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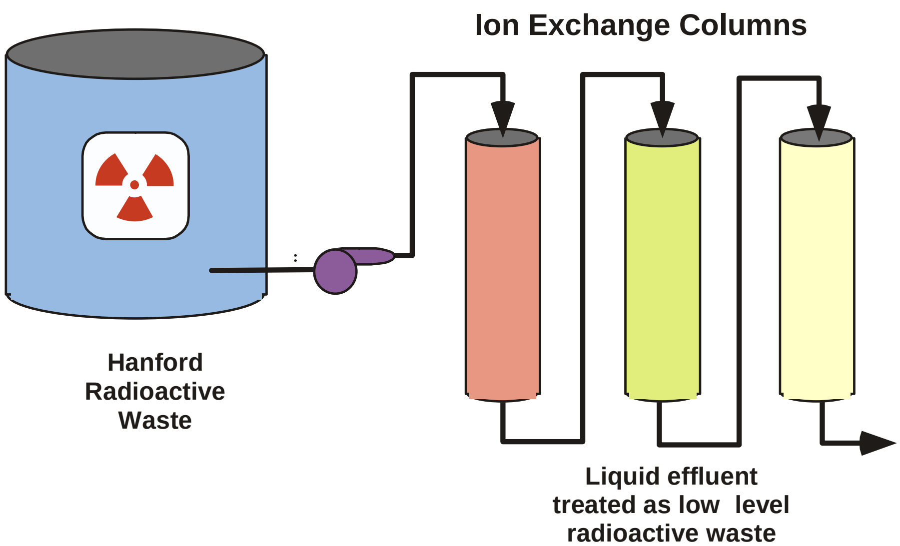


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# Ion Exchange Modeling of Cesium Removal from Hanford Waste Using Spherical Resorcinol-Formaldehyde Resin

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# 1.0 Executive Summary

This report discusses the expected performance of spherical Resorcinol-Formaldehyde (RF) ion exchange resin for the removal of cesium from alkaline Hanford radioactive waste. Predictions of full scale column performance in a carousel mode are made for the Hot Commissioning, Envelope B, and Subsequent Operations waste compositions under nominal operating conditions and for perturbations from the nominal. Only the loading phase of the process cycle is addressed in this report. Pertinent bench-scale column tests, kinetic experiments, and batch equilibrium experiments are used to estimate model parameters and to benchmark the ion-exchange model. The methodology and application presented in this report reflect the expected behavior of spherical RF resin manufactured at the intermediate-scale (i.e., approximately 100 gallon batch size; batch 5E-370/641). It is generally believed that scale-up to production-scale in resin manufacturing will result in similarly behaving resin batches whose chemical selectivity is unaffected while total capacity per gram of resin may vary some. As such, the full-scale facility predictions provided within this report should provide reasonable estimates of production-scale column performance.

## 1.1 Objectives

The primary objective of this work was, through modeling and verification based on experimental assessments, to predict the cesium removal performance of spherical RF resin for application in the full scale River Protection Program (RPP) Waste Treatment Plant (WTP) pretreatment facility. The scope of this task was provided in Test Specification 24590-PTF-TSP-RT-04-0004, Rev 1 (Meehan, 2005). The modeling scope was updated in Section III Activity I of the Task Technical and QA Plan issued by Nash (2006).

LAW feed variability was addressed by looking at three limiting/composite feed compositions referred to as Hot Commissioning Operation, Envelope B Operation, and Subsequent Operation. Feed compositions with the required product purity criteria were specified by Toth (2003). Only the performance of RF resin in the loading phase is addressed in this document.

The column performance predictions presented within this report reflect expected performance behavior for RF resin manufactured at the intermediate-scale 100 gallon batch size and in its spherical bead form. Data taken for earlier RF resin (ground material and spherical) were not incorporated into the final modeling assessment presented within this report (i.e., only data using the most current spherical RF resin was employed in establishing model parameter settings).

The specific objectives pertinent to this report, as outlined in the updated test specification for this activity, are:

| Test Objective | Objective Met | Discussion |
|---|---|---|
| Update an existing computer model that allows prediction of cesium sorption along with sorption of other cations under a wide variety of conditions, accounting for competitors (e.g., rubidium, potassium and sodium on the cesium resin), pH, ionic strength, particle size and temperature in the WTP ion-exchange column and in test columns. Both an isotherm and column transport model will be developed for spherical RF resin. | Yes | Experimental equilibrium distribution, particle loading kinetics, and material property measurements were employed in the model development phase of this effort. Appropriate/available data for the spherical bead form was used (i.e., no data for ground or earlier spherical RF resin was used). Limited algebraic isotherm models for specific feed compositions were developed using the most recent experimental data and feed stream definitions provided. |
| Modeling will be compared to column data from A-225, A-204, A-212 and the 24-inch column last cycle of A-215. | Yes | Column data from the A-225 (AZ-102), A-204 (AP-101) and A-212 (AN-102) tests were used to evaluate model performance. Data from A-215, where no cesium breakthrough was observed, could not be used to quantitatively evaluate the model. |
| Apply the model to evaluate full-scale WTP column performance with a matrix of 30 different feed conditions. | Yes | All 30 full-scale column simulations were completed. The nominal 3-column carousel configuration was considered to allow direct comparison with consistent analyses performed for SuperLig® 644 and previous RF resins. |

## 1.2 Test Exceptions

No official written test exceptions were imposed on this activity. Revisions to the modeling scope and objectives were made per WTP requests based on overall project needs and available databases.

## 1.3 Results and Performance Against Success Criteria

The success criteria for this task are listed in the following table.

| Success Criteria | Discussion |
|---|---|
| Creation and application of an isotherm model to support the prediction of resin loading performance under a wide variety of conditions, accounting for competitors (e.g., potassium on the cesium resin), ionic strength, and temperature where appropriate data exist. | Algebraic isotherm models for three specific feed compositions are provided based on the limited isotherm data and LAW feed stream definitions available. Insufficient isotherm data exists to establish parameter settings for all key aspects with a high level of confidence. Nevertheless, a methodology was developed where reasonable predictive isotherms were obtained for an appropriate range of operating conditions. |
| Creation and application of a column-transport model to support the prediction of ion-exchange column loading for RF resins under a wide variety of conditions, accounting for competitors (e.g., potassium on the cesium resin), pH, ionic strength, and temperature where appropriate data and understanding exist. | VERSE-LC model assessments are provided within this report. Assessments of small-scale column experiments and kinetics experiments were made for all pertinent tests available. The model was applied to simulate full-scale column operation under 30 different feed conditions. |

A summary is provided below to highlight specific modeling achievements and the results obtained during the course of this activity. The methodology employed was consistent with earlier RF analyses (Hardy et al., 2004) and earlier SuperLig® 644 analyses (Hamm et al., 2004).

- To achieve adequate batch contact "$K_d$" test data, sufficient contact time and agitation (i.e., mixing) is paramount. Using the most recent batch of RF resin in its spherical bead form, a limited set of batch contact tests and particle kinetics tests were performed in a manner consistent with the protocols employed for SuperLig® 644 resin testing. This limited database was used to establish key modeling parameter values (e.g., isotherm parameters and pore diffusivities). Through the modeling analysis, modest-to-significant variability was found in results obtained from the batch equilibrium, particle kinetics, and small column ion-exchange tests.

- A detailed thermodynamic equilibrium isotherm model was developed to correlate available batch contact data. Model parameters were adjusted to give a best fit to the experimental data. Isotherms calculated with the thermodynamic model were then fit to an algebraic isotherm model that could be used within the column transport model. A five-component (i.e., cesium, rubidium, potassium, sodium, and hydrogen) cation exchange isotherm model was created. Aleman and Hamm (2007) provide a detailed discussion of the detailed thermodynamic equilibrium isotherm model. The adequacy of this approach is verified by comparison to the available database and through use in column simulations/assessments.

- Full-scale column performance was simulated using "effective" single-component (cesium specific) isotherm and column transport models. Previous work has shown that for the cesium loading-phase, the "effective" single-component model is adequate for design purposes. Verification of this approach was performed further demonstrating its adequacy.

- In the order of estimated affinity, the five major cations competing for surface sites on RF resin considered are: hydrogen, cesium, rubidium, potassium, and sodium. For these cations, RF resin is most selective for $H^+$, then $Cs^+$, followed by $Rb^+$, followed by $K^+$, and then $Na^+$. Based on prior work with RF resin, $Cs^+$ capacity varies significantly with pH. In recent batch contact testing of spherical RF (Nash et al., 2006), an observed $OH^-$ dependence is again seen in batch equilibrium "$K_d$" test data for liquid solutions with varying pH values. Selectivity coefficients for RF resin are consistently lower than the corresponding values for SuperLig® 644 resin. Basically, RF resin is less selective for cesium than SuperLig® 644 resin. This comparison is valid for fresh resins and may not reflect the relative degradation aspects of the two resin types during multiple cycles of loading and eluting.

- Total cesium ion-exchange capacity for RF resin is pH dependent with a value of approximately 0.7 mmole/g at high OH concentration levels. This plateau value of 0.7 mmole/g for RF resin is approximately 26% higher than the 0.54 mmole/g value for SuperLig® 644 resin (i.e., based on fresh RF resin versus fresh SuperLig resin).

- Based on elution studies and simple simulant batch contact test studies it appears that the total sodium capacity of RF is around 6 mmole/g.

- The required parameter settings for the detailed thermodynamic equilibrium model were obtained from a series of selected batch contact tests (i.e., a total of 130 data points). All experimental cesium loading values were predicted to within ±20% while experimentally measured $K_d$ and equilibrium cesium concentrations in the liquid phase were generally predicted to within ±20%. For validation purposes, batch contact tests using the full recipe of AP-101 were not used in the non-linear regression analysis. Prediction of the 15, 25 and 45 ºC cesium isotherm data for the full recipe of AP-101, using the isotherm methodology, provided reasonable agreement with the data.

- Model simulations were run for several experimental column tests to assess the predictability of the methodology. In most cases, reasonable predictions were achieved for the cesium exit breakthrough curves. Both actual and simulant feed solutions were assessed.

- Based on this methodology, full-scale facility "best estimate" (i.e., nominal) simulations were run for three feed streams assuming a three-column carousel configuration. A cesium product concentration limit was imposed at the exit of the lag column. For all three feed streams, cesium removal performance exceeded minimum design specifications using "fresh" resin.

- When a $^{137}Cs$ inventory limit is imposed on the RF resin column loading, it limits the number of bed volumes for processing Envelope B and Subsequent Operations feed. Assuming an inventory limit of 75,000 Ci, VERSE-LC model predictions indicate that this limit is reached in about 30 bed volumes for the Envelope B Operations feed stream under nominal operating conditions. This result is consistent with earlier findings for RF and SL-644 resins.

Table 1-1 provides a brief summary of the number of bed volumes that can be processed for the first five cycles for each of the three feed compositions considered. The bed volumes in each cycle at 50% breakthrough are listed in parentheses following the breakthrough bed volumes. The number of bed volumes processed based on a cesium product criterion at the exit of the lag column and a total cesium inventory limit in the lead column were computed. The current design and operational strategy appear sufficient to achieve the desired decontamination factors (i.e., significant bed volumes of feed can be processed per operation cycle for all three feeds considered). Using 600 gallon ion-exchange columns, the 75,000 Ci limit for $^{137}Cs$ inventory in the lead column is reached for Envelope B feed at 30 bed volumes, independent of ion-exchange resin, compared with the current design requirement of 25 bed volumes. This curie limit is also reached for Subsequent Operations feed at 235 bed volumes with the current design requirement of 100 bed volumes.

The estimated RF resin cesium isotherms for each of the three feed compositions considered are shown in Figure 1-1 where resin capacity is for the $H^+$ form. Figures 1-2 through 1-4 show examples of the cesium breakthrough performance for each feed stream considered for columns packed with spherical RF resin. The results shown are for nominal feed conditions using a fresh resin bed. Very sharp mass transfer zones exist for each resin type when processing the Envelope B Operations feed. This is a direct result of the significantly higher cesium feed concentration along with the reduced feed flow rate (i.e., the non-linear isotherm has self-sharpening effects at the higher cesium feed concentration). Complete results for all case studies are presented in Section 10.

## 1.4 Quality Requirements

The Liquid Chromatography code VERSE-LC (Whitley and Wang, 1998) was used to perform the column performance assessments. Version 7.80 of VERSE-LC was used for verification purposes where several test cases (i.e., see certification package for VERSE-LC Version 7.80 by Hamm et al., 2000a) were checked to ensure its implementation on the stated PC platform. Further benchmarking was made by assessment to several key particle kinetics and column tests. Column test benchmarking is considered to be the ultimate check of the accuracy of the methodology employed. Column test benchmarking results are provided in Section 9 of this report where the cases considered demonstrated reasonably good predictive capability. Benchmarking of the detailed thermodynamic equilibrium model to a select number of batch contact tests was performed.

This work was conducted in accordance with the RPP-WTP QA requirements specified for work conducted by SRNL as identified in DOE IWO MOSRLE60. SRNL has provided matrices to WTP demonstrating compliance of the SRNL QA program with the requirements specified by WTP. Specific information regarding the compliance of the SRNL QA program with RW-0333P, Revision 16, NQA-1 1989, Part 1, *Basic and Supplementary Requirements* and NQA-2a 1990, Subpart 2.7 is contained in these matrices. The Test Specification also imposed WTP *QA*

*Project Plan for Testing Programs Generating Environmental Regulatory Data* (PL-24590-QA00001) for TCLP and spent resin organic analyses but did not impose QARD.

### 1.5 R&T Analysis Conditions

WTP provided three unique feed stream compositions to be considered. The RF resin analyses presented in this report are based on a limited database consistent with the programmatic needs associated with ion-exchange resin down selection activities. Data measuring RF resin behavior at the intermediate-scale (e.g., 100 gallon batch size) was used and the data was created using well-defined experimental protocols.

### 1.6 Simulant Use

This report contains modeling analysis and is not intended to report experimental data. However, experimental data using simulants is crucial to model development and benchmarking. In particular, the work and data from Nash et al. (2006) using AP-101 simulant plus variations about the nominal AP-101 composition for batch contact, batch kinetics, and small column ion-exchange experiments was used to develop and benchmark the isotherm and ion-exchange models described in this report. In addition, data from small column tests with simulants of AN-107 Sr/TRU filtrate (Nash et al., 2006), AN-102 (Fiskum et al., 2006b) and AZ-102 (Fiskum et al., 2006c) were also used to verify the models.

### 1.7 Discrepancies and Follow-on Analyses

In the process of performing this work, no significant discrepancies were observed. Full-scale facility performance was predicted to meet or exceed the design objectives Nevertheless, there are two issues worth noting:

- For Hot Commissioning Operation the predicted breakthrough values are about twice the current design specification (i.e., 130-140 bed volumes versus the 72 bed volumes in the system description based on processing 30,000 gallons in a 415 gallon bed). These are best estimate predictions which do not account for uncertainties. A lower bound estimate including uncertainties may not meet the design specifications.

- To predict plant performance, the behavior of the lag and guard columns at very low cesium concentrations is required. The isotherm model was modified as described in Section 4 to capture RF behavior at low cesium as well as possible using the limited batch contact testing performed in this regime. However, the model was not entirely successful in predicting the low cesium adsorption behavior and it would be desirable to have additional batch contact data at low cesium concentrations to confirm and extend the existing experimental results.

Table 1-1. Number of bed volumes required to reach lag column Cs breakthrough and 50% breakthrough during three-column carousel operation for Hot Commissioning, Envelope B, and Subsequent Operations feeds. 50% breakthrough bed volumes in parentheses.

| Cycle Number | Hot Commissioning Operation Feed (BV) | Envelope B Operations Feed (BV) | Subsequent Operations Feed (BV) |
|---|---|---|---|
| 1 | 206 (142) | 524 (276) [30][a] | 494 (326) [235][a] |
| 2 | 128 (80) | 276 (28) | 312 (158) |
| 3 | 131 (94) | 277 (27) | 319 (171) |
| 4 | 134 (107) | Not determined | 323 (178) |
| 5 | 138 (111) | Not determined | 323 (181) |

[a] Number of bed volumes to reach $^{137}Cs$ inventory limit of 75,000 Ci.

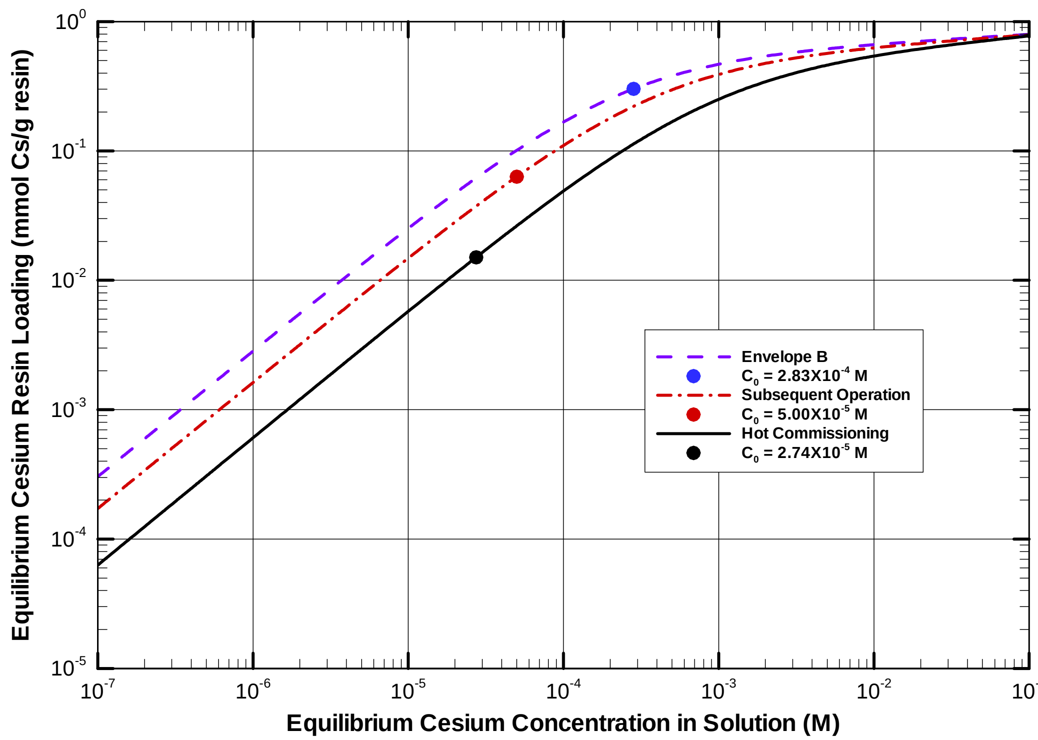


Figure 1-1. RF resin cesium isotherm curves for three feed compositions considered for column performance assessment (Hot Commissioning Operations, Envelope B Operations, and Subsequent Operations). Solid circles indicate the cesium concentration value for each feed (molar concentrations provided in legend).

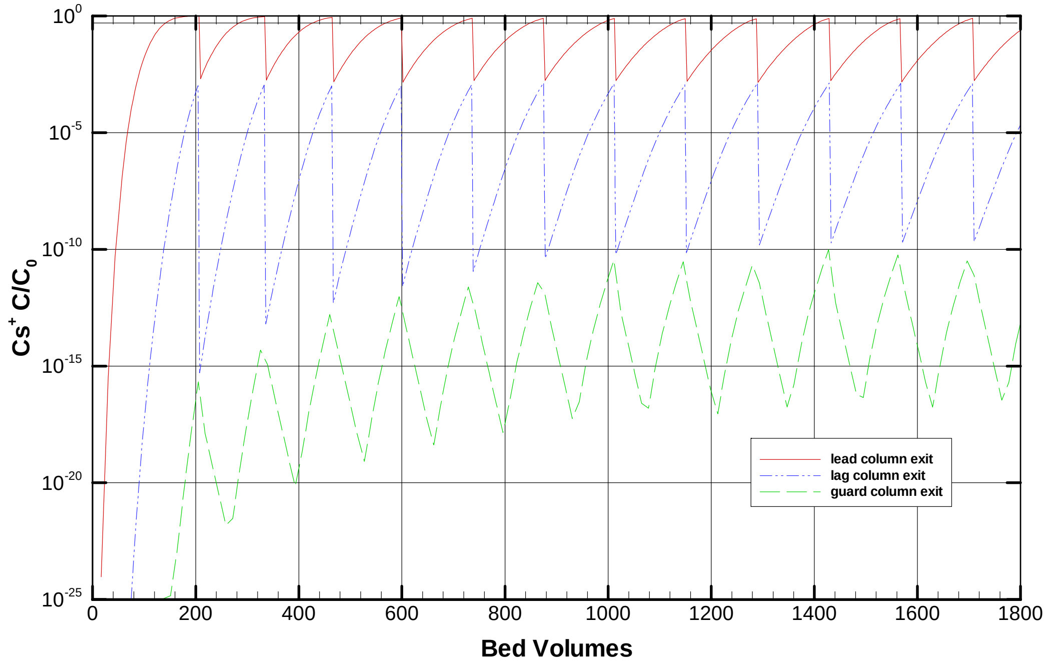


Figure 1-2. VERSE-LC RF resin cesium removal predictions for full-scale three column carousel under nominal Hot Commissioning Operations feed conditions. The figure shows lead, lag, and guard breakthrough behavior.

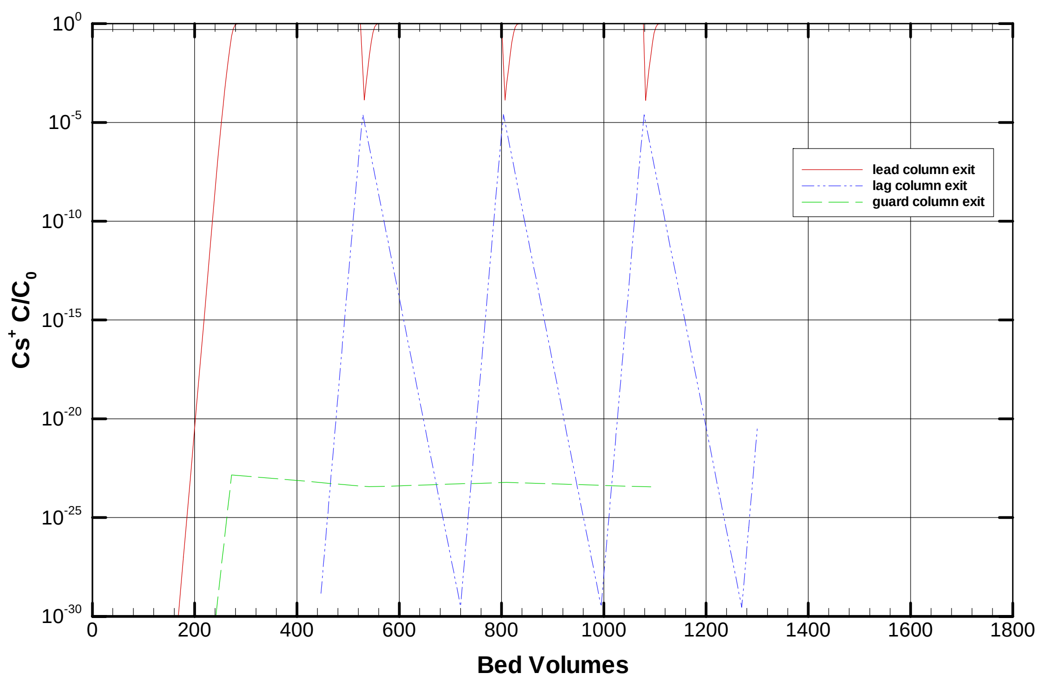


Figure 1-3. VERSE-LC RF resin cesium removal predictions for full-scale three column carousel under nominal Envelope B Operations feed conditions. The figure shows lead, lag, and guard breakthrough behavior.

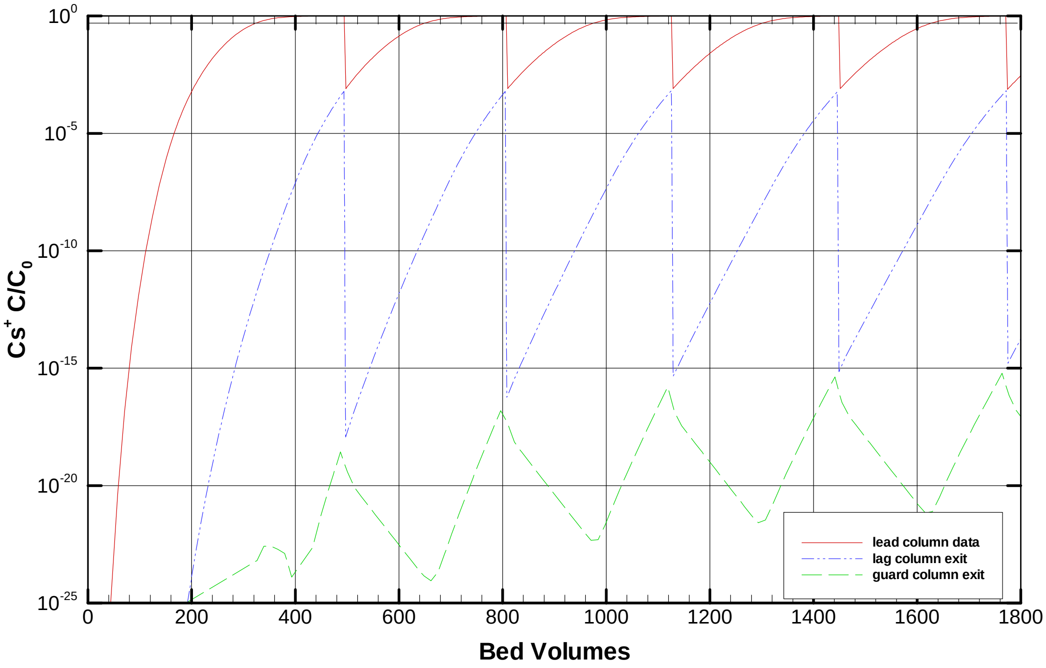


Figure 1-4. VERSE-LC RF resin cesium removal predictions for full-scale three column carousel under nominal Subsequent Operations feed conditions. The figure shows lead, lag, and guard breakthrough behavior.

# 2.0 Introduction and Background

A Waste Treatment Plant (WTP) is being designed for the immobilization of radioactive waste at the Hanford site. One process in the facility uses ion-exchange to remove radioactive cesium from a strongly alkaline aqueous phase. Ion-exchange will be used to separate cesium from ultra-filtered supernate originating in underground storage tanks at the Hanford site. Upon elution in acidic conditions, the separated cesium will be sent to the High-Level Waste (HLW) glass melter for vitrification. An elutable ion-exchange resin specifically designed with high selectivity for cesium under alkaline conditions is being investigated. The proposed design of the facility consists of four packed columns, with three columns used in series during loading (i.e., a lead column followed by a lag column then a guard column configuration). Each of the columns will be geometrically identical with only slight variations in bed sizes due to resin swelling/shrinkage effects. During operation, upon reaching the contract limit cesium breakthrough concentration at the exit of the lag column, the cesium-loaded lead column is processed (i.e., washed and eluted). The fourth standby column is switched to the guard position. The previous lag column is placed in the lead position (without eluting), the previous guard column is placed in the lag position, and the system is ready for use in the next cycle. The column train is to use a selective ion exchange resin to remove cesium having some isotopic fraction of $^{137}$Cs from the solution. RF resins are under consideration as ion exchangers and will be investigated through the analyses performed in this study. For a well designed process, the loading step should exceed the process time required to elute and place one column back into operation. Note that the original carousel design for the cesium ion exchange system used only two columns in series (i.e., a lead lag configuration) which was later revised to include a third column located after the lead and lag columns. The third column provides additional assurance that the target cesium concentration in the treated waste solution is not exceeded prior to meeting design objectives.

## 2.1 Ion Exchange Modeling

This ion-exchange system is one of many unit operations within the larger WTP process flowsheet. Experiments have been performed to characterize the resin and the ion-exchange process in support of the overall design. Modeling the ion-exchange process in detail provides key supporting information needed to establish the overall flowsheet. For example, cycle (time) average decontamination factors are required at the overall flowsheet level. Separate (off-line) detailed transient column modeling provides these average decontamination factors in a computational environment where the detail of the analysis is not restricted due to constraints imposed by the relatively large runtime and storage requirements of the complete flowsheet.

In addition, modeling:

- Reduces the overall number of experiments required;
- Provides guidance to experimental efforts and focuses attention on the critical parameters;
- Evaluates the adequacy and consistency of multiple data sets;
- Consolidates available information on a particular ion exchange system; and

- Establishes and confirms full-scale facility design and operational requirements.

## 2.2 Chosen Ion Exchange Material

Resorcinol-Formaldehyde (RF) cation-exchange resin was developed for the selective removal of cesium (containing some isotopic fraction of $^{137}Cs$) from highly alkaline supernates. The resin is prepared by condensation polymerization of resorcinol ($C_6H_6O_2$) and formaldehyde ($CH_2O$). The high selectivity has been attributed to the two weakly acidic hydroxyl groups on resorcinol, which ionize and become functional at high pH. Due to its weak acid nature, the resin has strong preference for $H^+$ and can be eluted using acid to remove $Cs^+$ and its competitors. Our current estimate for the relative affinities of RF resin for ion-exchange are $H^+ > Cs^+ > Rb^+ > K^+ > Na^+$. Resorcinol-formaldehyde has been manufactured in crushed or granular form, similar to SuperLig® 644, and in the spherical form. The experimental data used in this report, which includes the AP-101 batch contact, kinetics and small column experiments, were obtained using Batch Lot Number 5E-370/641 (with PNWD internal ID TI394-63) of spherical RF ion exchange resin purchased from Microbeads AS in Skedsmokorset, Norway (Nash, et al., 2006, Fiskum et al., 2006a).

## 2.3 Report Overview

This report focuses on the cesium-loading phase of a complete ion-exchange cycle. An analysis methodology is developed where as much of the available and pertinent data on the spherical form of Resorcinol-Formaldehyde is incorporated. The methodology can easily be updated as new information becomes available (e.g., measured bed and particle porosities). This document represents a report based on our current knowledge and capability to model the ion-exchange process for the cesium-spherical RF system under Hanford feed conditions. The methodology, its justification, assessment, and application to the proposed facility are discussed in the following sections.

Section 3 briefly discusses the transport model chosen for modeling column behavior. The governing equations and an appropriate simplification are presented. The VERSE-LC code (Berninger et al., 1991) was used for the modeling work presented in this report based on its availability and widespread (and accepted) use in this field and our earlier use of it in previous analysis efforts. Local equilibrium between the pore fluid and its neighboring surface sites is assumed where an equilibrium adsorption isotherm must be specified. The algebraic isotherm model used and the database employed in its creation are discussed in Section 4. A detailed thermodynamically based equilibrium model was developed as part of this work and is documented in the report by Aleman and Hamm (2007). Key column properties are addressed in Section 5 where the constraint imposed by bed porosity, particle porosity, and bed density is highlighted. Particle size distributions for spherical RF resins in sodium form are addressed in Section 6. The relationship between bulk and pore diffusion with an assessment against particle kinetics data is discussed in Section 7. In Section 8 the constitutive models for axial dispersion and film diffusion are presented. Headspace and short column impacts are also discussed where a correction factor is developed from limited literature data. Section 9 contains our laboratory-scale column assessments. Based on the current design specifications for the full-scale facility, Section 10 presents full-scale column predictions for three proposed inlet feed stream compositions, along with a series of sensitivity analyses. A list of the parameters specified for the full-scale column cases analyzed in this report is provided in Table 2-1.

Table 2-1. Full scale column simulation parameters.

| Case | Feed | Flow Rate gpm | Temp C | Potassium M | Sodium M | Cesium M | Free Hydroxide M | RF Diameter μm |
|---|---|---|---|---|---|---|---|---|
| HC_01 | Hot Commissioning | 15 | 25 | 0.48 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 460 |
| HC_02 | Hot Commissioning | 15 | 25 | 0.80 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 460 |
| HC_03 | Hot Commissioning | 15 | 25 | 0.30 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 460 |
| HC_04 | Hot Commissioning | 15 | 25 | 0.42 | 4.00 | $2.40 \times 10^{-5}$ | 1.62 | 460 |
| HC_05 | Hot Commissioning | 15 | 25 | 0.58 | 5.50 | $3.30 \times 10^{-5}$ | 2.23 | 460 |
| HC_06 | Hot Commissioning | 20 | 25 | 0.53 | 5.00 | $3.00 \times 10^{-5}$ | 2.02 | 460 |
| HC_07 | Hot Commissioning | 7.2 | 25 | 0.48 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 460 |
| HC_08 | Hot Commissioning | 20 | 25 | 0.48 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 460 |
| HC_09 | Hot Commissioning | 30 | 25 | 0.48 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 460 |
| HC_10 | Hot Commissioning | 15 | 35 | 0.48 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 460 |
| HC_11 | Hot Commissioning | 15 | 45 | 0.48 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 460 |
| HC_12 | Hot Commissioning | 20 | 25 | 0.48 | 4.57 | $2.74 \times 10^{-5}$ | 1.85 | 380 |
| HC_13 | Hot Commissioning | 15 | 25 | 0.48 | 4.57 | $5.50 \times 10^{-5}$ | 1.85 | 380 |
| HC_14 | Hot Commissioning | 22 | 25 | 0.48 | 4.57 | $5.50 \times 10^{-5}$ | 1.85 | 380 |
| EB_01 | Envelope B | 6.5 | 25 | 0.091 | 4.13 | $2.83 \times 10^{-4}$ | 1.28 | 460 |
| EB_02 | Envelope B | 10 | 25 | 0.091 | 4.13 | $2.83 \times 10^{-4}$ | 1.28 | 460 |
| SO_01 | Subsequent Operation | 20 | 25 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.80 | 460 |
| SO_02 | Subsequent Operation | 15 | 25 | 0.131 | 4.00 | $4.38 \times 10^{-5}$ | 0.80 | 460 |
| SO_03 | Subsequent Operation | 15 | 25 | 0.181 | 5.50 | $6.02 \times 10^{-5}$ | 0.963 | 460 |
| SO_04 | Subsequent Operation | 30 | 25 | 0.100 | 4.60 | $3.33 \times 10^{-5}$ | 2.067 | 460 |
| SO_05 | Subsequent Operation | 35 | 25 | 0.100 | 4.60 | $3.33 \times 10^{-5}$ | 2.067 | 460 |
| SO_06 | Subsequent Operation | 24 | 45 | 0.125 | 4.60 | $4.17 \times 10^{-5}$ | 1.433 | 460 |
| SO_07 | Subsequent Operation | 15 | 25 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.80 | 460 |
| SO_08 | Subsequent Operation | 15 | 25 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.60 | 460 |
| SO_09 | Subsequent Operation | 24 | 25 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.80 | 460 |
| SO_10 | Subsequent Operation | 30 | 25 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.80 | 460 |
| SO_11 | Subsequent Operation | 15 | 35 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.80 | 460 |
| SO_12 | Subsequent Operation | 15 | 45 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.80 | 460 |
| SO_13 | Subsequent Operation | 20 | 45 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.80 | 460 |
| SO_14 | Subsequent Operation | 20 | 25 | 0.150 | 4.60 | $5.00 \times 10^{-5}$ | 0.80 | 380 |

# 3.0 Column Model Formulations

The modeling of ion exchange columns is typically broken up into two basic categories:

- An equilibrium model generally highly empirical in nature, and
- A column model based on one-dimensional solute transport.

In this section, the equations for the multi-component and the simpler single-component ion exchange column models are addressed. Section 4 of this report addresses the equilibrium isotherm models. For details on VERSE-LC® and its application to modeling the cesium-RF ion exchange system see Hamm et al. (2000a, VERSE-LC® verification report), Hamm et al. (2000b, preliminary Cs removal performance using SuperLig® 644 report), Hamm et al. (2000c, preliminary Tc removal performance using SuperLig® 639 report), Hamm et al. (2002, Cs removal performance using CST report), and Hardy et al. (2004, Cs removal performance using RF report).

To account for the various mechanisms of transport and adsorption as ions travel down an ion exchange column, a porous particle solute transport formulation has gained widespread use and acceptability. For this class of column models, five basic aspects of the ion exchange column are addressed. In order of their importance with respect to predicting exit breakthrough curves for the cesium-RF system, they are:

- **Bed Definition** (high impact) – column size, geometry and resin mass have a direct impact on overall column performance (shifts entire breakthrough curve with respect to number of column volumes required to reach a specified concentration level) with particle geometry having a slightly less important impact. The nominal bed volume or column volume is defined as the volume occupied by the resin bed during the regeneration cycle (0.5 M NaOH solution). RF resin swelling is slightly less in 5 M [$Na^+$] salt solution which is associated with the feed conditions during the loading cycle.
- **Adsorption Isotherms** (high impact) – resin affinities for the various competing ions of interest have a very direct impact on overall column performance (shifts entire breakthrough curve with respect to number of column volumes required to reach a specified concentration level and for non-linear isotherms alters breakthrough curve shape as well as its sensitivity with respect to inlet feed conditions).
- **Pore Diffusion** (moderate impact) – intra-particle mass transport by pore diffusion to available surface sites has a moderate impact on overall column performance (alters the shape of exit breakthrough curves typically by a rotation about the ~50% relative concentration level with slight shifting) with particle geometry having a slightly less important impact.
- **Film Diffusion** (low impact) – liquid mass transport by film diffusion across the particle-to-bed boundary has a low impact on overall column performance (alters the shape of exit breakthrough curves typically by a rotation about the ~50% relative concentration level with slight shifting).

- **Axial Dispersion** (low impact) – mass transport along the column length by axial dispersion has a low impact on overall column performance (alters the shape of exit breakthrough curves typically by a rotation about the ~50% relative concentration level with slight shifting).

The levels of impact are based on sensitivity studies and are relative values. Mechanisms such as surface migration or adsorption kinetics are not included in our column model since their impacts were considered to be negligible or already indirectly incorporated into the other features during our parameter estimation process.

