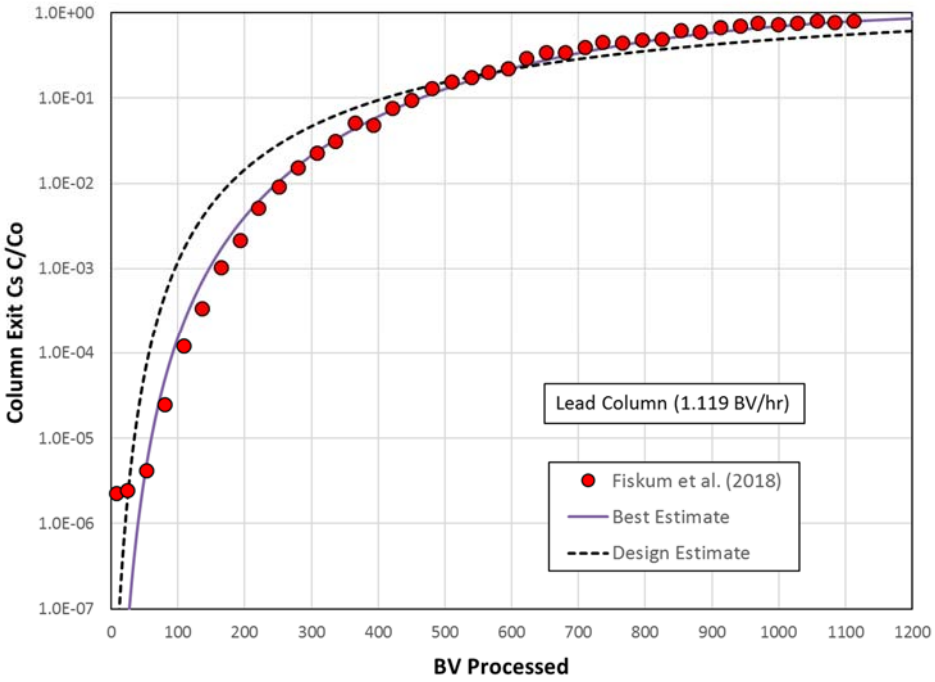

Figure E-5 VERSE-LC predicted breakthrough for red lead column using *design* and *best estimate* settings (1.19 BV/hr; semi-log scale plot).

As expected the VERSE-LC design estimate results show an earlier than measured Cs breakthrough curve. As such, column sizing employing the *design estimate* parameter settings will result in a conservative bed volume estimate. The *best estimate* results are in good agreement with the data, as expected since some degree of parameter adjustment was made in obtaining the tortuosity factor value of 4 (i.e., all other parameters remained fixed). As shown in Hamm et al. (2002) a tortuosity factor of 4 is within the historical range of values observed.

Using the same set of *best estimate* parameter settings, all three column cases (i.e., lead and lag Red, Blue, and Green cases) were run using VERSE-LC (i.e., basically the only variable changing was an increasing feed flowrate). Below the Cs breakthrough curves for both the lead and lag columns are compared to the data. Figures in linear and semi-log scales are provided as well.

Figures E-6 and E-7 show the VERSE-LC results versus the Red column Cs breakthrough data (i.e., 1.19 BV/hr flowrate).

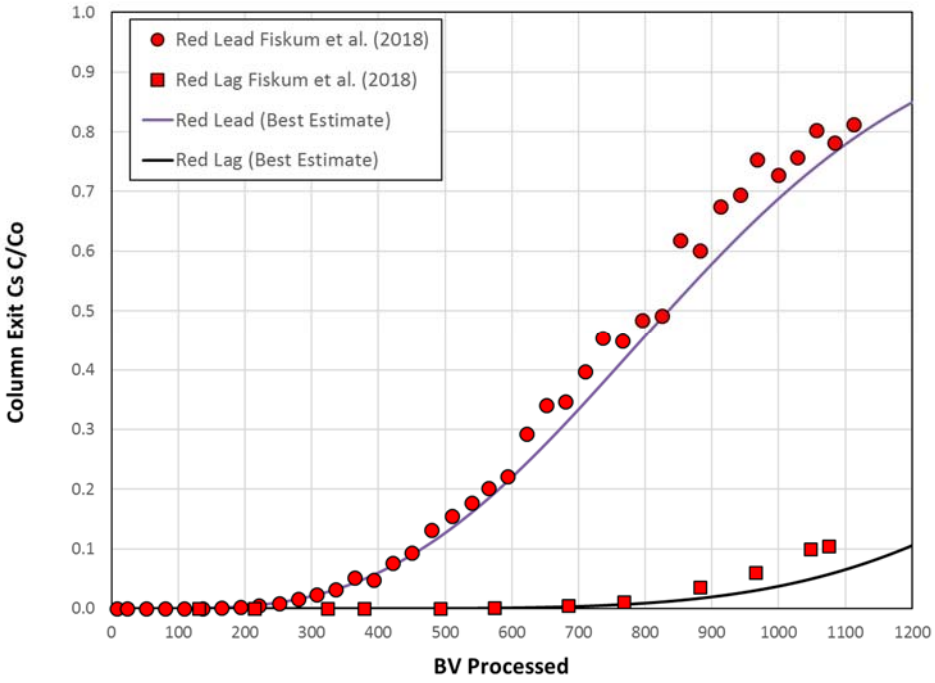

Figure E-6 VERSE-LC predicted breakthrough for red lead/lag column using *best estimate* settings (1.19 BV/hr; linear scale plot).

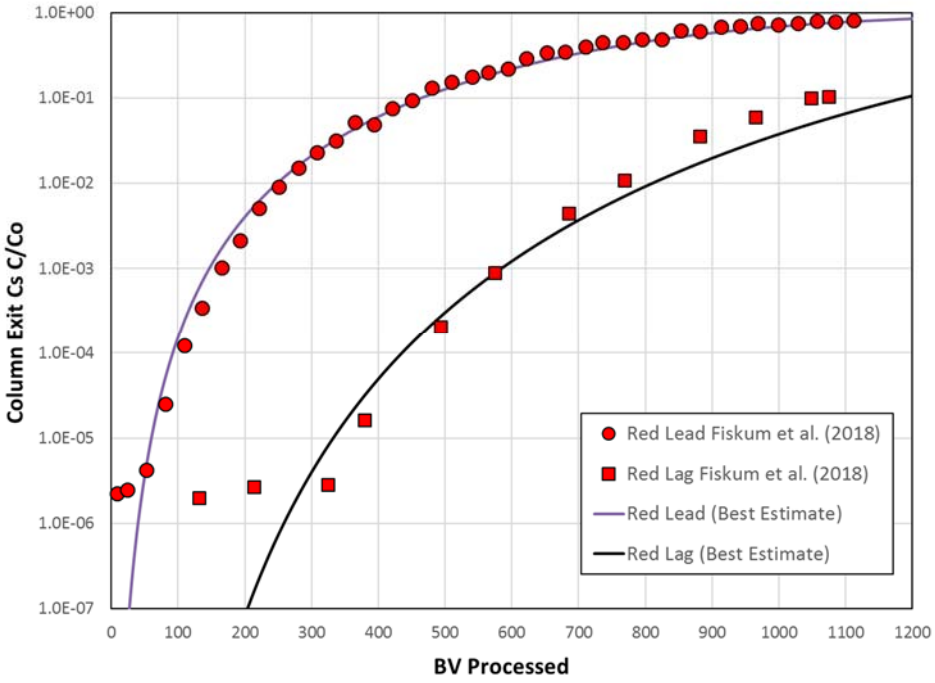

Figure E-7 VERSE-LC predicted breakthrough for red lead/lag column using *best estimate* settings (1.19 BV/hr; semi-log scale plot).

Figures E-8 and E-9 show the VERSE-LC results versus the Blue column Cs breakthrough data (i.e., 1.99 BV/hr flowrate).

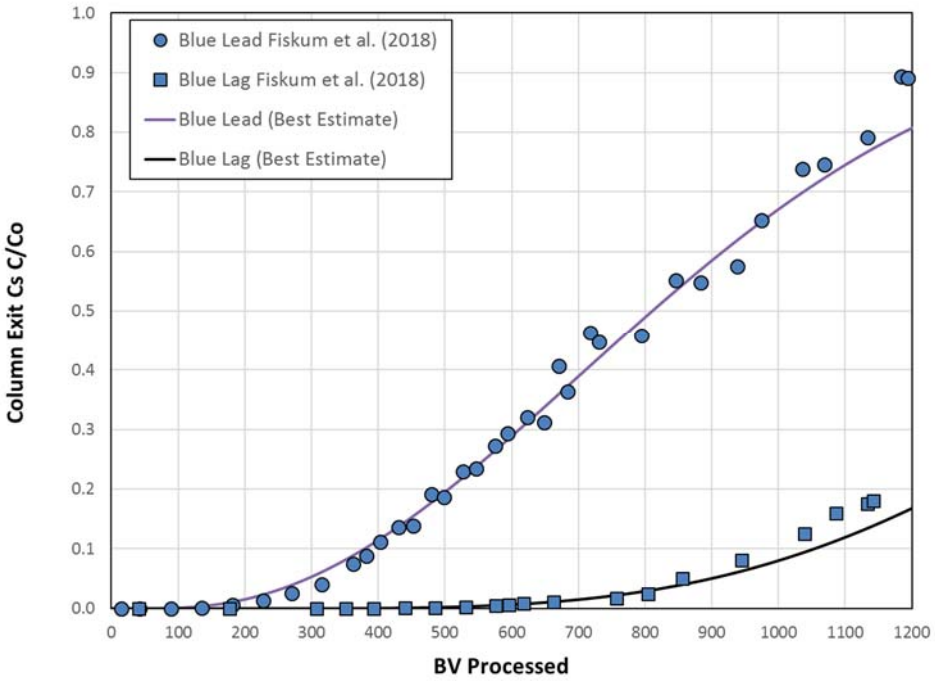

Figure E-8 VERSE-LC predicted breakthrough for blue lead/lag column using *best estimate* settings (1.99 BV/hr; linear scale plot).

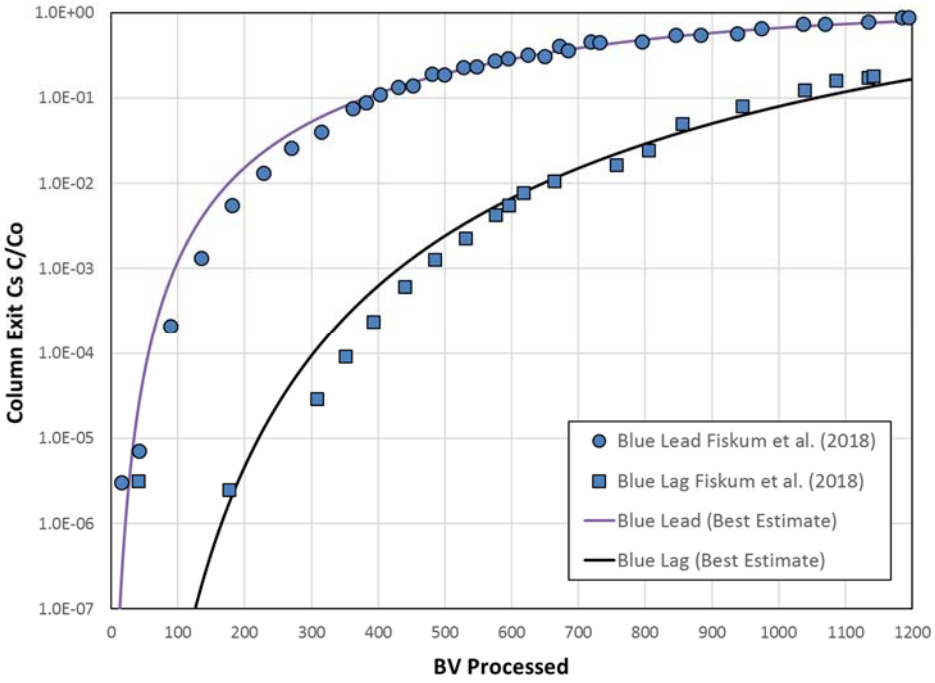

Figure E-9 VERSE-LC predicted breakthrough for blue lead/lag column using *best estimate* settings (1.99 BV/hr; semi-log scale plot).

Figures E-10 and E-11 show the VERSE-LC results versus the Green column Cs breakthrough data (i.e., 4.56 BV/hr flowrate).

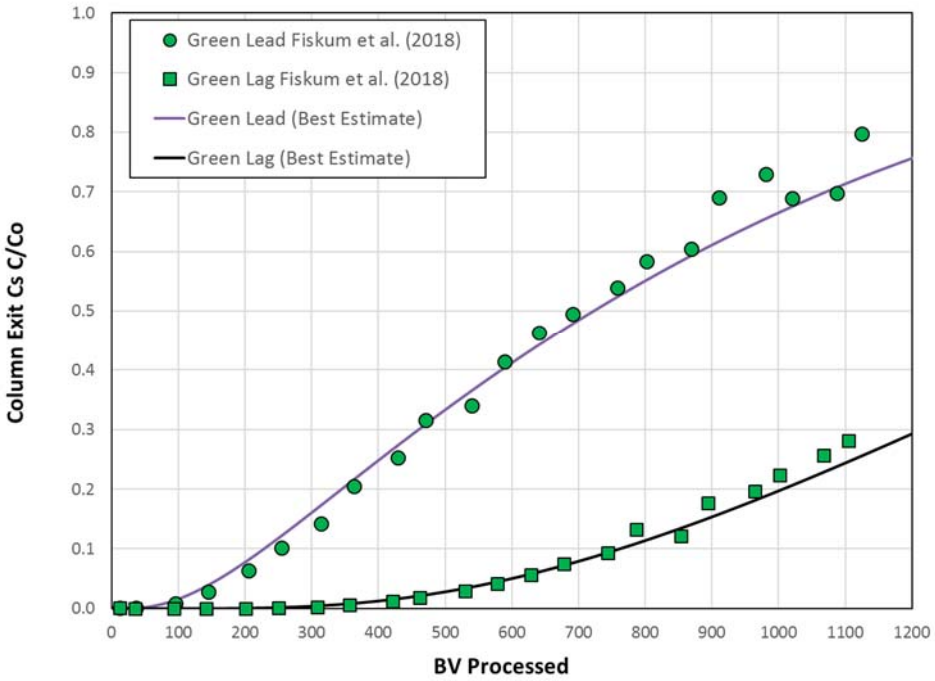

Figure E-10 VERSE-LC predicted breakthrough for green lead/lag column using *best estimate* settings (4.56 BV/hr; linear scale plot).

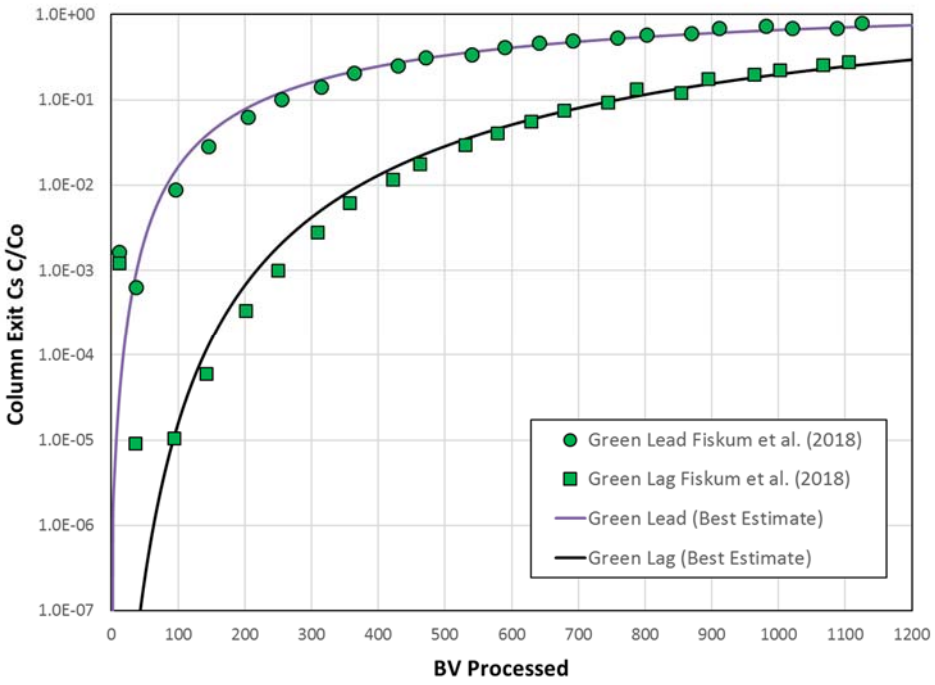

Figure E-11 VERSE-LC predicted breakthrough for green lead/lag column using *best estimate* settings (4.56 BV/hr; semi-log scale plot).

As the lead and lag Cs breakthrough comparisons indicate, the VERSE-LC *best estimate* results are in fairly good agreement for all three feed flowrates. These results provide some overall degree of confidence in the data sets provided by Fiskum et al. (2018) and the ZAM/VERSE methodology established by Hamm et al. (2002).

Fiskum et al. (2018) also performed gamma scanning axially down both the lead and lag columns as described in their report under Section 4.2. The point in the process when these gamma scans were performed is not provided but is assumed to have occurred at the end of simulant processing, followed by feed displacement. Thus, gamma scanning results are assumed to apply to both columns where:

- Red column configuration flowing at 1.19 BV/hr;
- Lead and lag columns initially fresh;
- 1112 BV of feed processed through both columns;
- Feed simulant washed completely from both columns;
- Only gamma emitting species are Cs isotopes; and
- Cs present only in solid phase.

A VERSE-LC simulation run was made using the *best estimate* parameter setting. The Cs liquid-phase radial concentration profiles within the CST beads were written out along the axial length of the lead and lag columns. These liquid-phase concentration profiles were written to file at the end of processing the 1112 BVs of feed. Within a spreadsheet these liquid-phase concentrations were converted over to local solid-phase profiles and then radially averaged to obtain the total Cs loading on the solid-phase as a function of axial distance down each column. A plot of these loading profiles is provided in Figure E-12. For comparison purposes, the gamma profiles, that infer Cs loading profiles, measured by Fiskum et al. (2018) are also plotted in Figure E-12 where a gamma scaling factor was employed to assist in the comparison.

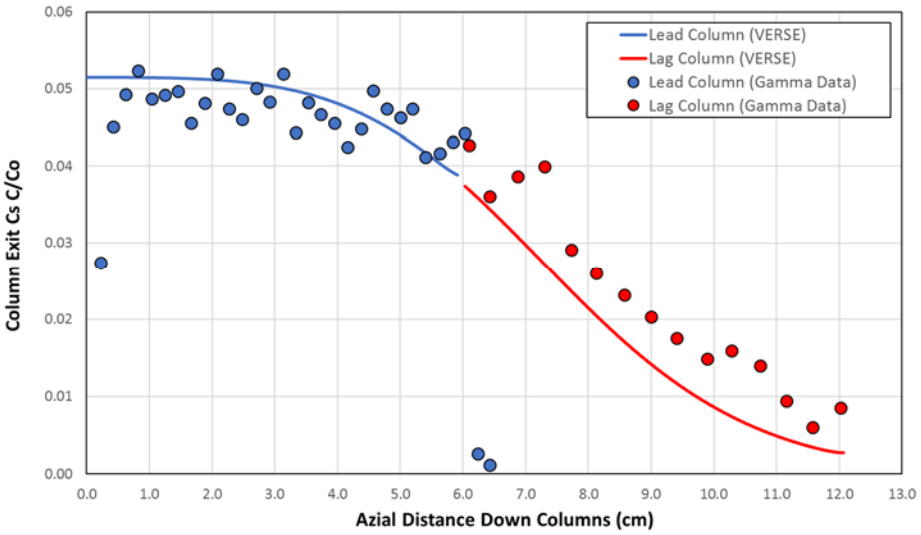

Figure E-12 VERSE-LC predicted total Cs solid-phase loading profiles for lead and lag columns using *best estimate* settings versus gamma data (Red 1.19 BV/hr; linear scale plot).

A single scaling factor was applied to both the lead and lag column data to convert the gamma measurements from counts/sec to C/Co units. The value used was 0.028.

Gamma measurements will have some level of axial smearing due to viewing angle limitations and that results in some degree of flattening out of the measured profiles. The VERSE-LC results appear slightly sharper consistent with this expectation. Overall the VERSE-LC predictions and the gamma data show very similar profile behavior.

17.0 Appendix F (Assessment of PNNL Actual AP-107 Waste Tests)

To evaluate the accuracy of using these parameters in the model a similar assessment was performed on the data sets provided by Rovira et al. (2018). That test utilized actual AP-107 tank waste and the same new CST batch (i.e., IONSIV™ R9140-B). Below both the batch contact and the column breakthrough data are reviewed where the SRNL ZAM/VERSE methodology is employed. The parameter settings that were established while assessing the simple simulant data (see Appendix E) were not altered during these assessments. Only those aspects that differ, such as feed composition, are updated. Thus, these comparisons are viewed as being confirmatory to the parameters and approach derived from the new data by Fiskum, et al. (2018).