## 3.1 The Multi-Component Model

For the cesium-RF resin system a porous particle multi-component ion exchange column model was considered. In this model we assume that kinetics associated with local ion exchange at an active resin surface site are very fast (faster than the various liquid mass transfer mechanisms that transport ions to that site). Assuming radial effects to be negligible within the active region of the packed bed (i.e., a large column-to-particle diameter ratio), a one-dimensional species (ion) transport equation for the mobile phase (within the bed) becomes:

$$\varepsilon_b \frac{\partial c_{bi}}{\partial t} + \varepsilon_b u \frac{\partial c_{bi}}{\partial z} = \varepsilon_b E_{bi} \frac{\partial^2 c_{bi}}{\partial z^2} - \left( \frac{3}{< R_p >} \right) (1 - \varepsilon_b) k_f \left( c_{bi} - c_{pi} \Big|_{r=R_p} \right), \tag{3-1a}$$

**storage** **advection** **axial dispersion** **liquid film diffusion (mass transfer)**

with boundary and initial conditions

$$z = 0, \qquad E_{bi} \frac{\partial c_{bi}}{\partial z} = u \left[ c_{bi} - c_{bi}^{feed}(t) \right], \tag{3-1b}$$

$$z = 1, \qquad \varepsilon_b E_{bi} \frac{\partial c_{bi}}{\partial z} = 0\,, \tag{3-1c}$$

$$t = 0, \qquad c_{bi} = c_{bi}(0, z). \tag{3-1d}$$

where

$\varepsilon_b$ ...................Bed porosity
$\varepsilon_p$ ...................Particle porosity
$u$......................Linear interstitial velocity, cm/min
$c_{bi}$ ..................Concentration of species i in bed fluid, M
$z$......................Axial coordinate, cm
$E_{bi}$ .................Species i axial dispersivity, $cm^2$/min
$< R_p >$ ...........Average particle radius, cm
$k_f$ ...................Liquid film mass transfer coefficient, cm/min
$c_{pi}$ ..................Concentration of species i in pore fluid, M
$r$ ......................Radial coordinate within average size particle, cm

t ......................Time, min

Assuming uniformly sized spherical particles with a homogeneous distribution of pores, a one-dimensional species transport equation for the pore phase (within an average sized particle of resin) becomes:

$$\varepsilon_p \frac{\partial c_{pi}}{\partial t} \quad + \quad (1-\varepsilon_p)\overline{C}_T \sum_{j=1}^{N_s}\left[\left(\frac{\partial q_i}{\partial c_{pj}}\right)\frac{\partial c_{pj}}{\partial t}\right] \quad = \quad \varepsilon_p D_{pi} \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial c_{pi}}{\partial r}\right], \tag{3-2a}$$

**storage** **surface adsorption** **Fickian pore diffusion**

with boundary and initial conditions

$$r = 0, \qquad \frac{\partial c_{pi}}{\partial r} = 0 \ , \tag{3-2b}$$

$$r = \langle R_p \rangle, \qquad \varepsilon_p D_{pi} \frac{\partial c_{pi}}{\partial r} = k_f \left(c_{bi} - c_{pi}\right) , \tag{3-2c}$$

$$t = 0, \qquad c_{pi} = c_{pi}(0, r) \ . \tag{3-2d}$$

where

$\overline{C}_T$ .................Total ion-exchange capacity of resin, moles/liter bed volume
$q_i$ ...................Species i fractional surface site loading
$D_{pi}$ .................Species i pore diffusion coefficient, $cm^2/min$

In Eq. (3-2) it is assumed that the pore diameters are large relative to the size of migrating ions of interest. Therefore, Fickian diffusion is acceptable and surface migration is considered to be small when compared to pore diffusion. Details of the above equations are given in Ma et al. (1996).

Assuming local equilibrium between the pore fluid and its neighboring surface sites, a multicomponent equilibrium isotherm model for the ion exchange between the pore and solid phases can be generically expressed as:

$$q_i = F_i\left(\overline{C}_T, c_{p1}, c_{p2}, \cdots, c_{pN_s}\right) , \quad i = 1 \ldots N_s, \tag{3-3}$$

where it has been assumed that surface loadings for the $i^{th}$ species can be explicitly related to the liquid concentrations locally. The number of species required to model the behavior of the $i^{th}$ species depends upon its dependence on other species through the functional form (i.e., $F_i$) of the isotherm model in Eq. (3-3). Specific application of Eq. (3-3) to the cesium-RF resin system is discussed in Section 4. Initial and boundary conditions for Eqs. (3-1) and (3-2) must also be specified. For further details on these equations and their solution in VERSE-LC see Berninger et al. (1991) and Ma et al. (1996). Helfferich and Carr (1993) provide an excellent review paper describing the behavior of non-linear waves in chromatography and also a brief listing of available algorithms (Table I.4, Helfferich and Carr, 1993). Their paper provides very clear insight into how the above equation set behaves for non-linear isotherms consistent with the system of interest discussed in this report.

For the modeling efforts presented in this report the VERSE-LC code was chosen (Berninger et al., 1991) based on its availability and widespread and accepted use in this field. Prior to applying VERSE-LC to the ion exchange modeling presented in this report a verification process was completed and the results of that effort are reported in Hamm et al. (2000a). The verification process provided us quality assurance that the installed PC Windows95™ version of VERSE-LC (Version 7.80) was capable of adequately solving the above mentioned equations and also helped us to better understand how to accurately use the VERSE-LC code (e.g., mesh refinement requirements and input/output options). For all column results presented in this report, numerical errors associated with the results of VERSE-LC should be very small when compared to the uncertainties associated with various model input parameters (bed density, particle radius, pore diffusion, etc.).

## 3.2 The Single-Component Model

Under certain situations the porous particle multi-component transport equations discussed in Section 3.1 can be adequately decoupled to a series of single-component transport equations. The reduction to single-component equations is:

- valid when the total ionic strength is the same between the column's native and feed solutions; or

- a reasonable approximation when one ion absorbs significantly more onto the resin than others.

Making the same basic assumptions as in Section 3.1 the single-component equations can be derived. For each species a one-dimensional species (ion) transport equation for the mobile phase (within the bed) becomes:

$$\varepsilon_b \frac{\partial c_b}{\partial t} + \varepsilon_b u \frac{\partial c_b}{\partial z} = \varepsilon_b E_b \frac{\partial^2 c_b}{\partial z^2} - \left(\frac{3}{< R_p >}\right)(1-\varepsilon_b) k_f \left( c_b - c_p\big|_{r=R_p} \right), \quad (3\text{-}4)$$

**storage** **advection** **axial dispersion** **liquid film diffusion (mass transfer)**

where initial and boundary conditions are consistent with Eqs. (3-1b, c, d). A one-dimensional species transport equation for the pore phase (within a particle of resin) becomes:

$$\varepsilon_p \frac{\partial c_p}{\partial t} + (1-\varepsilon_p)\overline{C}_T \left(\frac{\partial q}{\partial c_p}\right) \frac{\partial c_p}{\partial t} = \varepsilon_p D_p \frac{1}{r^2} \frac{\partial}{\partial r}\left[ r^2 \frac{\partial c_p}{\partial r} \right], \quad (3\text{-}5)$$

**storage** **surface adsorption** **Fickian pore diffusion**

where initial and boundary conditions are consistent with Eqs. (3-2b, c, d).

One example of a single-component equilibrium isotherm model for ion exchange between the pore fluid and solid phase is:

$$q = f(c) = \frac{c_p}{\beta + c_p} \quad , \tag{3-6}$$

where Eq. (3-6) is of the Langmuir form and β is a function of the feed conditions.

If we neglect axial dispersion in Eq. (3-4) and further assume that mass transfer between the liquid and solid phase is infinitely great, Eq. (3-4) can be simplified to:

$$\varepsilon_b \frac{\partial c_b}{\partial t} + \varepsilon_b u \frac{\partial c_b}{\partial z} + \rho_b \frac{\partial q}{\partial t} = 0 \, , \tag{3-7}$$

The last term in Eq. (3-7) represents the accumulation of material on the ion-exchange solid. Equation (3-7) can be rearranged to:

$$\left(1 + \frac{\rho_b}{\varepsilon_b} f'(c)\right) \frac{\partial c_b}{\partial t} + u \frac{\partial c_b}{\partial z} = 0 \, , \tag{3-8}$$

Equation (3-8) leads to the concept of a retarded velocity since it appears that material in the liquid phase is transported along the bed with the concentration wave velocity:

$$u_r = \frac{u}{1 + \frac{\rho_b}{\varepsilon_b} f'(c)} \quad , \tag{3-9}$$

The derivative of the function relating q to c is equivalent to the distribution coefficient $K_d$ yielding:

$$\frac{\partial c_b}{\partial t} + \frac{u}{\left(1 + \frac{\rho_b K_d(c)}{\varepsilon_b}\right)} \frac{\partial c_b}{\partial z} = 0 \, , \tag{3-10}$$

From Eq. (3-10), if $K_d$ is constant, propagation velocities will be independent of concentration and the wave front will maintain its shape as it moves down the column. If $K_d$ decreases with concentration, material at the leading edge of the wave front where liquid concentrations are lower (higher $K_d$) will move more slowly that material at the trailing edge where concentrations are higher (lower $K_d$). In this case, the wave will exhibit a "self sharpening" behavior as it moves down the column. As described in subsequent sections, this behavior occurs in the Cesium-RF system.

### 3.3 The Cesium-RF System

Based on our current understanding of the cesium-RF resin system, the competition for cation exchange loading at the resin sites is primarily between cesium, rubidium, potassium, and sodium. Prior to the loading phase the initial sodium and potassium levels in the resin pretreatment solution are approximately 0.1 M to 0.5 M and 0 M, respectively. During the loading phase these concentration levels increase to approximately 5.0 M sodium and 0.0 to 1.0 M potassium. Therefore, a total ionic concentration wave will pass through the column. Based on available batch equilibrium studies estimates for the relative affinities for adsorption have been computed as discussed in Section 4 (i.e., the resin affinities are $Cs^+ > Rb^+ > K^+ > Na^+$).

Given the above information, an accurate prediction of column performance during the early part of a cycle (say the first 5 to 10 column volumes or so) probably would require the use of the multi-component formulations of Section 3.1. On the other hand, long-term performance should be adequately handled using the simpler "effective" single-component formulations of Section 3.2. To check the validity of these statements, cesium exit breakthrough curves simulating the PNWD column experiment using actual AP-101 waste (Fiskum, et al., 2006a) at 26.5 °C were compared using both multi-component (4-component) and Cs "effective" single-component formulations. Very similar results for cesium breakthrough were obtained. To illustrate the differences in timing for the four ionic species, the exit breakthrough curves for each species are plotted in Figure 3-1 (with linear $C/C_0$ scale) and Figure 3-2 (with log $C/C_0$ scale) for the 4-component simulation of the experimental column test (i.e., $Cs^+$, $Rb^+$, $K^+$, and $Na^+$). As expected, sodium breakthrough is fastest, quickly followed by potassium, then somewhat later by rubidium, and an order of magnitude later by cesium. Slight shifts within the breakthrough curves can be seen as a less selective cation is replaced by the next one in line (e.g., $Na^+$ being selectively replaced by $K^+$ around 1.3 bed volumes).

When the single-component formulation is used, the cesium breakthrough curve is essentially indistinguishable from the 4-component model results as shown in Figures 3-3 and 3-4. Since significant CPU savings are achieved (i.e., factors greater than 500 times faster) when the single-component model is used and the differences in cesium breakthrough are well within our current predictive capabilities, the column analyses presented in this report were performed using only the single-component modeling approach.

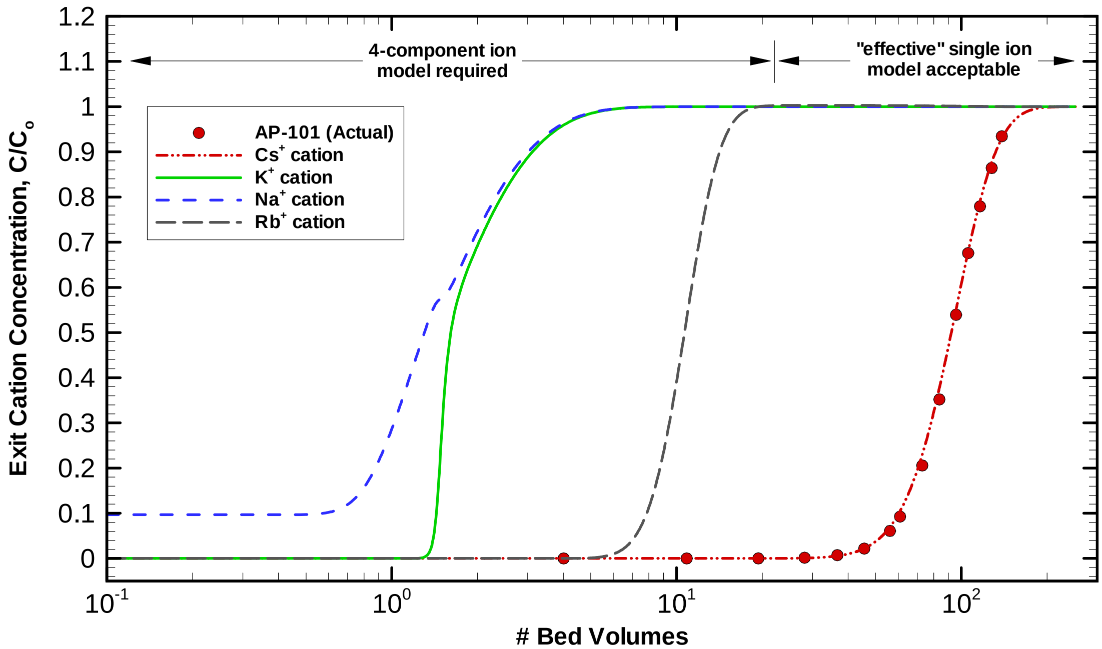


Figure 3-1. Linear scale plot of estimated sodium, potassium, rubidium and cesium exit breakthrough curves for PNWD small column experiment using actual AP-101 waste at 26.5 °C based on a 4-component ion exchange column model.

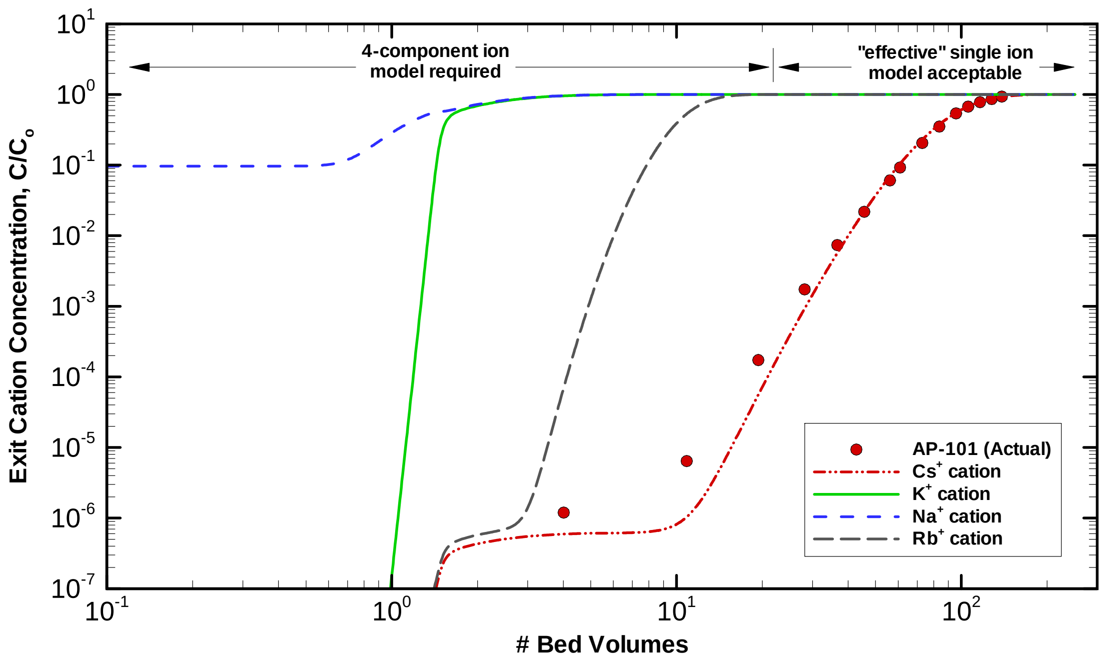


Figure 3-2. Log scale plot of estimated sodium, potassium, rubidium and cesium exit breakthrough curves for PNWD small column experiment using actual AP-101 waste at 26.5 °C based on a 4-component ion exchange column model.

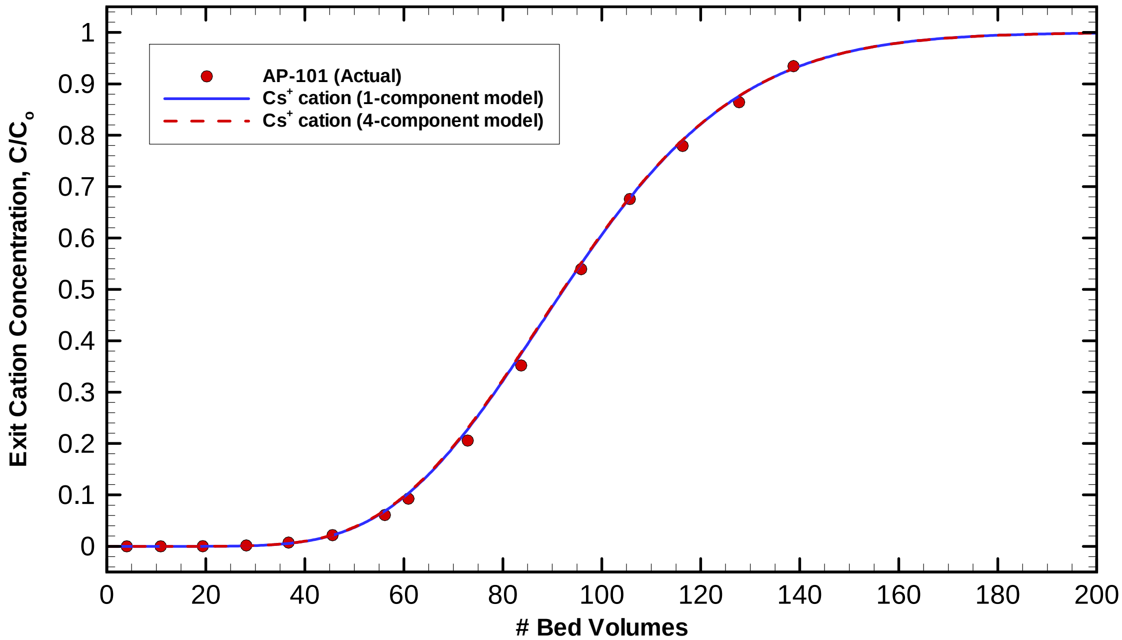


Figure 3-3. Linear scale plot of estimated cesium exit breakthrough curves for PNWD small column experiment using actual AP-101 waste at 26.5 °C based on the 4-component ion exchange column model, along with a comparison to predicted performance using its effective single component isotherm model.

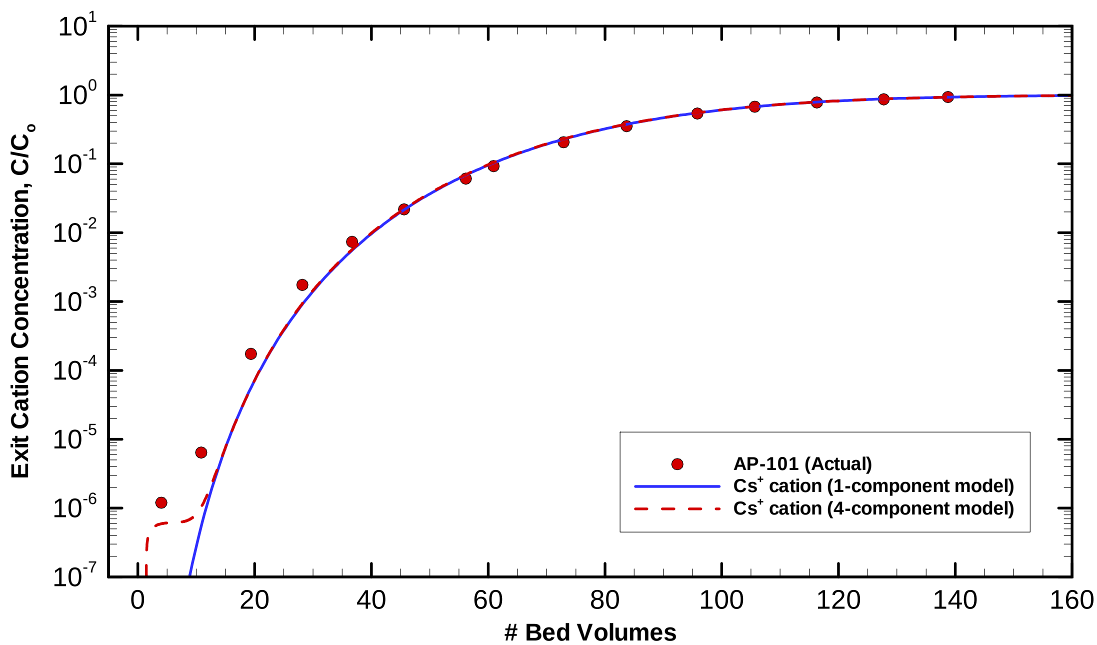


Figure 3-4. Log scale plot of estimated cesium exit breakthrough curves for PNWD small column experiment using actual AP-101 waste at 26.5 °C based on the 4-component ion exchange column model, along with a comparison to predicted performance using its effective single component isotherm model.

# 4.0 Equilibrium Cesium Isotherms

In column sizing one of two possible design strategies are typically considered: (1) bounding analysis where "worst case" feed compositions are used or (2) global optimization where best estimate feed compositions for each individual process batch are used. Each approach has its own advantages and disadvantages. For example, the bounding approach requires less analysis overall but it may be difficult to establish a reasonable bound that is not too restrictive. Since the amount of waste to be processed, flow rate, and key feed compositions depend significantly on which envelope is being considered, the global optimization strategy is generally preferred. However, to use a global optimization strategy, "best estimate" cesium isotherms for each of the WTP LAW batch feeds must be available. At the time of performing this work, a full set of LAW feed streams was not identified. Instead, only three operating feed streams were provided referred to as Hot Commissioning, Envelope B, and Subsequent Operation feeds. Details describing these three feed streams are provided by Toth (2003). Adsorption isotherms for each of the three feed streams for RF resin are required to perform the ion-exchange calculations. Isotherms are also required for the feed compositions used for column performance sensitivity analyses.

A detailed thermodynamic model was developed to generate cesium isotherm data for each feed composition. This simulated isotherm data was then fit to an appropriate algebraic isotherm model consistent with VERSE-LC input. Based on these considerations a binary homovalent isotherm model was developed and is presented in this section. Overall the algebraic isotherm model meets all of our objectives for this effort. A detailed discussion of the thermodynamic isotherm model that was used to create the algebraic isotherms is given in the separate report by Aleman and Hamm (2007). These isotherms are for the loading phase of the ion-exchange cycle only. The isotherm model discussed below closely follows the development presented by Hamm et al. (2000b) for the Cesium-SuperLig® 644 ion-exchange system.

In our column modeling, we assume that the rate of ion exchange at a surface site is very fast when compared to the rates of diffusion within the pore fluid and mass transfer across the liquid film at the outer boundaries of the particles. In other words, we assume that local equilibrium exists between the pore fluid and its neighboring surface sites. With this assumption, an algebraic expression relating ionic or species concentrations between the pore fluid and the solid Resorcinol-Formaldehyde resin surface sites (referred to as our "isotherm model") can be established for use in VERSE-LC column simulations. No explicit attempt is made in this report to verify this assumption. In an indirect manner, this assumption is either incorporated into some of the model parameters or verified by the comparison of model results to data. In addition, we assume that for each unique feed stream the total cesium capacity of the ion-exchange resin (active sites for cesium per gram of Resorcinol-Formaldehyde resin) remains independent of ionic strength and solution composition throughout the ion-exchange process.

## 4.1 Methodology

Under ideal conditions we would have sufficient isotherm data available (typically obtained from batch contact testing) corresponding to the feeds, resin, and column operating temperatures of interest. Such data would then be fitted to an algebraic isotherm model for use in VERSE-LC column simulations. For our monovalent cation-exchange resins, we have found that the Freundlich/Langmuir Hybrid isotherm model (one of the VERSE-LC options) can reasonably represent single or multicomponent isotherms. Unfortunately, in most situations we have not had sufficient isotherm data available to perform the above simple fitting process to obtain acceptable parameter settings for an algebraic model. Only limited batch contact data has typically been available. The data has been limited in temperature range, solution composition, cesium range, and in many cases modest-to-large measurement uncertainties have been observed.

In order to perform full-scale facility performance assessments, a methodology was established for the prediction of cesium isotherms at the temperatures and process feed compositions of interest. This methodology consists of:

- Using available batch contact data for a given resin batch, estimate key thermodynamic parameters associated with the liquid-solid equilibrium based on a "detailed thermodynamic equilibrium model" that describes the monovalent cation exchange process.
- For a particular process feed at a selected temperature, numerically generate batch contact data points using the detailed thermodynamic equilibrium model based on the prior estimated parameter values over a broad cesium concentration range.
- Using nonlinear regression, apply a least-squares algorithm to compute the two (or up to four) parameters associated with the algebraic Freundlich/Langmuir Hybrid isotherm model based on the numerical batch contact data points.

### 4.1.1 Detailed Thermodynamic Equilibrium Model

Restricting our attention to ion exchange of monovalent cations between an aqueous phase and RF resin, the following generic mass-action expression applies at chemical equilibrium:

$$[A_i]_{liquid} + [A_j]_{resin} \xleftrightarrow{K^e_{ij}} [A_i]_{resin} + [A_j]_{liquid} \; . \tag{4-1}$$

For spherical RF resin we currently believe that there are five dominant monovalent cations that are competing for "active" exchange sites with estimated resin affinities: $H^+ > Cs^+ > Rb^+ > K^+ > Na^+$. It is further thought that of these "active" exchange sites two types of sites exist with different pKa values in the pH range of 9 to 13. For each mass-action equation above (i.e., one for every ion pair competing for a particular site), the temperature dependent thermodynamic equilibrium constant can be expressed as:

$$K^e_{ij} \equiv \frac{1}{K^e_{ji}} = K^c_{ij} K^\gamma_{ij} \quad \text{and} \quad K^e_{ii} \equiv 1 \, , \tag{4-2}$$

where

$$K^c_{ij} = \frac{Q_i c_j}{Q_j c_i} \quad \text{and} \quad K^\gamma_{ij} = \frac{\hat{\gamma}_i \gamma_j}{\hat{\gamma}_j \gamma_i} \, . \tag{4-3}$$

and

$K^e_{ij}$ ..................thermodynamic equilibrium constant for ion i and ion j reaction

$K^c_{ij}$ ..................selectivity coefficient product for ion i and ion j reaction

$K^\gamma_{ij}$ ..................activity coefficient product for ion i and ion j reaction

$\hat{\gamma}_i$ ....................solid phase activity coefficient of ion i

$Q_i$ ...................solid-phase loading of ion i, mmol/g

$\gamma_i$ ....................liquid-phase activity coefficient of ion i

$c_i$ ....................liquid-phase concentration of ion i

The equilibrium constants are temperature dependent and this dependence can be obtained from the thermodynamic relationship (Van't Hoff equation):

$$\left(\frac{\partial \ln K^e_{ij}}{\partial T}\right)_p = \frac{\Delta H^o}{RT^2}, \tag{4-4}$$

where P and T are the temperature and pressure, $\Delta H^o$ is the heat or enthalpy change of the ion exchange reaction, and R is the gas constant. For a modest range in temperature, $\Delta H^o$ (a selected reference value) can be considered to be constant allowing a simple integration of Eq. (4-4) to be performed, yielding:

$$\ln K^e_{ij}(T) = \ln K^e_{ij}(T_{ref}) - \frac{\Delta H^o}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right), \tag{4-5}$$

where $T_{ref}$ is the chosen reference temperature and $K^e_{ij}(T_{ref})$ is the equilibrium constant at this reference temperature. Even though the equilibrium constant is a true constant for a given temperature (in practice the equilibrium constant may actually vary with composition due to approximations introduced by the Pitzer parameters), the selectivity coefficients are compositionally dependent since non-unity liquid-phase activity coefficients will exist. Fortunately, for a specified temperature and fixed feed composition (excluding cesium variations), the selectivity coefficients over a broad range of cesium concentrations only vary slightly. This allows simple algebraic isotherms to be generated that can represent the liquid-solid equilibrium at a given temperature with reasonable accuracy.

Note that for conditions where the equilibrium constants are true constants (i.e., fixed temperature and homogenous exchange sites) the algebraic isotherm becomes Langmuir in shape. The presence of solid-phase non-idealities (such as heterogeneous sites where site selectivity varies) the algebraic isotherm deviates from Langmuir. This is handled by using the more general Freundlich/Langmuir Hybrid isotherm model.

Currently, we handle the activity coefficients using a Pitzer activity coefficient model for ions within the liquid-phase. Non-idealities on the solid surface of the resin are handled using Wilson's model for solid-phase activity coefficients. This model uses the hydrated radius of each competitor ion ($Cs^+$, $Rb^+$, $K^+$ and $Na^+$) as input parameters. We assume that the hydrated radii for $Cs^+$ and $Rb^+$ are identical and that the hydrated radii for $K^+$ and $Na^+$ are identical. The ratio of these two radii was then used as an optimization parameter in the data fitting.

Spherical RF resin is an elutable resin with at least two pKa's where its total ionic exchange capacity is believed to vary based on changes in liquid-phase ionic strength and hydroxide concentration. Adsorption of neutral species such as NaOH is also possible. Based on elution studies, the total Na capacity of the RF resin appears to be about 6 mmole/g of resin (Nash et al., 2006). Modeling parameter estimation found a best estimate value of 6.75 mmol/g resin. For the modeling effort in this report, we are focusing on only those exchange sites that are assessable to all of the cation competitors listed earlier ($H^+$, $Cs^+$, $Rb^+$, $K^+$ and $Na^+$).

Assuming that the capacity for ion exchange for each ionic species is equivalent to the apparent total exchange capacity of the resin, the following empirical expression is used to account for the variation in ionic capacity with ionic strength and solution pH:

$$Q_A\left(I, c_{OH}\right) = \frac{I\,C_T + \delta\,Q_D}{I + \delta}, \qquad (4\text{-}6)$$

where

$Q_A$..................total apparent ionic capacity, mmol/g resin
$Q_D$..................sum of all active ionic capacities, mmol/g resin
$C_T$ ..................total ionic capacity (active and inactive sites), mmol/g resin
I .....................ionic strength of solution
$\delta$.....................ionic strength parameter

Equation (4-6) is plotted in Figure 4-1 and compared to available sodium loading data. The solid red, green and blue lines are model predictions for the RF-641 resin. Parameter values were estimated by fitting to the green and blue data points. The resin capacity $C_T$ is estimated to be 6.75 mmol/g.

Based on Eqs. (4-1) – (4-6), to have a working detailed thermodynamic equilibrium model for addressing cesium loading on RF resin the following key parameters must be determined from batch contact data:

$$\left[K^e_{12}, K^e_{13}, K^e_{14}, K^e_{15}, C_T, \delta, \Delta H^o, T_{ref}\right]$$

where 1-$Cs^+$, 2-$K^+$, 3-$Na^+$, 4-$Rb^+$, and 5-$H^+$. Once these parameter values have been estimated, numerical batch contact data points can be generated over a range of temperatures and feed compositions. Using the estimate of the apparent capacity $C_T$ derived from the fitting shown in Figure 4-1, the thermodynamic model was run to optimize for the other remaining parameters using the batch contact data at 25 and 45 °C. Further details of the thermodynamic equilibrium model briefly discussed above are provided by Aleman and Hamm (2007).

### 4.1.2 Available Batch Contact Data

A series of batch contact tests were performed to provide benchmarking data to assist in establishing and validating our isotherm model approach to be used in VERSE-LC column simulations. The batch contact experimental database was obtained using Batch Lot Number 5E-370/641 (PNWD internal ID TI394-63) of spherical RF ion exchange resin (sometimes referred to as RF-641) purchased from Microbeads AS in Skedsmokorset, Norway. The details and results of these batch contact tests are provided by Nash, et al. (2006). A brief summary of the batch contact test matrix is provided in Tables 4-1 and 4-2. A total of 18 types of batch contact tests were performed using the following simulants:

- Nominal recipe AP-101 simulant without the toxic metals and aluminum
- Full recipe AP-101 simulant including the toxic metals and aluminum
- Modified recipe Nominal recipe where one of the key ions has been altered
- Simple recipe Very simple recipe where hydroxide concentration is varied

Since planned operation of the WTP ion-exchange facility will be at cesium feed conditions where the isotherm will experience non-linear behavior, several points along an isotherm were required for testing. Four points along the isotherm were measured for the baseline simulants (i.e., simulants S01, S02 and S03 in Table 4-1). For parameter estimation requirements of the detailed thermodynamic equilibrium model, seven additional modified simulant test sets were performed (i.e., S04, S05, S06, S07, S08, S09 and S10 in Table 4-1). As listed in Table 4-1, these seven sets address primarily the competitor effects associated with $Na^+$, $K^+$, and $Rb^+$ versus $Cs^+$ on the RF resin within a simulated AP-101 solution. For these tests, only the lowest and highest points along the isotherm used in the other tests were measured.

Additional batch contact tests were performed using a very simple simulant where primarily the hydroxide concentration was varied (i.e., S11 through S18 in Table 4-2). These eight additional tests were performed, as listed in Table 4-2, to address the change in $Cs^+$ capacity of the RF resin with respect to $OH^-$ concentration (i.e., pH effect).

Temperature effects were addressed by running almost the full set of experiments at both 25 and 45 °C with one set also run at 15 °C. For the first ten simulant compositions 70 batch contact tests were performed while for the second eight simulant compositions 60 batch contact tests were performed. The batch contact database of 130 data points was used in estimating the key parameters required in the detailed thermodynamic isotherm model.

### 4.1.3 Parameter Estimation for Detailed Thermodynamic Equilibrium Model

As mentioned above, to have a working detailed thermodynamic equilibrium model for addressing cesium loading on RF resin the following key parameters must be determined (or chosen) based on available batch contact data:

$$\left[K^e_{12}, K^e_{13}, K^e_{14}, K^e_{15}, C_T, \delta, \Delta H^o, T_{ref}\right]$$

where 1-$Cs^+$, 2-$K^+$, 3-$Na^+$, 4-$Rb^+$, and 5-$H^+$. An optimization algorithm was employed where some of these parameters were estimated using the following cost function:

$$\Phi \equiv \frac{1}{2}\sum_k \left[ \frac{w_k (K_{d,k}^{exp} - K_{d,k}^{mod})}{K_{d,k}^{exp}} \right]^2 , \qquad (4\text{-}7)$$

where

$w_k$ ..................weighting factor typically set to unity

The experimental and model $K_d$'s in Eq. (4-7) are defined to be:

$$K_{d,k}^{exp} = \frac{Q_k^{exp}}{c_k^{exp}} \quad \text{and} \quad K_{d,k}^{mod} = \frac{Q_k^{mod}}{c_k^{mod}}$$

The CERMOD code (Aleman and Hamm, 2007) performs numerical batch contact simulations where input initial liquid cesium concentration and the resin to liquid phase ratio are used to estimate the final liquid concentration and solid loading of cesium. From the computed liquid concentration and solid loading of cesium, a $K_d$ value is calculated using the above expression.

The experimentally measured cesium $K_d$ values for S01, S03 through S13, and S16 through S18 with a total of 70 data points at 25 °C and 60 data points at 45 °C were used in the cost function. S02 was left out to be used for verification purposes since it represents the closest set of isotherm data to an actual waste feed and also was measured over the broadest temperature range (i.e., 15, 25 and 45 °C). S14 and S15 were left out due to the very low hydroxide concentrations [0.05 and 0.01 M, respectively] used in their testing. The results from S14 and S15 are under evaluation as to their accuracy. Additional modeling effort may also be required to address neutral species adsorption when $OH^-$ levels drop below 0.05 M.

During the initial parameter estimation process, it was recognized that the available batch contact database would not sufficiently pin down some of the required parameters in a statistically unique manner (i.e., a high degree of correlation exists among certain parameters). As such, certain parameters were fixed to values believed to be reasonable based on assessments made when looking at subsets of the database and prior experience with earlier resin materials. The final parameter estimations are summarized in Table 4-3. The reference temperature was set to 25 °C. The existing batch contact database was unable to adequately establish thermodynamic equilibrium constants for $Rb^+$. For $Rb^+$ its value was estimated from the limited breakthrough curve data provided in the SRNL small column test using AP-101 simulant at 45 °C.

Using the parameter settings provided in Table 4-3, a direct comparison is made of the numerical estimates generated from the detailed thermodynamic equilibrium model versus the experimentally measured $K_d$, $Cs^+$ loading on the resin in $H^+$ form, and $Cs^+$ concentration in solution in Figures 4-2 through 4-4 for tests at 25 °C and in Figures 4-5 through 4-7 for tests at 45 °C. Also provided on these figures are ±20% error bands to illustrate the level of fit achieved with the numerical model. Comparisons between model calculated and experimentally measured $K_d$, cesium concentration in the liquid and resin loading at equilibrium for each batch contact data point are also tabulated in Tables A-1 through A-6 in Appendix A. Equilibrium concentrations of $Na^+$, $K^+$, $Rb^+$, $Cs^+$ and $OH^-$ are tabulated in Appendix B.

As illustrated in Figures 4-3 and 4-6 and by the data listed in Tables A-2 and A-5 in Appendix A, the numerical model can estimate cesium loadings on the RF resin within 20% for the entire 130 data points that range over: 25 to 45 °C, 4.0 to 6.0 M Sodium, 0 to 0.71 M Potassium and 0.05 to 2.0 M Hydroxide. Over this broad range of conditions, cesium loading predictions within 20% are considered quite acceptable. Given the theoretical foundation of the detailed thermodynamic equilibrium model, extrapolation of conditions beyond this database should provide reasonable estimates with perhaps acceptable error growth. One such example will be seen below where a validation effort for the methodology is discussed. Examination of Figures 4-2 and 4-5 and Tables A-1 and A-4 in Appendix A also shows that the isotherm model correctly predicts higher $K_d$ values at lower cesium concentrations in agreement with the experimental data.