Batch Contact Tests

Rovira et al. (2018) performed three sets of batch contact tests: one for 48 hours, one for 51 hours, and one for 91 hours. Temperature ranged from 26.9°C to 27.4°C (average around 27°C). Following our standard methodology for creating an isotherm using ZAM, a series of numerical batch contact runs were made employing the composition listed in Table 2-1. The results from these runs were also fitted to Eq. (D-1) resulting in:

$$\beta = 3.7377 \text{x} 10^{-4} \quad [\text{M}]$$

Even though several factors differed between the simple simulant and the AP-107 solution (e.g., composition such as Sr^{++} being present and higher temperatures), we see that this beta-factor ended up being only 20% larger than the value computed for the simple simulant.

The ZAM predicted Langmuir isotherm for the AP-107 solution is shown in Figure F-1, along with the batch contact data. Also shown is the batch contact data for the simple simulant indicating how similar its

behavior is to the AP-107 data. For comparison purposes the batch contact data taken by King et al. (2018) with SRS Average simulant (at 23.2°C) is shown along with the ZAM predicted Langmuir isotherm. As expected the SRS Avg simulant has less competitors (primarily K^+) and results in a higher isotherm than either of the other two solutions.

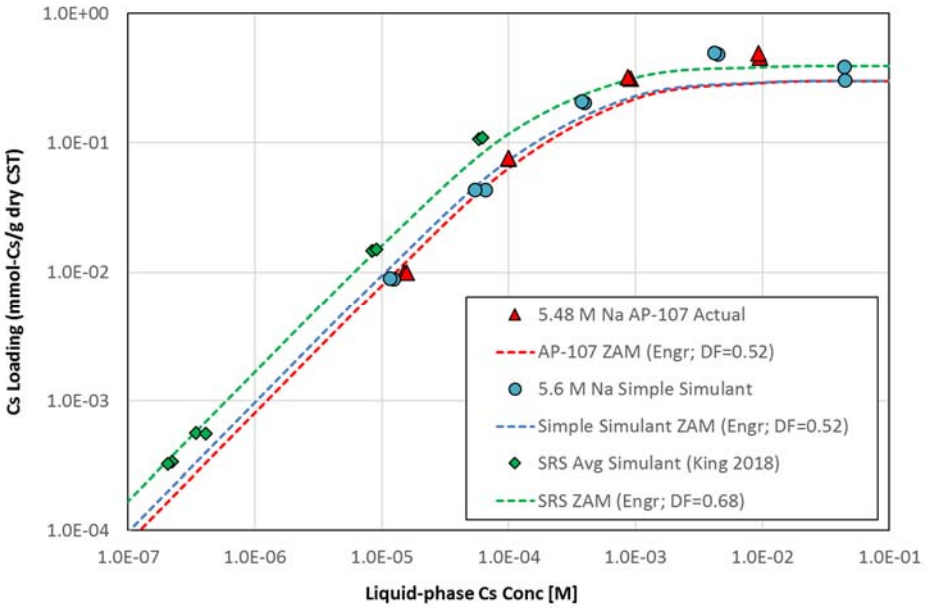

Figure F-1 ZAM generated Langmuir fits to actual AP-107 Waste at 27°C.

Since Rovira et al. (2018) ran their column runs at the lower temperature range of 24°C to 26°C, a new ZAM-based isotherm was created at the average temperature of 25°C. The results from these runs were also fitted to Eq. (D-1) resulting in:

$$\beta = 3.6327\text{x}10^{-4} \quad [\text{M}]$$

This beta-factor corresponds to a 25°C isotherm and was used in the following column simulations.

Lead/Lag Column Test

Rovira et al. (2018) ran two equally sized ~10 ml columns in series. Each column had headspaces above their packed CST beds. Each column was stated to be 1.44 cm in ID. From their legend to their Eq. (4.1) the total amount of dry CST mass per column was ~9.7919 g. We assume that the dry bulk bed density is 1.0 g/ml. This results in bed lengths of 6.14 cm each. The two columns operated at ambient conditions within the Hot Cell assumed to be about 25°C (i.e., 24°C to 26°C). Only the initial feed flowrate of 2.2 BV/hr was considered in these analyses. During these tests one carousel action was taken at about 500 BVs into the testing where the lead column was removed from the system, the lag column was transferred to the lead position, and fresh lag column was installed. Since we are only interested in breakthrough performance of a fresh lead column, no carousel action analyses were considered here.

For this actual AP-107 waste solution at the average temperature of 25°C, the OLI code (which employs significantly improved methods) computed the following property values required as input to VERSE-LC:

$D_{\infty,Cs} = 7.46\text{x}10^{-4}$ (cm^2/min)	(effective Cs binary diffusivity)
$\rho_f = 1.223$ (g/ml)	(liquid-phase solution density)
$\mu_f = 2.260$ (cP)	(absolute viscosity of the solution)

The two different tortuosity factor settings that were considered in the simple simulant assessment were employed here making this a confirmation study:

- $\tau = 10$ (-) (for *design estimate* purposes)
- $\tau = 4$ (-) (for *best estimate* purposes)

VERSE-LC runs were made for the initial column configuration (i.e., fresh lead and lag columns operating at 2.2 BV/hr) where all parameters were at nominal settings based on our current methodology. Both *design* and *best estimate* runs were made. VERSE-LC runs were extended out to ~1000 BVs (i.e., about 500 BVs beyond when an actual carousel action was taken). VERSE-LC predicted Cs breakthrough curves are compared to the data in Figure F-2.

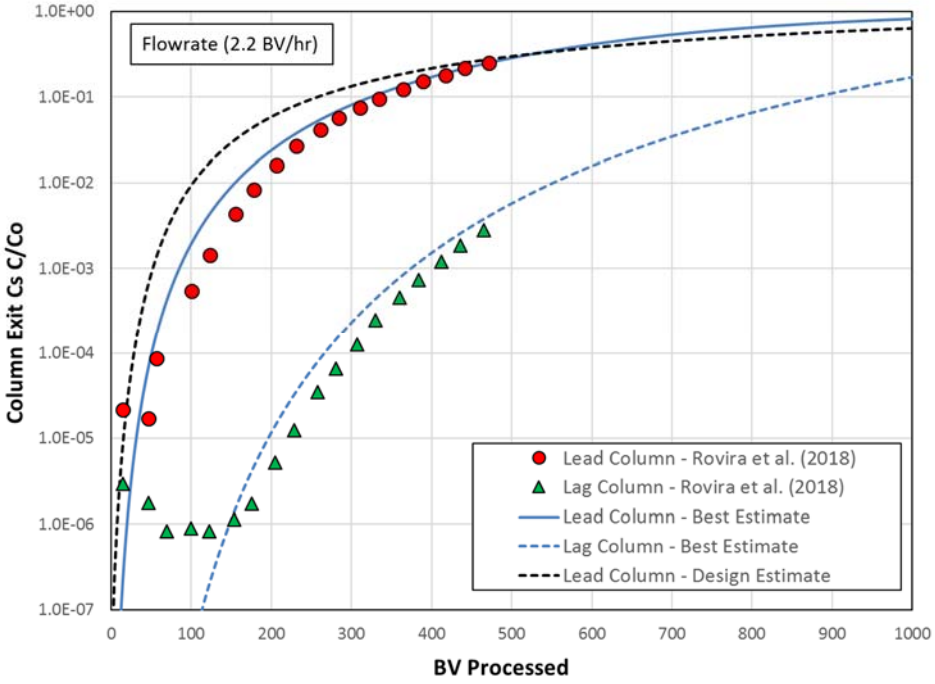

Figure F-2 VERSE-LC predicted breakthrough for lead/lag column using *design* and *best estimate* settings (semi-log scale plot).

As observed for the simple simulant VERSE-LC runs: (1) the *design estimated* breakthrough is conservative with respect to the data and (2) the *best estimate* results are fairly consistent (but slightly conservative) with respect to the data.

As mentioned earlier SRNL and PNNL employ differing protocols when drying out their CST media. This can lead to dry bulk bed densities that are perhaps in inaccurate. To see the possible effect of having less dry CST media within these columns, VERSE-LC runs were redone using a bed density of 0.75 g/ml (based on the 75% F-Factor that was measured). With this lower bed density, the tortuosity factor was lowered from 4 to 2 in order to see how well the VERSE-LC predictions would remain. These altered parameter settings were made, and the VERSE-LC results are shown in Figure F-3.

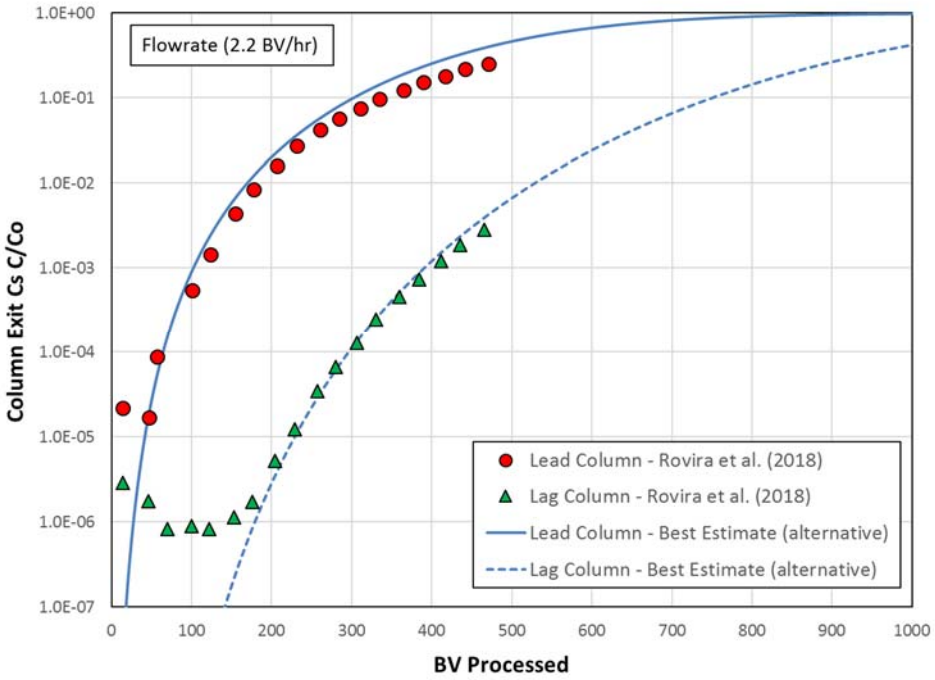

Figure F-3 VERSE-LC predicted breakthrough for lead/lag column using altered *best estimate* settings (semi-log scale plot).

As a comparison between Figures F-2 and F-3 show, similar predictive capability can be achieved but consistency in measuring the amount of truly dry CST media within the bed should be of high priority.

17.1 This example illustrates how certain parameters are interrelated. This implies that one type of data set (e.g., column data) cannot alone provide definitive parameters settings. The ideal case is to run for a specific batch contact tests, kinetic tests, and column tests. From the three data types the various key parameters settings can be confidently isolated. Appendix G (ZAM Analysis Details)

The following are the ZAM input and output files for a subset of the batch contact cases considered. In the creation of a ZAM generated isotherm, a series of numerical batch contact runs are made. Each numerical batch contact run presents a baseline solution composition where CsCl is being added to trace out the isotherm. Nine initial Cs concentrations varying from $1.0x10^{-9}$ to 0.1 M are considered where in each case a very large phase ratio is employed (i.e., $\phi = 1.0x10^{5}$).

- Case1 – $1.0x10^{-9}$
- Case2 – $1.0x10^{-8}$
- Case3 – $1.0x10^{-7}$
- Case4 – $1.0x10^{-6}$
- Case5 – $1.0x10^{-5}$
- Case6 – $1.0x10^{-4}$
- Case7 – $1.0x10^{-3}$
- Case8 – $1.0x10^{-2}$
- Case9 – $1.0x10^{-1}$

All ZAM runs made in the course of this effort have been saved and archived onto SRNL servers that can be retrieved at a later date, if requested. For details on the input values provided see Hamm et al. (2002) for additional information and comparison to input decks provided there. Primarily version 4.0 of ZAM

was used. Only a few limited version 5.0 cases were run to verify the results when Sr was present in the solution.

Only one case for each isotherm of interest will be provided below. Specifically, Case5 where the initial Cs concentration is $1.0x10^{-5}$ [M] case.

17.2 TBI Feed Isotherms

Two TBI isotherms at 22°C were generated: (1) one without Sr being present and (2) one with Sr present in the feed. Below the input and output files for each is provided. Note that ZAM results are identical for the Sr present case when either it is brought in as Sr^{+2} or as $SrOH^{+}$. At these OH^{-} and Sr^{++} concentration levels one would expect near identical results as were observed in the ZAM runs.

Input: 22C – TBI Feed – No Sr present

```
1, 295.15
Hanford TBI project: Temperature Effect @ 22C
7, 10
1244
 3, 6,  1,  5,  4, 40, 13
13, 9, 27, 15, 19,  2, 20, 28, 25  1
96.0107
6.046186       1.0E-05 1.0E-14 0.0     0.143996       0.0     0.0
1.128881       1.951459       1.236809       0.040287       0.533244       0.078146
       0.037274       0.515168       0.0     0.020844
1, 0.00001
0
.9
```

Output: 22C – TBI Feed – No Sr present

```
 Solution:  Hanford TBI project: Temperature
**********INPUT**********

  Density=  .1244E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .6046E+01
Cs+.....        132.9054          1.       .1000E-04
H+......          1.0079          1.       .1000E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .1440E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1129E+01
NO3-....         62.0049         -1.       .1951E+01
NO2-....         46.0000         -1.       .1237E+01
SO4--...         96.0636         -2.       .4029E-01
CO3--...         60.0092         -2.       .5332E+00
Cl-.....         35.4527         -1.       .7815E-01
PO4---..         94.9712         -3.       .3727E-01
Al(OH)4-         95.0000         -1.       .5152E+00
Other--.         96.0107         -2.       .0000E+00
F-......         18.9984         -1.       .2084E-01

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

 Material: Na Form


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

 Ionic Strength=           9.002453498063479 mol/kg
```

```
        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .1568E-01      .1000E-01      .1568E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .0000E+00      .0000E+00      .0000E+00
  K         .4987E+00      .1440E+03      .3463E+01
```

Input: 22C – TBI Feed – Sr present

```
1, 295.15
Hanford TBI project: Temperature Effect @ 22C
7, 10
1244
 3, 6,  1,  5,  4, 40, 13
13, 9, 27, 15, 19,  2, 20, 28, 25  1
96.0107
6.046186       1.0E-05 1.0E-14 0.0     0.143996       0.0    8.19e-6
1.128881       1.951459       1.236809       0.040287       0.533244       0.078146
       0.037274       0.515168       0.0     0.020844
1, 0.00001
0
.9
```

Output: 22C – TBI Feed – Sr present

```
   Solution:  Hanford TBI project: Temperature
  **********************INPUT************************

    Density=  .1244E+04 kg/m3

                Molecular Wt.    Valance    Molarity(mol/L)
  Na+.....         22.9898          1.       .6046E+01
  Cs+.....        132.9054          1.       .1000E-04
  H+......          1.0079          1.       .1000E-13
  Rb+.....         85.4678          1.       .0000E+00
  K+......         39.0983          1.       .1440E+00
  SrOH+...        105.0000          1.       .0000E+00
  Sr++....         87.6200          2.       .8190E-05
  OH-.....         17.0073         -1.       .1129E+01
  NO3-....         62.0049         -1.       .1951E+01
  NO2-....         46.0000         -1.       .1237E+01
  SO4--...         96.0636         -2.       .4029E-01
  CO3--...         60.0092         -2.       .5332E+00
  Cl-.....         35.4527         -1.       .7815E-01
  PO4---..         94.9712         -3.       .3727E-01
  Al(OH)4-         95.0000         -1.       .5152E+00
  Other--.         96.0107         -2.       .0000E+00
  F-......         18.9984         -1.       .2084E-01

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

   Material: Na Form


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

   Ionic Strength=           9.002473347999935 mol/kg

          Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
  Cs        .1041E-01      .1000E-01      .1041E+04
  Rb        .0000E+00      .0000E+00      .0000E+00
  Sr        .2100E+00      .8188E-02      .2564E+05
  K         .5686E+00      .1440E+03      .3949E+01
```

17.3 5.6 M Na Simple Simulant Feed Isotherm

Two isotherms were generated for the Simple Simulant studied by Fiskum et al. (2018): one at 24ºC and the other at 20ºC. The 24ºC isotherm was for comparison to their batch contact data while the 20ºC isotherm was employed in the column simulations. Sr^{+2} was not present in the simple simulant solution employed (however, trace amounts may have been present due to purity aspects of reagents employed).

Input: 24C – 5.6 M Na Simple Simulant Feed – No Sr present

```
1, 297.15
PNNL Testing for TBI project: Temperature Effect @ 24C
7, 10
1227
 3, 6,  1,  5,  4, 40, 13
13, 9, 27, 15, 19,  2, 20, 28, 25  1
96.0107
5.570000       1.0E-05 1.0E-14 0.0     0.122000       0.0     0.0
1.410000       1.780000       1.020000       0.066000       0.468000       0.117870
       0.043400       0.166000       0.0     0.000000
1, 0.00001
0
.9
```

Output: 24C – 5.6 M Na Simple Simulant Feed – No Sr present

```
 Solution:  PNNL Testing for TBI project: Te
**********INPUT**********

  Density=  .1227E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .5570E+01
Cs+.....        132.9054          1.       .1000E-04
H+......          1.0079          1.       .1000E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .1220E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1410E+01
NO3-....         62.0049         -1.       .1780E+01
NO2-....         46.0000         -1.       .1020E+01
SO4--...         96.0636         -2.       .6600E-01
CO3--...         60.0092         -2.       .4680E+00
Cl-.....         35.4527         -1.       .1179E+00
PO4---..         94.9712         -3.       .4340E-01
Al(OH)4-         95.0000         -1.       .1660E+00
Other--.         96.0107         -2.       .0000E+00
F-......         18.9984         -1.       .0000E+00

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

 Material: Na Form


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

 Ionic Strength=           7.900198300082176 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .1804E-01      .1000E-01      .1804E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .4925E+00      .1220E+03      .4037E+01
```

Input: 20C – 5.6 M Na Simple Simulant Feed – No Sr present

```
1, 293.15
PNNL Testing for TBI project: Temperature Effect @ 20C
7, 10
1230
 3, 6,  1,  5,  4, 40, 13
13, 9, 27, 15, 19,  2, 20, 28, 25  1
96.0107
5.570000       1.0E-05 1.0E-14 0.0     0.122000       0.0     0.0
1.410000       1.780000       1.020000       0.066000       0.468000       0.117870
       0.043400       0.166000       0.0     0.000000
1, 0.00001
0
.9
```

Output: 20C – 5.6 M Na Simple Simulant Feed – No Sr present

```
 Solution:  PNNL Testing for TBI project: Te
**********INPUT**********

  Density=  .1230E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .5570E+01
Cs+.....        132.9054          1.       .1000E-04
H+......          1.0079          1.       .1000E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .1220E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .0000E+00
OH-.....         17.0073         -1.       .1410E+01
NO3-....         62.0049         -1.       .1780E+01
NO2-....         46.0000         -1.       .1020E+01
SO4--...         96.0636         -2.       .6600E-01
CO3--...         60.0092         -2.       .4680E+00
Cl-.....         35.4527         -1.       .1179E+00
PO4---..         94.9712         -3.       .4340E-01
Al(OH)4-         95.0000         -1.       .1660E+00
Other--.         96.0107         -2.       .0000E+00
F-......         18.9984         -1.       .0000E+00

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

 Material: Na Form


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

 Ionic Strength=           7.872211469078249 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .1935E-01      .1000E-01      .1935E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .0000E+00      .0000E+00      .0000E+00
K         .5187E+00      .1220E+03      .4252E+01
```

17.4 Actual AP-107 Waste Isotherm

Two isotherms were generated for the actual AP-107 waste studied by Rovira et al. (2018): one at 27ºC and the other at 25ºC. The 27ºC isotherm was for comparison to their batch contact data while the 25ºC isotherm was employed in the column simulations. Sr^{+2} was present in the actual AP-107 waste solution employed.