### 4.1.4 Verification of Numerical Isotherm Methodology

To assess the isotherm methodology one set of batch contact tests was not employed in the determination of the any of the parameters required by the detailed thermodynamic equilibrium model. Simulant number S02 in Table 4-1 was chosen for the verification data since it represents the full recipe of AP-101 in simulant form. This simulant solution includes the toxic metals and aluminum. Batch contact tests were performed at three temperatures (15, 25 and 45 °C). At each temperature, loading measurements were made in duplicate at four different points along each isotherm. Each point represents an equilibrium liquid-phase cesium concentration level. In the discussion below, data points 1, 2, 3 and 4 refer to the low, medium, medium high and high cesium concentrations, respectively. For each temperature a series of numerical batch contact tests were performed over a broad range of cesium concentrations using the thermodynamic equilibrium model. The numerical results (shown as lines) are compared to the experimental data (shown as symbols) in Figure 4-8. Resin loading is based on the dry hydrogen form.

This comparison provides some degree of verification of the isotherm methodology being employed. Overall the predictions are fairly consistent with the available data. Excellent agreement between the numerical and experimental results are observed for data point 2 (medium Cs) as shown in Figure 4-8. The relative shift in magnitude for cesium loading due to increasing temperature appears to be consistent between the numerical and experimental data. Note also that the 15 °C predictions are beyond the above database used to estimate the parameters required by the detailed thermodynamic equilibrium model. The numerically estimated apparent capacity of the resin is just under 0.69 mmole/g of resin in dry sodium form. As shown in Figure 4-8, for all three temperatures the numerical results over-predict cesium loading near data point 3 (medium-high Cs) and under-predict cesium loading near data point 1 (low Cs). That is, at lower cesium concentrations, the experimental data appears to have a smaller slope on the log-log plot than is predicted by the model. As described below in Section 4.1.5, the isotherm model has been modified from the version used in all previous work to allow a log-log slope that is different from unity. However, using parameter values optimized by fitting the isotherm model over the entire set of batch contact data (excluding validation set S02), the model still predicts a slope that is only slightly less than one at liquid cesium concentrations below about $3 x 10^{-4}$ M for the S02 data. The isotherm model does predict a slope less than one in agreement with the data trend; however, the model fails to capture the magnitude of the slope in the S02 experimental data. Uncertainty in the experimental data may account for some of this difference. Review of the experimental data indicates that analytical errors may have occurred during the gamma counting for batch contact data with loadings near 0.1 mmole/g (data point 3). No apparent explanation exists for the discrepancies at the low Cs concentration (data point 1) where the numerically generated isotherm is lower than the experimental data.

Isotherms for the other batch contact data sets are plotted in Figures 4-9 through 4-22. Resin loading is based on dry hydrogen form. As shown in Figure 4-9, the model and data are in very good agreement for the S01 data. However, in general, for the other batch contact experiments, the model under predicts resin loading a low cesium concentration. Assuming that the experimental data is a better reflection of the true isotherm within that region, VERSE-LC column predictions employing the lower isotherm will yield earlier leading edge breakthrough in the column. As such, some degree of conservatism will occur in the column modeling calculations and actual columns may perform better at low cesium concentrations than predicted by the model. Note that the S15 data shown in Figure 4-22 was not used to isotherm fit model parameters because this data, taken at very low hydroxide, is significantly different from other experimental results.

In the next subsection the "effective" cesium isotherm model is discussed based on a general ion-exchange process and in the following subsection its specific application to the Resorcinol-Formaldehyde ion-exchange system is discussed.

### 4.1.5 Algebraic Isotherm Model

An ion-exchange isotherm represents the local thermodynamic equilibrium at the liquid-solid interface as a function of the solid and liquid-phase ion concentrations at one specified temperature. Generally these expressions can be defined with the liquid-phase concentration as an explicit function of solid-phase concentrations. However, for typical transport analyses (e.g., VERSE-LC code) these expressions need to be inverted. Only in certain limited cases can unique algebraic forms be obtained.

An algebraic multi-component isotherm model expressing solid-phase loadings as an explicit function of the liquid-phase concentrations can be explicitly derived from the mass-action Eqs. (4-1) under the following assumptions:

1. Cation competitors are monovalent.
2. Active sites are homogeneous and every competitor has access to all active sites (i.e., individual ionic capacities all are equal to the total ionic capacity).
3. Selectivity coefficients, $K_{ji}^{c}$, are constant over the composition range of interest.

Making use of the above assumptions the following generic algebraic multi-component isotherm model is obtained:

$$Q_i = F^{-1}(\bar{c}, T) = \eta_{df}\left[\frac{\overline{C}_T c_i}{c_i + [\sum_{j \neq i} K^c_{ji} c_j]}\right], \tag{4-8}$$

where

$Q_i$ ...................species i solid loading, mmol/g
$\overline{C}_T$ .................total ion-exchange capacity of resin, mmol/g
$\eta_{df}$ ................isotherm chemical degradation factor
$c_i$ ...................species i concentration in liquid-phase bed fluid, [M]
$K^c_{ji}$ ................selectivity coefficient between species j and i
T ....................specified temperature of isotherm

The chemical degradation factor accounts for aging effects to the resin as it continually passes through loading-elution cycles (i.e., continual loss of active exchange sites). The algebraic isotherm model defined by Eq. (4-8) is also thermodynamically consistent.

More generally, relaxing assumption 3, selectivity coefficients are composition and temperature dependent:

$$K^c_{ij}(\bar{c}, T) \equiv \frac{1}{K^c_{ji}(\bar{c}, T)} = \frac{K^e_{ij}(T)}{K^\gamma_{ij}(\bar{c}, T)} \quad \text{and} \quad K^c_{ii} \equiv 1, \tag{4-9}$$

Fortunately, for the typical LAW feed compositions of interest we find that for a given recipe the selectivity coefficients only vary marginally with respect to cesium concentrations over a broad range. For the spherical RF resin there are five dominant cation competitors. For this five component monovalent system the surface loading for cesium on the RF material can be expressed using Eq. (4-8) as:

$$Q_{Cs} = \frac{\eta_{df}\overline{C}_T c_{Cs}}{c_{Cs} + [K^c_{21}c_K + K^c_{31}c_{Na} + K^c_{41}c_{Rb} + K^c_{51}c_H]}, \tag{4-10}$$

where the labeling of cations are 1 for $Cs^+$, 2 for $K^+$, 3 for $Na^+$, 4 for $Rb^+$, and 5 for $H^+$.

As demonstrated by Hamm et al. (2000b) for SuperLig® 644 resins and also for spherical RF resin in Figure 3-1, for ion exchange competitors with affinities significantly less than the value for cesium, a single-component model is adequate for predicting column performance for the cesium loading phase. Using a single component model, computational demands for VERSE-LC simulations can be reduced by a factor greater than 500, with very little loss in accuracy of the predicted breakthrough behavior for cesium.

To perform spherical RF resin single-component transport simulations, an "effective" binary isotherm model in an algebraic form, consistent with Eq. (4-10), must be available for use in the

VERSE-LC code. The multi-component cesium isotherm given by Eq. (4-10) can be reduced to the following "effective" binary isotherm model:

$$Q_{Cs} = \eta_{df}\left[\frac{\overline{C}_T\ c_{Cs}}{c_{Cs} + \beta_{Cs}}\right], \tag{4-11}$$

$$\beta_{Cs} = K^c_{21}c_K + K^c_{31}c_{Na} + K^c_{41}c_{Rb} + K^c_{51}c_H, \tag{4-12}$$

where

$\beta_{Cs}$ ................isotherm parameter for cesium, [M]

Equation (4-12) indicates that the beta parameter for cesium will vary based on local concentrations of the other competing cations. As shown in Figure 3-1, the concentrations for all of the other competing cations, excluding cesium, have completely broken through the column and are at their saturation values (i.e., feed values) after approximately 10 to 20 bed volumes. Beyond this point the beta parameter given by Eq. (4-12) becomes constant.

Equation (4-11) is in the form of a Langmuir isotherm. A somewhat empirical extension of this to the Freundlich/Langmuir form introduces powers on the concentration terms to obtain:

$$Q_{Cs} = \eta_{df}\left[\frac{\overline{C}_T\ c_{Cs}^{M_{aCs}}}{\beta_{Cs} + c_{Cs}^{M_{bCs}}}\right], \tag{4-13}$$

$$\beta_{Cs} = K^c_{21}c_K^{M_{bK}} + K^c_{31}c_{Na}^{M_{bNa}} + K^c_{41}c_{Rb}^{M_{bRb}} + K^c_{51}c_H^{M_{bH}}, \tag{4-14}$$

The beta parameter for cesium is dependent upon the feed concentrations of the other ionic competitors for Resorcinol-Formaldehyde adsorption ($K^+$, $Na^+$, $Rb^+$ and $H^+$). The beta parameter contains the selectivity coefficients making it dependent upon temperature and liquid composition of all of the ionic species in solution. Therefore, the beta parameter for cesium will be unique for each waste feed considered at a particular operating temperature. The larger the beta parameter the less favorable the isotherm at lower cesium concentrations with correspondingly lower cesium loadings. The degradation factor ($\eta_{df}$) is unity when considering a fresh resin and becomes less than unity following chemical exposure (i.e., cycling). Given a fixed degradation factor, Eq. (4-13) contains four free parameters (i.e., a total cesium capacity, a beta value, and the two powers $M_{aCs}$ and $M_{bCs}$) that need to be specified. For each particular feed stream and operating temperature, these four parameters are estimated by fitting Eq. (4-13) to data simulated using the detailed thermodynamic model as described by Aleman and Hamm (2007).

To demonstrate and validate the assumptions being made for reducing the multi-component isotherm down to the more simple "effective" cesium binary algebraic isotherm model of Eq. (4-13), a comparison of the numerically generated isotherm versus the algebraic isotherm has been performed. The full recipe AP-101 simulant at 25 ºC was chosen for the comparison. The comparison is shown in Figure 4-23 where the experimental batch contact data points are provided as well (shown as green diamond symbols). The numerically generated batch contact points (i.e., from the detailed thermodynamic equilibrium model) are shown as red circles. The blue solid line represents the fitted Eq. (4-13) algebraic isotherm model. The excellent fit of the numerical data to the algebraic model over the entire cesium range, supports the main assumption that the selectivity coefficients over this range are reasonably constant.

### 4.1.6 Isotherm Model for VERSE-LC Application

In order to perform column transport simulations, the algebraic model given by Eq. (4-13) must be converted into one of the available VERSE-LC isotherm modeling options. Based on our previous experience using VERSE-LC modeling SuperLig® 644 (Hamm et al., 2000b), SuperLig® 639 resins (Hamm et al., 2000c), and CST resins (Hamm et al., 2002), the VERSE-LC Freundlich/Langmuir Hybrid isotherm model option was chosen. See Section 4 of Hamm et al. (2000b) for further description of the multi-component homovalent isotherm approach.

For a five-component homovalent isotherm, the VERSE-LC Freundlich/Langmuir Hybrid model is expressed in general as:

$$\overline{C}_{pi} = \frac{a_i c_{pi}^{M_{ai}}}{\beta_i + b_1 c_{p1}^{M_{b1}} + b_2 c_{p2}^{M_{b2}} + b_3 c_{p3}^{M_{b3}} + b_4 c_{p4}^{M_{b4}}} \qquad \text{for} \quad i = 1 \ldots 4, \tag{4-15}$$

where

$\overline{C}_{pi}$ .............species i solid surface concentration based on bed volume, gmole/L-BV

$c_{pi}$ ..............species i concentration in pore fluid, M

$\beta_i, a_i, b_i$ .......Fruendlich/Langmuir Hybrid model coefficients for species i

$M_{ai}, M_{bi}$ .....Freundlich/Langmuir Hybrid model exponents for species i

The model parameters ($a_i$, $b_i$, $M_{ai}$, $M_{bi}$, and $\beta_i$ for i=1…4) can be determined from the parameter values associated with the five-component homovalent model in Eqs. (4-13) and (4-14).

The Freundlich/Langmuir Hybrid model can also be used for an "effective" single-component case. Here the potassium, sodium, rubidium, and hydrogen (actually hydroxide) concentrations throughout the column are assumed to be at their feed concentration levels. For an "effective" single-component total cesium isotherm, Eq. (4-15) under these conditions reduces to:

$$\overline{C}_{p1} = \frac{a_1 c_{p1}^{M_{a1}}}{\left[\beta_i + b_2 c_{p2}^{M_{b2}} + b_3 c_{p3}^{M_{b3}} + b_4 c_{p4}^{M_{b4}} + b_4 c_{p5}^{M_{b5}}\right] + b_1 c_{p1}^{M_{b1}}} \Rightarrow \frac{a_1 c_{p1}^{M_{a1}}}{\hat{\beta}_1 + b_1 c_{p1}^{M_{b1}}}, \tag{4-16}$$

where $\hat{\beta}_1$ is the Fruendlich/Langmuir "effective" single-component isotherm constant.

The beta parameter for cesium is dependent upon the potassium, sodium, rubidium, and hydrogen feed concentrations.

Without loss of generality, we can divide the numerator and denominator of Eq. (4-16) by $b_1$ to obtain:

$$\overline{C}_{p1} = \frac{a_1' \, c_{p1}^{M_{a1}}}{\beta_1' + c_{p1}^{M_{b1}}}, \tag{4-17}$$

Equation (4-17) is then equivalent to Eq. (4-13) with the exception that the VERSE-LC resin capacity is expressed in terms of mmol per liter of bed volume whereas the resin capacity $Q_{Cs}$ is in mmol per gram resin. The VERSE-LC parameter $a_1'$ in Eq. (4-17) is therefore computed as:

$$a_1' = \rho_b \, \eta_{df} \, \overline{C}_T, \tag{4-18}$$

where $\rho_b$ is the bed density of the active column in sodium form, g/ml. The final form of the isotherm model as used in VERSE-LC is then:

$$\overline{C}_{pCs} = \eta_{df} \left[ \frac{\rho_b \, \overline{C}_T \, c_{pCs}^{M_{aCs}}}{\beta_{Cs} + c_{pCs}^{M_{bCs}}} \right], \tag{4-19}$$

where the prime on $\beta$ has been dropped to simplify the notation.

It is assumed that the binary selectivity coefficients are not composition dependent, but are true constants (i.e., note that the selectivity coefficients actually contain the true equilibrium constants and liquid/solid phase activity coefficients; see Aleman and Hamm (2007) for details). This assumption appears to be adequate when considering different feeds within the same envelope (i.e., generally only small variations are observed in selectivity coefficients within a given envelope), but should not be used between envelopes or different temperatures. The composite impact on cesium loading from the other cation competitors is summed up in the beta parameter as shown above in Eq. (4-14). As mentioned earlier, the chemical degradation factor, $\eta_{df}$, is set to unity for fresh resin behavior and less than unity to account for chemical degradation effects.

Modeling parameter values for cesium single-component isotherms are listed in Table 4-11 for the 17 unique ion-exchange LAW feed stream compositions used in this study for addressing full-scale operations.

## 4.2 LAW Batch Feed Compositions

To assess the overall performance of the spherical RF-641 resin operating within a carousel of three full-scale columns, three proposed LAW feeds have been established by Toth (2003). In order to generate the cesium loading isotherm databases using the detailed thermodynamic isotherm model, the proposed LAW feed compositions for the three candidate batch feeds had to be slightly altered to enforce a charge balance. The original feed compositions for each feed stream were supplied by Toth (2003). For each feed stream overall charge balancing was achieved by adjusting the anion concentrations for nitrite and nitrate while maintaining the nitrite to nitrate ratio constant. The nominal feed compositions for each feed stream are provided in Table 4-4 after achieving a charge balance.

Additional LAW feed streams under the off-nominal settings specified by Thorson (2006) were used for sensitivity studies to determine competitor impacts on column performance. Hot Commissioning feed compositions derived from variation about the nominal potassium and sodium concentrations are provided in Tables 4-5 and 4-6, respectively. Subsequent Operation feed compositions derived from variation about sodium and hydroxide concentrations and the addition of caustic leach solution are provided in Tables 4-7 and 4-8, respectively. The off-nominal feed compositions were obtained by varying each competitor along with the anions nitrite and nitrate to maintain charge balance while keeping the nitrite to nitrate ratio constant.

## 4.3 Simulant Compositions

AP-101 simulant was used by SRNL personnel (Nash et al., 2006) to conduct batch contact, particle kinetics, and small column testing. AP-101 simulant and actual AP-101 waste were used by PNWD personnel (Fiskum et al., 2006a) to perform small scale column tests. Table 4-9 provides the compositions for actual AP-101 waste and AP-101 simulant at approximately 5 M sodium. Trace ions that are not supported by the detailed thermodynamic isotherm model are excluded. In addition, a simulant of AN-107 Sr/TRU filtrate was used for a small column test at SRNL (Nash et al., 2006) and a simulant of AZ-102 was used for a small column test at PNWD (Fiskum et al., 2006c). Compositions of these simulants for the major analytes are given in Table 4-10.

## 4.4 The Total Capacity and Beta Parameter Values

For each of the LAW batch feed compositions discussed above and presented in Tables 4-4 through 4-8, isotherm data was generated using the detailed thermodynamic equilibrium isotherm model. As discussed above, the detailed isotherm model was established and benchmarked using the AP-101 batch contact experimental data (Nash et al, 2006). For each unique feed, a nonlinear regression analysis was used to determine the total cesium exchange capacity and beta value, as defined in Eqs. (4-13 and 4-14). The parameter estimation results from these regression analyses are provided in Table 4-11.

Isotherms for the three nominal feed streams are plotted in Figure 4-24 where capacity is calculated for the resin in $H^+$ form. The Hot Commissioning Operation isotherm is the least favorable isotherm for cesium ion-exchange. The impact of variations in competitor ions on the nominal Hot Commissioning Operation feed stream $Cs^+$ isotherm is shown in Figures 4-25 and 4-26 for potassium and sodium, respectively. The effect of temperature over the range 25 to 45 °C on the cesium isotherms with nominal Hot Commissioning feed is shown in Figure 4-27. Higher temperatures decrease the RF resin cesium capacity. Similar results for Subsequent Operation feed are plotted in Figures 4-28 through 4-31. The impact of variations in sodium and hydroxide on the nominal Subsequent Operation feed stream $Cs^+$ isotherm is shown in Figures 4-28 and 4-29, respectively. The effect of varying the composition of Subsequent Operation feed from running the caustic leaching process is shown in Figure 4-30. In Figure 4-30, the case with 20% added sodium was run at 45 °C, which lowers resin capacity, while the other two cases were run at 25 °C. The effect of temperature over the range 25 to 45 °C on the cesium isotherms with nominal Subsequent Operation feed is shown in Figure 4-31. In all of the isotherm plots resin capacity is for the resin in $H^+$ form.

Table 4-1. Baseline batch contact test matrix for addressing sorption behavior of spherical RF-641 resin using a simulated AP-101 solution (i.e., nominal simulant and various variations in support of isotherm modeling needs).

| AP 101 Simulant Recipe[b] | Label | $Na^+$ [M] | $K^+$ [M] | $Rb^+$ [M] | $OH^-$ [M] | Cs[a] | 15 °C | 25 °C | 45 °C |
|---|---|---|---|---|---|---|---|---|---|
| Nominal | S01 | 5.0 | 0.71 | $5.85 \times 10^{-5}$ | 1.94 | 4-pt. | - | 3X | 2X |
| Full Recipe | S02 | 5.0 | 0.71 | $4.80 \times 10^{-5}$ | 1.94 | 4-pt. | 2X | 2X | 2X |
| No Rubidium | S03 | 5.0 | 0.71 | 0.0 | 1.94 | 4-pt. | - | 2X | 2X |
| Modified | S04 | 6.0 | 0.71 | $5.85 \times 10^{-5}$ | 1.94 | 2-pt. | - | 2X | 2X |
| Modified | S05 | 4.0 | 0.71 | $5.85 \times 10^{-5}$ | 1.94 | 2-pt. | - | 2X | 2X |
| Modified | S06 | 6.0 | 0.0 | $5.85 \times 10^{-5}$ | 1.94 | 2-pt. | - | 2X | 2X |
| Modified | S07 | 5.0 | 0.0 | $5.85 \times 10^{-5}$ | 1.94 | 2-pt. | - | 2X | 2X |
| Modified | S08 | 5.0 | 0.71 | $5.85 \times 10^{-5}$ | 0.8 | 2-pt. | - | 2X | 2X |
| Modified | S09 | 5.0 | 0.71 | $5.85 \times 10^{-5}$ | 0.2 | 2-pt. | - | 2X | 2X |
| Modified | S10 | 4.0 | 0.0 | $5.85 \times 10^{-5}$ | 1.94 | 2-pt. | - | 2X | 2X |

[a] 4-pt. cases have Cs concentrations near $6 \times 10^{-3}$, $3.4 \times 10^{-2}$, $2.2 \times 10^{-1}$, and 1.3 g/L. The 2-pt. cases focuses on just the lower and upper concentration values. The actual simulant Cs concentrations vary to some degree from the number provided here (Nash, et al., 2006).

[b] The Nominal simulant listed is for the simple AP-101 recipe without toxic metals included, as well as aluminum omitted. Full Recipe has the these other species added back into the recipe. No rubidium represents the Nominal case where rubidium has been omitted. Modified Recipe represents the Nominal simple recipe where either $Na^+$, $K^+$, or $OH^-$ has been altered to provided isotherm modeling support.

Table 4-2. Additional batch contact tests designed specially to address capacity of spherical RF-641 resin with a very simple solution by varying pH.

| Simple Recipe | Label | $Na^+$ [M] | $K^+$ [M] | $Rb^+$ [M] | $OH^-$ [M] | $Cl^-$ [M] | Cs[a] | 25 °C | 45 °C |
|---|---|---|---|---|---|---|---|---|---|
| Simple | S11 | 5.0 | 0.0 | 0.0 | 2.0 | 3.0 | 2-pt. | X | X |
| Simple | S12 | 5.0 | 0.0 | 0.0 | 1.0 | 4.0 | 2-pt. | X | X |
| Simple | S13 | 5.0 | 0.0 | 0.0 | 0.1 | 4.9 | 2-pt. | X | X |
| Simple | S14 | 5.0 | 0.0 | 0.0 | 0.05 | 4.95 | 2-pt. | X | X |
| Simple | S15 | 5.0 | 0.0 | 0.0 | 0.01 | 4.99 | 2-pt. | X | X |
| Simple | S16 | 5.0 | 0.0 | 0.0 | 2.0 | 3.0 | 1-pt. | X | - |
| Simple | S17 | 5.0 | 0.0 | 0.0 | 1.0 | 4.0 | 1-pt. | X | - |
| Simple | S18 | 5.0 | 0.0 | 0.0 | 0.1 | 4.9 | 1-pt. | X | - |

[a] 2-pt. cases have Cs concentrations near $6 \times 10^{-3}$ and 1.5 g/L. The 1-pt. cases have Cs concentrations near $1 \times 10^{-4}$ g/L. The actual simulant Cs concentrations vary to some degree from the number provided here (Nash, et al., 2006).

Table 4-3. Best estimate parameter settings to be used in the detailed thermodynamic equilibrium model for the spherical RF-641 resin.

| Cation-Pair | Parameter[b] | Value[a] | Units |
|---|---|---|---|
| | $T_{ref}$ | 25 | ºC |
| | $C_T$ | 6.75 | mmol/g resin $H^+$ form |
| | ε | 0.112 | - |
| | δ | 1.79 | - |
| $Cs^+$ - $Rb^+$ (1-4) | $K^e_{14}$ | 8.0 | - |
| | $\Delta H^o_{14}$ | -18,533.0 | J/gmole |
| $Cs^+$ - $K^+$ (1-2) | $K^e_{12}$ | 308.1 | - |
| | $\Delta H^o_{12}$ | -17,621.0 | J/gmole |
| $Cs^+$ - $Na^+$ (1-3) | $K^e_{13}$ | 41,733.2 | - |
| | $\Delta H^o_{13}$ | -29,468.0 | J/gmole |
| $K^+$ - $Na^+$ (2-3) | $K^e_{23}$ | 135.4 | - |
| | $\Delta H^o_{23}$ | -11,874.0 | J/gmole |

[a] Selectivity coefficients provided at reference temperature 25 °C.
Negative numbers for heats of reaction imply exothermic reactions.

Table 4-4. Waste compositions used to represent ion exchange performance during selected operating time periods (nominal charge balanced values).

| Ion Category | Species | Hot Commissioning Operation Projection (M) | Envelope B Operation Projection (M) | Subsequent Operation Projection (M) |
|---|---|---|---|---|
| **Cations** | **$Na^+$** | 4.57 | 4.13 | 4.60 |
| | **$K^+$** | 0.48 | 0.091 | 0.15 |
| | **Total $Cs^+$** | 2.74E-05 | 2.83E-04 | 5.00E-05 |
| | **$^{137}Cs^+$ (Ci/L)** | 0.072 | 1.18 | 0.14 |
| | **g $^{137}Cs^+$/g Total $Cs^+$** | 0.22 | 0.35 | 0.24 |
| **Anions** | **$SO_4^{2-}$** | 0.032 | 0.129 | 0.030 |
| | **$OH^-$ (free)** | 1.85 | 1.28 | 0.80 |
| | **$NO_2^-$** | 0.523 | 0.921 | 0.750 |
| | **$NO_3^-$** | 1.393 | 0.882 | 2.340 |
| | **$CO_3^{2-}$** | 0.61 | 0.44 | 0.40 |

Table 4-5. Hot Commissioning Operation waste composition with variation about nominal value in potassium concentration.

| Ion Category | Species | Hot Commissioning 0.8 M $K^+$ (M) | Hot Commissioning 0.3 M $K^+$ (M) |
|---|---|---|---|
| **Cations** | **$Na^+$** | 4.57 | 4.57 |
| | **$K^+$** | 0.80 | 0.30 |
| | **Total $Cs^+$** | 2.74E-05 | 2.74E-05 |
| | **$^{137}Cs^+$ (Ci/L)** | 0.072 | 0.072 |
| | **g $^{137}Cs^+$/g Total $Cs^+$** | 0.22 | 0.22 |
| **Anions** | **$SO_4^{2-}$** | 0.032 | 0.032 |
| | **$OH^-$ (free)** | 1.85 | 1.85 |
| | **$NO_2^-$** | 0.610 | 0.473 |
| | **$NO_3^-$** | 1.626 | 1.263 |
| | **$CO_3^{2-}$** | 0.61 | 0.61 |

Table 4-6. Hot Commissioning Operation waste composition with variation about nominal value in sodium concentration.

| Ion Category | Species | Hot Commissioning 4 M $Na^+$ (M) | Hot Commissioning 5 M $Na^+$ (M) | Hot Commissioning 5.5 M $Na^+$ (M) |
|---|---|---|---|---|
| **Cations** | **$Na^+$** | 4.00 | 5.00 | 5.50 |
| | **$K^+$** | 0.420 | 0.525 | 0.578 |
| | **Total $Cs^+$** | 2.74E-05 | 2.74E-05 | 2.74E-05 |
| | **$^{137}Cs^+$ (Ci/L)** | 0.072 | 0.072 | 0.072 |
| | **g $^{137}Cs^+$/g Total $Cs^+$** | 0.22 | 0.22 | 0.22 |
| **Anions** | **$SO_4^{2-}$** | 0.0280 | 0.0350 | 0.0385 |
| | **$OH^-$ (free)** | 1.619 | 2.024 | 2.265 |
| | **$NO_2^-$** | 0.457 | 0.572 | 0.629 |
| | **$NO_3^-$** | 1.220 | 1.525 | 1.677 |
| | **$CO_3^{2-}$** | 0.610 | 0.667 | 0.734 |

Table 4-7. Subsequent Operation waste composition with variation about nominal value in sodium and hydroxide concentration.

| Ion Category | Species | Subsequent Operation 4 M $Na^+$ (M) | Subsequent Operation 5.5 M $Na^+$ (M) | Subsequent Operation 0.6 M $OH^-$ (M) |
|---|---|---|---|---|
| Cations | $Na^+$ | 4.00 | 5.50 | 4.60 |
| | $K^+$ | 0.130 | 0.179 | 0.15 |
| | Total $Cs^+$ | 2.74E-05 | 2.74E-05 | 2.74E-05 |
| | $^{137}Cs^+$ (Ci/L) | 0.072 | 0.072 | 0.072 |
| | g $^{137}Cs^+$/g Total $Cs^+$ | 0.22 | 0.22 | 0.22 |
| Anions | $SO_4^{2-}$ | 0.0261 | 0.0359 | 0.0300 |
| | $OH^-$ (free) | 0.696 | 0.957 | 0.600 |
| | $NO_2^-$ | 0.652 | 0.897 | 0.799 |
| | $NO_3^-$ | 2.035 | 2.780 | 2.491 |
| | $CO_3^{2-}$ | 0.348 | 0.478 | 0.400 |

Table 4-8. Subsequent Operation waste composition with variation about nominal feed value for caustic leach cases.

| Ion Category | Species | Subsequent Operation 50% added Na from NaOH (M) | Subsequent Operation 20% added Na from NaOH (M) |
|---|---|---|---|
| Cations | $Na^+$ | 4.60 | 4.60 |
| | $K^+$ | 0.100 | 0.125 |
| | Total $Cs^+$ | 2.192E-05 | 2.74E-05 |
| | $^{137}Cs^+$ (Ci/L) | 0.0576 | 0.072 |
| | g $^{137}Cs^+$/g Total $Cs^+$ | 0.22 | 0.22 |
| Anions | $SO_4^{2-}$ | 0.030 | 0.030 |
| | $OH^-$ (free) | 2.067 | 1.433 |
| | $NO_2^-$ | 0.430 | 0.590 |
| | $NO_3^-$ | 1.343 | 1.842 |
| | $CO_3^{2-}$ | 0.40 | 0.40 |

Table 4-9. Compositions of AP-101 simulant and actual AP-101 diluted feed.

| Ion Category | Species | AP-101 Simulant (M) | Actual AP-101 DF (M) |
|---|---|---|---|
| **Cations** | $Na^+$ | 4.89 | 5.13 |
| | $K^+$ | 0.679 | 0.737 |
| | $Cs^+$ | 4.37E-05 | 4.45E-05 |
| **Anions** | $Al(OH)_4^-$ | 0.245 | 0.253 |
| | $Cl^-$ | 0.0502 | 0.0423 |
| | $CO_3^{2-}$ | 0.458 | 0 |
| | $NO_2^-$ | 0.732 | 0.824 |
| | $NO_3^-$ | 1.72 | 1.82 |
| | $OH^-$ (free) | 1.89 | 1.98 |
| | $PO_4^{2-}$ | 0.0116 | 0 |
| | $SO_4^{2-}$ | 0.0373 | 0.0344 |

Table 4-10. Compositions of AN-107 Sr/TRU filtrate simulant and AZ-102 simulant.

| Ion Category | Species | AN-107 Simulant (M) | AZ-102 Simulant (M) |
|---|---|---|---|
| **Cations** | $Na^+$ | 5.58 | 5.18 |
| | $K^+$ | 0.0284 | 0.145 |
| | $Cs^+$ | 6.94E-05 | 3.92E-04 |
| **Anions** | $Al(OH)_4^-$ | 0 | 0 |
| | $Cl^-$ | 0 | <7.5E-05 |
| | $CO_3^{2-}$ | 0.755 | 0.95 |
| | $NO_2^-$ | 0.80 | 1.22 |
| | $NO_3^-$ | 2.36 | 0.473 |
| | $OH^-$ (free) | 0.70 | 0.454 |
| | $PO_4^{2-}$ | 0.007 | 0.0102 |
| | $SO_4^{2-}$ | 0.052 | 0.309 |

Table 4-11. Four-parameter fit of algebraic isotherm parameters for spherical Resorcinol-Formaldehyde.

| LAW IX Operating Time Period | Variability | $C_T$ (mmol/g resin $H^+$ form) | β [M] | $M_{aCs}$ | $M_{bCs}$ |
|---|---|---|---|---|---|
| Hot Commissioning | Nominal | 1.0268 | 2.0762E-3 | 0.9850 | 0.8695 |
| Hot Commissioning | 0.8 M $K^+$ | 1.0600 | 3.2807E-3 | 0.9900 | 0.8527 |
| Hot Commissioning | 0.3 M $K^+$ | 0.9993 | 1.3825E-3 | 0.9808 | 0.8816 |
| Hot Commissioning | 4.0 M $Na^+$ | 1.0139 | 1.7776E-3 | 0.9833 | 0.8744 |
| Hot Commissioning | 5.5 M $Na^+$ | 1.0454 | 2.6072E-3 | 0.9875 | 0.8615 |
| Hot Commissioning | 5.0 M $Na^+$ | 1.0357 | 2.3142E-3 | 0.9862 | 0.8658 |
| Hot Commissioning | 35 °C | 1.0447 | 2.6458E-3 | 0.9877 | 0.8609 |
| Hot Commissioning | 45 °C | 1.0611 | 3.2821E-3 | 0.9900 | 0.8525 |
| Envelope B | Nominal | 0.9369 | 4.7832E-4 | 0.9727 | 0.9042 |
| Subsequent Operation | Nominal | 0.9591 | 8.1745E-4 | 0.9761 | 0.8941 |
| Subsequent Operation | 4.0 M $Na^+$ | 0.9454 | 6.8877E-4 | 0.9749 | 0.8976 |
| Subsequent Operation | 5.5 M $Na^+$ | 0.9768 | 1.0342E-3 | 0.9781 | 0.8889 |
| Subsequent Operation | 50% $Na^+$ from NaOH | 0.9465 | 5.2812E-4 | 0.9733 | 0.9024 |
| Subsequent Operation | 20% $Na^+$ from NaOH, 45 °C | 0.9867 | 1.1684E-3 | 0.9792 | 0.8859 |
| Subsequent Operation | 0.6 M $OH^-$ | 0.9556 | 8.3660E-4 | 0.9763 | 0.8936 |
| Subsequent Operation | 35 °C | 0.9762 | 1.1035E-3 | 0.9786 | 0.8874 |
| Subsequent Operation | 45 °C | 0.9930 | 1.4451E-3 | 0.9812 | 0.8804 |

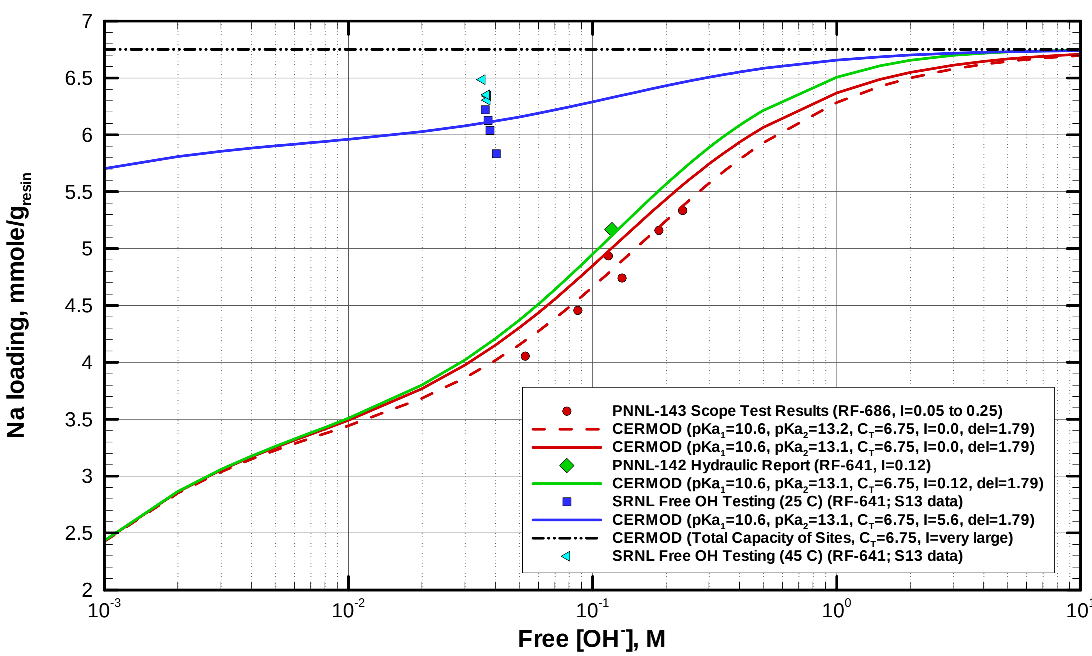


Figure 4-1. Comparison of detailed thermodynamic model's prediction of apparent and measured $Na^+$ loadings versus hydroxide level and ionic strength on spherical RF-641 and RF-686 resins near 25°C for the full recipe AP-101 simulant.

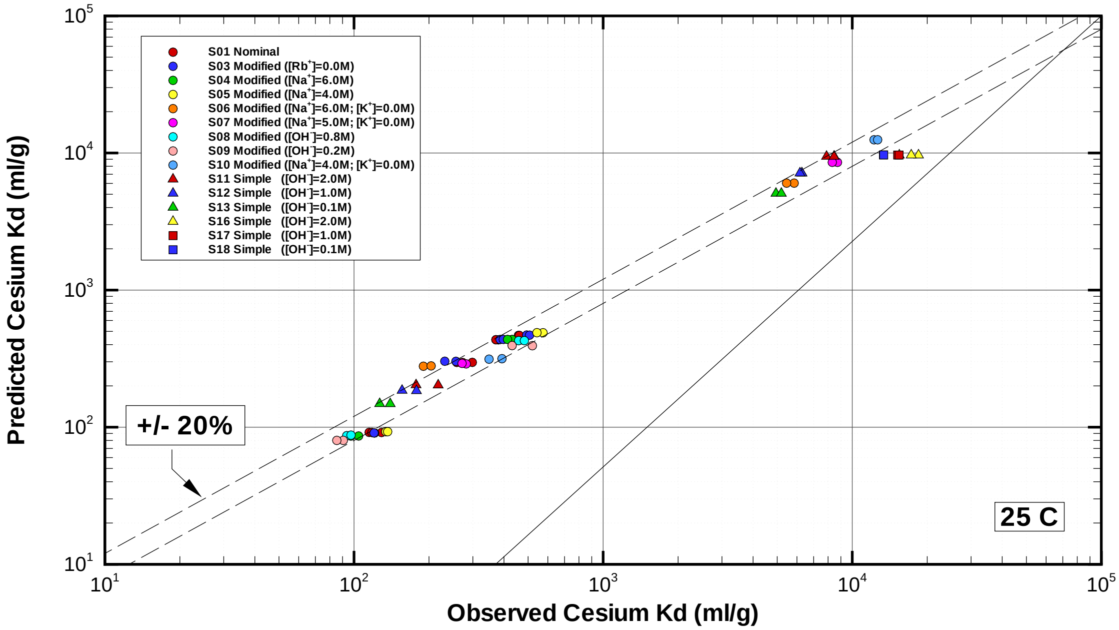


Figure 4-2. Performance of detailed thermodynamic model's prediction of $Cs^+$ $K_d$ on spherical RF-641 resin versus measured $K_d$ at 25°C for various simulants (i.e., AP-101 Nominal and Modified, as well as very Simple recipes).