Input: 27C – Actual AP-107 waste Feed – Sr present

```
1, 300.15
PNNL Testing of Actual AP-107: Temperature Effect @ 27C
7, 10
```

```
1222
 3, 6,  1,  5,  4, 40, 13
13, 9, 27, 15, 19,  2, 20, 28, 25  1
96.0107
5.480715       1.0E-05 1.0E-14 0.0     0.100004       0.0     3.77768E-06
0.990000       1.709542       1.143342       0.015928       0.635833       0.019670
       0.016531       0.365065       0.0     0.000000
1, 0.00001
0
.9
```

Output: 27C – Actual AP-107 waste Feed – Sr present

```
 Solution:  PNNL Testing of Actual AP-107: T
**********INPUT**********

  Density=  .1222E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .5481E+01
Cs+.....        132.9054          1.       .1000E-04
H+......          1.0079          1.       .1000E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .1000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .3778E-05
OH-.....         17.0073         -1.       .9900E+00
NO3-....         62.0049         -1.       .1710E+01
NO2-....         46.0000         -1.       .1143E+01
SO4--...         96.0636         -2.       .1593E-01
CO3--...         60.0092         -2.       .6358E+00
Cl-.....         35.4527         -1.       .1967E-01
PO4---..         94.9712         -3.       .1653E-01
Al(OH)4-         95.0000         -1.       .3651E+00
Other--.         96.0107         -2.       .0000E+00
F-......         18.9984         -1.       .0000E+00

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

 Material: Na Form


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

 Ionic Strength=           7.996981618976492 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .1511E-01      .1000E-01      .1511E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .1266E+00      .3776E-02      .3352E+05
K         .4702E+00      .1000E+03      .4702E+01
```

Input: 25C – Actual AP-107 waste Feed – Sr present

```
1, 298.15
PNNL Testing of Actual AP-107: Temperature Effect @ 25C
7, 10
1223
 3, 6,  1,  5,  4, 40, 13
13, 9, 27, 15, 19,  2, 20, 28, 25  1
96.0107
5.480715       1.0E-05 1.0E-14 0.0     0.100004       0.0     3.77768E-06
0.990000       1.709542       1.143342       0.015928       0.635833       0.019670
       0.016531       0.365065       0.0     0.000000
1, 0.00001
0
.9
```

Output: 25C – Actual AP-107 waste Feed – Sr present

```
 Solution:  PNNL Testing of Actual AP-107: T
**********************INPUT************************

  Density=  .1223E+04 kg/m3

              Molecular Wt.    Valance    Molarity(mol/L)
Na+.....         22.9898          1.       .5481E+01
Cs+.....        132.9054          1.       .1000E-04
H+......          1.0079          1.       .1000E-13
Rb+.....         85.4678          1.       .0000E+00
K+......         39.0983          1.       .1000E+00
SrOH+...        105.0000          1.       .0000E+00
Sr++....         87.6200          2.       .3778E-05
OH-.....         17.0073         -1.       .9900E+00
NO3-....         62.0049         -1.       .1710E+01
NO2-....         46.0000         -1.       .1143E+01
SO4--...         96.0636         -2.       .1593E-01
CO3--...         60.0092         -2.       .6358E+00
Cl-.....         35.4527         -1.       .1967E-01
PO4---..         94.9712         -3.       .1653E-01
Al(OH)4-         95.0000         -1.       .3651E+00
Other--.         96.0107         -2.       .0000E+00
F-......         18.9984         -1.       .0000E+00

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

 Material: Na Form



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

 Ionic Strength=           7.987339567930459 mol/kg

        Q (mmol/gCST)    C (mmol/L)    Kd (ml/gCST)
Cs        .1554E-01      .1000E-01      .1554E+04
Rb        .0000E+00      .0000E+00      .0000E+00
Sr        .1289E+00      .3776E-02      .3412E+05
K         .4827E+00      .1000E+03      .4827E+01
```

18.0 Appendix H (VERSE-LC Analysis Details)

VERSE-LC runs were made under a variety of conditions.

For the TBI study a single column was assumed where a headspace was applied at both the frontend and backend of the CST bed. Both nominal cases, as well as, sensitivity studies about nominal settings were considered. A range of bed volume sizes were considered under nominal conditions. The sensitivity cases (i.e., feed flowrate and mean particle size) focused only on the 20 gallon bed volume.

For the simple simulant and actual AP-107 waste a lead and lag column configuration were assumed. Headspaces were applied above and below each CST bed. No carousel actions were considered.

18.1 TBI Nominal Conditions – Best Estimate – No Sr present

Six different bed volumes were considered (16, 18, 20, 21, 25, 27). Only the 20 gallon case is provided here.

Input: TBI Feed – No Sr present

```
[Full-Scale] Simulation of Cs removal on TBI Baseline CST material lead column
1 component (Cs) isotherm (Na 5.06 M) (Hanford TBI: Nominal Case)
1, 50, 3, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNA                           isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                           input-only,perfusable,feed-equil,datafile.yio
```

```
MM                              comp-conc units
103.63, 30.48, 3785.412, 18904.0 Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0       part-rad(um), bed-void, part-void, sorb-cap()
  0.0                           initial concentrations (M)
S                               COMMAND - conc step change
1, 0.0, 5.06d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                               COMMAND - viscosity/density change
0.02695, 1.244                  fluid viscosity(posie), density(g/cm^3)
h                               COMMAND - effluent history dump
1, 1.0, 1.0, 0.25, 0.1          unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1          unit op#, ptscale(1-4) filtering
D
-1,    500.0, 1, 0.0
D
-1,   1000.0, 1, 0.0
D
-1,   1500.0, 1, 0.0
D
-1,   2000.0, 1, 0.0
-                               end of commands
2100.0, 1.0                     end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                  abs-tol, rel-tol
-                               non-negative conc constraint
1.0d0                           size exclusion factor
1.5125d-4                       part-pore diffusivities(cm^2/min) tortuosity factor = 10.0
6.050d-4                        Brownian diffusivities(cm^2/min)
0.3016                          Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0 g/ml
1.0                             Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                             Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580
1.0                             Freundlich/Langmuir Hybrid Mb   (-)
3.600d-4                        Freundlich/Langmuir Hybrid beta (-) "eff" isotherm Na = 5.06 M
```

Output: TBI Feed – No Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ================================================================================
 Input file: case
 [Full-Scale] Simulation of Cs removal on TBI Baseline CST material lead col
 1 component (Cs) isotherm (Na 5.06 M) (Hanford TBI: Nominal Case)
 Begin Run:  15:10:22 on 08-07-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  1610
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ================================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =   2100.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    103.63000 cm          D              =     30.48000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =  75614.53832 mL
 F              =   3785.41200 mL/min      Uo (linear)    =      9.46701 cm/min
 R              =    286.50000 microns     L/R            =   3617.10297
 Bed Void frac. =       .54800            Pcl. Porosity  =       .24000
 Spec. Area     =     47.32984 1/cm        Time/BV        =     10.94644 min
 Vol CSTRs      =  18904.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .14471E+01
 Dp  [cm2/min]  =  .15125E-03
 Doo [cm2/min]  =  .60500E-03
 kf  [cm/min]   =  .16572E+00
 Ds  [cm2/min]  =  .00000E+00
```

```
Dimensionless Groups:
Re             =  .22870E+00
Sc(i)          =  .21485E+04
Peb(i)         =  .67794E+03
Bi(i)          =  .13080E+03
Nf(i)          =  .15668E+03
Np(i)          =  .48409E+00
Pep(i)         =  .74719E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .30160E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .36000E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
================================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5060E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2695E-01 poise and density to 1.244     g/cm3
  3: Monitor conc. history at stream  1.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  4: Monitor conc. history at stream  2.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Dump full profile file at  500.0     min
     Execute   1 times, every .0000     mins.
  6: Dump full profile file at  1000.     min
     Execute   1 times, every .0000     mins.
  7: Dump full profile file at  1500.     min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  2000.     min
     Execute   1 times, every .0000     mins.
================================================================================
VERSE-LC finished in   404 steps.  Average step size 5.198     minutes
End run:  15:10:38 on 08-07-2018
Integrated Areas in History Files:
case.h01                   .106004
case.h02                   .241912E-04
```

18.2 TBI Nominal Conditions – Design Estimate – No Sr present

Five different bed volumes were considered (18, 20, 21, 25, 27). Only the 20 gallon case is provided here.

Input: TBI Feed – No Sr present

```
[Full-Scale] Simulation of Cs removal on TBI Baseline CST material lead column
1 component (Cs) isotherm (Na 5.06 M) (Hanford TBI: Nominal Case)
1, 50, 3, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                            input-only,perfusable,feed-equil,datafile.yio
MM                               comp-conc units
103.63, 30.48, 3785.412, 18904.0 Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
  0.0                            initial concentrations (M)
S                                COMMAND - conc step change
1, 0.0, 5.06d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02695, 1.244                   fluid viscosity(posie), density(g/cm^3)
h                                COMMAND - effluent history dump
1, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
D
```

```
-1,    500.0, 1, 0.0
D
-1,   1000.0, 1, 0.0
D
-1,   1500.0, 1, 0.0
D
-1,   2000.0, 1, 0.0
-                              end of commands
2100.0, 1.0                    end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                 abs-tol, rel-tol
-                              non-negative conc constraint
1.0d0                          size exclusion factor
6.0500d-5                      part-pore diffusivities(cm^2/min) tortuosity factor = 10.0
6.0500d-4                      Brownian diffusivities(cm^2/min)
0.3944                         Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0 g/ml
1.0                            Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                            Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580
1.0                            Freundlich/Langmuir Hybrid Mb   (-)
3.600d-4                       Freundlich/Langmuir Hybrid beta (-) "eff" isotherm Na = 5.06 M
```

Output: TBI Feed – No Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ================================================================================
 Input file: case
 [Full-Scale] Simulation of Cs removal on TBI Baseline CST material lead col
 1 component (Cs) isotherm (Na 5.06 M) (Hanford TBI: Nominal Case)
 Begin Run:  15:14:52 on 08-07-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  1610
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ================================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =   2100.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    103.63000 cm          D              =     30.48000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =  75614.53832 mL
 F              =   3785.41200 mL/min      Uo (linear)    =      9.46701 cm/min
 R              =    286.50000 microns     L/R            =   3617.10297
 Bed Void frac. =       .54800            Pcl. Porosity  =       .24000
 Spec. Area     =     47.32984 1/cm        Time/BV        =     10.94644 min
 Vol CSTRs      =  18904.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .14471E+01
 Dp  [cm2/min]  =  .60500E-04
 Doo [cm2/min]  =  .60500E-03
 kf  [cm/min]   =  .16572E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .22870E+00
 Sc(i)          =  .21485E+04
 Peb(i)         =  .67794E+03
 Bi(i)          =  .32699E+03
 Nf(i)          =  .15668E+03
 Np(i)          =  .19364E+00
 Pep(i)         =  .18680E+05

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .39440E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .10000E+01
```

```
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .36000E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
================================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5060E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2695E-01 poise and density to 1.244     g/cm3
  3: Monitor conc. history at stream  1.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  4: Monitor conc. history at stream  2.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Dump full profile file at  500.0     min
     Execute   1 times, every .0000     mins.
  6: Dump full profile file at  1000.     min
     Execute   1 times, every .0000     mins.
  7: Dump full profile file at  1500.     min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  2000.     min
     Execute   1 times, every .0000     mins.
================================================================================
VERSE-LC finished in   393 steps.  Average step size 5.344     minutes
End run:  15:15:08 on 08-07-2018
Integrated Areas in History Files:
case.h01                   .106003
case.h02                   .327822E-03
```

18.3 TBI Nominal Conditions – Best Estimate – Sr present

Five different bed volumes were considered (18, 20, 21, 25 27). Only the 20 gallon case is provided here.

Input: TBI Feed – With Sr present

```
[Full-Scale] Simulation of Cs removal on TBI Baseline CST material lead column
1 component (Cs) isotherm (Na 5.06 M) (Hanford TBI: Nominal Case)
1, 50, 3, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                            input-only,perfusable,feed-equil,datafile.yio
MM                               comp-conc units
103.63, 30.48, 3785.412, 18904.0 Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
  0.0                            initial concentrations (M)
S                                COMMAND - conc step change
1, 0.0, 5.06d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02695, 1.244                   fluid viscosity(posie), density(g/cm^3)
h                                COMMAND - effluent history dump
1, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
D
-1,    500.0, 1, 0.0
D
-1,   1000.0, 1, 0.0
D
-1,   1500.0, 1, 0.0
D
-1,   2000.0, 1, 0.0
-                                end of commands
2100.0, 1.0                      end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
```

```
1.5125d-4                       part-pore diffusivities(cm^2/min) tortuosity factor = 10.0
6.050d-4                        Brownian diffusivities(cm^2/min)
0.3016                          Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0 g/ml
1.0                             Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                             Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580
1.0                             Freundlich/Langmuir Hybrid Mb   (-)
5.472d-4                        Freundlich/Langmuir Hybrid beta (-) "eff" isotherm Na = 5.06 M
```

Output: TBI Feed – With Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: case
 [Full-Scale] Simulation of Cs removal on TBI Baseline CST material lead col
 1 component (Cs) isotherm (Na 5.06 M) (Hanford TBI: Nominal Case)
 Begin Run:  15:41:46 on 08-15-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  1610
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =   2100.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    103.63000 cm          D              =     30.48000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =  75614.53832 mL
 F              =   3785.41200 mL/min      Uo (linear)    =      9.46701 cm/min
 R              =    286.50000 microns     L/R            =   3617.10297
 Bed Void frac. =       .54800            Pcl. Porosity  =       .24000
 Spec. Area     =     47.32984 1/cm        Time/BV        =     10.94644 min
 Vol CSTRs      =  18904.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .14471E+01
 Dp  [cm2/min]  =  .15125E-03
 Doo [cm2/min]  =  .60500E-03
 kf  [cm/min]   =  .16572E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .22870E+00
 Sc(i)          =  .21485E+04
 Peb(i)         =  .67794E+03
 Bi(i)          =  .13080E+03
 Nf(i)          =  .15668E+03
 Np(i)          =  .48409E+00
 Pep(i)         =  .74719E+04

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .30160E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .10000E+01
 Iso. Const. 4  =  .10000E+01
 Iso. Const. 5  =  .54720E-03
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units           M
 ===============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .5060E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .2695E-01 poise and density to 1.244     g/cm3
   3: Monitor conc. history at stream  1.  Filename = case.h01
      Output density adjustments:
```

```
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .25    *default force w/ conc delta, .10    *default force w/o conc delta
   4: Monitor conc. history at stream  2.  Filename = case.h02
      Output density adjustments:
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .25    *default force w/ conc delta, .10    *default force w/o conc delta
   5: Dump full profile file at  500.0     min
      Execute   1 times, every .0000     mins.
   6: Dump full profile file at  1000.     min
      Execute   1 times, every .0000     mins.
   7: Dump full profile file at  1500.     min
      Execute   1 times, every .0000     mins.
   8: Dump full profile file at  2000.     min
      Execute   1 times, every .0000     mins.
 ================================================================================
 VERSE-LC finished in   398 steps.  Average step size 5.276     minutes
 End run:  15:42:02 on 08-15-2018
 Integrated Areas in History Files:
 case.h01                   .106003
 case.h02                   .221259E-03
```

18.4 TBI Nominal Conditions – Design Estimate – Sr present

Seven different bed volumes were considered (18, 20, 21, 25, 27, 30, 35). Only the 20 gallon case is provided here.

Input: TBI Feed – with Sr present

```
[Full-Scale] Simulation of Cs removal on TBI Baseline CST material lead column
1 component (Cs) isotherm (Na 5.06 M) (Hanford TBI: Nominal Case)
1, 50, 3, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                            input-only,perfusable,feed-equil,datafile.yio
MM                               comp-conc units
103.63, 30.48, 3785.412, 18904.0 Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
  0.0                            initial concentrations (M)
S                                COMMAND - conc step change
1, 0.0, 5.06d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02695, 1.244                   fluid viscosity(posie), density(g/cm^3)
h                                COMMAND - effluent history dump
1, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
D
-1,    500.0, 1, 0.0
D
-1,   1000.0, 1, 0.0
D
-1,   1500.0, 1, 0.0
D
-1,   2000.0, 1, 0.0
-                                end of commands
2100.0, 1.0                      end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
6.0500d-5                        part-pore diffusivities(cm^2/min) tortuosity factor = 10.0
6.0500d-4                        Brownian diffusivities(cm^2/min)
0.3944                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0 g/ml
1.0                              Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
5.472d-4                         Freundlich/Langmuir Hybrid beta (-) "eff" isotherm Na = 5.06 M
```

Output: TBI Feed – With Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: case
 [Full-Scale] Simulation of Cs removal on TBI Baseline CST material lead col
 1 component (Cs) isotherm (Na 5.06 M) (Hanford TBI: Nominal Case)
 Begin Run:  16:21:56 on 08-15-2018   running under Windows 95/8
 Finite elements    - axial: 50  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  1610
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =   2100.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    103.63000 cm          D              =     30.48000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =  75614.53832 mL
 F              =   3785.41200 mL/min      Uo (linear)    =      9.46701 cm/min
 R              =    286.50000 microns     L/R            =   3617.10297
 Bed Void frac. =       .54800            Pcl. Porosity  =       .24000
 Spec. Area     =     47.32984 1/cm        Time/BV        =     10.94644 min
 Vol CSTRs      =  18904.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .14471E+01
 Dp  [cm2/min]  =  .60500E-04
 Doo [cm2/min]  =  .60500E-03
 kf  [cm/min]   =  .16572E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .22870E+00
 Sc(i)          =  .21485E+04
 Peb(i)         =  .67794E+03
 Bi(i)          =  .32699E+03
 Nf(i)          =  .15668E+03
 Np(i)          =  .19364E+00
 Pep(i)         =  .18680E+05

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .39440E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .10000E+01
 Iso. Const. 4  =  .10000E+01
 Iso. Const. 5  =  .54720E-03
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units           M
 ===============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .5060E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .2695E-01 poise and density to 1.244     g/cm3
   3: Monitor conc. history at stream  1.  Filename = case.h01
      Output density adjustments:
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .25    *default force w/ conc delta, .10    *default force w/o conc delta
   4: Monitor conc. history at stream  2.  Filename = case.h02
      Output density adjustments:
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .25    *default force w/ conc delta, .10    *default force w/o conc delta
   5: Dump full profile file at  500.0     min
      Execute   1 times, every .0000     mins.
   6: Dump full profile file at  1000.     min
      Execute   1 times, every .0000     mins.
   7: Dump full profile file at  1500.     min
      Execute   1 times, every .0000     mins.
```

```
  8: Dump full profile file at  2000.     min
     Execute   1 times, every .0000     mins.
 ================================================================================
 VERSE-LC finished in   393 steps.  Average step size 5.344     minutes
 End run:  16:22:12 on 08-15-2018
 Integrated Areas in History Files:
 case.h01                   .106003
 case.h02                   .136126E-02
```

18.5 5.6M Na Simple Simulant

Three separate lead/lag column cases here where the flowrate was increased. Fiskum et al. (2018) labeled these as Red, Blue, and Green cases.

Input: Simple Simulant – Red Columns – Best Estimate - No Sr present

```
[Lab-Scale] PNNL 5.6 M Na simple Simulant at Cs removal on Baseline CST material lead/lag columns
1 component (Cs) isotherm (Na 5.0 M) (5.6 M Na simple Simulant 20C isotherm)
1, 100, 3, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
MM                                comp-conc units
12.0704,  1.44, 0.19494, 4.9145   Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
  0.0, 0.0                        initial concentrations (M)
S                                 COMMAND - conc step change
1, 0.0, 5.970d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.0239095, 1.227                  fluid viscosity(posie), density(g/cm^3)
m                                 COMMAND - subcolumns
50, 100, 0, 1, 5.970d+8, 0.0, 900000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
D
-1,   4000.0, 1, 0.0
D
-1,  15125.0, 1, 0.0
D
-1,  30250.0, 1, 0.0
D
-1,  45375.0, 1, 0.0
D
-1,  60500.0, 1, 0.0
-                                 end of commands
60500.0, 1.0                      end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                    abs-tol, rel-tol
-                                 non-negative conc constraint
1.0d0                             size exclusion factor
1.485d-4                          part-pore diffusivities(cm^2/min)  4x factor
5.940d-4                          Brownian diffusivities(cm^2/min)
0.3016                      Freundlich/Langmuir Hybrid a (moles/L B.V.) rhob=1.0, DF=0.52,QT=0.58
1.0                               Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                               Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580, DF=0.988
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
2.8982d-4                         Freundlich/Langmuir Hybrid beta (-) 20C isotherm
```

Output: Simple Simulant – Red Columns – Best Estimate - No Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ================================================================================
 Input file: case
 [Lab-Scale] PNNL 5.6 M Na simple Simulant at Cs removal on Baseline CST mat
 1 component (Cs) isotherm (Na 5.0 M) (5.6 M Na simple Simulant 20C isotherm
 Begin Run:  14:04:51 on 08-28-2018   running under Windows 95/8
 Finite elements    - axial:100  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  3219
```

```
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Axial Dispersion and CSTR
================================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        =  60500.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =     12.07040 cm          D              =      1.44000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     19.65787 mL
F              =       .19494 mL/min      Uo (linear)    =       .21843 cm/min
R              =    286.50000 microns     L/R            =    421.30541
Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
Spec. Area     =     47.32984 1/cm        Time/BV        =     27.63033 min
Vol CSTRs      =      4.91450 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .34134E-01
Dp  [cm2/min]  =  .14850E-03
Doo [cm2/min]  =  .59400E-03
kf  [cm/min]   =  .46605E-01
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .58663E-02
Sc(i)          =  .19683E+04
Peb(i)         =  .38620E+02
Bi(i)          =  .37464E+02
Nf(i)          =  .11122E+03
Np(i)          =  .11997E+01
Pep(i)         =  .17559E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .30160E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .28982E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
================================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5970E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2391E-01 poise and density to 1.227     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .9000E+06 min.
     When comp.  1 reaches .5970E+09 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  6: Dump full profile file at  4000.     min
     Execute   1 times, every .0000     mins.
  7: Dump full profile file at  .1513E+05 min
     Execute   1 times, every .0000     mins.
  8: Dump full profile file at  .3025E+05 min
     Execute   1 times, every .0000     mins.
  9: Dump full profile file at  .4538E+05 min
     Execute   1 times, every .0000     mins.
 10: Dump full profile file at  .6050E+05 min
     Execute   1 times, every .0000     mins.
================================================================================
```