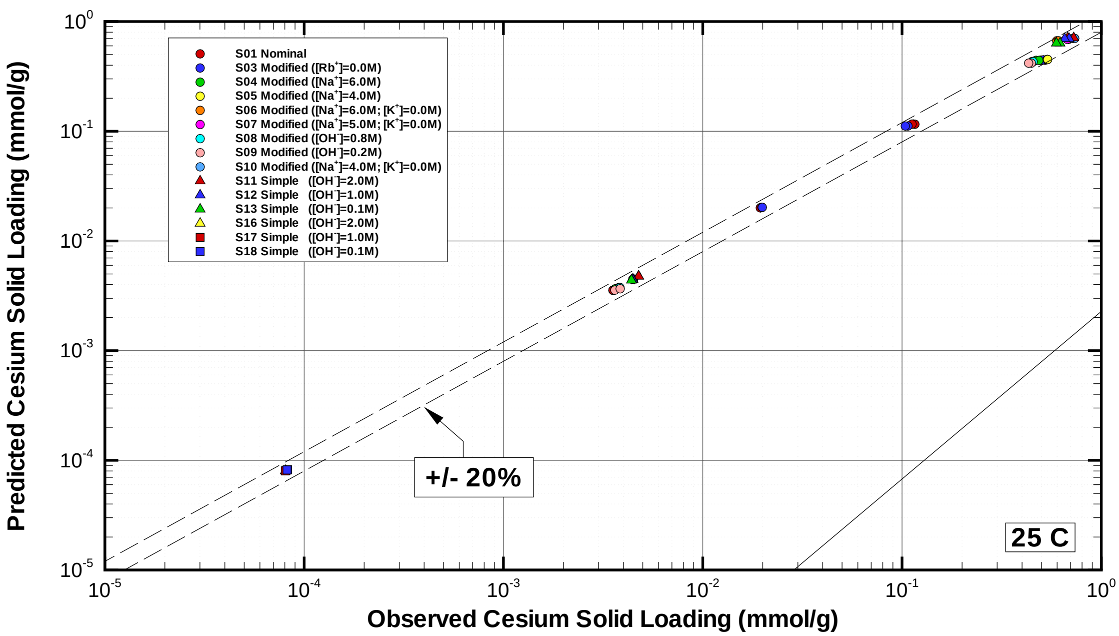


Figure 4-3. Performance of detailed thermodynamic model's prediction of $Cs^+$ loading on spherical RF-641 resin versus measured loading at 25°C for various simulants (i.e., AP-101 Nominal and Modified, as well as very Simple recipes).

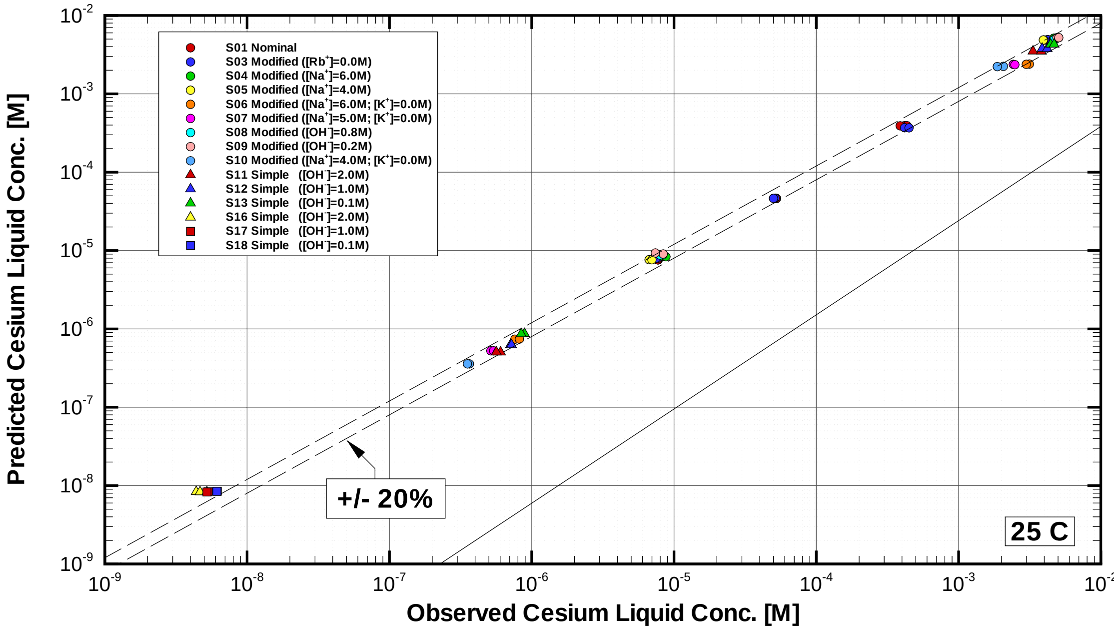


Figure 4-4. Performance of detailed thermodynamic model's prediction of $Cs^+$ concentration on spherical RF-641 resin versus measured concentration at 25°C for various simulants (i.e., AP-101 Nominal and Modified, as well as very Simple recipes).

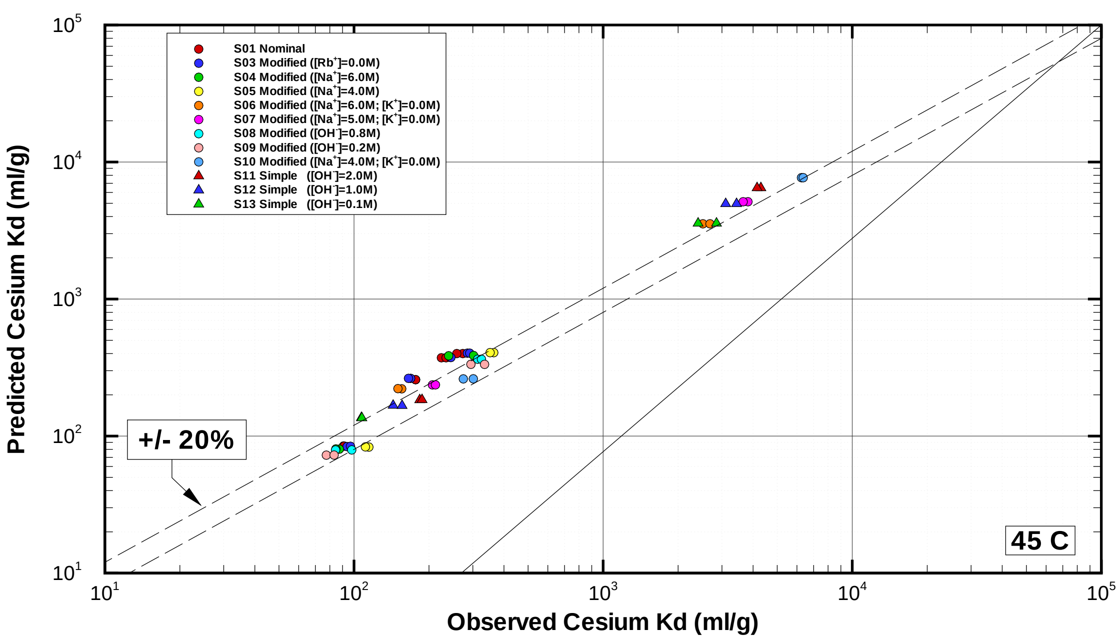


Figure 4-5. Performance of detailed thermodynamic model's prediction of $Cs^+$ $K_d$ on spherical RF-641 resin versus measured $K_d$ at 45°C for various simulants (i.e., AP-101 Nominal and Modified, as well as very Simple recipes).

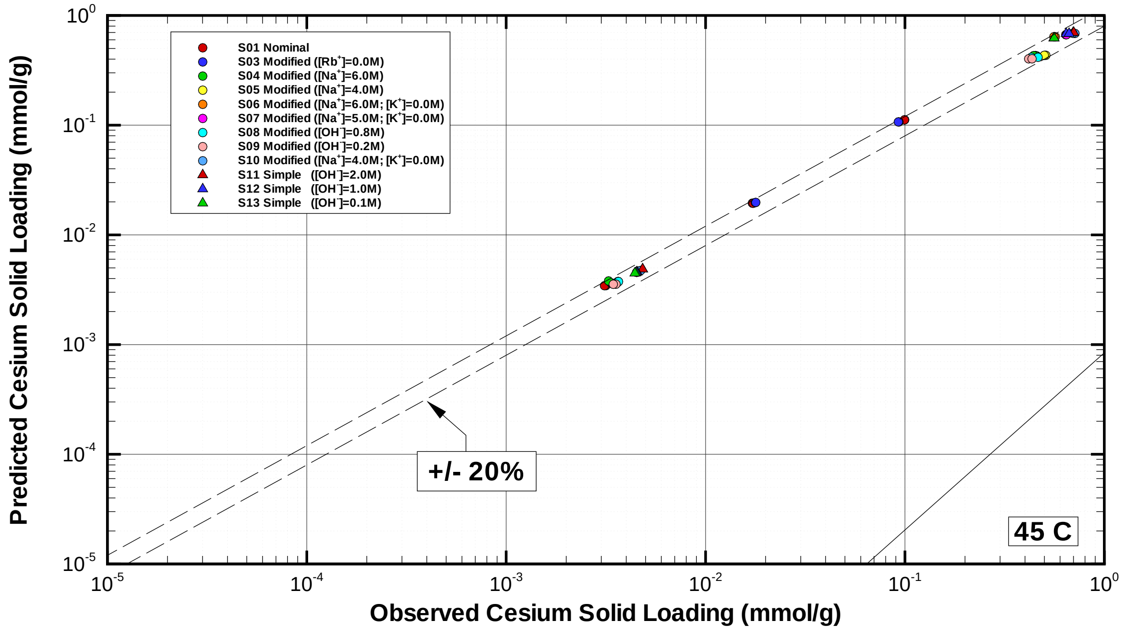


Figure 4-6. Performance of detailed thermodynamic model's prediction of $Cs^+$ loading on spherical RF-641 resin versus measured loading at 45°C for various simulants (i.e., AP-101 Nominal and Modified, as well as very Simple recipes).

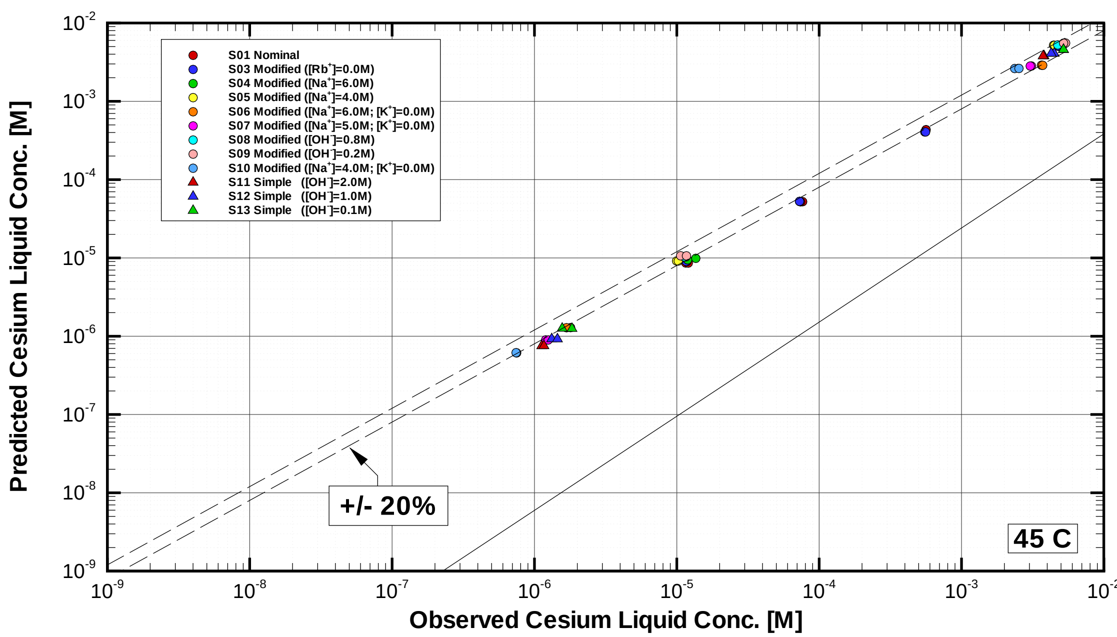


Figure 4-7. Performance of detailed thermodynamic model's prediction of $Cs^+$ concentration on spherical RF-641 resin versus measured concentration at 45°C for various simulants (i.e., AP-101 Nominal and Modified, as well as very Simple recipes).

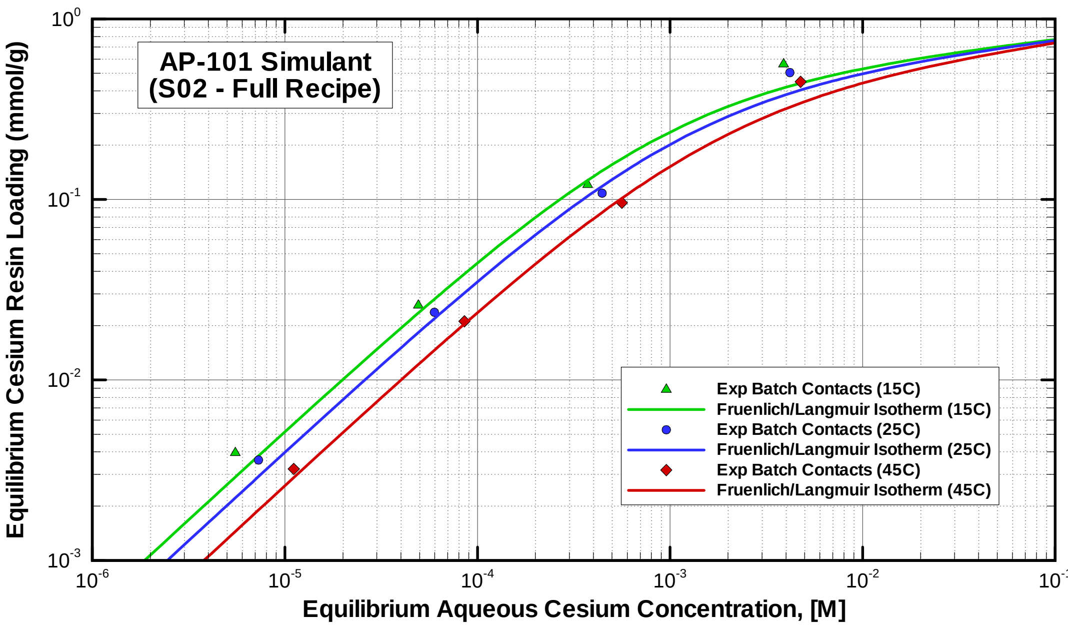


Figure 4-8. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S02 at 15, 25, and 45°C (i.e., AP-101 Full Recipe simulant used as a validation case).

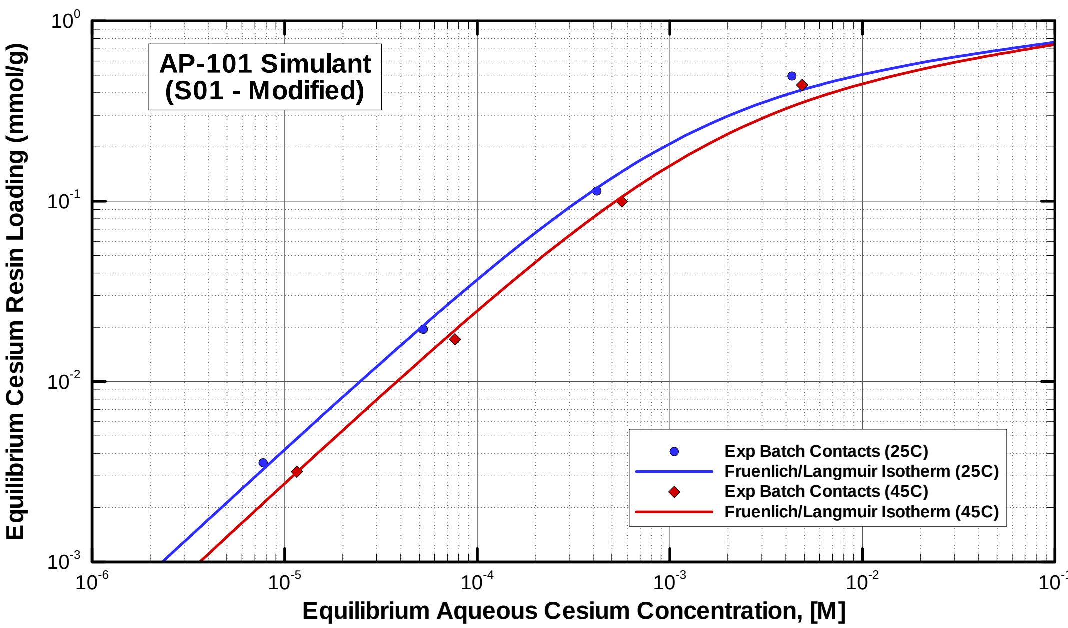


Figure 4-9. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S01 at 25 and 45°C (i.e., AP-101 Modified Recipe simulant with $Rb^+$ present).

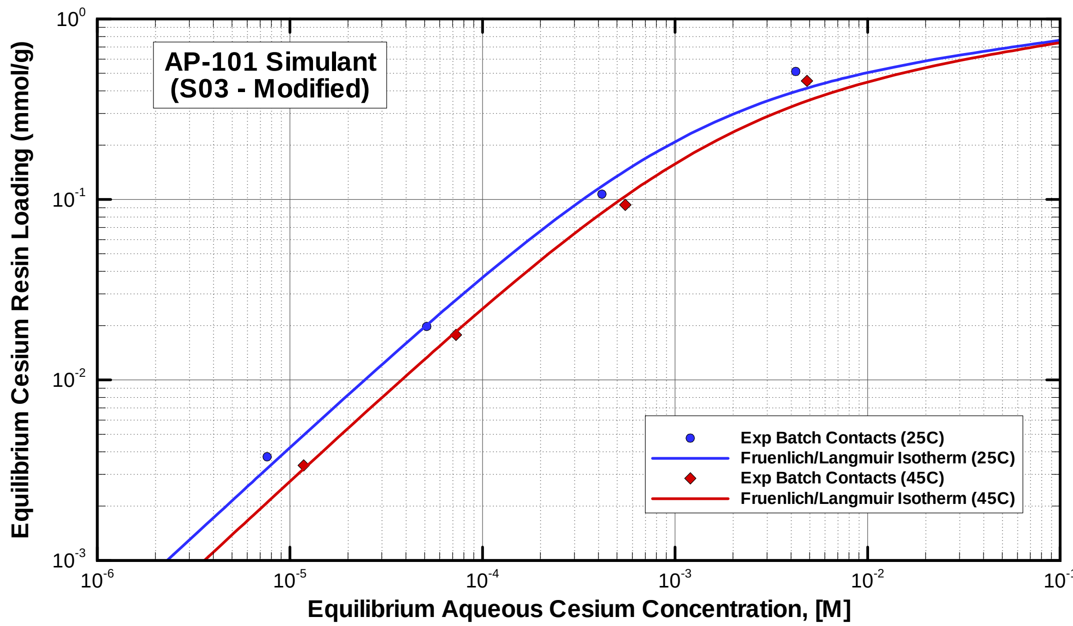


Figure 4-10. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S03 at 25 and 45°C (i.e., AP-101 Modified Recipe simulant without $Rb^+$ present).

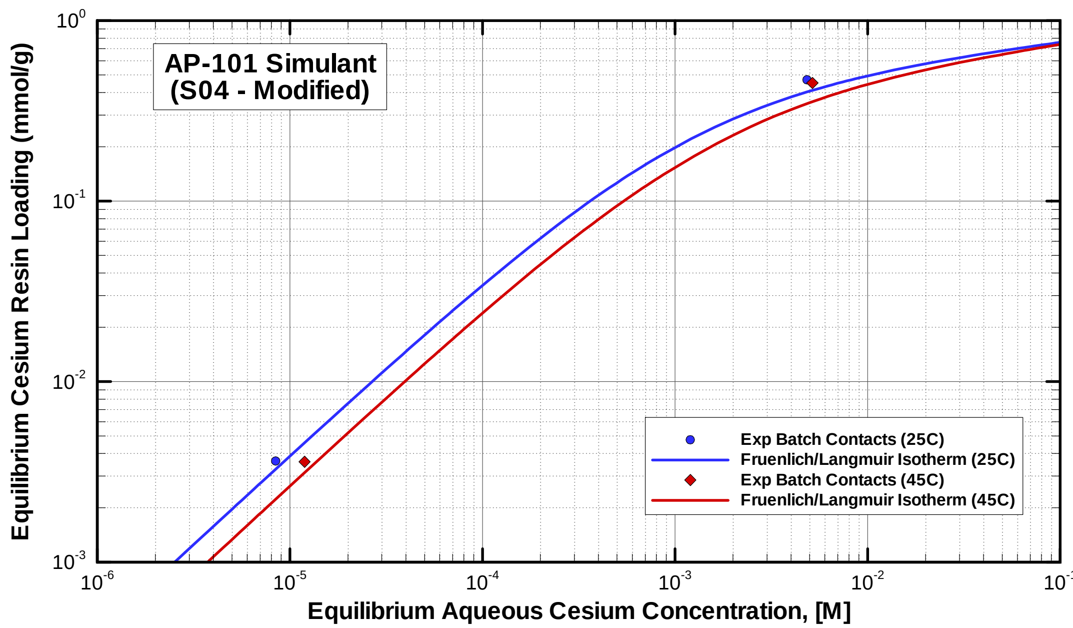


Figure 4-11. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S04 at 25 and 45°C (i.e., AP-101 Modified Recipe simulant with $Na^+$ at 6M).

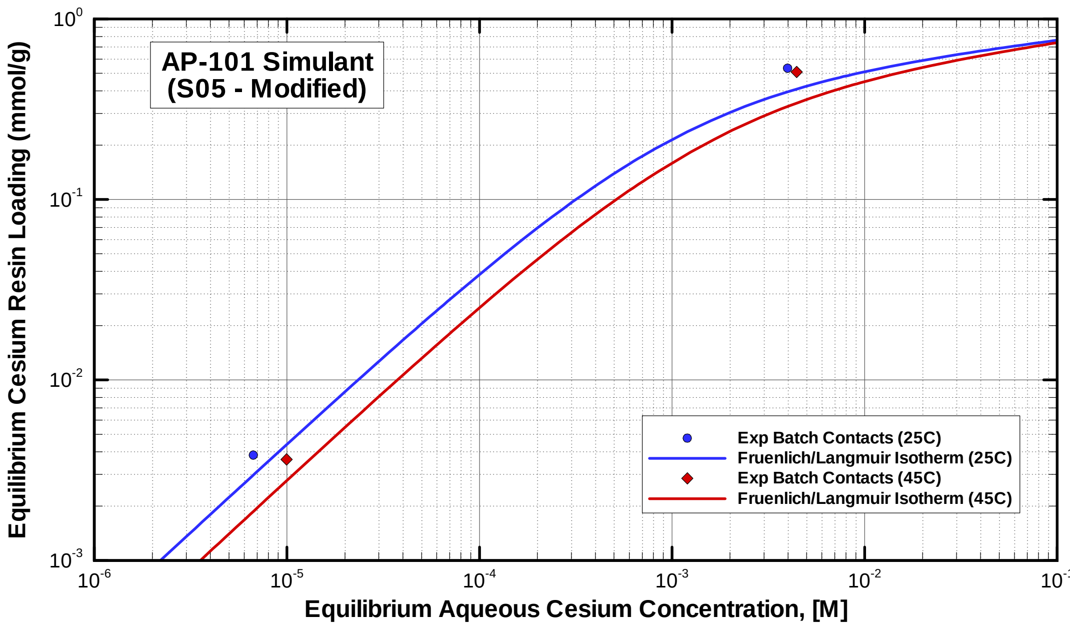


Figure 4-12. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S05 at 25 and 45°C (i.e., AP-101 Modified Recipe simulant with $Na^+$ at 4M).

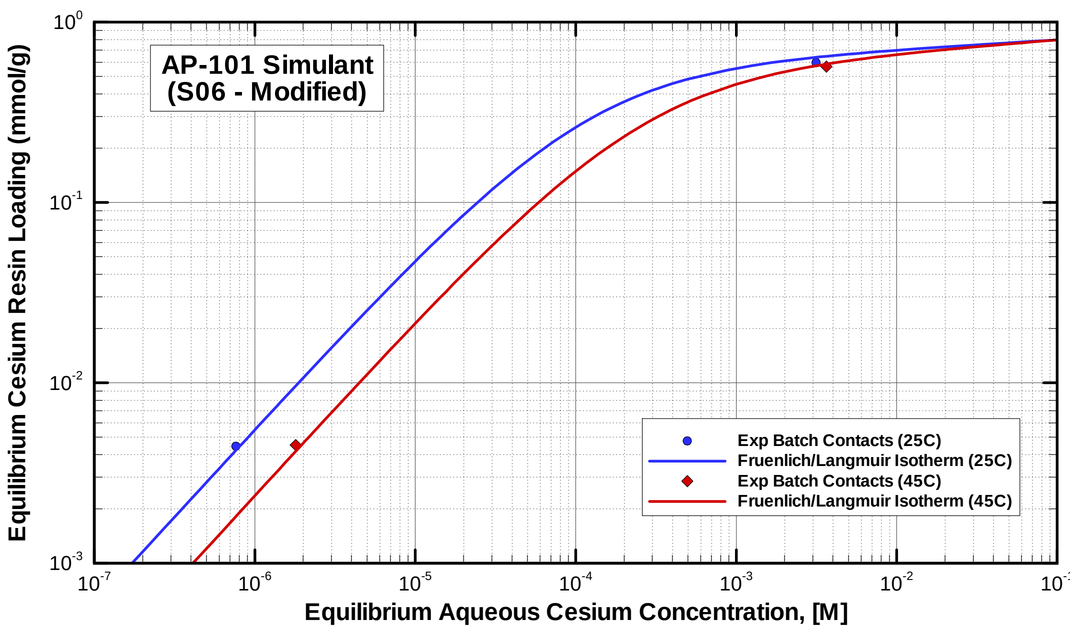


Figure 4-13. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S06 at 25 and 45°C (i.e., AP-101 Modified Recipe simulant with $Na^+$ at 6M and no $K^+$ present).

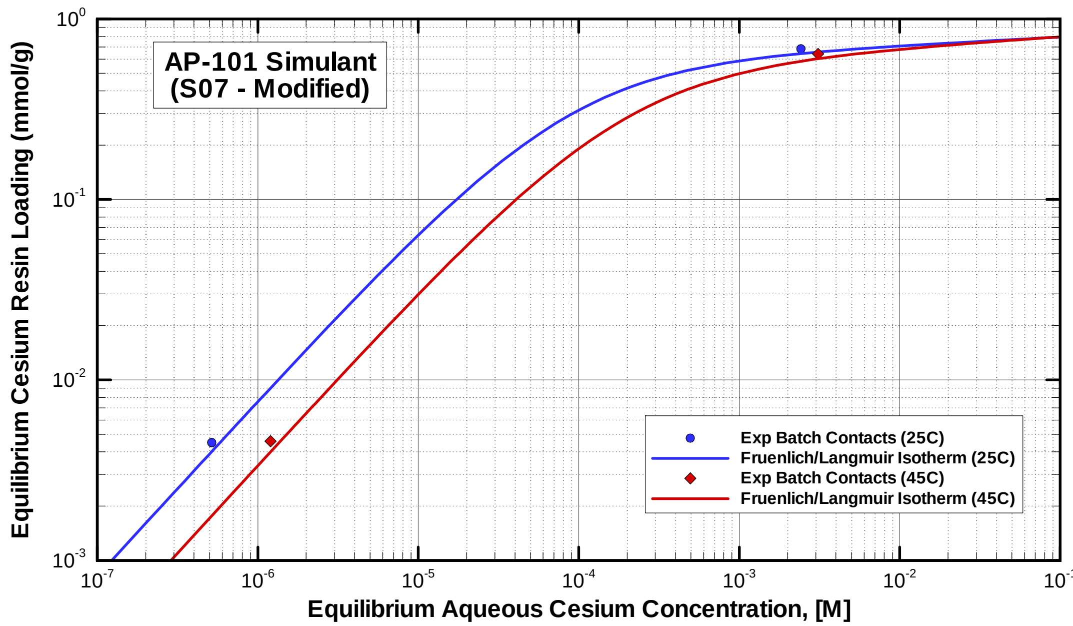


Figure 4-14. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S07 at 25 and 45°C (i.e., AP-101 Modified Recipe simulant with no $K^+$ present).

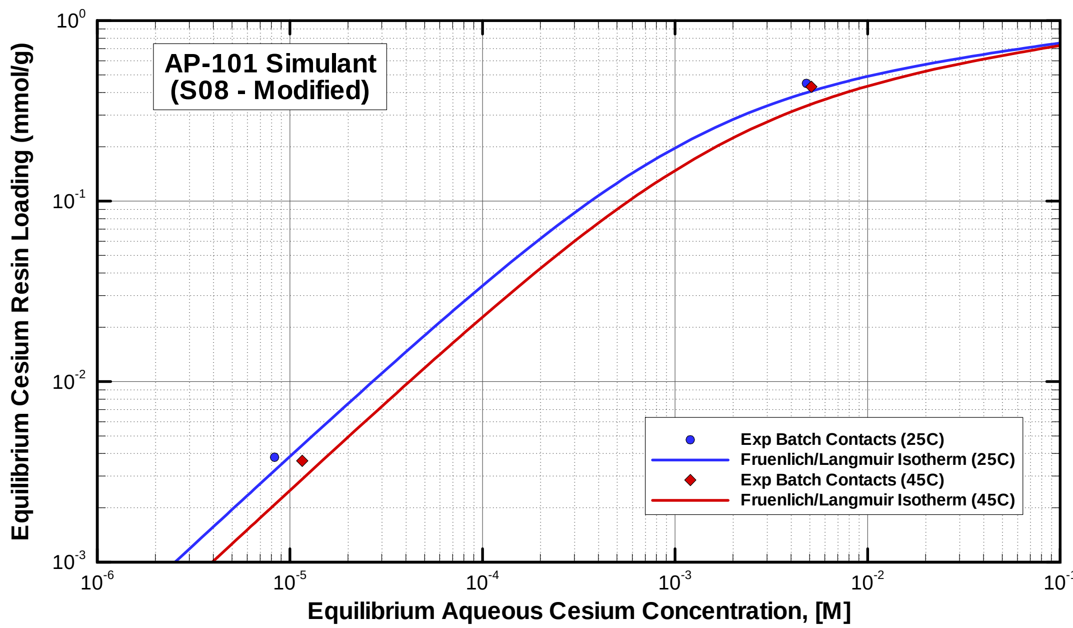


Figure 4-15. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S08 at 25 and 45°C (i.e., AP-101 Modified Recipe simulant with $OH^-$ at 0.8M).

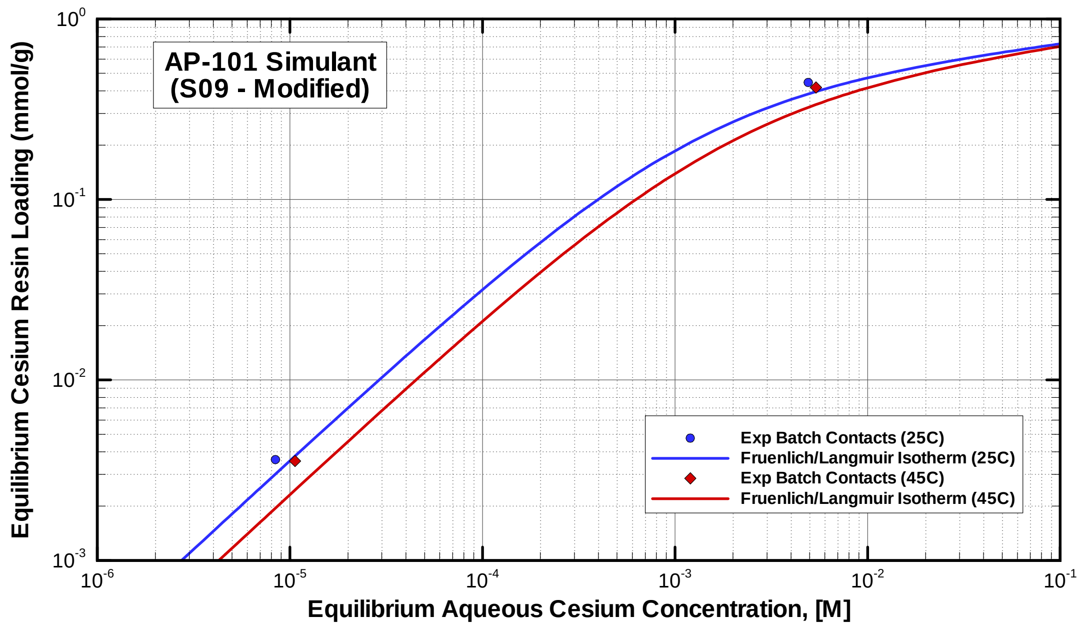


Figure 4-16. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S09 at 25 and 45°C (i.e., AP-101 Modified Recipe simulant with $OH^-$ at 0.2M).

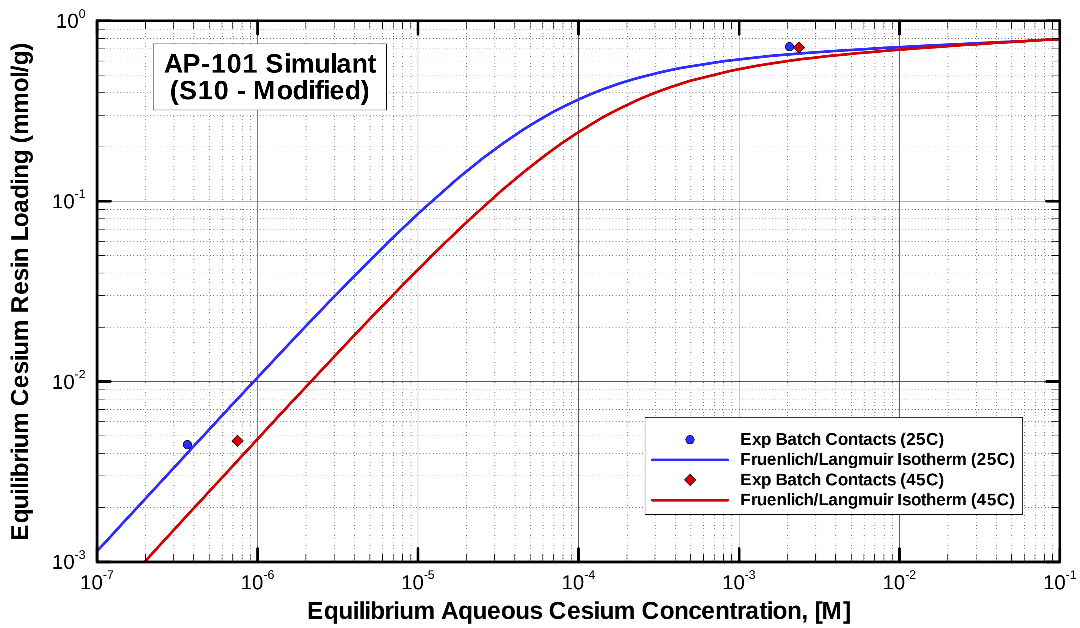


Figure 4-17. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S10 at 25 and 45°C (i.e., AP-101 simplified simulant with $Na^+$ at 4M and no $K^+$ present).

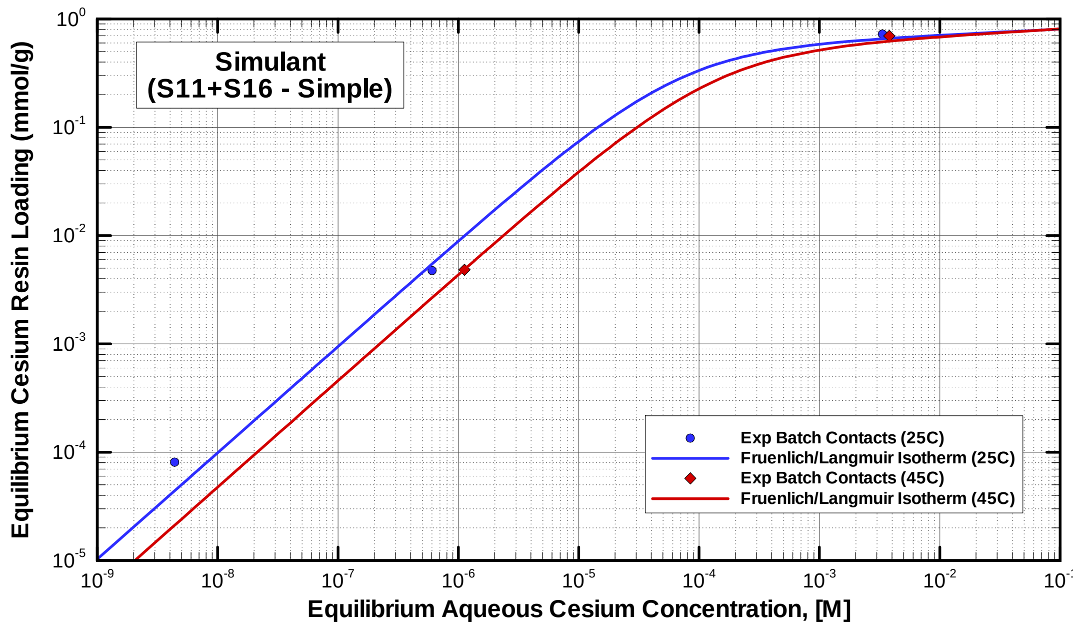


Figure 4-18. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S11 and S16 at 25 and 45°C (i.e., Simplified simulant with $OH^-$ at 2M).