```
 VERSE-LC finished in  2280 steps.  Average step size 26.54     minutes
 End run:  14:05:15 on 08-28-2018
 Integrated Areas in History Files:
 case.h01                   1.11120
 case.h02                   .558929E-01
```

Input: Simple Simulant – Blue Columns – Best Estimate - No Sr present

```
[Lab-Scale] PNNL 5.6 M Na simple Simulant at Cs removal on Baseline CST material lead/lag columns
1 component (Cs) isotherm (Na 5.0 M) (5.6 M Na simple Simulant 20C isotherm)
1, 100, 3, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
MM                                comp-conc units
12.0704,  1.44, 0.32599, 4.9145   Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
  0.0, 0.0                        initial concentrations (M)
S                                 COMMAND - conc step change
1, 0.0, 5.970d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.0239095, 1.227                  fluid viscosity(posie), density(g/cm^3)
m                                 COMMAND - subcolumns
50, 100, 0, 1, 5.970d+8, 0.0, 900000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
-                                 end of commands
36200.0, 1.0                      end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                    abs-tol, rel-tol
-                                 non-negative conc constraint
1.0d0                             size exclusion factor
1.485d-4                          part-pore diffusivities(cm^2/min)  4x factor
6.610d-4                          Brownian diffusivities(cm^2/min)
0.3016                   Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0, DF=0.52,QT=0.58
1.0                               Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                               Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580, DF=0.988
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
2.8982d-4                         Freundlich/Langmuir Hybrid beta (-) 20C isotherm
```

Output: Simple Simulant – Blue Columns – Best Estimate - No Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
================================================================================
 Input file: case
 [Lab-Scale] PNNL 5.6 M Na simple Simulant at Cs removal on Baseline CST mat
 1 component (Cs) isotherm (Na 5.0 M) (5.6 M Na simple Simulant 20C isotherm
 Begin Run:  15:43:42 on 08-28-2018   running under Windows 95/8
 Finite elements    - axial:100  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  3219
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Axial Dispersion and CSTR
================================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  36200.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =     12.07040 cm          D              =     1.44000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     19.65787 mL
 F              =       .32599 mL/min      Uo (linear)    =       .36527 cm/min
 R              =    286.50000 microns     L/R            =    421.30541
 Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
 Spec. Area     =     47.32984 1/cm        Time/BV        =     16.52277 min
 Vol CSTRs      =      4.91450 mL
```

```
Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .57007E-01
Dp  [cm2/min]  =  .14850E-03
Doo [cm2/min]  =  .66100E-03
kf  [cm/min]   =  .59403E-01
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .98100E-02
Sc(i)          =  .17688E+04
Peb(i)         =  .38670E+02
Bi(i)          =  .47752E+02
Nf(i)          =  .84770E+02
Np(i)          =  .71742E+00
Pep(i)         =  .29363E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .30160E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .28982E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units            M
================================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5970E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2391E-01 poise and density to 1.227     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .9000E+06 min.
     When comp.  1 reaches .5970E+09 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
================================================================================
VERSE-LC finished in  2320 steps.  Average step size 15.60     minutes
End run:  15:44:10 on 08-28-2018
Integrated Areas in History Files:
case.h01                   .711226
case.h02                   .694942E-01
```

Input: Simple Simulant – Green Columns – Best Estimate - No Sr present

```
[Lab-Scale] PNNL 5.6 M Na simple Simulant at Cs removal on Baseline CST material lead/lag columns
1 component (Cs) isotherm (Na 5.0 M) (5.6 M Na simple Simulant 20C isotherm)
1, 100, 3, 6                    ncomp, nelem, ncol-bed, ncol-part
FCWNA                           isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                           input-only,perfusable,feed-equil,datafile.yio
MM                              comp-conc units
12.0704,  1.44, 0.74700, 4.9145  Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0       part-rad(um), bed-void, part-void, sorb-cap()
  0.0, 0.0                      initial concentrations (M)
S                               COMMAND - conc step change
1, 0.0, 5.970d-5, 1, 0.0        spec id, time(min), conc(M), freq, dt(min)
V                               COMMAND - viscosity/density change
0.0239095, 1.227                fluid viscosity(posie), density(g/cm^3)
m                               COMMAND - subcolumns
50, 100, 0, 1, 5.970d+8, 0.0, 900000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                               COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1          unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1          unit op#, ptscale(1-4) filtering
```

```
-                                 end of commands
15800.0, 1.0                      end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                    abs-tol, rel-tol
-                                 non-negative conc constraint
1.0d0                             size exclusion factor
1.485d-4                          part-pore diffusivities(cm^2/min)  4x factor
6.610d-4                          Brownian diffusivities(cm^2/min)
0.3016                    Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0, DF=0.52,QT=0.58
1.0                               Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                               Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580, DF=0.988
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
2.8982d-4                         Freundlich/Langmuir Hybrid beta (-) 20C isotherm
```

Output: Simple Simulant – Green Columns – Best Estimate - No Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
================================================================================
 Input file: case
 [Lab-Scale] PNNL 5.6 M Na simple Simulant at Cs removal on Baseline CST mat
 1 component (Cs) isotherm (Na 5.0 M) (5.6 M Na simple Simulant 20C isotherm
 Begin Run:  15:46:46 on 08-28-2018   running under Windows 95/8
 Finite elements    - axial:100  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  3219
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Axial Dispersion and CSTR
================================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  15800.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =     12.07040 cm          D              =      1.44000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     19.65787 mL
 F              =       .74700 mL/min      Uo (linear)    =       .83700 cm/min
 R              =    286.50000 microns     L/R            =    421.30541
 Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
 Spec. Area     =     47.32984 1/cm        Time/BV        =      7.21052 min
 Vol CSTRs      =      4.91450 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .13025E+00
 Dp  [cm2/min]  =  .14850E-03
 Doo [cm2/min]  =  .66100E-03
 kf  [cm/min]   =  .78315E-01
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .22479E-01
 Sc(i)          =  .17688E+04
 Peb(i)         =  .38782E+02
 Bi(i)          =  .62955E+02
 Nf(i)          =  .48772E+02
 Np(i)          =  .31308E+00
 Pep(i)         =  .67284E+03

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .30160E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .10000E+01
 Iso. Const. 4  =  .10000E+01
 Iso. Const. 5  =  .28982E-03
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units           M
================================================================================
 COMMAND LIST:
```

```
   1: Step conc. of component 1 at .0000     min to .5970E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .2391E-01 poise and density to 1.227     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .9000E+06 min.
      When comp.  1 reaches .5970E+09 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  2.  Filename = case.h01
      Output density adjustments:
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .25    *default force w/ conc delta, .10    *default force w/o conc delta
   5: Monitor conc. history at stream  4.  Filename = case.h02
      Output density adjustments:
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .25    *default force w/ conc delta, .10    *default force w/o conc delta
 ================================================================================
 VERSE-LC finished in  2358 steps.  Average step size 6.701     minutes
 End run:  15:47:21 on 08-28-2018
 Integrated Areas in History Files:
 case.h01                   .366137
 case.h02                   .811163E-01
```

Input: Simple Simulant – Red Columns – Design Estimate - No Sr present

```
[Lab-Scale] PNNL 5.6 M Na simple Simulant at Cs removal on Baseline CST material lead/lag columns
1 component (Cs) isotherm (Na 5.0 M) (5.6 M Na simple Simulant 20C isotherm)
1, 100, 3, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                            input-only,perfusable,feed-equil,datafile.yio
MM                               comp-conc units
12.0704,  1.44, 0.19494, 4.9145  Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
  0.0, 0.0                       initial concentrations (M)
S                                COMMAND - conc step change
1, 0.0, 5.970d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.0239095, 1.227                 fluid viscosity(posie), density(g/cm^3)
m                                COMMAND - subcolumns
50, 100, 0, 1, 5.970d+8, 0.0, 900000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
D
-1,   4000.0, 1, 0.0
D
-1,  15125.0, 1, 0.0
D
-1,  30250.0, 1, 0.0
D
-1,  45375.0, 1, 0.0
D
-1,  60500.0, 1, 0.0
-                                end of commands
60500.0, 1.0                     end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
5.940d-5                         part-pore diffusivities(cm^2/min) 10x factor
5.940d-4                         Brownian diffusivities(cm^2/min)
0.3944                        Freundlich/Langmuir Hybrid a (moles/L BV) rhob=1.0, DF=0.68,CT=0.58
1.0                              Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580, DF=0.988
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
2.8982d-4                        Freundlich/Langmuir Hybrid beta (-) 20C isotherm
```

Output: Simple Simulant – Red Columns – Design Estimate - No Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
```

```
================================================================================
Input file: case
[Lab-Scale] PNNL 5.6 M Na simple Simulant at Cs removal on Baseline CST mat
1 component (Cs) isotherm (Na 5.0 M) (5.6 M Na simple Simulant 20C isotherm
Begin Run:  14:52:46 on 08-28-2018   running under Windows 95/8
Finite elements    - axial:100  particle: 1
Collocation points - axial:  3  particle: 6 => Number of eqns:  3219
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Axial Dispersion and CSTR
================================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        =  60500.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =     12.07040 cm          D              =      1.44000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     19.65787 mL
F              =       .19494 mL/min      Uo (linear)    =       .21843 cm/min
R              =    286.50000 microns     L/R            =    421.30541
Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
Spec. Area     =     47.32984 1/cm        Time/BV        =     27.63033 min
Vol CSTRs      =      4.91450 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .34134E-01
Dp  [cm2/min]  =  .59400E-04
Doo [cm2/min]  =  .59400E-03
kf  [cm/min]   =  .46605E-01
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .58663E-02
Sc(i)          =  .19683E+04
Peb(i)         =  .38620E+02
Bi(i)          =  .93660E+02
Nf(i)          =  .11122E+03
Np(i)          =  .47988E+00
Pep(i)         =  .43897E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .39440E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .28982E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
================================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5970E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2391E-01 poise and density to 1.227     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .9000E+06 min.
     When comp.  1 reaches .5970E+09 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  6: Dump full profile file at  4000.     min
     Execute   1 times, every .0000     mins.
  7: Dump full profile file at  .1513E+05 min
     Execute   1 times, every .0000     mins.
```

```
   8: Dump full profile file at  .3025E+05 min
      Execute   1 times, every .0000     mins.
   9: Dump full profile file at  .4538E+05 min
      Execute   1 times, every .0000     mins.
  10: Dump full profile file at  .6050E+05 min
      Execute   1 times, every .0000     mins.
 ================================================================================
 VERSE-LC finished in  2340 steps.  Average step size 25.85     minutes
 End run:  14:53:18 on 08-28-2018
 Integrated Areas in History Files:
 case.h01                   .880345
 case.h02                   .691059E-01
```

18.6 Actual AP-107 Waste

One lead/lag column case was considered at design estimate and best estimate settings. Rovira et al. (2018) ran this configuration and had one carousel action during the overall processing period. Only the initial phase was modeled with VERSE-LC. Even though the actual system performed a carousel action at ~500 BVs, the VERSE-LC run was allowed to run out to ~1000 BVs without this carousel action to see more of the Cs breakthrough curves. One additional VERSE-LC run was made where the dry mass of CST in the bed was reduced to 75% of its stated amount and the tortuosity factor was decreased to 2.