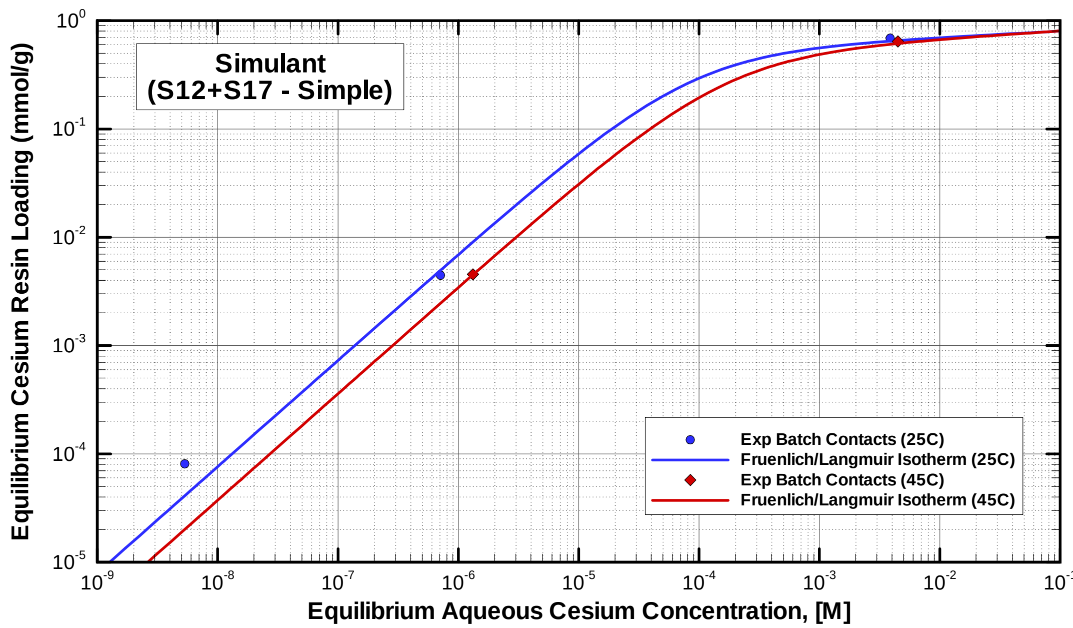


Figure 4-19. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S12 and S17 at 25 and 45°C (i.e., Simplified simulant with $OH^-$ at 1M).

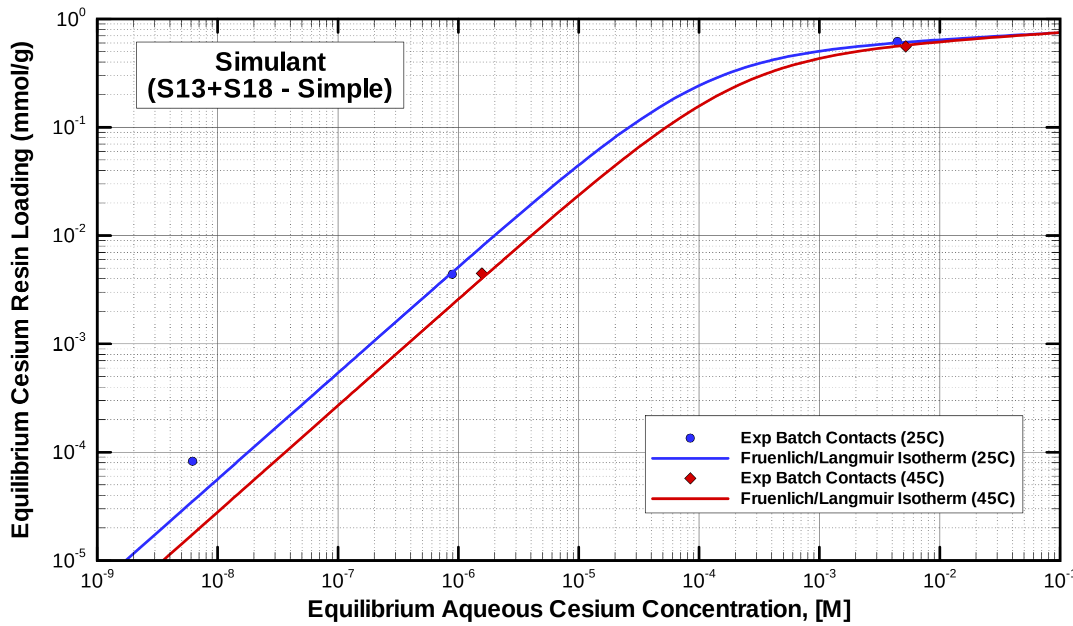


Figure 4-20. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulants S13 and S18 at 25 and 45°C (i.e., Simplified simulant with $OH^-$ at 0.1M).

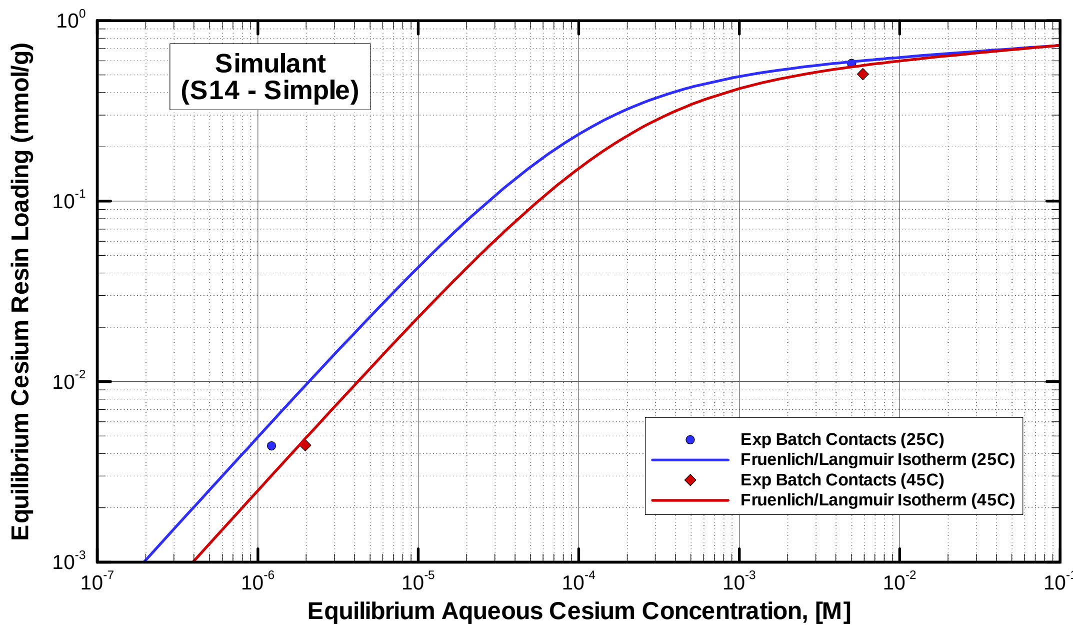


Figure 4-21. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S14 at 25 and 45°C (i.e., Simplified simulant with $OH^-$ at 0.05M).

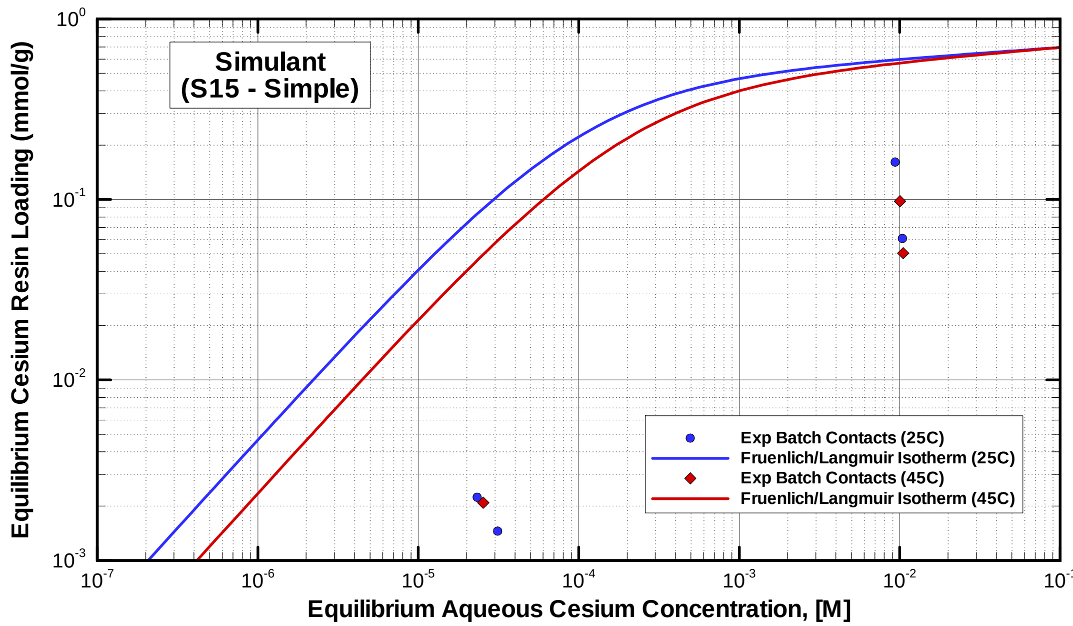


Figure 4-22. Comparison of predicted Fruenlich/Langmuir isotherm versus measured loadings on spherical RF-641 resin for simulant S15 at 25 and 45°C (i.e., Simplified simulant with $OH^-$ at 0.01M).

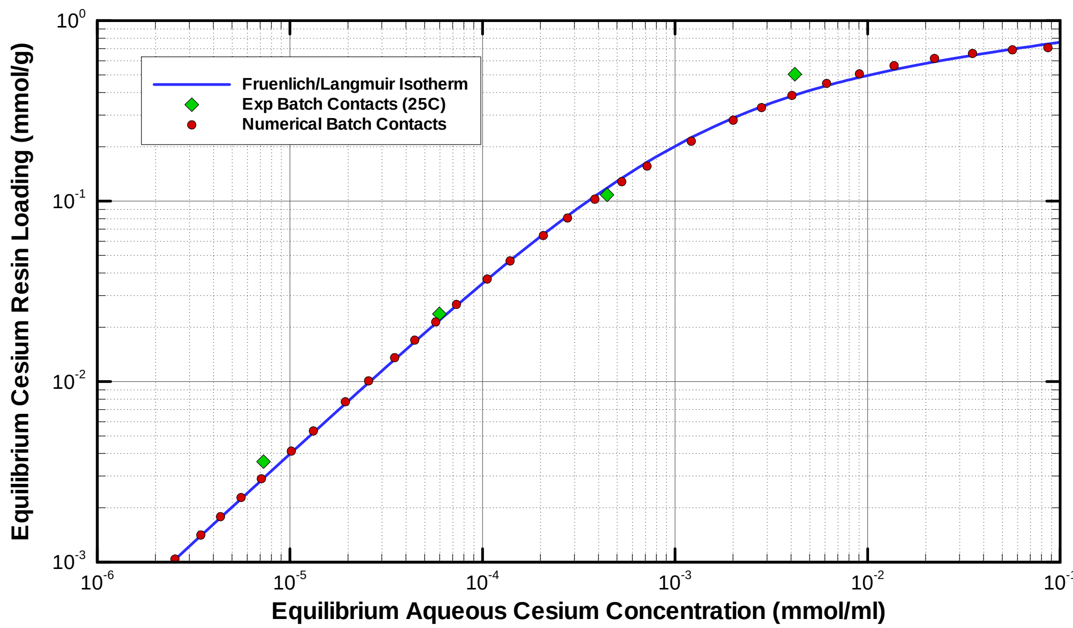


Figure 4-23. Comparison of algebraic isotherm model fit to numerically generated batch contact data using detailed thermodynamic model for the prediction of $Cs^+$ loading on spherical RF-641 resin at 25°C for the full recipe AP-101 simulant.

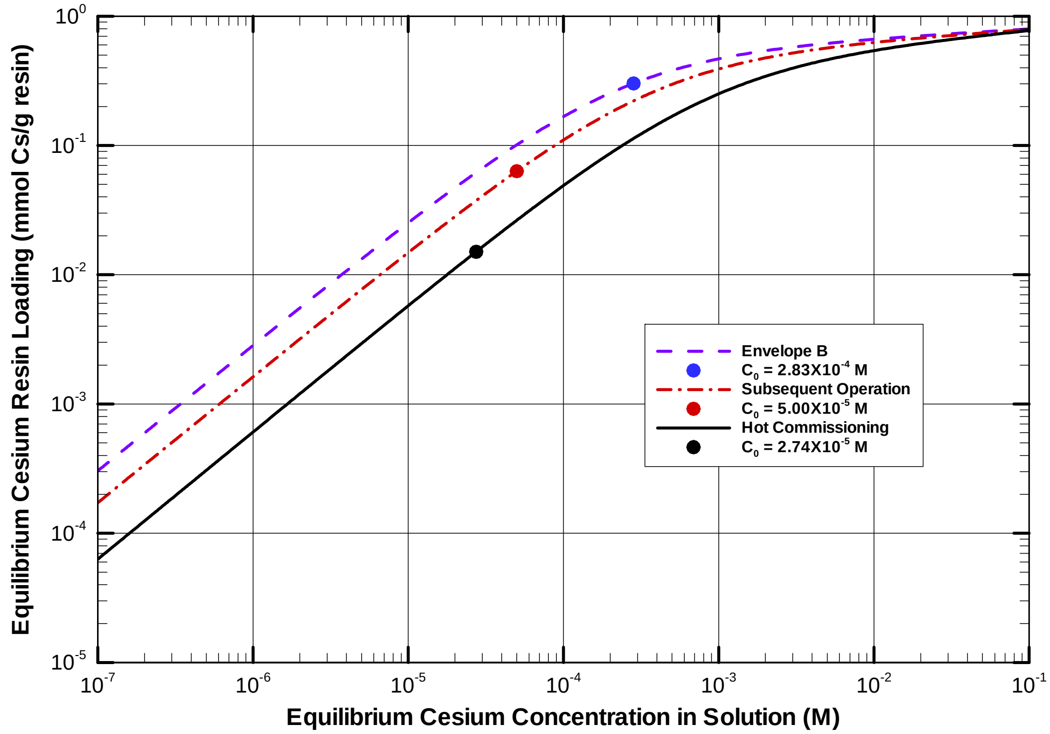


Figure 4-24. Hot Commissioning, Envelope B and Subsequent Operation cesium isotherms for fresh Resorcinol-Formaldehyde resin.

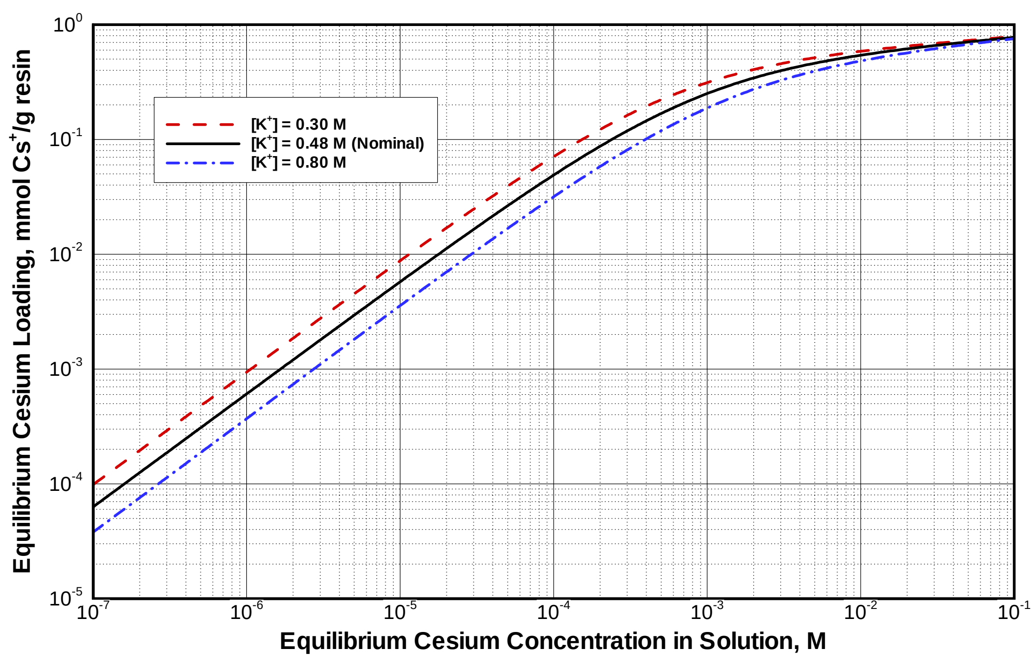


Figure 4-25. Hot Commissioning Operation cesium isotherms with variation in potassium concentration.

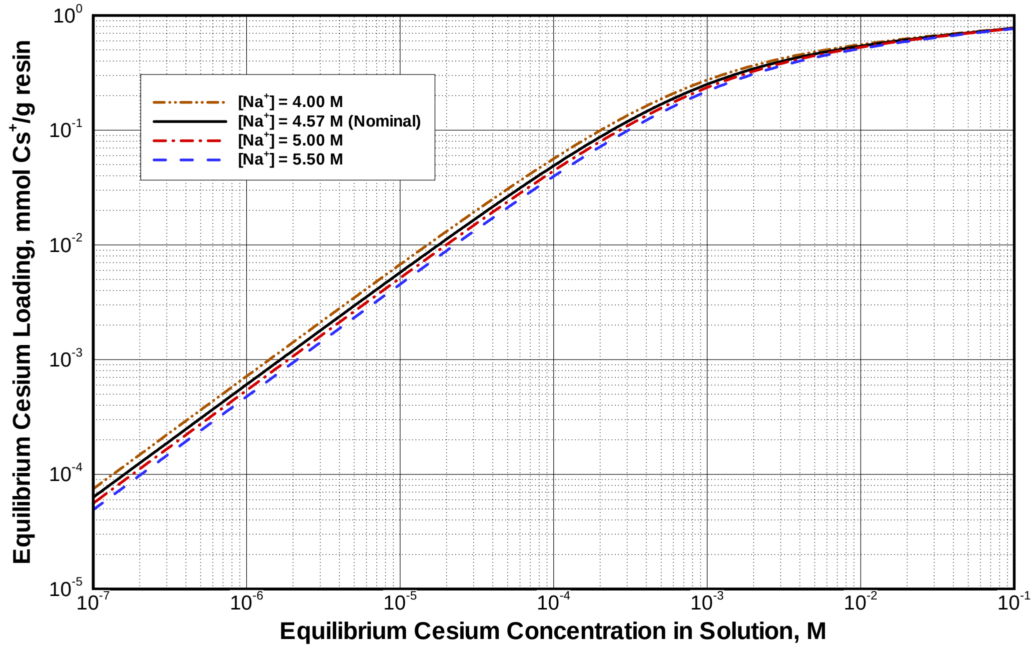


Figure 4-26. Hot Commissioning Operation cesium isotherms with variation in sodium concentration.

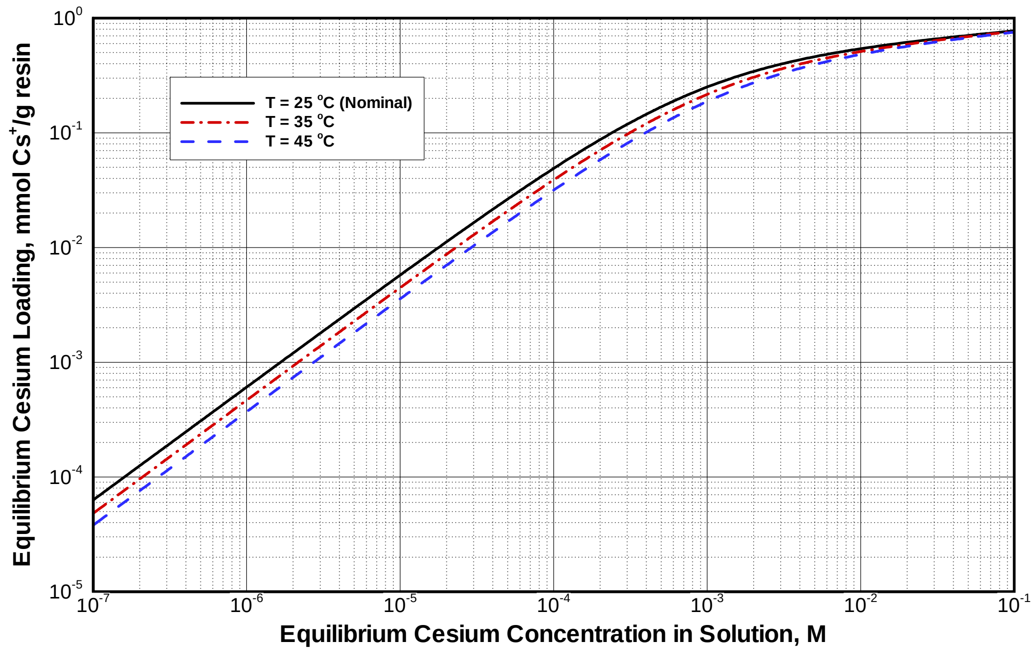


Figure 4-27. Hot Commissioning Operation cesium isotherms with variation in temperature.

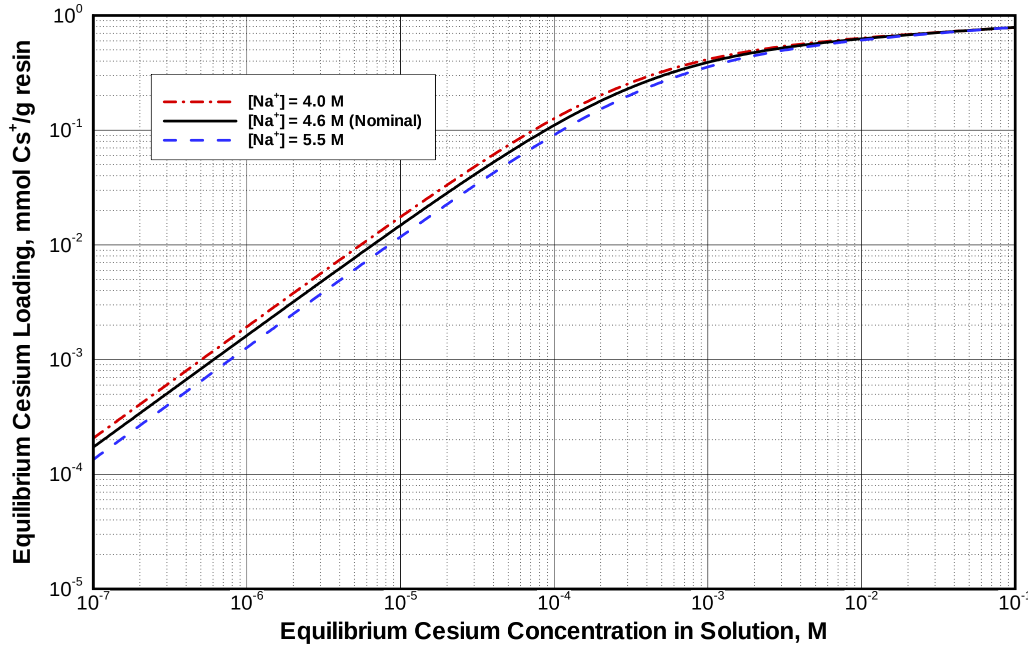


Figure 4-28. Subsequent Operation cesium isotherm variation for in sodium concentration.

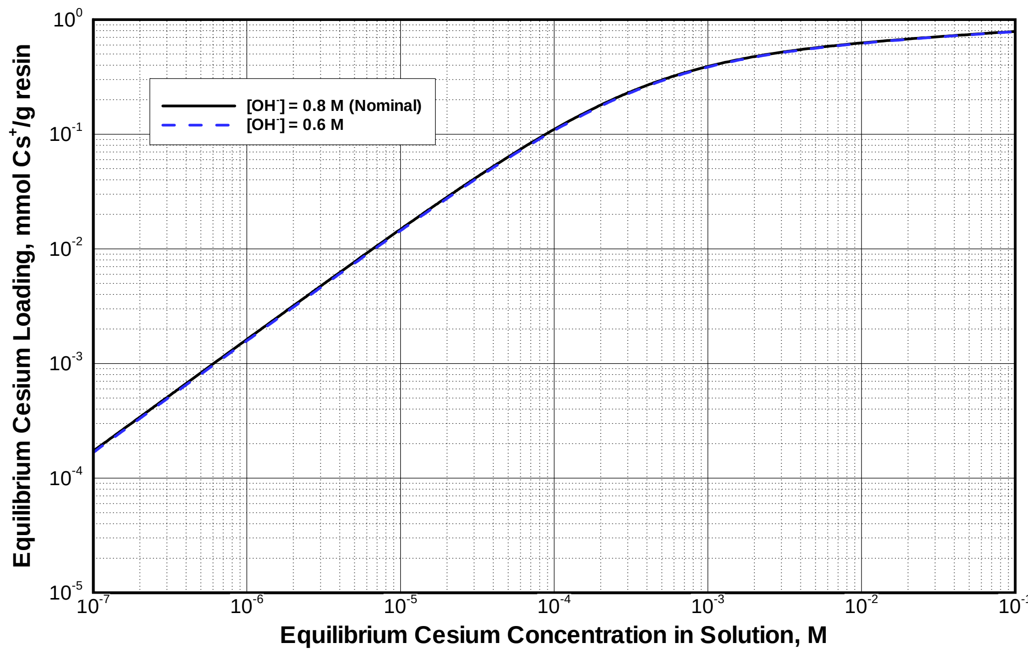


Figure 4-29. Subsequent Operation cesium isotherm variation in free hydroxide concentration.

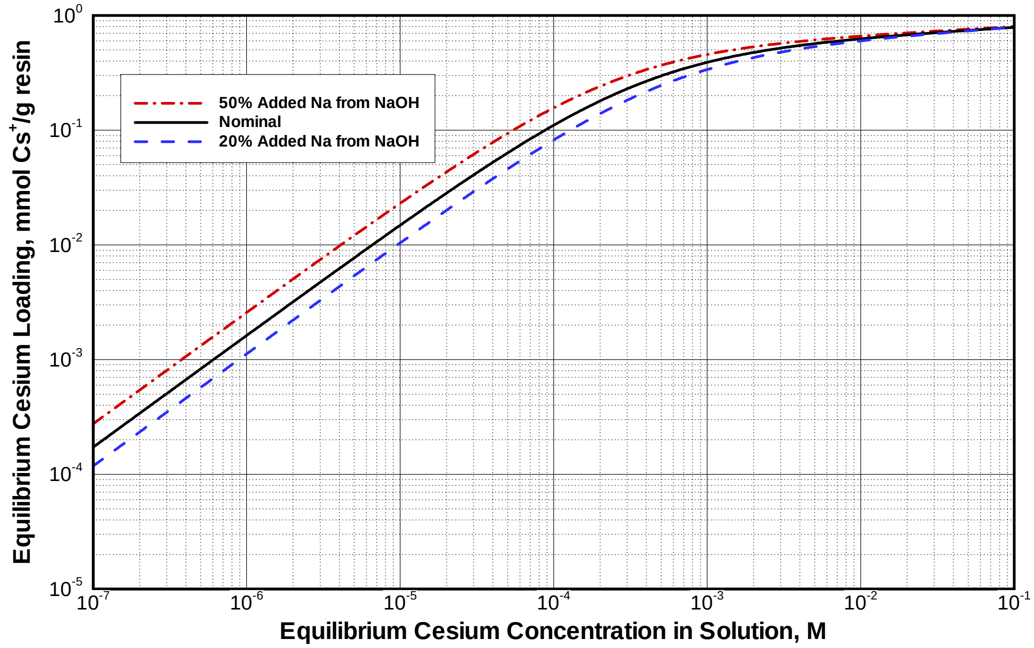


Figure 4-30. Subsequent Operation cesium isotherm variation for caustic leach cases.

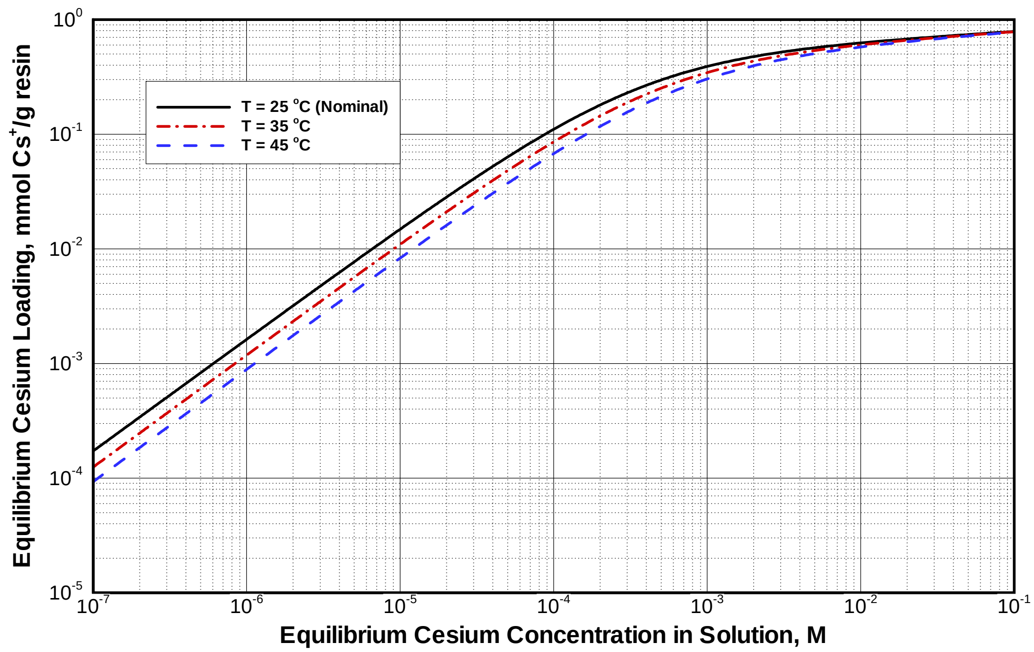


Figure 4-31. Subsequent Operation cesium isotherms with variation in temperature.

# 5.0 Column Properties

Certain material properties (such as, resin density and total ionic capacity) are unique to the ion-exchange material and vary only between batches. On the other hand, composite properties associated with an ion-exchange column (such as, bed density and porosities) are inherently column specific. Even when different columns are made from the same batch of resin, column properties can vary. During operational cycles where a significant variation in total ionic strength of the feed occurs, the active bed size of a column can change as much as 100% (see King et al., 2000). The discussion that follows focuses on the column properties required to perform column transport simulations during the loading phase of a column cycle.

For additional details on column properties required to perform a VERSE-LC column performance analysis see Hamm et al. (2000b, preliminary Cs removal performance using SuperLig® 644 report), Hamm et al. (2000c, preliminary Tc removal performance using SuperLig® 639 report), and Hamm et al. (2002, Cs removal performance using CST report)

## 5.1 Basic Constraint Functions

Based on geometrical considerations not all densities and porosities are independent. The following two expressions place constraints on the densities and porosities:

$$\varepsilon_t = \varepsilon_b + (1-\varepsilon_b)\varepsilon_p , \tag{5-1}$$

and

$$\rho_b = \rho_s(1-\varepsilon_t) = \rho_s(1-\varepsilon_b)(1-\varepsilon_p) , \tag{5-2}$$

where

$\varepsilon_t$ ..................total porosity of active column, [-]

$\varepsilon_b$ ..................bed porosity of active column, [-]

$\varepsilon_p$ ..................pore porosity of resin particles, [-]

$\rho_b$ ..................bed density of active column, g/ml

$\rho_s$ ..................solid (particle) density of resin, g/ml

For the five variables listed above only three are independent. The various porosities used in Eq. (5-1) are defined as:

$$\varepsilon_b = \frac{V_{void} - V_{pore}}{V_{bed}}; \quad \varepsilon_p = \frac{V_{pore}}{V_{part}}; \quad \varepsilon_t = \frac{V_{void}}{V_{bed}} = \frac{V_{bed} - V_{sld}}{V_{bed}} \tag{5-3}$$

where

$V_{bed}$ ...............total volume of active (bed) column, ml

$V_{void}$ ..............total volume of voids within active column, ml

$V_{pore}$ ..............total volume of pores within particles, ml

$V_{part}$ ...............total volume of particles within active column, ml

$V_{sld}$ ................total volume of solid resin within active column, ml

## 5.2 Densities

The particle ("skeletal") density of the resin in sodium form was measured during pilot scale hydraulic testing by Adamson et al. (2006). A summary of their results (extracted from Table 15 in the original report) is given in Table 5-1. For the column modeling presented in this report the average particle density of 1.615 g/ml listed in Table 5-1 for $Na^+$-form RF was employed.

The actual amount of resin present within a column is a parameter of prime importance with respect to column performance (i.e., exit breakthrough curves). For the column studies assessed in this report, an estimate of column bed density was derived from data reported in the study by Nash et al. (2006). In that study, the dry mass of RF resin in $H^+$-form (2.886 g) and the bed volume during loading (11.26 ml) were measured. The column bed density is then computed as:

$$\rho_b = \frac{m_{resin}}{V_{bed}} = \frac{2.886}{11.26} = 0.2563\,\text{g/ml} \tag{5-4}$$

The bed density calculated in Eq. (5-4) represents our nominal value with the resin in $H^+$-form. A factor of 1.25 (Nash et al., 2006) can be applied to convert the resin mass from $H^+$-form to $Na^+$-form.

## 5.3 Porosities

The drainable void fraction for a nominal sample of RF resin was provided by Thorson (personal communication):

$$\varepsilon_b = \frac{V_{void} - V_{pore}}{V_{bed}} = 0.42 \tag{5-5}$$

The bed porosity given in Eq. (5-5) represents our nominal value. The average measured porosity for dense packing of mono-sized hard spheres is 0.363 as reported by German (1989). Greater packing fractions (or smaller bed porosities) can be achieved when multi-sized spheres are employed. The particle size distribution for the spherical RF material was quite narrow with the bulk of the distribution in the range 400 to 600 microns so a void volume somewhat greater than that for uniform hard spheres is reasonable.

Based on Eq. (5-2) the pore porosity of the resin particles is known once the particle density, bed density and bed porosity are specified. Using the values presented in the above subsections, the pore porosity of the resin particles becomes:

$$\varepsilon_p = 1 - \rho_b / \rho_s (1 - \varepsilon_b) = 1 - 1.25 \text{x} 0.2563 / 1.615(1 - 0.42) = 0.6579 \qquad (5\text{-}6)$$

The pore porosity computed by Eq. (5-6) represents our nominal value.

Table 5-1. Measured skeletal densities of spherical Resorcinol-Formaldehyde resin in $Na^+$ form.

| **EDL Resin Sample** | **Particle Density (g/ml)** |
|---|---|
| Ten total Cycles from the Column Core Sample | 1.589 |
| Sixteen total Cycles the Column Core Sample | 1.602 |
| Sixteen total Cycles top layer dark particles | 1.637 |
| PNWD 3” IX Column new RF, Batch 5E-370/641 | 1.630 |
| Average | 1.615 |

# 6.0 Particle Size Distribution

The particle size distribution of spherical RF resin from batch 5E-370/641 was characterized in hydrogen and sodium form using a Microtrac® S3000 at both Battelle-Pacific Northwest Division (PNWD) and SRNL. Results from the PNWD and SRNL measurements are summarized in Fiskum et al. (2006a) and Adamson et al. (2006), respectively. For ion-exchange column modeling, the particle size in sodium form is required.

For further details on particle size distribution properties required to perform a VERSE-LC column performance analysis see Hamm et al. (2000b, preliminary Cs removal performance using SuperLig® 644 report), Hamm et al. (2000c, preliminary Tc removal performance using SuperLig® 639 report), and Hamm et al. (2002, Cs removal performance using CST report).

## 6.1 Spherical Resorcinol-Formaldehyde Resin

Microtrac® particle size data (volume-based) for spherical RF in sodium form was measured by Adamson et al. (2006) with the results summarized in Table 6-1. The bulk of the particle size distribution fell in the 400 to 600 micron range. PNWD (Fiskum, 2006a) reports an average particle diameter of 452 μm for spherical RF in sodium form while SRNL measured an average particle diameter of 461 μm in AP-101 simulant. The average of these two values, 457 μm, was used as the RF particle diameter in the VERSE-LC calculations for the small scale column and batch kinetics experiments reported in Sections 7 and 9. WTP (Thorson, 2006) specified a nominal particle diameter of 460 μm for the large column simulations reported in Section 10. This value is not significantly different from the experimentally determined average diameter.

A log-normal cumulative distribution function was applied to the Microtrac® particle size analysis (volume-based) for spherical RF in sodium form. The log-normal cumulative distribution function has been used extensively to represent particle size distributions of aerosols. Table 6-2 summarizes the log-normal cumulative and probability distribution functions. From the SRNL data, the log-normal geometric mass mean diameter was estimated to be $\overline{x}_g = 455$ μm and the geometric standard deviation as $\sigma_g = 1.19$. Figure 6-1 shows a plot of the Microtrac® particle size analysis data and log-normal cumulative distributions. The log-normal cumulative distribution represents the particle size distribution of the spherical RF sample very closely and the mass mean diameter is not significantly different from the average Microtrac® measured diameter. Since both estimates of the RF particle diameter are in good agreement, the average measured value was used for calculation purposes.

Table 6-1. Microtrac® particle size analysis data for pretreated spherical RF resin, sodium form in simulant (volume-based data).

| Channel Size (microns) | % PASS | % CHAN |
|---|---|---|
| 296.0 | 0.06 | 0.06 |
| 352.0 | 2.54 | 2.48 |
| 418.6 | 28.87 | 26.33 |
| 497.8 | 74.47 | 45.60 |
| 592.0 | 95.52 | 21.05 |
| 704.0 | 99.51 | 3.99 |
| 837.2 | 99.97 | 0.46 |
| 995.6 | 100.00 | 0.03 |

Table 6-2. Log-normal cumulative and probability distribution functions.

| Function | Basis | Equation |
|---|---|---|
| cdf | weight | $W(x)=\frac{1}{2}\left\{1+\operatorname{erf}\left(\frac{\ln(x/\bar{x}_g)}{\sqrt{2}\ln\sigma_g}\right)\right\}$ |
| pdf | weight | $w(x)=\frac{dW(x)}{dx}=\frac{1}{x\sqrt{2\pi}\ln\sigma_g}\exp\left[-\left(\frac{\ln(x/\bar{x}_g)}{\sqrt{2}\ln\sigma_g}\right)^2\right]$ |
| pdf | number | $n(x)=w(x)/f(x)\sigma(x)x^3$ |

where

$\bar{x}_g$ ..................geometric mass mean diameter, $x_{50}$

$\sigma_g$ ..................geometric standard deviation, $x_{84}/x_{50}=x_{50}/x_{16}=\sqrt{x_{84}/x_{16}}$

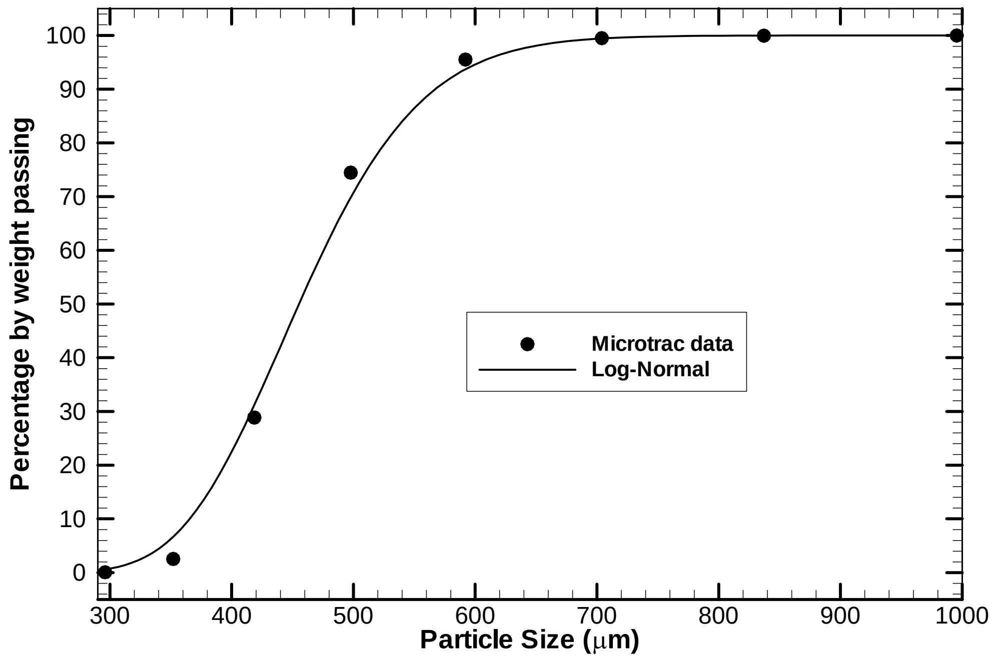


Figure 6-1. Microtrac® data and log-normal cumulative distribution for spherical RF resin from batch 5E-370/641 in sodium form.

# 7.0 Pore Diffusion

A series of VERSE-LC simulations were performed to identify a best estimate value for the effective diffusivity of cesium ions in RF ion-exchange resin pores from experimental data measuring adsorption kinetics. Once the value of this parameter was established, the consistency of the model was tested by comparing its predictions with data from small column experiments. For the set of experimental data available in this study, it was found that the results were not consistent between the kinetics and small column experiments. This required adjustment of the estimated pore diffusion to bring model simulations into better agreement with the overall data. All of the kinetics tests shown in this section were performed using the SRNL kinetics rig and are discussed by Nash et al. (2006).

## 7.1 Waste Solution Density and Viscosity

Two other physical properties needed for VERSE-LC simulations are the density and viscosity of the bulk liquid phase. Waste solution density and viscosity vary depending on temperature and composition (primarily through the sodium concentration). The density and viscosity of the various simulants and LAW IX feeds used in the VERSE-LC calculations were computed using OLI Systems, Inc. Stream Analyzer Version 2.0. In the previous modeling study for RF resin by Hardy et al. (2004) diffusivities were also calculated using the OLI software. In this study we have reverted to using a methodology developed earlier that may better represent values at high ionic strength. Calculated values of physical properties for the LAW IX feeds used in the large column simulations in this study are listed in Table 7-1.

## 7.2 Molecular Diffusion Coefficients

Binary diffusion (sometimes referred to as free stream or Brownian motion) coefficients of electrolytes originating from a single salt in solution under dilute conditions can be reasonably estimated using the Nernst-Haskell equation (Reid et al., 1977):

$$D_{\pm}^{\infty} = \left(\frac{RT}{\mathcal{F}^2}\right)\left[\frac{\frac{1}{z_+}+\frac{1}{z_-}}{\frac{1}{\lambda_+^o}+\frac{1}{\lambda_-^o}}\right], \qquad (7\text{-}1)$$

where

- $D_{\pm}^{\infty}$ - binary diffusion coefficient at infinite dilution, $cm^2/s$
- $\lambda_+^o, \lambda_-^o$ - limiting ionic conductivity for cation and anion, mhos/equivalent
- $z_+, z_-$ - valences of cation and anion, respectively
- $\mathcal{F}$ - Faraday constant, 96,500 C/g-equivalent
- R - gas constant, 8.314 J/gmole-K
- T - absolute temperature, K

Limiting ionic conductivities at 25 °C and infinite dilution for the various ions of interest in this study are tabulated in Table 7-2. Most of the conductivities were calculated using the correlation shown in Eq. (7-2) which is from Anderko and Lencka (1997):

$$\ln\left[\lambda^0(T)\eta(T)\right] = A + B/T, \tag{7-2}$$

where

A, B - correlation coefficients
$\eta(T)$ - viscosity of pure water in Pa-s (cP/1000)

The correlation coefficients A and B are listed in Table 7-2. In a few instances where the anion was not included in the Anderko correlation, literature values of the ionic conductivity (Reid et al., 1977; Perry, 1973, Glasstone and Lewis, 1960) were used.

Using Eq. (7-1) and the limiting ionic conductivities provided in Table 7-2, the binary molecular diffusion coefficient for certain single salts within an aqueous phase can be computed. To account for fluid property differences between a waste solution and pure water, a correction factor is applied. Based on hydrodynamic theory, the following expression, typically referred to as the Stokes-Einstein equation, is obtained (Bird et al., 1960, page 514):

$$\frac{D_{AB}\,\mu_B}{\kappa T} = \frac{1}{6\pi R_A}, \tag{7-3}$$

where

$D_{AB}$ - binary diffusion coefficient for A diffusing through solvent B
$\mu_B$ - dynamic viscosity of solvent mixture
$R_A$ - radius of diffusing particle
$\kappa$ - Boltzmann's constant

Based on Eq. (7-3), the ratio of the dynamic viscosity of pure water (representing conditions at infinite dilution) to that of the waste solution is a correction factor that can be applied to the molecular diffusion coefficients computed from Eq. (7-1) to estimate binary diffusion coefficients in the waste solution.

Binary pairs for the dominant cation-anion pairs (i.e., cesium paired with an individual anion) where the anions considered are based on the composition of the various wastes and their computed binary molecular diffusion coefficients are listed in Table 7-3 at 25 °C. The viscosity corrected values for AP-101 waste at 5 M sodium are also provided in Table 7-3. An overall diffusion coefficient for cesium was estimated as the average of the individual cesium pair diffusion coefficients weighted by the mole fraction of each pair in solution. The diffusion coefficients calculated using this method for the LAW IX large column simulations are listed in Table 7-1.

In Cussler (1984) the "effective" binary ionic diffusion coefficient of cesium in essentially pure water is $1.236\text{x}10^{-3}$ cm$^2$/min at 25 °C, which is within 16% of the estimated value computed from Eq. (7-1). Some other values based on Cussler (1984) at 25 °C are $7.98\text{x}10^{-4}$ cm$^2$/min for

$Na^+$, 1.176x10$^{-3}$ cm$^2$/min for $K^+$, and 5.586x10$^{-3}$ cm$^2$/min for $H^+$. The ionic radii of sodium and potassium are 0.95 and 1.33 angstroms with average hydration numbers of 4 and 3, respectively. All metal cations are hydrated in aqueous media, where, for example, sodium migrates perhaps in the form $Na(H_2O)_4^+$. Reasonable values for the radii of the hydrated alkali metal ions sodium and potassium are ~2.76 and ~2.32 angstroms (Peters et al., 1974), respectively. Therefore, sodium is bigger and slower moving than potassium in aqueous solutions consistent with the predictions listed in Table 7-3. Anions are characteristically less heavily hydrated, suggesting that the cations set the overall rate of diffusion.

Molecular diffusion coefficients are important in determining key dimensionless numbers (e.g., Schmidt Number, Sc) used in various constitutive law correlations pertinent to column transport modeling. They also provide an upper bound for pore diffusion coefficients.

## 7.3 Particle Kinetics Parameters

The rate of cesium uptake controls the transient behavior of the column. As the rate of cesium uptake by the resin is increased, the breakthrough curve becomes sharper (steeper) and utilization of the resin is increased. Thus, a proper evaluation of the parameters that control the rate of cesium uptake is essential for modeling column performance. For Resorcinol-Formaldehyde resin, we assume that the rate of chemical adsorption (i.e. exchange of ions at a surface site) is very fast when compared to the rates of diffusion within the pore fluid and mass transfer across the liquid film at the outer boundary of the particles. Hence, within the resin particles, the rate of cesium uptake is dominated by intra-particle diffusion. Diffusion within the particles is governed by the pore diffusivity, particle porosity, and size of the particles. Externally, the rate of cesium transport from the inter-particle fluid to the particle surface depends upon the film mass transfer coefficient. Due to their influence on the rate of cesium uptake and, thus, the transient behavior of the column, the particle porosity, pore diffusivity, particle radius and the film mass transfer coefficient are referred to as kinetics parameters.

In VERSE-LC the film mass transfer coefficient is calculated from a correlation developed by Wilson and Geankoplis (1966). The particle porosity is available from the data presented in Section 5. Therefore, of the kinetics parameters, the pore diffusivity and diffusion length remain to be determined. In the VERSE-LC code, the model for intra-particle diffusion assumes that the particles are spheres of uniform radius. The spherical Resorcinol-Formaldehyde particles have a relatively narrow distribution of particle sizes as shown in Section 6. To apply the VERSE-LC model to the spherical Resorcinol-Formaldehyde resin it is therefore necessary to determine an average radius for the particle size distribution and an effective pore diffusivity. In this approach, the particle radius or pore diffusion length is expressed as

$$\langle r_p \rangle = \frac{\langle d_p \rangle}{2} \tag{7-4}$$

where

$\langle r_p \rangle$ .............average particle radius or pore diffusion length, μm

$\langle d_p \rangle$ ............average particle diameter, μm

As shown in Section 6, we have chosen to use an average volume mean diameter of 457 μm for the average particle diameter so the equivalent average particle radius is 228.5 μm.

Specific information on the actual pore sizes present in the RF resin is not available. We assume that the pore sizes are large relative to the size of the migrating ions of interest and that pore diffusion coefficients should not be significantly lower than their bulk or free stream values. However, some level of reduced diffusion in the pores is expected resulting from bends along the pore paths that are generally accounted for by a particle tortuosity factor defined as

$$D_p = \frac{D_\infty}{\tau} \tag{7-5}$$

where

$D_p$ .................pore diffusivity of $Cs^+$ in the particle pore, $cm^2/min$

$D_\infty$ ................bulk diffusivity of $Cs^+$ in the free stream, $cm^2/min$

$\tau$ .....................particle tortuosity factor

## 7.4 SRNL Particle Kinetics Testing

The SRNL particle kinetics rig is a closed loop differential column with temperature control. The recirculation device contained 120 ml of simulant and produced bed flow rates of 0.5, 30 and 90 ml/min. At these flow rates, film mass transfer resistance is negligible relative to that for diffusion in the pores of the particle (Biot numbers range from 13 to 73). In this way, the effect of the film mass transfer coefficient was eliminated and the data showed only the effect of $< r_p >$ and $\tau$.

Three experiments were conducted using spherical RF contacted with AP-101 simulant (Nash et al., 2006). The experiments were conducted at temperatures of 15, 25 and 45 °C to ascertain the impact of temperature on the particle kinetics. The flow rate was held constant at 30 ml/min in all three experiments. The isotherm parameters for AP-101 simulant and spherical Resorcinol-Formaldehyde resin were calculated using the thermodynamic model described by Aleman and Hamm (2007). However, the capacity was adjusted to better match the equilibrium experimental value. A series of VERSE-LC calculations were executed varying the tortuosity factor between 1.0 and 4.0 using a volume mean diameter of 457 μm.

Figure 7-1 shows a comparison of the transient aqueous cesium concentration for the Experiment at 15 °C to the VERSE-LC simulation for various tortuosity factors set to 1.0, 2.0, 3.0 and 4.0. The VERSE-LC simulation represents the transient cesium concentration exiting the CSTR upstream of the differential column. The resin capacity was increased to 110% of the model predicted value to better match the apparent experimental conditions at equilibrium. The VERSE-LC simulation using a tortuosity factor of 4.0 provides the closest agreement with the data from this experiment. However, none of the simulations match the kinetic data very closely. Results for the kinetics experiment conducted at 25 °C are plotted against VERSE-LC simulated results in Figure 7-2. Here it is seen that using a tortuosity factor of 3.0 gives good agreement between the calculation and the data. Similar results are obtained for the experiment conducted at 45 °C as shown in Figure 7-3. In both of these cases, the resin loading capacity was again increased to 110% of the model predicted value to better match the apparent experimental conditions at equilibrium.

The kinetics data suggests using a tortuosity factor of 3.0 to 4.0 which implies that pore diffusion will be 33% to 25% of that in the bulk liquid phase. In a previous study (Hardy, et al., 2004) using granular and spherical RF resin, the tortuosity factor was estimated to be 1.5 which produced good agreement between VERSE-LC calculations and data from both batch kinetics and small column ion-exchange experiments. In this study using a tortuosity factor of 4.0 did not lead to good agreement between VERSE-LC calculations and small column ion-exchange experimental data. The small column data suggested that a smaller tortuosity should apply. As a compromise, a tortuosity factor of 3.0 was chosen as the best estimate value considering all of the experimental data. This value is also in much better agreement with the result for RF resin obtained previously.

Table 7-1. Physical properties of LAW IX feed solutions.

| **Feed** | **Composition Variability** | **Diffusivity ($cm^2$/min)** | **Density (g/ml)** | **Viscosity (cP)** |
|---|---|---|---|---|
| Hot Commissioning | Nominal | 4.935E-04 | 1.2181 | 2.5032 |
| Hot Commissioning | 0.8 M $K^+$ | 4.737E-04 | 1.2354 | 2.5832 |
| Hot Commissioning | 0.3 M $K^+$ | 5.050E-04 | 1.2084 | 2.4612 |
| Hot Commissioning | 4.0 M $Na^+$ | 5.785E-04 | 1.1923 | 2.1357 |
| Hot Commissioning | 5.5 M $Na^+$ | 3.751E-04 | 1.2598 | 3.2938 |
| Hot Commissioning | 5.0 M $Na^+$ | 4.355E-04 | 1.2375 | 2.8368 |
| Hot Commissioning | 35 °C | 6.150E-04 | 1.2113 | 1.9702 |
| Hot Commissioning | 45 °C | 7.389E-04 | 1.2050 | 1.6135 |
| Envelope B | Nominal | 6.087E-04 | 1.1822 | 1.9695 |
| Subsequent Operation | Nominal | 5.706E-04 | 1.2178 | 1.9791 |
| Subsequent Operation | 4.0 M $Na^+$ | 6.516E-04 | 1.1908 | 1.7332 |
| Subsequent Operation | 5.5 M $Na^+$ | 4.610E-04 | 1.2575 | 2.4496 |
| Subsequent Operation | 50% $Na^+$ from NaOH | 5.458E-05 | 1.1971 | 2.3203 |
| Subsequent Operation | 20% $Na^+$ from NaOH | 8.287E-04 | 1.1948 | 1.4066 |
| Subsequent Operation | 0.6 M $OH^-$ | 5.737E-04 | 1.2206 | 1.9274 |
| Subsequent Operation | 35 °C | 6.927E-04 | 1.2106 | 1.5961 |
| Subsequent Operation | 45 °C | 8.209E-04 | 1.2034 | 1.3232 |

Table 7-2. Limiting ionic conductivity fitting coefficients and calculated conductivities in water at 25 °C.

| Ion | | Ionic valance | A | B | Limiting ionic conductivity MHOS/equivalent |
|---|---|---|---|---|---|
| **Cations** | $H^{+}$ | 1 | -3.9726 | 837.79 | 351.05 |
| | $Na^{+}$ | 1 | -3.3594 | 75.492 | 50.27 |
| | $K^{+}$ | 1 | -3.5730 | 254.36 | 73.97 |
| | $Rb^{+}$ | 1 | -3.6517 | 294.79 | 78.34 |
| | $Cs^{+}$ | 1 | -3.6512 | 291.42 | 77.46 |
| **Anions** | $OH^{-}$ | -1 | -3.3346 | 468.13 | 192.30 |
| | $NO_3^{-}$ | -1 | -3.6743 | 277.43 | 72.22 |
| | $NO_2^{-}$ | -1 | | | 72.00[b] |
| | $F^{-}$ | -1 | | | 55.40[b] |
| | $Cl^{--}$ | -1 | -3.4051 | 216.03 | 76.94 |
| | $I^{-}$ | -1 | -3.5660 | 265.28 | 77.27 |
| | $CO_3^{-2}$ | -2 | | | 69.30[b] |
| | $SO_4^{-2}$ | -2 | -2.9457 | 90.983 | 80.08 |
| | $PO_4^{-2}$ | -2 | | | 75.00[a] |
| | $Al(OH)_4^{-}$ | -1 | | | 70.00[a] |

[a] Estimated value, [b]Literature value

Table 7-3. Best estimate binary molecular[a] diffusion coefficients at 25 °C for a solution containing essentially only cesium cations and anion of one particular species.

| Cesium Ion Pairs | Molecular diffusion coef. in water ($cm^2$/min) | Molecular diffusion coef. in 5 M Na AP-101 waste ($cm^2$/min) |
|---|---|---|
| $Cs^{+}$ - $OH^{-}$ | 1.764E-03 | 5.006E-04 |
| $Cs^{+}$ - $NO_3^{-}$ | 1.194E-03 | 3.388E-04 |
| $Cs^{+}$ - $NO_2^{-}$ | 1.192E-03 | 3.383E-04 |
| $Cs^{+}$ - $Al(OH)_4^{-}$ | 1.175E-03 | 3.333E-04 |
| $Cs^{+}$ - $CO_3^{-2}$ | 8.763E-04 | 2.487E-04 |
| $Cs^{+}$ - $SO_4^{-2}$ | 9.433E-04 | 2.677E-04 |
| $Cs^{+}$ - $PO_4^{-2}$ | 9.129E-04 | 2.591E-04 |
| $Cs^{+}$ - $Cl^{-}$ | 1.233E-03 | 3.499E-04 |
| $Cs^{+}$ - $F^{-}$ | 1.032E-03 | 2.928E-04 |
| $Cs^{+}$ - $I^{-}$ | 1.236E-03 | 3.507E-04 |

[a] The molecular diffusion coefficient is sometimes referred to as the “free” or “Brownian” motion diffusion coefficient.

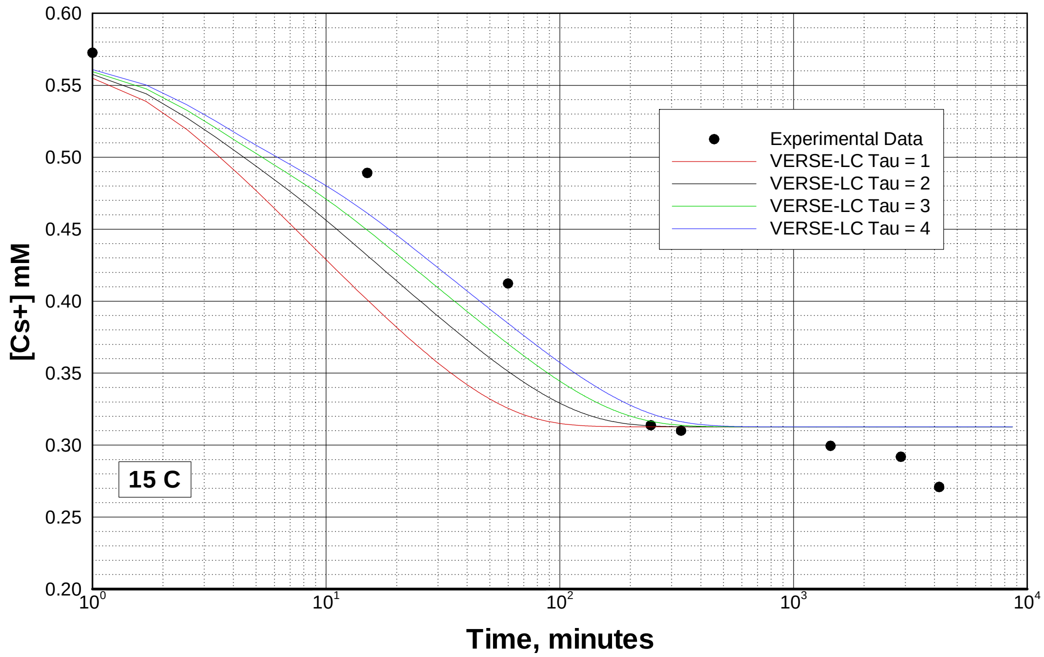


Figure 7-1. Transient cesium aqueous concentration during SRNL experiment with spherical Resorcinol-Formaldehyde resin in AP-101 simulant at 15 °C with tortuosity factors from 1.0 to 4.0 and bed flow rate set to 30 ml/min.

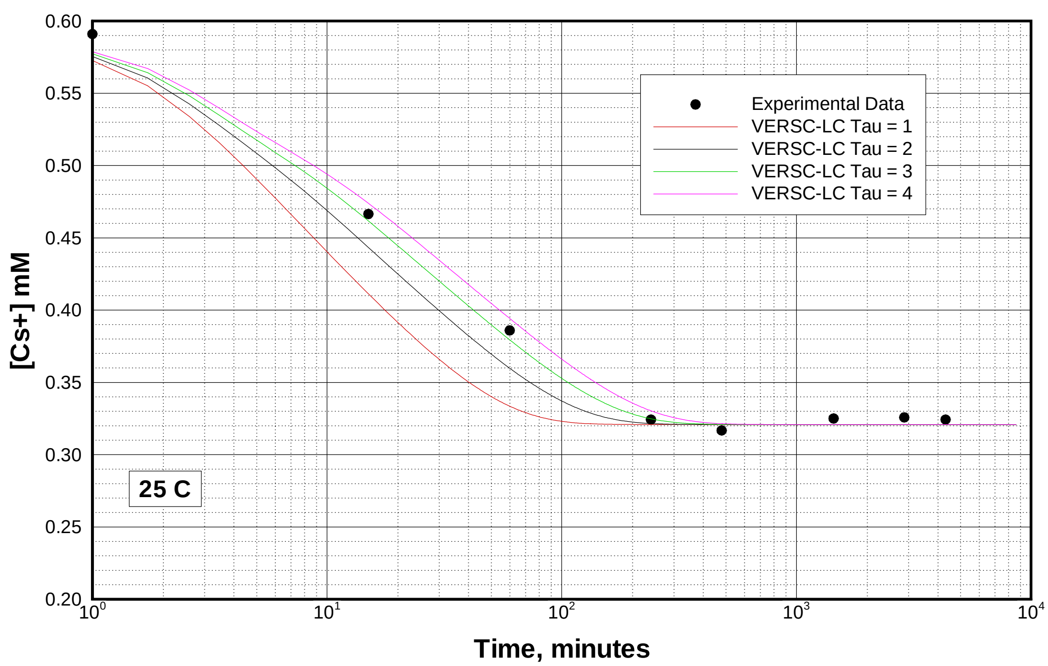


Figure 7-2. Transient cesium aqueous concentration during SRNL experiment with spherical Resorcinol-Formaldehyde resin in AP-101 simulant at 25 °C with tortuosity factors from 1.0 to 4.0 and bed flow rate set to 30 ml/min.

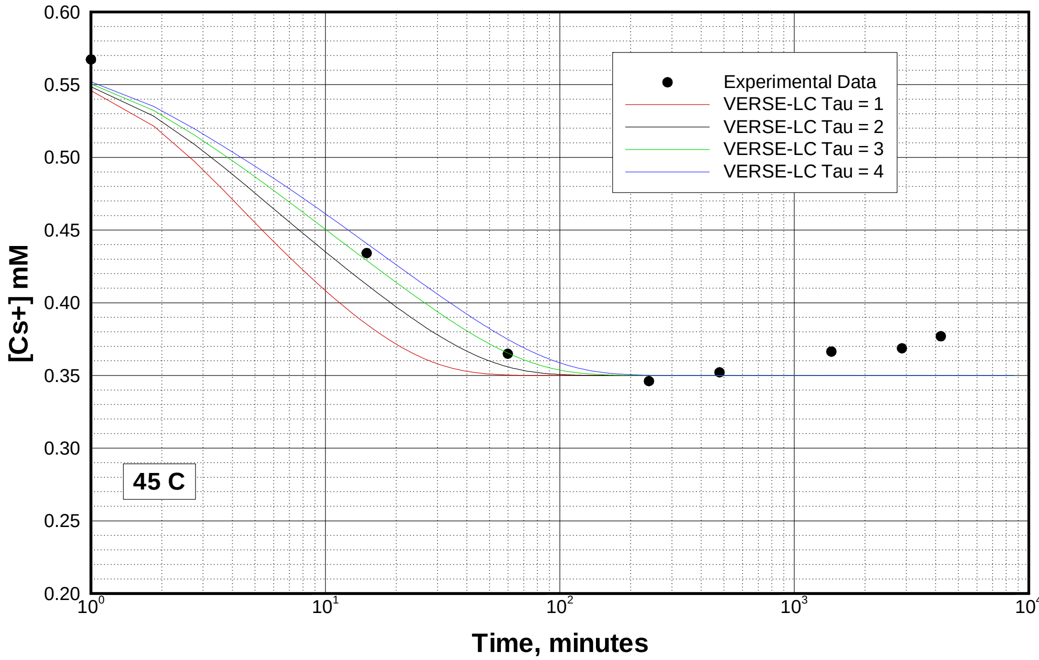


Figure 7-3. Transient cesium aqueous concentration during SRNL experiment with spherical Resorcinol-Formaldehyde resin in AP-101 simulant at 45 °C with tortuosity factors from 1.0 to 4.0 and bed flow rate set to 30 ml/min.

# 8.0 Film Diffusion and Axial Dispersion

For details on axial dispersion and film diffusion correlation values required to perform a VERSE-LC column performance analysis see Hamm et al. (2000b, preliminary Cs removal performance using SuperLig® 644 report), Hamm et al. (2000c, preliminary Tc removal performance using SuperLig® 639 report), and Hamm et al. (2002, Cs removal performance using CST report).

In this section we present the correlations used to define: (1) mass transfer across the liquid film separating the bed fluid from its neighboring particle pore fluid and (2) axial dispersion along the bed length.

## 8.1 Film Diffusion

For the laboratory-scale column tests and proposed full-scale facility the Reynolds number range is approximately 0.1 to 1.0. With respect to published literature this is a very low Reynolds number range. Numerous mass transfer correlations exist as discussed by Foo and Rice (1975, see their Figure 2). One of the correlations compared in Foo and Rice (1975) is one developed by Wilson and Geankoplis (1966) based on low Reynolds number data. Large variations between correlations can be seen; however, our sensitivity to the film coefficient is low as shown in the section discussing sensitivities. Since VERSE-LC has the Wilson and Geankoplis (1966) correlation as an option and this correlation falls somewhat within the spread of available low Reynolds number data we have chosen it for all the column simulations in this report. For each ion species considered, the Wilson and Geankoplis (1966) correlation is expressed as:

$$J \equiv \left[\frac{k_{fi}}{u\varepsilon_b}\right] Sc_i^{2/3} = \frac{1.09}{\varepsilon_b} Re^{-2/3} . \tag{8-1}$$

In Eq. (8-1), the Reynolds number is defined as:

$$Re \equiv \frac{2R_p \rho_w u \varepsilon_b}{\mu_w},$$

and the Schmidt number for each species is defined as:

$$Sc_i \equiv \frac{\mu_w}{\rho_w D_i^{\infty}} .$$

A standard deviation of approximately 25% is reported for Eq. (8-1) by Wilson and Geankoplis (1966), while from comparison to the various correlations presented by Foo and Rice (1975) a standard deviation of 100% to 200% is observed.

## 8.2 Axial Dispersion

Axial dispersion in packed columns is the result of mechanical dispersion added onto molecular diffusion. For practical flow rates mechanical dispersion dominates. For well-packed columns of sufficient diameter such that wall effects (i.e., channeling) are minimal a variety of correlations exist for long column performance. A brief discussion of minimum column sizing is presented in Brooks (1994).

In the low Reynolds number range of interest, the Chung and Wen (1968) correlation is applicable for sufficiently large columns (i.e., large diameter and length). The axial dispersion coefficient $E_b$ (cm$^2$/min) is expressed as:

$$E_b = \frac{2R_p u \varepsilon_b}{0.2 + 0.011 Re^{0.48}}, \quad (8\text{-}2)$$

where the standard deviation of this correlation based on all available data points was reported to be 46%. Equation (8-2) applies for only sufficiently large columns and correction factors must be considered for columns with small diameters and/or short active bed lengths.

### 8.2.1 Radial Flow Maldistribution

Flow maldistribution is caused by packing irregularities. As such the bed porosity varies over the cross-section of a column and increases as the outer wall is approached even in well-packed columns. "Channeling" near the wall becomes more serious for smaller column diameters and larger particle sizes. As a "rule of thumb" Helfferich (1962) states that this effect becomes significant when the bed diameter is less than thirty times the particle diameter.

The experimental and mathematical basis for this rule of thumb stems from the work of Schwartz and Smith (1953) and Morales et al. (1951). Their experimental efforts were for uniform packing of either spheres or cylinders using air-flow rates in the range of 145 to 547 cm/min. Over the range of their database they concluded that:

- The radial velocity profile (normalized) is independent of total flow rate and
- The divergence of the radial velocity profile from uniform behavior is less than 20% for column diameter to particle diameter ratios greater than 30.

A measure of the degree of non-uniformity in the radial velocity profiles can be made by looking at the ratio of peak-to-average velocity. Based on the limited database of Schwartz and Smith (1953) this peak-to-average velocity ratio is plotted versus column-to-particle diameter ratio in Figure 8-1. As illustrated in Figure 8-1 velocity ratios greater than 100% can occur for column-to-particle diameter ratios less than 10 and beyond ~50 the impact is negligible. Also shown in Figure 8-1 is a least squares fit of the data in the power law form:

$$\frac{u_{peak}}{u_{CL}} = \begin{cases} 4.3786\left(\dfrac{D}{2 < R_p >}\right)^{-0.372935} & \text{for } \dfrac{D}{2 < R_p >} < 52.44 \\ 1.0 & \text{for } \dfrac{D}{2 < R_p >} \geq 52.44 \end{cases} . \quad (8\text{-}3)$$

Note that Eq. (8-3) is based on packed beds with uniformly shaped cylinders and air-flow rates in the range of 145 to 547 cm/min. This correlation may be suspect for liquid flows in the range of 0.5 to 12 cm/min as applies to the various column tests considered in this report. Dorweiler and Fahien (1959) performed similar experiments that agreed with Schwartz and Smith (1953) and went to flow rates as low as 30 cm/min. In a later study by Fahien and Smith (1955) significant radial effects were observed for column-to-particle diameters less than 20.

The small scale experimental columns used in this study typically have column to particle diameter ratios of about 30 (1.5 cm/457 μm). This places them at the point where radial flow distribution is just expected to become a factor. No attempt was made to adjust the experimental data for this effect.

### 8.2.2 Headspace and Short Column Impacts

Liles and Geankoplis (1960) conducted experiments to ascertain the impact that short column lengths and void headspaces have on axial dispersion in packed bed columns. When end effects were eliminated they concluded that no effects of length on axial dispersion were observed. However, in the presence of end effects such as void headspaces significant effects of length can result. A summary of their data is presented in Figure 8-2 illustrating that the impact can become significant for columns under ~20 cm. Also shown in Figure 8-2 is a least squares fit of the data in the power law form:

$$\frac{E_b(L)}{E_b(L \to \infty)} = 1.0 + 61.4988L^{-1.20799} , \quad (8\text{-}4)$$

where column length is in units of cm.

The small lab-scale experimental columns fall into the region where end effects can significantly alter axial dispersion. We assume that maintaining a volume of liquid above the column, as was done in all of the small-scale experiments, eliminates column end effects and no correction to axial dispersion is applied.

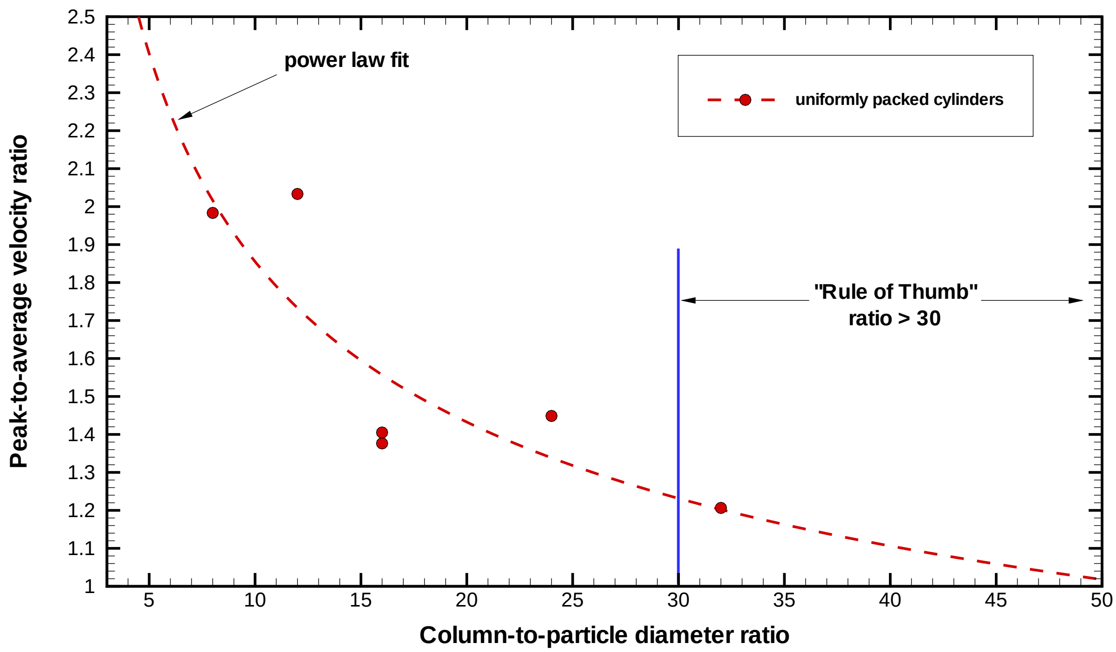


Figure 8-1. Estimated impact of column-to-particle diameter ratios on radial velocity profile based on the limited data by Schwartz and Smith (1953).

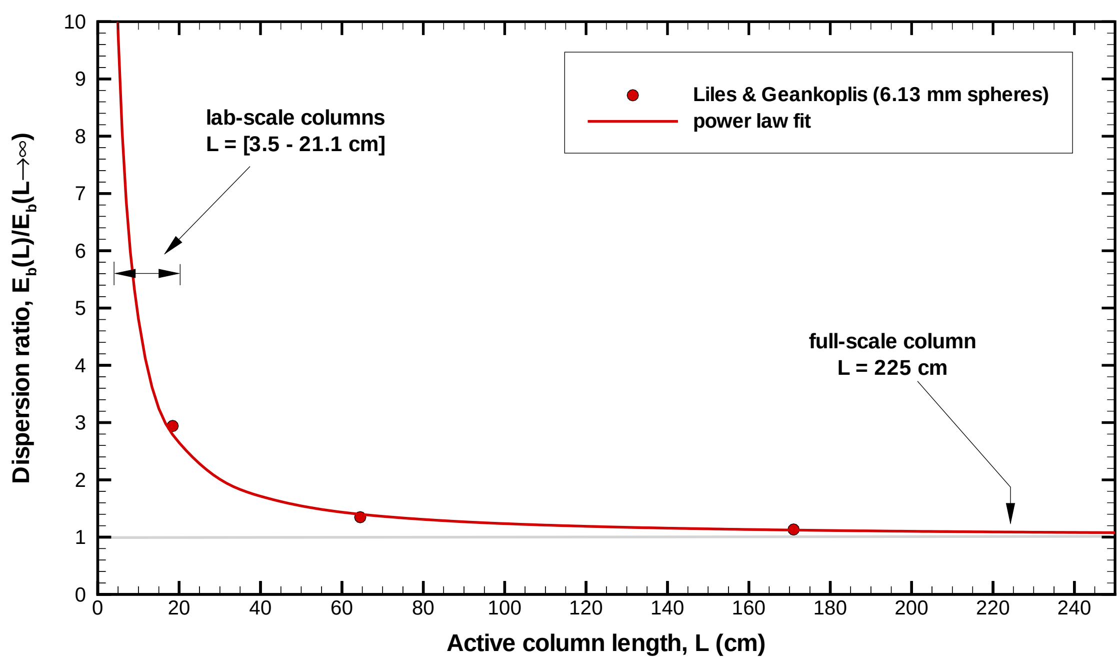


Figure 8-2. Estimation of the impact from end effects and short columns on axial dispersion based on the limited data by Liles and Geankoplis (1960).