Input: AP-107 – Nominal conditions – Best Estimate - Sr present

```
[Lab-Scale] PNNL 5.48 M Na Ap-107 at Cs removal on Baseline CST material lead/lag columns
1 component (Cs) isotherm (Na 5.0 M) (5.48 M Na AP-107 Actual 25C isotherm)
1, 100, 3, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                            input-only,perfusable,feed-equil,datafile.yio
MM                               comp-conc units
12.2800,  1.44, 0.36665, 5.0     Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
  0.0, 0.0                       initial concentrations (M)
S                                COMMAND - conc step change
1, 0.0, 6.390d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.0226, 1.223                    fluid viscosity(posie), density(g/cm^3)
m                                COMMAND - subcolumns
50, 100, 0, 1, 6.390d+8, 0.0, 900000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
-                                end of commands
30000.0, 1.0                     end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                   abs-tol, rel-tol
-                                non-negative conc constraint
1.0d0                            size exclusion factor
1.865d-4                         part-pore diffusivities(cm^2/min)  4x factor
7.460d-4                         Brownian diffusivities(cm^2/min)
0.3016                           Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0,
DF=0.52,QT=0.58
1.0                              Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                              Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580, DF=0.988
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
3.6327d-4                        Freundlich/Langmuir Hybrid beta (-) "eff" isotherm Na = 5.0 M
```

Output: AP-107 – Nominal conditions – Best Estimate - Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ================================================================================
 Input file: case
 [Lab-Scale] PNNL 5.48 M Na Ap-107 at Cs removal on Baseline CST material le
 1 component (Cs) isotherm (Na 5.0 M) (5.48 M Na AP-107 Actual 25C isotherm)
 Begin Run:  12:44:16 on 08-29-2018   running under Windows 95/8
 Finite elements    - axial:100  particle: 1
```

```
Collocation points - axial:  3  particle: 6 => Number of eqns:  3219
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? N   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
Sub-Column Boundary Conditions: Axial Dispersion and CSTR
================================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        =  30000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =     12.28000 cm          D              =      1.44000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     19.99923 mL
F              =       .36665 mL/min      Uo (linear)    =       .41082 cm/min
R              =    286.50000 microns     L/R            =    428.62129
Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
Spec. Area     =     47.32984 1/cm        Time/BV        =     14.94556 min
Vol CSTRs      =      5.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .64085E-01
Dp  [cm2/min]  =  .18650E-03
Doo [cm2/min]  =  .74600E-03
kf  [cm/min]   =  .66965E-01
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .11635E-01
Sc(i)          =  .14863E+04
Peb(i)         =  .39361E+02
Bi(i)          =  .42863E+02
Nf(i)          =  .86440E+02
Np(i)          =  .81499E+00
Pep(i)         =  .26296E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .30160E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .36327E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
================================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .6390E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2260E-01 poise and density to 1.223     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .9000E+06 min.
     When comp.  1 reaches .6390E+09 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
================================================================================
VERSE-LC finished in  2127 steps.  Average step size 14.10     minutes
End run:  12:44:42 on 08-29-2018
Integrated Areas in History Files:
case.h01                   .730655
case.h02                   .907559E-01
```

Input: AP-107 – Nominal conditions – Design Estimate - Sr present

```
       [Lab-Scale] PNNL 5.48 M Na Ap-107 at Cs removal on Baseline CST material lead/lag columns
1 component (Cs) isotherm (Na 5.0 M) (5.48 M Na AP-107 Actual 25C isotherm)
1, 100, 3, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
MM                                comp-conc units
12.2800,  1.44, 0.36665, 5.0      Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
  0.0, 0.0                        initial concentrations (M)
S                                 COMMAND - conc step change
1, 0.0, 6.390d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.0226, 1.223                     fluid viscosity(posie), density(g/cm^3)
m                                 COMMAND - subcolumns
50, 100, 0, 1, 6.390d+8, 0.0, 900000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
-                                 end of commands
30000.0, 1.0                      end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                    abs-tol, rel-tol
-                                 non-negative conc constraint
1.0d0                             size exclusion factor
7.460d-5                          part-pore diffusivities(cm^2/min) 10x factor
7.460d-4                          Brownian diffusivities(cm^2/min)
0.3944                            Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0
1.0                               Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                               Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580, DF=0.988
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
3.6327d-4                         Freundlich/Langmuir Hybrid beta (-) 25C
```

Output: AP-107 – Nominal conditions – Design Estimate - Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ================================================================================
 Input file: case
 [Lab-Scale] PNNL 5.48 M Na Ap-107 at Cs removal on Baseline CST material le
 1 component (Cs) isotherm (Na 5.0 M) (5.48 M Na AP-107 Actual 25C isotherm)
 Begin Run:  13:15:33 on 08-29-2018   running under Windows 95/8
 Finite elements    - axial:100  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  3219
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Axial Dispersion and CSTR
 ================================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  30000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =     12.28000 cm          D              =      1.44000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     19.99923 mL
 F              =       .36665 mL/min      Uo (linear)    =       .41082 cm/min
 R              =    286.50000 microns     L/R            =    428.62129
 Bed Void frac. =       .54800            Pcl. Porosity  =       .24000
 Spec. Area     =     47.32984 1/cm        Time/BV        =     14.94556 min
 Vol CSTRs      =      5.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .64085E-01
 Dp  [cm2/min]  =  .74600E-04
 Doo [cm2/min]  =  .74600E-03
 kf  [cm/min]   =  .66965E-01
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
```

```
Re             =  .11635E-01
Sc(i)          =  .14863E+04
Peb(i)         =  .39361E+02
Bi(i)          =  .10716E+03
Nf(i)          =  .86440E+02
Np(i)          =  .32600E+00
Pep(i)         =  .65740E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .39440E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .36327E-03
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
================================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .6390E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2260E-01 poise and density to 1.223     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .9000E+06 min.
     When comp.  1 reaches .6390E+09 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
================================================================================
VERSE-LC finished in  2176 steps.  Average step size 13.79     minutes
End run:  13:16:07 on 08-29-2018
Integrated Areas in History Files:
case.h01                   .627282
case.h02                   .103534
```

Input: AP-107 – Reduced dry mass – Best Estimate - Sr present

```
[Lab-Scale] PNNL 5.48 M Na Ap-107 at Cs removal on Baseline CST material lead/lag columns
1 component (Cs) isotherm (Na 5.0 M) (5.48 M Na AP-107 Actual 25C isotherm)
1, 100, 3, 6                    ncomp, nelem, ncol-bed, ncol-part
FCWNA                           isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNNN                           input-only,perfusable,feed-equil,datafile.yio
MM                              comp-conc units
12.2800,  1.44, 0.36665, 5.0    Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
286.5, 0.548, 0.240,  0.0       part-rad(um), bed-void, part-void, sorb-cap()
  0.0, 0.0                      initial concentrations (M)
S                               COMMAND - conc step change
1, 0.0, 6.390d-5, 1, 0.0        spec id, time(min), conc(M), freq, dt(min)
V                               COMMAND - viscosity/density change
0.0226, 1.223                   fluid viscosity(posie), density(g/cm^3)
m                               COMMAND - subcolumns
50, 100, 0, 1, 6.390d+8, 0.0, 900000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                               COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1          unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1          unit op#, ptscale(1-4) filtering
-                               end of commands
30000.0, 1.0                    end time(min), max dt in B.V.s
1.0d-7, 1.0d-4                  abs-tol, rel-tol
-                               non-negative conc constraint
1.0d0                           size exclusion factor
3.730d-4                        part-pore diffusivities(cm^2/min)  2x factor
7.460d-4                        Brownian diffusivities(cm^2/min)
0.2262                          Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=1.0,
DF=0.52,QT=0.58
```

```
1.0                             Freundlich/Langmuir Hybrid b    (1/M)  Batch specific isotherm
1.0                             Freundlich/Langmuir Hybrid Ma   (-)    ccap=0.580, DF=0.988
1.0                             Freundlich/Langmuir Hybrid Mb   (-)
3.6327d-4                       Freundlich/Langmuir Hybrid beta (-) "eff" isotherm Na = 5.0 M
```

Output: AP-107 – Reduced dry mass – Best Estimate - Sr present

```
================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
================================================================================
 Input file: case
 [Lab-Scale] PNNL 5.48 M Na Ap-107 at Cs removal on Baseline CST material le
 1 component (Cs) isotherm (Na 5.0 M) (5.48 M Na AP-107 Actual 25C isotherm)
 Begin Run:  13:23:52 on 08-29-2018   running under Windows 95/8
 Finite elements    - axial:100  particle: 1
 Collocation points - axial:  3  particle: 6 => Number of eqns:  3219
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? N   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 Sub-Column Boundary Conditions: Axial Dispersion and CSTR
================================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =  30000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =     12.28000 cm          D              =      1.44000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     19.99923 mL
 F              =       .36665 mL/min      Uo (linear)    =       .41082 cm/min
 R              =    286.50000 microns     L/R            =    428.62129
 Bed Void frac. =       .54800             Pcl. Porosity  =       .24000
 Spec. Area     =     47.32984 1/cm        Time/BV        =     14.94556 min
 Vol CSTRs      =      5.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .64085E-01
 Dp  [cm2/min]  =  .37300E-03
 Doo [cm2/min]  =  .74600E-03
 kf  [cm/min]   =  .66965E-01
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .11635E-01
 Sc(i)          =  .14863E+04
 Peb(i)         =  .39361E+02
 Bi(i)          =  .21431E+02
 Nf(i)          =  .86440E+02
 Np(i)          =  .16300E+01
 Pep(i)         =  .13148E+03

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .22620E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .10000E+01
 Iso. Const. 4  =  .10000E+01
 Iso. Const. 5  =  .36327E-03
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units           M
================================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .6390E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .2260E-01 poise and density to 1.223     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .9000E+06 min.
      When comp.  1 reaches .6390E+09 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  2.  Filename = case.h01
      Output density adjustments:
```

```
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
 ================================================================================
 VERSE-LC finished in  2093 steps.  Average step size 14.33     minutes
 End run:  13:24:13 on 08-29-2018
 Integrated Areas in History Files:
 case.h01                   .993207
 case.h02                   .208513
```

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