# 9.0 Laboratory-Scale Column Assessments

Several laboratory-scale column experiments have been performed to measure cesium removal capability of Resorcinol-Formaldehyde resin for feed conditions typical of Hanford wastes. VERSE-LC was used to model three of the small column experiments for AP-101 waste where cesium breakthrough curves were experimentally measured by PNWD (Fiskum et al., 2006a) and SRNL (Nash et al., 2006) using batch 5E-370/641 spherical Resorcinol-Formaldehyde. This is the same batch of resin used in the batch contact and kinetics experiments that supplied the data used to establish isotherm parameters and pore tortuosity as described above. One of the PNWD experiments used actual AP-101 waste material while the other PNWD experiment and the SRNL experiment used a simulant of AP-101 waste. VERSE-LC was also used to model two small column experiments using simulants of Hanford waste types AZ-102 and AN-107 and one experiment using actual AN-102 waste. PNWD (Fiskum et al., 2006c) used an earlier RF resin batch (6C-370/745) in the experiment with AZ-102 simulant. Based on prior AP-101 studies with various resin batches it was expected that its performance would be similar to that of batch 5E-370/641.

A VERSE-LC calculation was also performed for the SRNL experiment conducted with AP-101 simulant on a 24" diameter column and compared to the results summarized by Fiskum et al. (2006c). Neither of the two cycles where data is reported for the 24" column (Fig 12.4 in Fiskum et al. 2006c) show cesium breakthrough before the tests were terminated after processing 52 bed volumes of feed. The VERSE-LC model calculation predicted that $C/C_0$ would exceed $10^{-4}$, which was the measurement limit for this experiment, at just over 50 bed volumes. As shown by Eq. (8-1), the higher flow velocity in the large diameter column reduces film resistance and improves breakthrough performance over that observed in small diameter columns. This qualitative observation is in agreement with the experimental data.

Experimental parameters for the small column experiments are listed in Table 9-1. All three AP-101 experiments used essentially the same size column and mass of RF resin (listed mass is $H^+$ form). However, temperature varied from 19 °C to 45 °C between these experiments. Table 9-2 lists the physical properties calculated for the small column feed solutions at the given column temperatures. Table 9-3 lists the isotherm parameters calculated using the thermodynamic model described by Aleman and Hamm (2007) for the small column ion-exchange experiments. Figures 9-1 through 9-6 show comparisons of VERSE-LC model calculations to experimental data for each of the three AP-101 experiments. Two plots are shown for each experiment with the model calculated breakthrough curve and experimental data plotted using both linear and log concentration scales. Figures 9-7 and 9-8 show a similar comparison of the VERSE-LC prediction to the limited cesium breakthrough data obtained from the AN-107 waste experiment. Figures 9-9 and 9-10 show model predictions that bound the cesium breakthrough curve measured in the PNWD experiment using actual AN-102 waste. Figures 9-11 and 9-12 show a comparison of the VERSE-LC predictions of cesium breakthrough for AZ-102 waste using three estimates of the bed density compared to the experimentally measured result.

## 9.1 PNWD Column Data with Actual AP-101 Waste

A VERSE-LC model calculation was compared to data collected from the PNWD small column experiment using spherical RF resin (batch 5E-370/641) with actual AP-101 diluted feed as shown in Figures 9-1 and 9-2. A full description of the test is reported by Fiskum et al. (2006a). The feed composition is listed in Table 4-9. The experiment collected nominally 2 ml samples from both the lead and lag columns at nominally 10 bed volume increments. The hot cell temperature ranged from 26 °C to 27 °C during the loading phase of the experiment and an average temperature of 26.5 °C was used in the VERSE-LC calculation. Isotherm parameters used in the model calculations are given in Table 9-3. The bulk diffusivity of $Cs^+$ in AP-101 is given in Table 9-2 also at 26.5 °C. The tortuosity factor of 3.0, given in Section 7, was used to compute pore diffusivity. Bed and particle porosity values were taken from Section 5. The factor used to convert from a dry H-form resin mass to a dry Na-form resin mass was 1.25, based on data from Nash et al. (2006). The average particle radius was assumed to be 228.5 μm.

From Figures 9-1 and 9-2, it can be seen that the model is in good agreement with the data for both the lead and lag columns even at very low cesium concentrations ($C_0$ for this experiment was $4.48\times10^{-5}$ so $C/C_0 = 10^{-4}$ corresponds to a cesium concentration $C = 4.48\times10^{-9}$). Both model and data predict 50% breakthrough in the lead column at approximately 95 bed volumes. Model parameters used in this simulation were computed using the methods described in the preceding sections of this report.

In Section 3, this experiment was also modeled using a 4-component (i.e., $Cs^+$, $K^+$, $Rb^+$, and $Na^+$) isotherm model. The VERSE-LC results obtained using the four component approach are shown in Figure 3-2. To validate the use of an "effective" Cs only modeling approach, the 4-component modeling results were compared to the 1-component approach in Figures 3-3 and 3-4 for cesium breakthrough. As Figures 3-3 and 3-4 illustrate, the "effective" Cs only modeling approach provides excellent breakthrough curve approximation when compared to the more complex 4-component approach.

## 9.2 PNWD Column Data with AP-101 Simulant

PNWD also tested spherical Resorcinol-Formaldehyde resin (batch 5E-370/641) using an AP-101 simulant. A full description of the test is reported by Fiskum et al. (2006a). The feed composition is listed in Table 4-9. The experiment again collected nominally 2 ml samples from both lead and lag columns at nominally 10 bed volume increments. The experiment was not temperature controlled and ambient temperature ranged from 19 °C to 25 °C over the course of the experiment. Unfortunately, this is a relatively large temperature variation over which isotherm parameters and solution properties can change significantly. Trial runs indicated that the best agreement between model predictions and the experimental data was obtained by running the calculations at 19 °C.

The VERSE-LC model calculation at 19 °C is compared to data collected from this experiment in Figures 9-3 and 9-4. The model used the AP-101 cesium isotherm parameters given in Table 9-3 calculated at 19 °C. The bulk diffusivity of $Cs^+$ in AP-101 simulant is given in Table 9-2 at 19 °C. The tortuosity factor of 3.0, given in Section 7, was used to compute the pore diffusivity.

Bed and particle porosity values were from Section 5. The factor for converting from a dry H-form resin mass to a dry Na-form resin mass was 1.25, based on data from Nash et al. (2006). The average particle radius was assumed to be 228.5 μm.

The VERSE-LC cesium breakthrough curve falls above the experimental data for cesium $C/C_0 > 10^{-3}$ and rises faster than the data beyond 50% breakthrough which indicates better particle kinetics in the model. In this case, using a higher tortuosity in the VERSE-LC calculation would allow the calculation to better match the slope of the experimental data. The experimental data shows 50% breakthrough in the lead column at about 120 bed volumes while the model predicts that 50% breakthrough will occur at about 112 bed volumes. The model estimate of resin capacity is therefore less than the experimentally observed value. Since resin capacity decreases with temperature, model calculations at 25 °C fall even further to the left of the experimental data. Cesium concentrations exiting the lag column are all very small in this experiment and as shown in Figure 9-4 are captured fairly well by the model calculation. A value of $C/C_0$ around $10^{-5}$ appears to be the detection limit in this experiment.

### 9.3 SRNL Column Data with AP-101 Simulant

SRNL tested spherical Resorcinol-Formaldehyde resin (batch 5E-370/641) with the same AP-101 simulant formulation as PNWD (i.e., full recipe). A full description of the test is provided by Nash et al. (2006). The experiment only used a single column which allowed collecting all of the column effluent in nominally 8 ml aliquots. The experiment was temperature controlled by jacketing the ion-exchange column to maintain a column temperature of 45 °C over the course of the experiment. Both cesium and rubidium breakthrough measurements were made.

The VERSE-LC model calculation at 45 °C is compared to data collected from this experiment in Figures 9-5 and 9-6. The isotherm parameters for an "effective" single component Cs isotherm model are provided in Tables 9-3 and 9-4. The bulk diffusivities of $Cs^+$ and $Rb^+$ in AP-101 simulant at 45 °C are given in Table 9-2. The tortuosity factor of 3.0, derived in Section 7, was used to compute the pore diffusivity. Bed and particle porosity values were taken from Section 5. The factor for converting from a dry H-form resin mass to a dry Na-form resin mass was 1.25, based on data from Nash et al. (2006). The average particle radius was assumed to be 228.5 μm. Since this experiment measured rubidium breakthrough, a second calculation was also made using the binary cesium and rubidium isotherm parameters given in Table 9-4 calculated at 45 °C to allow modeling the rubidium breakthrough.

The VERSE-LC model predicts earlier cesium breakthrough than the experimental data and has approximately the same slope (and shape) throughout the transient. The matching slope indicates that using a value of 3.0 for the pore tortuosity in the VERSE-LC calculation is a good estimate. The experimental data shows 50% breakthrough in the column at about 76 bed volumes while the model predicts that 50% breakthrough will occur at about 68 bed volumes. Either increasing the resin capacity in the model ($C_T$) by about 5% or decreasing the β factor by 5% would bring the model calculation into good agreement with the experimental data.

The VERSE-LC model predicts a slightly sharper breakthrough curve for rubidium, but overall the prediction follows the data quite well. It is this set of rubidium data that was used to assist in establishing the thermodynamic equilibrium coefficient for the $Cs^+$ to $Rb^+$ mass-action ion exchange reaction. As mentioned in Section 4, the limited batch contact data with rubidium present was not sufficient to accurately determine the equilibrium coefficient.

## 9.4 SRNL Column Data with AN-107 Simulant

SRNL tested spherical Resorcinol-Formaldehyde resin from batch 5E-370/641 with a simulant of AN-107 Sr/TRU filtrate. A full description of the test is reported by Nash et al. (2006). The experiment used a single column which allowed collecting all of the column effluent in nominally 8 ml aliquots. The experiment was temperature controlled by jacketing the ion-exchange column to maintain a column temperature of 25 °C over the course of the experiment. Unfortunately, the experiment was terminated after only about 7% cesium breakthrough.

The VERSE-LC model calculation at 25 °C is compared to data collected from the AN-107 experiment in Figures 9-7 and 9-8. The tortuosity factor of 3.0, given in Section 7, was used to compute the pore diffusivity. Bed and particle porosity values were from Section 5. The factor for converting from a dry H-form resin mass to a dry Na-form resin mass was 1.25, based on data from Nash et al. (2006). The average particle radius was assumed to be 228.5 μm. The bed volume in this experiment was 10.76 ml and the flow rate 0.246 ml/min.

The VERSE-LC model predicts breakthrough considerably later than is observed experimentally with initial breakthrough in the model calculation occurring at about 300 bed volumes compared to 200 bed volumes in the experimental data. As shown in the figures, reducing the resin capacity to 60% of the nominal value allows the model to approach the experimental data.

## 9.5 PNWD Column Data with Actual AN-102 Waste

PNWD tested spherical Resorcinol-Formaldehyde resin from batch 5E-370/641 with a composite sample of actual AN-102 Hanford waste. The waste was treated to simulate pretreatment prior to ion-exchange. A full description of the test is reported by Fiskum et al. (2006b). The experiment collected nominally 2 ml samples from both lead and lag columns at nominally 10 bed volume increments. The experiment was not temperature controlled but was conducted in hot cells where the ambient temperature remained between 26 °C and 27 °C. The average temperature of 26.5 °C was used for the model calculations. The lead column in this experiment had served as the lag column in a previous experiment with AP-101 waste and was therefore partially loaded with cesium.

The VERSE-LC model calculation of cesium breakthrough is compared to data collected from the AN-102 experiment in Figures 9-9 and 9-10. The dashed curves in each figure (black for lead column blue for lag) show results from a VERSE-LC calculation assuming that the column starts with our best estimate of the initial cesium loading. As can be seen in Figure 9-9, this best estimate would predict cesium breakthrough in the lead column at the start of the AN-102 experiment which clearly did not occur. The solid curves in Figures 9-9 and 9-10 show results from a VERSE-LC model prediction assuming that the column initially contains no cesium. These results predict considerably later breakthrough than is observed experimentally. The experiments show some measurable cesium breakthrough at about 100 bed volumes whereas the model predicts initial cesium breakthrough at about 350 bed volumes when starting with a clean column. The experimental behavior falls between the model predictions for a preloaded and a clean column but closer to the preloaded results. A likely explanation is that some of the loaded cesium was eluted from the column during the 11 days storage and handling between the time it served as the lag column in the AP-101 experiment and the lead column in the AN-102 test. Unfortunately, this experiment was also terminated prematurely with only about 10% cesium breakthrough which makes an exact comparison with the model predictions difficult.

## 9.6 PNWD Column Data with Simulated AZ-102 Waste

PNWD tested spherical Resorcinol-Formaldehyde resin using an earlier batch (6C-370/745) and a simulant of AZ-102 Hanford waste (i.e., an Envelope B waste stream). A description of the test results reported by Fiskum et al. (2006c) where cesium breakthrough curves for several spherical RF resin batches with AP-101 feeds show relatively similar behavior. As such, it was believed that the cesium breakthrough for this earlier batch and the one used in our prior assessment activities would also behavior similarly under an AZ-102 feed. The experiment was run in a single column where the temperature was not controlled and the ambient temperature varied between 19 °C to 24 °C. The average temperature of 22 °C was used for the model calculations.

VERSE-LC model calculations of cesium breakthrough are compared to the data collected from the AZ-102 experiment in Figures 9-11 and 9-12 where the solid curves show VERSE-LC model predictions at different bed densities. The black curve at the far right was obtained using the reported bed density of 0.36 g resin/ml. The blue curve on the far left was obtained using a nominal bed density (0.26 g resin/ml bed) that applies for the other experiments. The red curve in the middle assumes 120% of the nominal bed density (0.31 g resin/ml). Even though this is a different batch of RF resin, the reported bed density appears to be somewhat high. It may be that the bed density is actually higher but that the resin ion-exchange capacity is lower for this batch. Batch contact data would be needed to accurately determine these parameters. The shape of the predicted breakthrough suggests that a larger tau factor also applies for this resin batch ($\tau = 3.0$ was used in all of the VERSE-LC calculations).

Table 9-1. Small column experimental parameters.

| Experiment | Temperature (C) | Volume (ml) | Diameter (cm) | Length (cm) | Resin Mass (g $H^+$ form) | Flow rate (ml/min) |
|---|---|---|---|---|---|---|
| Actual AP-101 Diluted Feed | 26-27 (26.5) | 11 | 1.5 | 6.225 | 2.8697 | 0.530 |
| PNWD AP-101 Simulant | 19-25 (19) | 11 | 1.5 | 6.225 | 2.8697 | 0.539 |
| SRNL AP-101 Simulant | 45 | 11.06 | 1.574 | 5.684 | 2.8859 | 0.240 |
| SRNL AN-107 Simulant | 25 | 10.76 | 1.571 | 5.551 | 2.8915 | 0.246 |
| PNWD Actual AN-102 | 26.5 | 11 | 1.5 | 6.225 | 2.87 | 0.530 |
| PNWD AZ-102 Simulant | 22 | 19.8 | 2.0 | 6.3025 | 7.19 | 0.495 |

Table 9-2. Physical properties of small column experimental solutions.

| Feed | Cs Diffusivity ($cm^2$/min) | Rb Diffusivity ($cm^2$/min) | Density (g/ml) | Viscosity (cP) |
|---|---|---|---|---|
| Actual AP-101 Diluted Feed, 26.5 °C | 4.136E-04 | - | 1.255 | 2.954 |
| PNWD AP-101 Simulant, 19 °C | 3.577E-04 | - | 1.253 | 3.486 |
| SRNL AP-101 Simulant, 45 °C | 6.205E-04 | 6.243E-04 | 1.236 | 1.904 |
| SRNL AN-107 Simulant, 25 °C | 3.610E-04 | - | 1.274 | 3.020 |
| PNWD Actual AN-102, 26.5 °C | 5.031E-04 | - | 1.230 | 2.289 |
| PNWD AZ-102 Simulant, 22 °C | 9.817E-04 | - | 1.239 | 3.336 |

Table 9-3. Four-parameter fit of isotherm parameters for small column experiments ($H^+$ form basis for $\rho_b$ and $C_T$).

| LAW IX Operating Time Period | $\rho_b C_T$ (mmol/ml BV) | β [M] | $M_a$ | $M_b$ |
|---|---|---|---|---|
| Actual AP-101 Diluted Feed, 26.5 °C | 0.2756 | 3.1317E-3 | 0.9896 | 0.8550 |
| PNWD AP-101 Simulant, 19 °C | 0.2714 | 2.5528E-3 | 0.9874 | 0.8630 |
| SRNL AP-101 Simulant, 45 °C | 0.2822 | 4.4400E-4 | 0.9933 | 0.8404 |
| SRNL AN-107 Simulant, 25 °C | 0.2494 | 4.3138E-4 | 0.9721 | 0.9060 |
| PNWD Actual AN-102, 26.5 °C | 0.2390 | 3.3350E-4 | 0.9718 | 0.9120 |
| PNWD AZ-102 Simulant, 22 °C | 0.3469 | 8.4835E-4 | 0.9764 | 0.8933 |

Table 9-4. Parameter settings for the binary and 'Effective" single-component Freundlich/Langmuir Hybrid equilibrium isotherm models for cesium and rubidium on RF-641 resin for AP-101 simulant (full recipe) at 45 ºC.

| Parameter[a] | Cesium (component 1) | Rubidium (component 2) | Cesium ("effective" single component) |
|---|---|---|---|
| $a_i$ (gmoles/$L_{CV}$) [b] | 0.2822 | $2.6616 \times 10^{-2}$ | 0.2822 |
| $b_i$ ($M^{-1}$) | 1.0 | $9.6006 \times 10^{-2}$ | 1.0 |
| $M_{ai}$ (-) | 0.9933 | 1.0 | 0.9933 |
| $M_{bi}$ (-) | 0.8404 | 1.0 | 0.8404 |
| $\beta_i$ (-) | $4.4400 \times 10^{-4}$ | $5.2545 \times 10^{-3}$ | $4.4400 \times 10^{-4}$ |

[a] The parameters for components 1 and 2 refer to cesium and rubidium, respectively. The impact from the competitors sodium, hydrogen, and potassium are embedded within the beta parameters.

[b] These values are based on a bed density of 0.2563 g/ml and total ionic capacity of 0.6832 mmole/g.

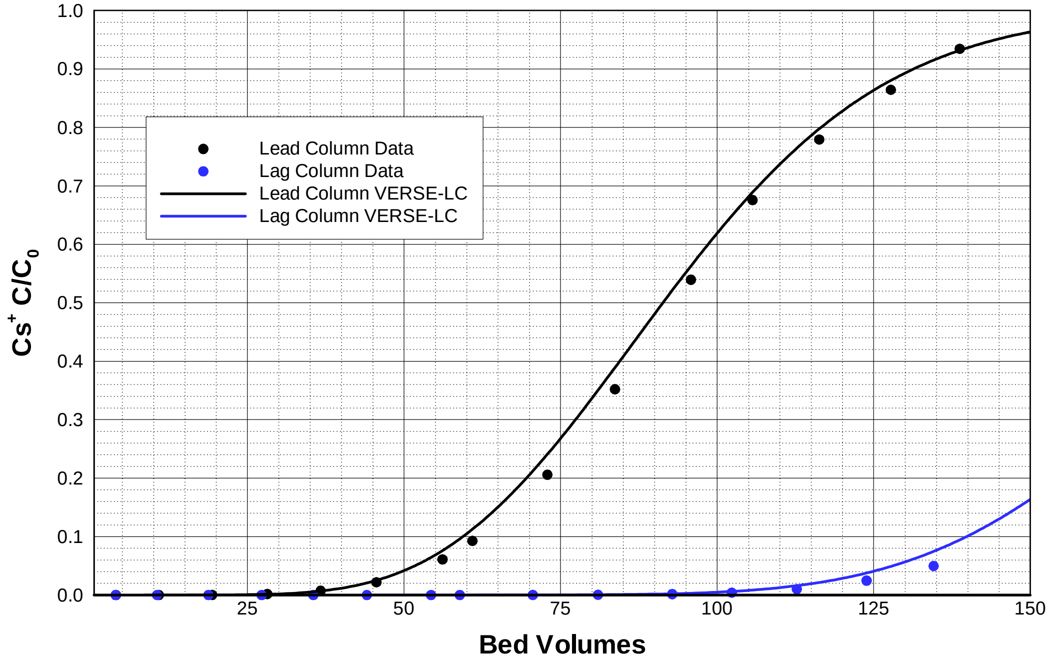


Figure 9-1. Comparison of VERSE-LC cesium breakthrough predictions with data from PNWD small column test using actual AP-101 waste at 26.5 °C, linear scale.

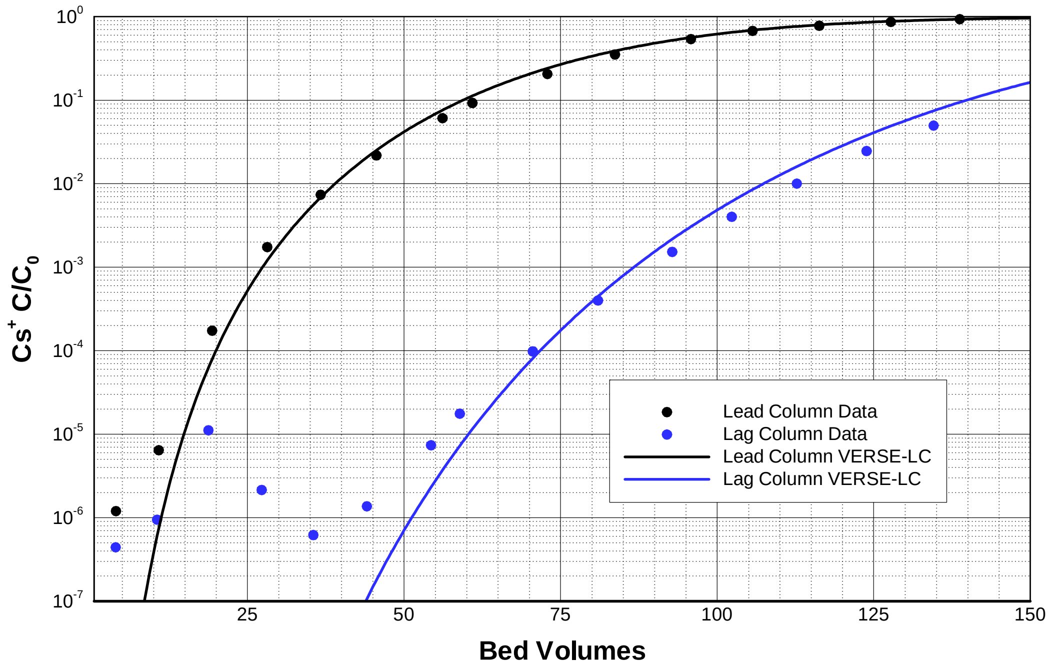


Figure 9-2. Comparison of VERSE-LC cesium breakthrough predictions with data from PNWD small column test using actual AP-101 waste at 26.5 °C, log scale.

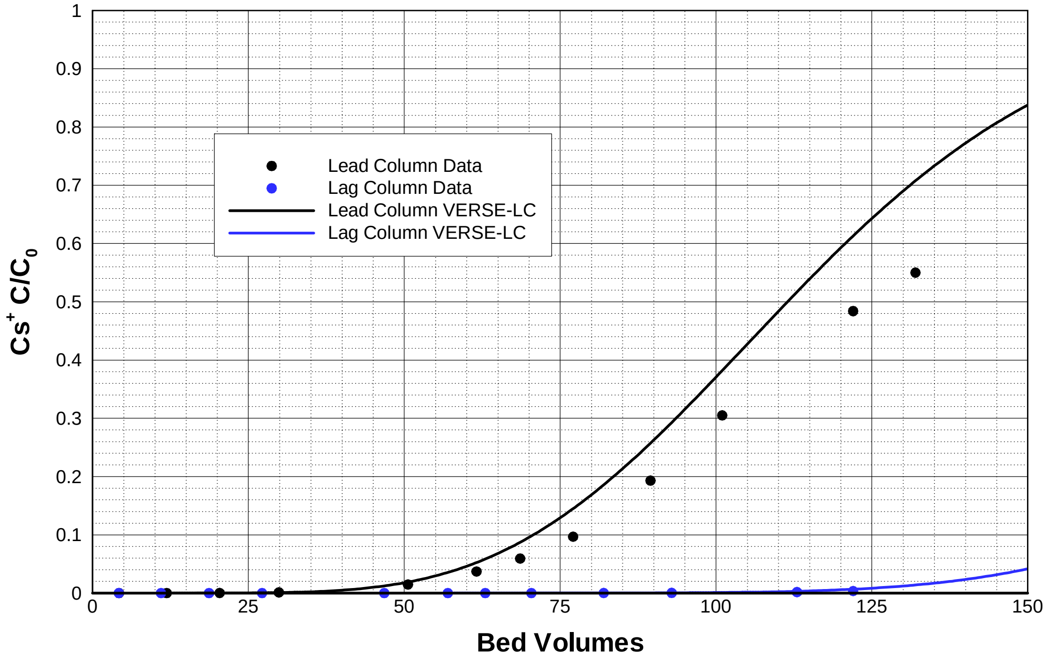


Figure 9-3. Comparison of VERSE-LC cesium breakthrough predictions with data from PNWD small column test using AP-101 simulant at 19 °C, linear scale.

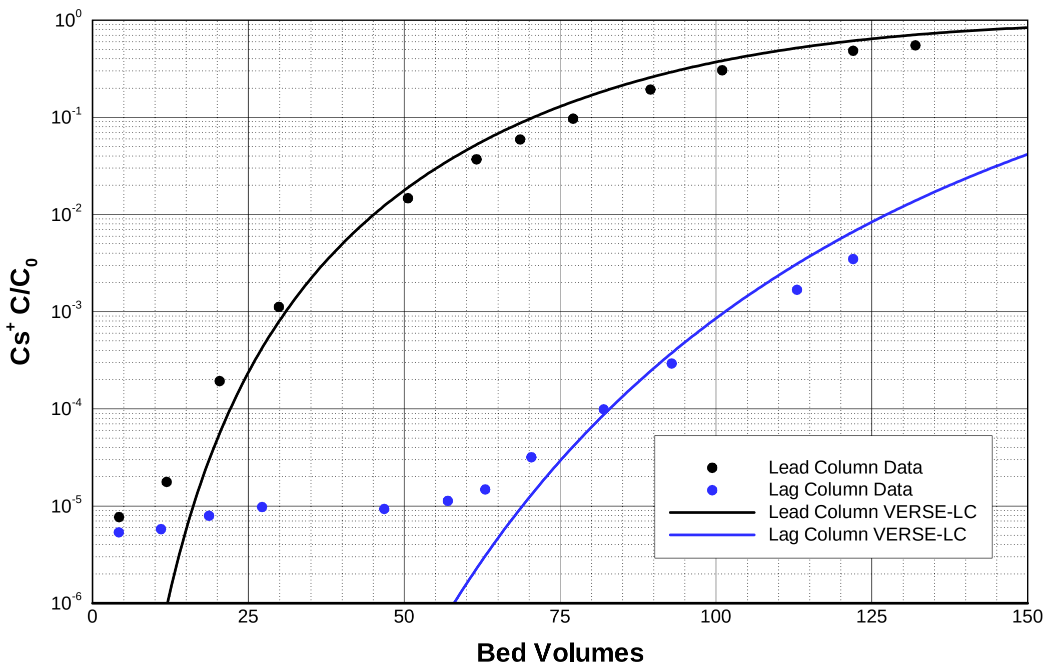


Figure 9-4. Comparison of VERSE-LC cesium breakthrough predictions with data from PNWD small column test using AP-101 simulant at 19 °C, log scale.

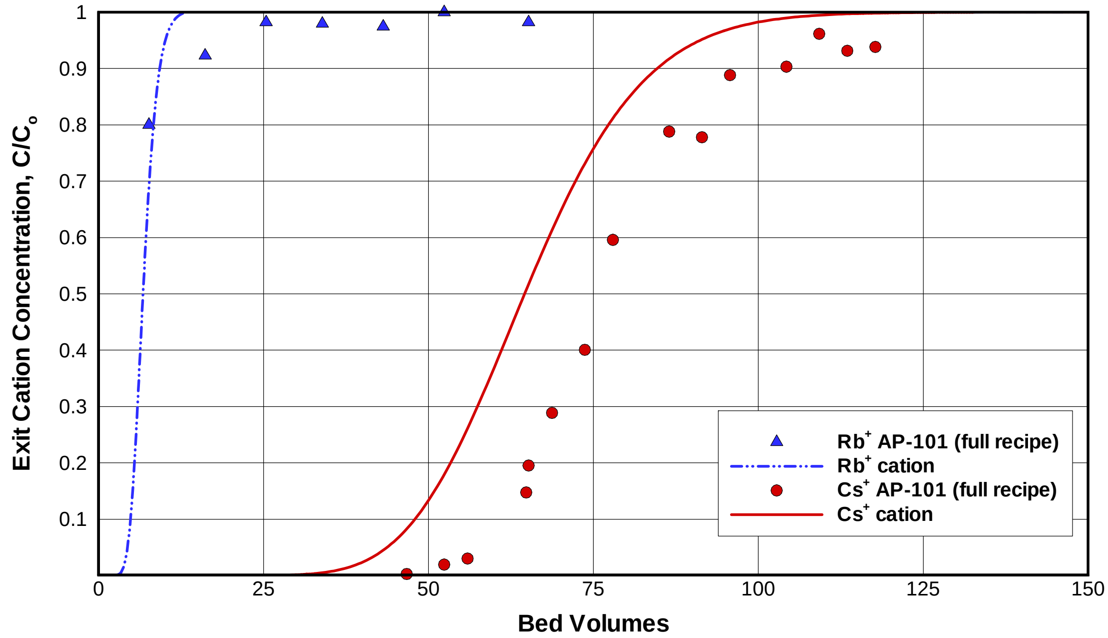


Figure 9-5. Comparison of VERSE-LC cesium breakthrough predictions with data from SRNL small column test using AP-101 simulant (full recipe) at 45 °C, linear scale.

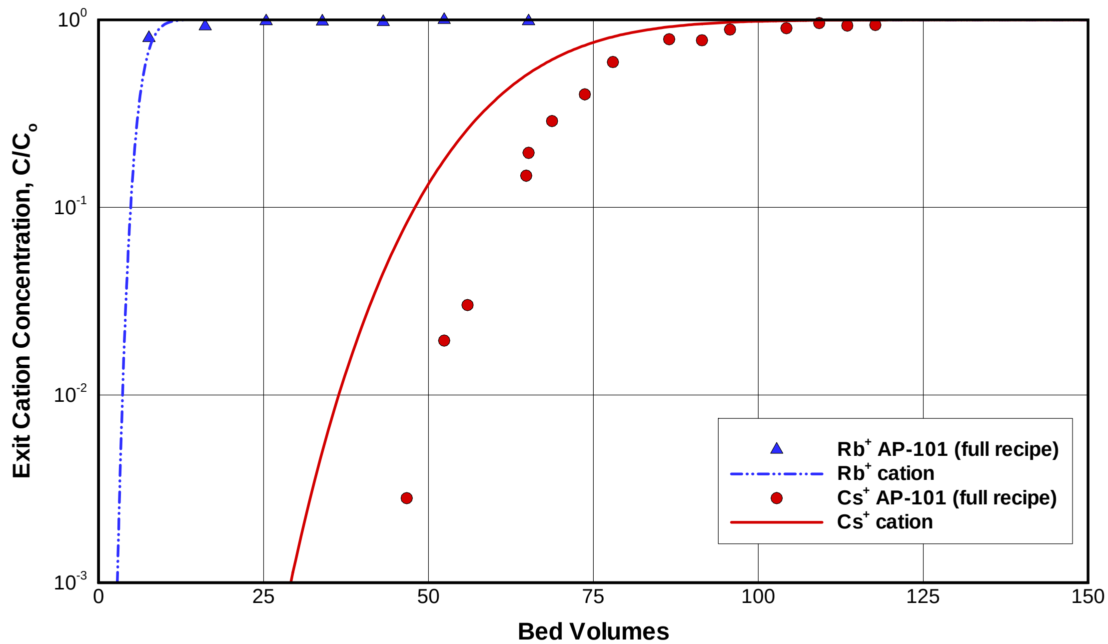


Figure 9-6. Comparison of VERSE-LC cesium breakthrough predictions with data from SRNL small column test using AP-101 simulant (full recipe) at 45 °C, log scale.

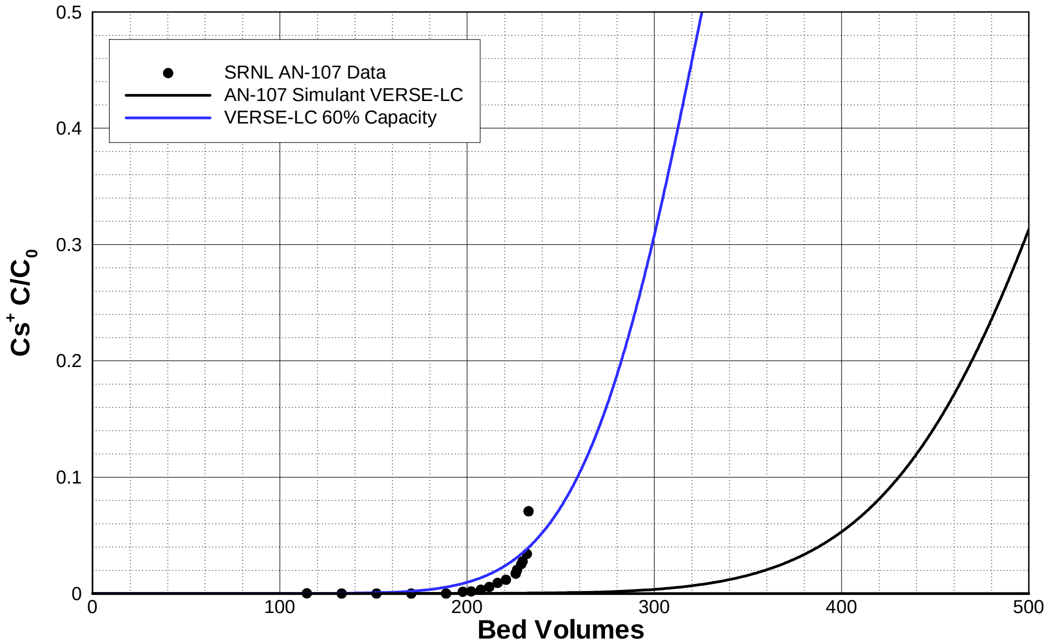


Figure 9-7. Comparison of VERSE-LC cesium breakthrough predictions with data from SRNL small column test using AN-107 simulant at 25 °C, linear scale.

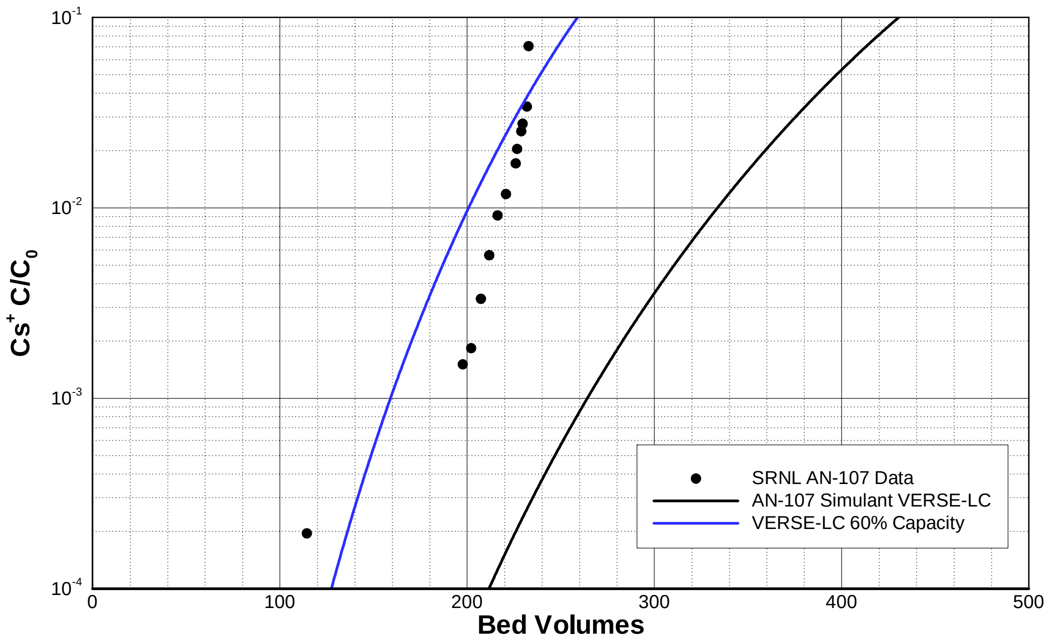


Figure 9-8. Comparison of VERSE-LC cesium breakthrough predictions with data from SRNL small column test using AN-107 simulant at 25 °C, log scale.

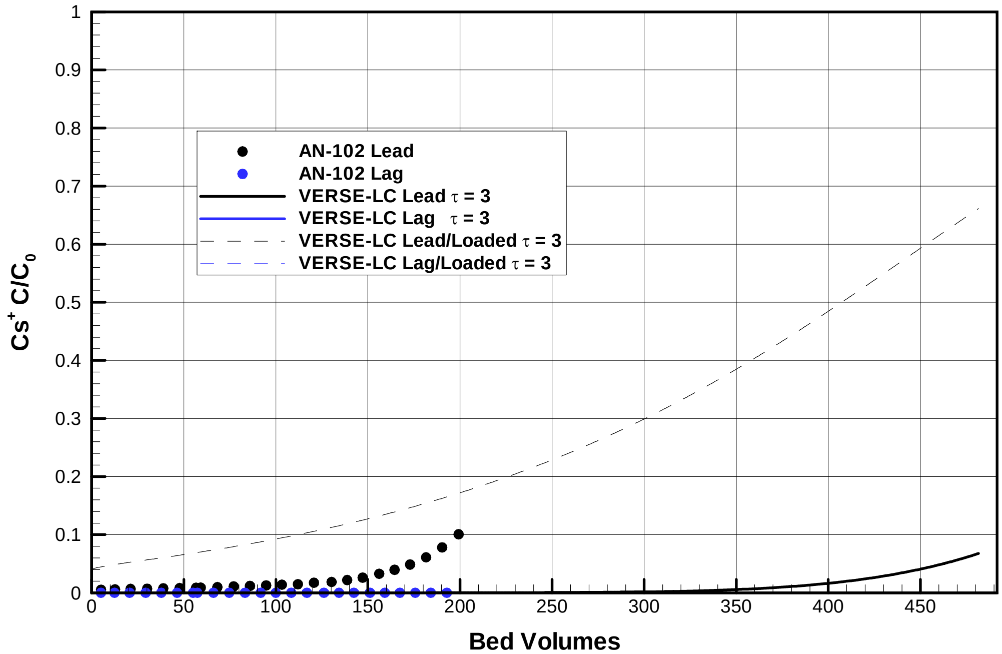


Figure 9-9. Comparison of VERSE-LC cesium breakthrough predictions with data from PNWD small column test using actual AN-102 waste at 26.5 °C where the column was partially pre-loaded with cesium, linear scale.

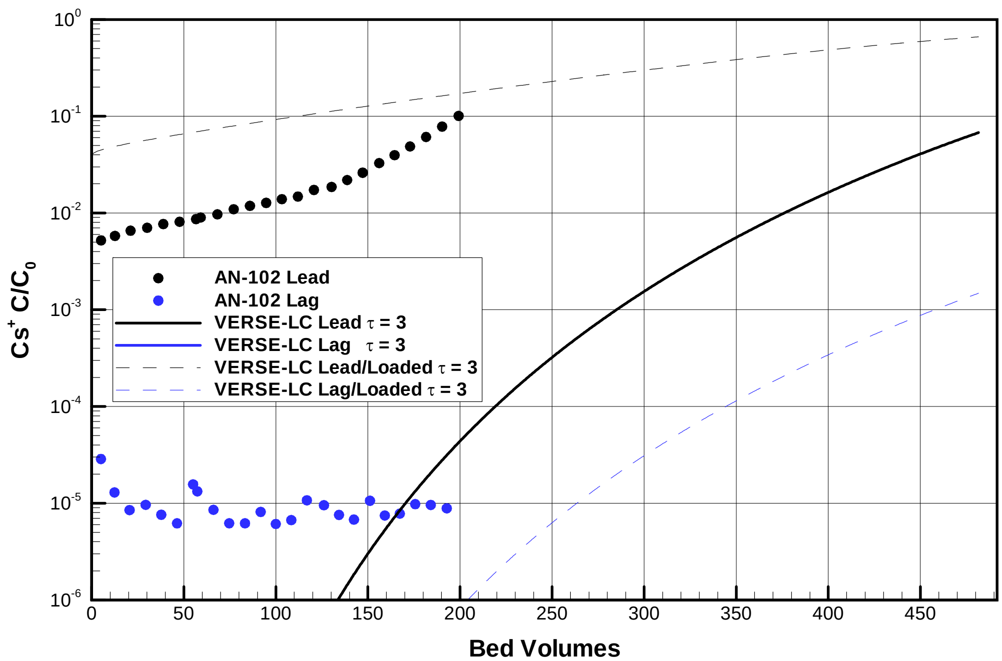


Figure 9-10. Comparison of VERSE-LC cesium breakthrough predictions with data from PNWD small column test using actual AN-102 waste at 26.5 °C where the column was partially pre-loaded with cesium, log scale.

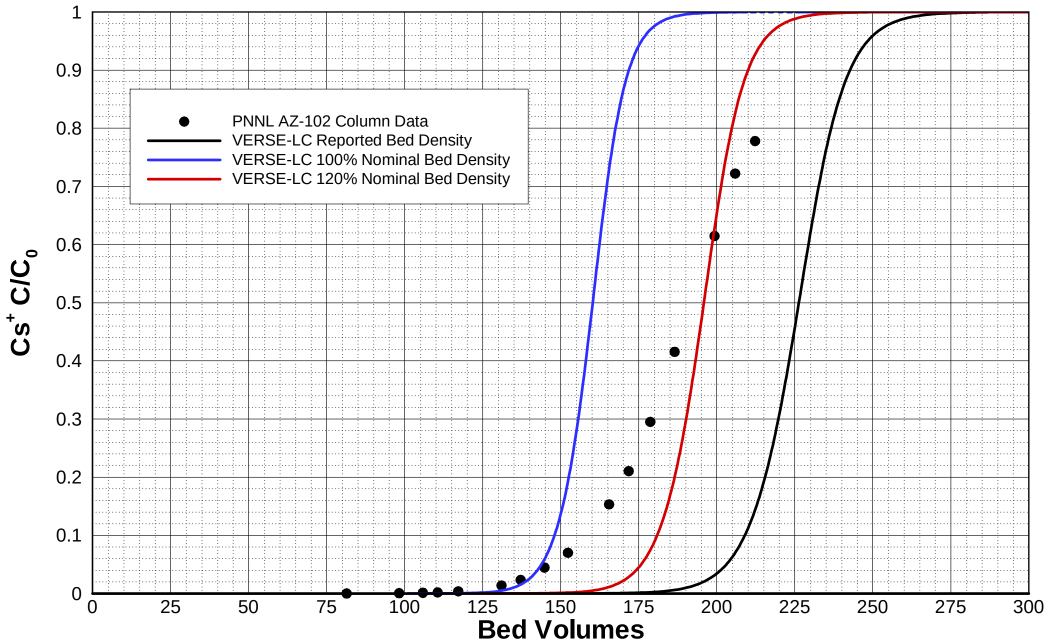


Figure 9-11. Comparison of VERSE-LC cesium breakthrough predictions with data from PNWD small single column test using simulated AZ-102 waste at an average temperature of ~22 °C, linear scale.

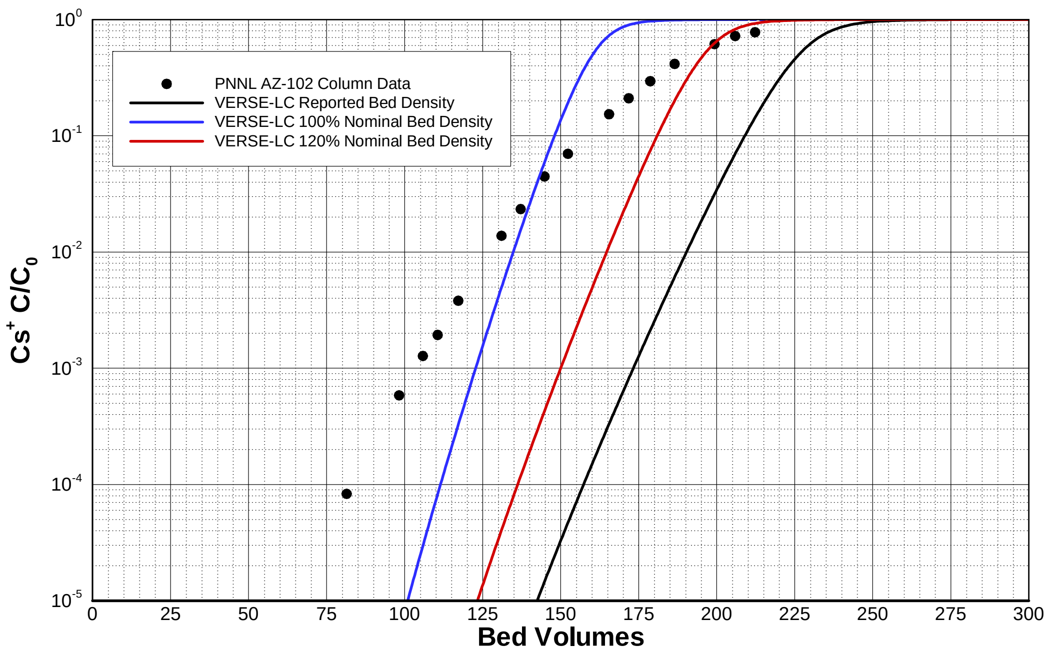


Figure 9-12. Comparison of VERSE-LC cesium breakthrough predictions with data from PNWD small single column test using simulated AZ-102 waste at an average temperature of ~22 °C, log scale.

# 10.0 Full-Scale Column Predictions

A series of VERSE-LC simulations were performed to predict the cesium removal performance of a full-scale facility consisting of a three-column carousel configuration. The resin bed contained within each single column was 53.0 inches in diameter and 62.8 inches high. A total bed volume of 600 gallons of resin was assumed with a head space of 500 gallons. The dimensions and operating parameters for the columns were specified by WTP (Thorson, 2006). Nominal operating conditions for "Hot Commissioning", "Envelope B" and "Subsequent Operations" were investigated. In addition, sensitivity studies specified by WTP were made for each of the feeds. A list of the parameters used for each of the full-scale column case runs is provided in Table 10-1. Note that a nominal RF particle radius of 230 μm was specified for the full-scale column simulations which is slightly larger than the best estimate value of 228.5 μm used in the experimental verification calculations. Column switching during carousel operation was performed based on the cesium concentration at the exit of the lag column reaching the contract limit specified by Toth (2003). For these carousel analyses, no safety limit on the total amount of $^{137}$Cs inventory within a given column was imposed. All of the calculations assume fresh RF resin.

The number of bed volumes processed for the first five cycles when the cesium criterion at the exit of the lag column is reached and bed volumes at 50% breakthrough are given in Tables 10-2 through 10-4 for column operation under nominal parameter settings for the three feed streams. The 50% breakthrough point is defined as the point where the cesium concentration at the exit from the lead column is 50% of the feed concentration. Similar bed volume results are provided in Tables 10-5 and 10-6 for the various sensitivity simulations performed for Hot Commissioning feed, in Table 10-7 for the two Envelope B simulations, and in Tables 10-8 and 10-9 for the sensitivity simulations performed for Subsequent Operation feed.

When a $^{137}$Cs inventory limit is imposed on column loading, the number of bed volumes processed with the Envelope B and Subsequent Operations feed streams become limited prior to reaching the lag column exit concentration criterion. An LAW loading limit of 75,000 Ci was specified by Toth (2003). VERSE calculations predict that this inventory limit is reached in about 30 bed volumes for the nominal Envelope B and in 235 bed volumes for the nominal Subsequent Operations feed streams. In contrast, the concentration limit at the lag column exit was reached in 524 bed volumes with the nominal Envelope B and in 494 bed volumes with the nominal Subsequent Operations feed streams. Table 10-10 summarizes the number of bed volumes required to reach the LAW Loading Limit (LLL), Limiting Condition for Operation (LCO) limit and Technical Safety Limit (TSL) of 75000, 125000 and 150000 Ci, respectively. The greatest impact from imposing a curie loading limit is on Envelope B feed since it has the highest cesium concentration.

## 10.1 Carousel Cycles for Hot Commissioning Operations

Figures 10-1 through 10-28 show cesium breakthrough predictions for full-scale three column carousel operation with Hot Commissioning feed assuming fresh RF resin. The figures are presented as pairs where the first figure (e.g. 10-1) plots the cesium concentration ratio ($C/C_0$) on a linear scale and the second figure (e.g. 10-2) plots the concentration on a log scale to better show the behavior at low concentrations.. Complete specification of simulation parameters for each run are given in Table 10-1. Breakthrough volumes for the first seven cycles for these cases are listed in Tables 10-5 and 10-6. Figures 10-1 and 10-2 shows full-scale carousel operation with Hot Commissioning feed under nominal operating conditions. Breakthrough bed volumes for the first five cycles during nominal Hot Commissioning operations are also listed in Table 10-2.

Figures 10-3 and 10-4 show full-scale carousel operation using Hot Commissioning feed with the potassium concentration increased from 0.48 M to 0.8 M. As expected, the increased potassium reduces the cesium loading capacity on the resin and increases the carousel cycling frequency. Figures 10-5 and 10-6 show full-scale carousel operation using Hot Commissioning feed with the potassium concentration reduced from 0.48 M to 0.3 M. The reduced potassium increases the cesium loading capacity of the resin and reduces the frequency of carousel cycling. Except for hydrogen and cesium, potassium has the greatest affinity for RF ion-exchange sites.

Figures 10-7 and 10-8 show full-scale carousel operation with Hot Commissioning feed diluted from 4.57 M to 4 M sodium. Diluting the feed reduces the concentrations of cesium, potassium and sodium by the same ratio and thereby increases the bed volumes of feed that are processed. Breakthrough in the first cycle with nominal Hot Commissioning feed occurs at 206 bed volumes. Using a simple concentration ratio predicts column breakthrough at 206 x 4.57/4 = 235 bed volumes. Secondary effects from reduced liquid viscosity and increased cesium diffusivity (see Table 7-1) act to increase the cesium loading slightly more to 251 bed volumes. Figures 10-9 and 10-10 show full-scale carousel operation with Hot Commissioning feed concentrated from 4.57 to 5.5 M sodium. Concentrating the feed increases the concentration of all ion-exchange cations by the same ratio and thereby reduces the bed volumes that can be processed. Again the effect is somewhat greater than a simple ratio would predict (151 bed volumes to first breakthrough versus 206 x 4.57/5.5 = 171). Figures 10-11 and 10-12 show full-scale carousel operation with Hot Commissioning feed concentrated to 5 M sodium and with the flow rate increased to 20 gpm. Both the higher feed concentration and higher flow tend to reduce the number of bed volumes that can be processed before the contract limit breakthrough is reached at the lag column exit.

Figures 10-13 and 10-14 show full-scale carousel operation with nominal Hot Commissioning feed at a reduced flow rate of 7.2 gpm. Lowering the flow rate allows more time for equilibration which increases column loading and increases the number of bed volumes that can be processed before the contract limit breakthrough is reached at the lag column exit. The effect is relatively small (230 bed volumes to the first breakthrough versus 206 bed volumes at 15 gpm). At half the flow it will take twice as long to process a given volume of feed so the approximately 10% increase in bed volumes per ion-exchange column may not be worth the extra processing cost. Figures 10-15 and 10-16 show full-scale carousel operation with nominal Hot Commissioning feed at an increased flow rate of 20 gpm. Increasing the feed flow rate from 15 gpm to 20 gpm reduces the bed volumes to the first breakthrough point from 206 to 191. However, this 5% reduction in column capacity is offset by the 33% increase in production rate. Similarly, Figures 10-17 and 10-18 show full-scale carousel operation with nominal Hot

Commissioning feed at a flow rate of 30 gpm. Lag column breakthrough in the first cycle occurs when 171 bed volumes have been processed through the lead column.

Figures 10-19 and 10-20 show full-scale carousel operation with the nominal Hot Commissioning feed composition at a temperature of 35 °C while Figures 10-21 and 10-22 shows results for a column temperature of 45 °C. As can be seen from the isotherm plots in Section 4 (e.g. Figure 4-8), cesium capacity decreases with increasing temperature. Breakthrough bed volumes for the lead column in the first cycle decrease from 206 at 25 °C to 166 at 35 °C and to 134 at 45 °C.

Figures 10-23 and 10-24 show full-scale carousel operation with nominal Hot Commissioning feed using a smaller RF resin particle diameter at a feed flow rate of 20 gpm. Comparing this result to Figures 10-15 and 10-16, shows that, as expected, a smaller particle size reduces transport resistance and allows more bed volumes of feed to be processed before breakthrough. However, the effect is relatively small. For the initial cycle, breakthrough occurs after 191 bed volumes have been processed through the lead column with the nominal RF particle size while the smaller resin particle allows 209 bed volumes to be processed.

Figures 10-25 and 10-26 show cesium breakthrough predictions for full-scale carousel operation with Hot Commissioning feed having twice the nominal cesium concentration and using the smaller RF particle size at a feed flow of 15 gpm. Figures 10-27 and 10-28 also show cesium breakthrough predictions for full-scale carousel operation with Hot Commissioning feed having twice the nominal cesium concentration and using the smaller RF particle size at a feed flow of 22 gpm. As in previous results, a higher feed flow leads to breakthrough after slightly fewer bed volumes. The difference is only about 5% in this case.

## 10.2 Carousel Cycles for Envelope B Operations

Figures 10-29 through 10-32 show cesium breakthrough predictions for full-scale three column carousel operation with nominal Envelope B feed assuming fresh RF resin. Full specification of simulation parameters for both runs are listed in Table 10-1 where it is seen that the only difference between the two Envelope B cases is an increase in feed flow rate from 6.5 gpm in Figures 10-29 and 10-30 to 10 gpm in Figures 10-31 and 10-32. At the lower flow rate, breakthrough in the first cycle occurs after 524 bed volumes of feed have been processed while at the higher flow rate breakthrough occurs after 523 bed volumes. This less than 1% decrease in capacity would appear to be more than offset by the 50% increase in processing rate. However, these results should be treated with caution because of the significant impact on Envelope B processing if curie limits are imposed on the ion-exchange columns. As shown in Table 10-10, the number of bed volumes that can be processed for Envelope B is significantly decreased when curie limits are imposed.

## 10.3 Carousel Cycles for Subsequent Operations

Figures 10-33 through 10-60 show cesium breakthrough predictions for a full-scale three column carousel under Subsequent Operations feed assuming fresh RF resin. Full specification of simulation parameters for each run are listed in Table 10-1. Breakthrough volumes for the first seven cycles for these cases are listed in Tables 10-8 and 10-9. Figures 10-33 and 10-34 show full-scale carousel operation with Subsequent Operations feed under nominal operating conditions. Breakthrough bed volumes for the first five cycles during nominal Subsequent Operations are also listed in Table 10-4.

Figure 10-35 and 10-36 show full-scale carousel operation with Subsequent Operations feed diluted from the nominal value of 4.6 M to 4 M sodium and with the feed flow rate reduced from 20 gpm to 15 gpm. Dilution alone would increase the number of bed volumes that can be processed during each cycle. As seen with Hot Commissioning feed, the effect of dilution is somewhat greater than what is predicted by using a simple concentration ratio. Decreasing the flow also tends to increase the number of bed volumes processed before breakthrough. The combination of the two effects increases the breakthrough volume for the first cycle from 494 to 635 bed volumes. Figures 10-37 and 10-38 show full-scale carousel operation with Subsequent Operations feed concentrated to 5.5 M sodium with a feed flow rate of 15 gpm. The concentration effect alone would predict a reduction in bed volumes processed at breakthrough from the 635 bed volumes, shown in Figures 10-35 and 10-36, to 461 (635 X 4/5.5). As seen with Hot Commissioning feed, the effect is somewhat greater from the concentration dependence of isotherm parameters, cesium diffusivity, and solution density and viscosity. The VERSE-LC model predicts that breakthrough during the first cycle will occur at 390 bed volumes.

Figures 10-39 through 10-44 show results for full-scale carousel operation with Subsequent Operations feed adjusted for caustic leach processing. Figures 10-39 and 10-40 show results for a caustic leaching process where 50% of the sodium in the ion-exchange feed stream is from NaOH with a feed flow of 30 gpm. Figures 10-41 and 10-42 show this same case with the ion-exchange feed flow increase to 35 gpm. As before, increasing the flow rate slightly decreases the number of bed volumes that can be processed before breakthrough. The calculation presented in Figures 10-43 and 10-44 used a different feed composition, lower feed flow rate and higher column temperature so it is difficult to compare with the other results.

Figures 10-45 and 10-46 show full-scale carousel operation with nominal Subsequent Operations feed at a feed flow rate of 15 gpm. This may be compared directly with the results shown in Figures 10-33 and 10-34 that used a higher feed flow rate of 20 gpm. The lower feed flow rate increases the number of bed volumes that can be processed from 494 to 517 for the first cycle. However, this 3% increase in bed volumes is obtained with a 25% decrease in flow rate and corresponding increase in processing time.

Figures 10-47 and 10-48 show full-scale carousel operation with Subsequent Operations feed under the same conditions as those in Figure 10-45 and 10-46 but with the free hydroxide concentration reduced from 0.6 M to 0.8 M. As shown by Aleman and Hamm (2007), the effective capacity of the ion-exchange resin is a function of the hydroxide concentration. At the reduced hydroxide concentration, the number of bed volumes of feed that can be processed before breakthrough during the first cycle is reduced by about 1% from 517 to 509.

Figures 10-49 and 10-50 show results for full-scale carousel operation with nominal Subsequent Operations feed at feed flow rate of 24 gpm. Figures 10-51 and 10-52 show results for full-scale carousel operation with nominal Subsequent Operations feed at feed flow rates of 30 gpm. When compared to results for the nominal flow rate of 20 gpm shown in Figures 10-33 and 10-

34, increasing the flow rate to 24 gpm reduces the number of bed volumes processed in the first cycle from 494 to 474. Increasing the flow rate to 30 gpm further reduces the bed volumes processed in the first cycle to 448. However, at a feed rate of 30 gpm, a 50% increase in processing rate has been achieved with only about a 10% decrease in the waste volume processed.

Figures 10-53 and 10-54 show full-scale carousel operation with the nominal Subsequent Operations feed composition at a temperature of 35 °C and a flow rate of 15 gpm while Figures 10-55 and 10-56 show results at the same flow rate with a column temperature of 45 °C. As can be seen from Figure 4-8, cesium capacity decreases with increasing temperature. Breakthrough bed volumes for the lead column during the first cycle decrease from 517 at 25 °C (case SO_07) to 398 at 35 °C and 312 at 45 °C. Figures 10-57 and 10-58 show full-scale carousel operation with the nominal Subsequent Operations feed composition at a temperature of 45 °C and a flow rate of 20 gpm which can be compared to Figures 10-33 and 10-34 to determine the temperature effect. As before raising the temperature decreases the cesium capacity of the RF resin. At a feed flow rate of 20 gpm, increasing the temperature from 25 °C to 45 °C decreases the bed volumes processing in the first carousel cycle from 494 to 297.

Figures 10-59 and 10-60 show full-scale carousel operation with Subsequent Operations feed at nominal conditions using a smaller RF particle size. As before, a reduced resin particle enhances equilibration between the fluid and the ion-exchange resin. For this case, the number of bed volumes that can be processed in the first cycle increases from 494 to 533 when using smaller resin particles.

## 10.4 Breakthrough Curves for Hot Commissioning Operations

Figures 10-61 through 10-68 show cesium breakthrough predictions for the lead column in a three column carousel during the first operating cycle with Hot Commissioning Operations feed assuming fresh RF resin. The plots are designed to indicate sensitivity to the parameters varied in the case studies.

Figure 10-61 shows the impact on cesium breakthrough with variation in potassium concentration for the lead column with Hot Commissioning feed during the first cycle. The order of breakthrough is from high to low potassium concentration. Since potassium is a strong competitor with cesium for ion-exchange sites, lower potassium leads to significantly greater cesium adsorption. Similarly, Figure 10-62 shows the impact on cesium breakthrough with variation in sodium concentration for the lead column with Hot Commissioning feed during the first cycle. The order of breakthrough is from high to low sodium concentration. Like potassium, sodium is a competitor with cesium for ion-exchange sites and lower sodium leads to greater cesium adsorption. Sodium is a weaker competitor than potassium so varying the sodium concentration from 4 M to 5.5 M has less impact on cesium adsorption than varying the potassium concentration from 0.3 M to 0.8 M.

Figures 10-63 (linear $C/C_0$) and 10-64 (log $C/C_0$) show the impact on cesium breakthrough with variation in feed flow rate for the lead column with Hot Commissioning feed at twice the nominal cesium during the first cycle. These breakthrough curves also apply for the smaller RF particle radius of 190 μm. The sharper breakthrough curve occurs at the lower flow rate. Figures 10-65 (linear $C/C_0$) and 10-66 (log $C/C_0$) show the impact on cesium breakthrough with variation in feed flow rate for the lead column with nominal Hot Commissioning feed and nominal RF particle size during the first cycle. As the flow rate decreases, the breakthrough curves become sharper. The nominal feed flow rate is 15 gpm. Unlike changing the concentration of competing cations which shifts the breakthrough curves, decreasing the feed flow rate simply sharpens the adsorption front but does not alter the midpoint for breakthrough.

Figure 10-67 shows the impact on cesium breakthrough with variation in temperature for the lead column with nominal Hot Commissioning feed during the first cycle. The order of breakthrough is from high to low temperature. This is consistent with Figure 4-8 which shows a decrease in cesium capacity as temperature increases. Increasing the ion-exchange column operating temperature from 25 °C to 45 °C decreases the number of bed volumes processed at 50% breakthrough from about 142 to 91. Operating temperature will have a significant impact on ion-exchange column performance.

Figure 10-68 shows the impact on cesium breakthrough with variation in RF resin particle radius for the lead column with nominal Hot Commissioning feed during the first cycle at a feed flow rate of 20 gpm. As with variations in flow rate, decreasing the ion-exchange particle radius sharpens the adsorption front but does not translate the breakthrough curve.

## 10.5 Breakthrough Curves for Envelope B Operations

Figures 10-69 (linear $C/C_0$) and 10-70 (log $C/C_0$) show cesium breakthrough predictions for the lead column in a three column carousel with nominal Envelope B Operations feed assuming fresh RF resin. The plot shows the impact on breakthrough with variation in liquid flow rate for the first cycle. As before, lowering the flow rate through the column leads to a sharper breakthrough front.

## 10.6 Breakthrough Curves for Subsequent Operations

Figures 10-71 through 10-77 show cesium breakthrough predictions for the lead column in a three column carousel during the first operating cycle with Subsequent Operations feed assuming fresh RF resin. The plots are designed to show sensitivity to the parameters varied in the case studies.

Figure 10-71 shows the impact on cesium breakthrough with variation in sodium concentration for the lead column with Subsequent Operations feed during the first cycle. The order of breakthrough is from high to low sodium concentration. Sodium is a competitor with cesium for ion-exchange sites and lower sodium leads to greater cesium adsorption. Although sodium is a weaker competitor than potassium the sodium concentration still has a significant impact on the cesium adsorption. As the sodium concentration varies from 4 M to 5.5 M the number of bed volumes at 50% breakthrough decreases from about 386 to 259.

Figure 10-72 shows the impact on cesium breakthrough for three cases simulating operation of the caustic leaching process. Results are for the lead column with nominal Subsequent

Operations feed during the first cycle. These are cases SO_04, SO_05 and SO_06 in Table 10-1. Cases SO_04 and SO_05 both assume that 50% of the sodium in the feed is from NaOH while case SO_06 assumes that 20% of the sodium is from NaOH. The only difference between cases SO_04 and SO_05 is that the feed flow rate is 30 gpm for case SO_04 and 35 gpm for case SO_05. Results from these two cases are the two intersecting breakthrough curves with 50% breakthrough at about 512 bed volumes. The relatively high flow rates used for these two cases leads to broad breakthrough curves. Case SO_06 has different concentrations, flow rate and temperature from the other cases. Combined effects from the increase in operating temperature from 25 °C to 45 °C along with increases in cesium and potassium concentrations (see Table 10-1) make for a much faster and sharper breakthrough curve.

Figures 10-73 (linear $C/C_0$) and 10-74 (log $C/C_0$) show the impact on cesium breakthrough with variation in feed flow rate for the lead column with nominal Subsequent Operations feed during the first cycle. The nominal feed flow rate for Subsequent Operations feed is 20 gpm. Unlike changing the concentration of competing cations which shifts the breakthrough curves, decreasing the feed flow rate simply sharpens the adsorption front but does not alter the midpoint for breakthrough.

Figure 10-75 shows the impact on cesium breakthrough with variation in RF resin particle radius for the lead column with nominal Subsequent Operations feed during the first cycle at a feed flow rate of 20 gpm. As with variations in flow rate, decreasing the ion-exchange particle radius sharpens the adsorption front but does not translate the breakthrough curve.

Figure 10-76 shows the impact on cesium breakthrough with variation in temperature at a feed flow rate of 15 gpm for the lead column with nominal Subsequent Operations feed during the first cycle. The order of breakthrough is from high to low temperature. The results are consistent with Figure 4-8 which shows a decrease in cesium capacity as temperature increases. Increasing the ion-exchange column operating temperature from 25 °C to 45 °C decreases the number of bed volumes processed at 50% breakthrough from about 327 to 195.

Figure 10-77 shows the impact on cesium breakthrough with variation in temperature at a feed flow rate of 20 gpm for the lead column with nominal Subsequent Operations feed during the first cycle. The order of breakthrough is from high to low temperature. The results are again consistent with Figure 4-8 which shows a decrease in cesium capacity as temperature increases. Increasing the ion-exchange column operating temperature from 25 °C to 45 °C decreases the number of bed volumes processed at 50% breakthrough from about 326 to 193.

In summary, over the range of values tested, cesium loading on spherical RF resin is most sensitive to the potassium concentration in the feed followed by temperature and sodium concentration. Smaller resin particles and lower flow rates can be used to sharpen the breakthrough front and thereby make more use of the resin's capacity to store cesium. However, using a lower flow rate to more completely load the resin will increase processing time.

Table 10-1. Full scale column simulation parameters.

| Case | Flow Rate gpm | Temp C | K+ M | Na+ M | Cs+ M | Free OH- M | RF Diameter μm | Solution Diffusivity[1] $cm^2/min$ | Resin Capacity[2] mmol/l |
|---|---|---|---|---|---|---|---|---|---|
| HC_01 | 15 | 25 | 0.48 | 4.57 | $2.74x10^{-5}$ | 1.85 | 460 | $4.935x10^{-4}$ | $3.865x10^{-3}$ |
| HC_02 | 15 | 25 | 0.80 | 4.57 | $2.74x10^{-5}$ | 1.85 | 460 | $4.737x10^{-4}$ | $2.425x10^{-3}$ |
| HC_03 | 15 | 25 | 0.30 | 4.57 | $2.74x10^{-5}$ | 1.85 | 460 | $5.050x10^{-4}$ | $5.811x10^{-3}$ |
| HC_04 | 15 | 25 | 0.42 | 4.00 | $2.40x10^{-5}$ | 1.62 | 460 | $5.785x10^{-4}$ | $3.986x10^{-3}$ |
| HC_05 | 15 | 25 | 0.58 | 5.50 | $3.30x10^{-5}$ | 2.23 | 460 | $3.751x10^{-4}$ | $3.665x10^{-3}$ |
| HC_06 | 20 | 25 | 0.53 | 5.00 | $3.00x10^{-5}$ | 2.02 | 460 | $4.355x10^{-4}$ | $3.775x10^{-3}$ |
| HC_07 | 7.2 | 25 | 0.48 | 4.57 | $2.74x10^{-5}$ | 1.85 | 460 | $4.935x10^{-4}$ | $3.865x10^{-3}$ |
| HC_08 | 20 | 25 | 0.48 | 4.57 | $2.74x10^{-5}$ | 1.85 | 460 | $4.935x10^{-4}$ | $3.865x10^{-3}$ |
| HC_09 | 30 | 25 | 0.48 | 4.57 | $2.74x10^{-5}$ | 1.85 | 460 | $4.935x10^{-4}$ | $3.865x10^{-3}$ |
| HC_10 | 15 | 35 | 0.48 | 4.57 | $2.74x10^{-5}$ | 1.85 | 460 | $6.150x10^{-4}$ | $3.021x10^{-3}$ |
| HC_11 | 15 | 45 | 0.48 | 4.57 | $2.74x10^{-5}$ | 1.85 | 460 | $7.389x10^{-4}$ | $2.427x10^{-3}$ |
| HC_12 | 20 | 25 | 0.48 | 4.57 | $2.74x10^{-5}$ | 1.85 | 380 | $4.935x10^{-4}$ | $3.865x10^{-3}$ |
| HC_13 | 15 | 25 | 0.48 | 4.57 | $5.50x10^{-5}$ | 1.85 | 380 | $4.935x10^{-4}$ | $7.374x10^{-3}$ |
| HC_14 | 22 | 25 | 0.48 | 4.57 | $5.50x10^{-5}$ | 1.85 | 380 | $4.935x10^{-4}$ | $7.374x10^{-3}$ |
| EB_01 | 6.5 | 25 | 0.091 | 4.13 | $2.83x10^{-4}$ | 1.28 | 460 | $6.087x10^{-4}$ | $7.740x10^{-2}$ |
| EB_02 | 10 | 25 | 0.091 | 4.13 | $2.83x10^{-4}$ | 1.28 | 460 | $6.087x10^{-4}$ | $7.740x10^{-2}$ |
| SO_01 | 20 | 25 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.80 | 460 | $5.706x10^{-4}$ | $1.622x10^{-2}$ |
| SO_02 | 15 | 25 | 0.131 | 4.00 | $4.38x10^{-5}$ | 0.80 | 460 | $6.516x10^{-4}$ | $1.685x10^{-2}$ |
| SO_03 | 15 | 25 | 0.181 | 5.50 | $6.02x10^{-5}$ | 0.963 | 460 | $4.610x10^{-4}$ | $1.539x10^{-2}$ |
| SO_04 | 30 | 25 | 0.100 | 4.60 | $3.33x10^{-5}$ | 2.067 | 460 | $5.458x10^{-4}$ | $1.718x10^{-2}$ |
| SO_05 | 35 | 25 | 0.100 | 4.60 | $3.33x10^{-5}$ | 2.067 | 460 | $5.458x10^{-4}$ | $1.718x10^{-2}$ |
| SO_06 | 24 | 45 | 0.125 | 4.60 | $4.17x10^{-5}$ | 1.433 | 460 | $8.287x10^{-4}$ | $1.000x10^{-2}$ |
| SO_07 | 15 | 25 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.80 | 460 | $5.706x10^{-4}$ | $1.622x10^{-2}$ |
| SO_08 | 15 | 25 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.60 | 460 | $5.737x10^{-4}$ | $1.580x10^{-2}$ |
| SO_09 | 24 | 25 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.80 | 460 | $5.706x10^{-4}$ | $1.622x10^{-2}$ |
| SO_10 | 30 | 25 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.80 | 460 | $5.706x10^{-4}$ | $1.622x10^{-2}$ |
| SO_11 | 15 | 35 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.80 | 460 | $6.927x10^{-4}$ | $1.231x10^{-2}$ |
| SO_12 | 15 | 45 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.80 | 460 | $8.209x10^{-4}$ | $0.953x10^{-2}$ |
| SO_13 | 20 | 45 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.80 | 460 | $8.209x10^{-4}$ | $0.953x10^{-2}$ |
| SO_14 | 20 | 25 | 0.150 | 4.60 | $5.00x10^{-5}$ | 0.80 | 380 | $5.706x10^{-4}$ | $1.622x10^{-2}$ |

1 In all cases, the particle or pore cesium diffusivity is equal to one third of the solution or free stream diffusivity listed in the table.

2 The resin capacity is given as mmol cesium per liter of bed volume. The resin capacity is calculated from the isotherm equation as: $Q = a\,[Cs]^{Ma}/(\beta + [Cs]^{Mb})$ using the feed cesium composition. The capacity is the maximum bed loading that can be achieved with the feed solution. A bed density of 0.2563 g resin ($H^+$ form)/liter BV, obtained from SRNL experimental data, was used to convert from mmol/g resin to mmol/liter of bed volume.

Table 10-2. Number of bed volumes required to reach lag column Cs breakthrough and 50% breakthrough during three-column carousel operation for nominal Hot Commissioning Operations.

| Cycle Number | Lead Column Exit to Feed Concentration Ratio (%) | Number of bed volumes required to reach lag column exit criterion (BV) | Number of bed volumes required to reach 50% breakthrough (BV) |
|---|---|---|---|
| 1 | 100 | 206 | 142 |
| 2 | 94 | 128 | 80 |
| 3 | 87 | 131 | 94 |
| 4 | 80 | 134 | 107 |
| 5 | 76 | 138 | 111 |

Table 10-3. Number of bed volumes required to reach lag column Cs breakthrough during three-column carousel operation for nominal Envelope B Operations.

| Cycle Number | Lead Column Exit to Feed Concentration Ratio (%) | Number of bed volumes required to reach lag column exit criterion (BV) | Number of bed volumes required to reach 50% breakthrough (BV) |
|---|---|---|---|
| 1 | 100 | 524 | 276 |
| 2 | 100 | 276 | 28 |
| 3 | 100 | 277 | 27 |

Table 10-4. Number of bed volumes required to reach lag column Cs breakthrough during three-column carousel operation for nominal Subsequent Operations.

| Cycle Number | Lead Column Exit to Feed Concentration Ratio (%) | Number of bed volumes required to reach lag column exit criterion (BV) | Number of bed volumes required to reach 50% breakthrough (BV) |
|---|---|---|---|
| 1 | 100 | 494 | 326 |
| 2 | 100 | 312 | 158 |
| 3 | 99 | 319 | 171 |
| 4 | 99 | 323 | 178 |
| 5 | 99 | 323 | 181 |

Table 10-5. Number of bed volumes required to reach lag column Cs breakthrough and 50% breakthrough during three-column carousel operation for Hot Commissioning Operations cases. 50% breakthrough bed volumes in parentheses.

| Cycle Number | HC_01 Nominal | HC_02 | HC_03 | HC_04 | HC_05 | HC_06 | HC_07 | HC_08 |
|---|---|---|---|---|---|---|---|---|
| 1 | 206 (142) | 126 (89) | 315 (214) | 251 (167) | 151 (114) | 165 (128) | 230 (144) | 191 (144) |
| 2 | 128 ( 80) | 77 (54) | 198 (114) | 155 ( 84) | 98 ( 74) | 111 ( 91) | 138 ( 57) | 128 ( 94) |
| 3 | 131 ( 94) | 80 (67) | 202 (128) | 154 ( 97) | 101 ( 87) | 111 (104) | 138 ( 60) | 128 (107) |
| 4 | 134 (107) | 84 (74) | 205 (141) | 161 (111) | 104 ( 97) | 117 (114) | 138 ( 67) | 131 (117) |
| 5 | 138 (111) | 84 (77) | 208 (148) | 161 (117) | 104 ( 97) | 118 (114) | 141 ( 70) | 134 (124) |
| 6 | 138 (114) | 87 (80) | 208 (151) | 165 (121) | 107 (101) | 121 (114) | 141 ( 74) | 138 (124) |
| 7 | 138 (114) | 84 (81) | 208 (155) | 165 (125) | 104 (101) | 118 (114) | 141 ( 74) | 134 (124) |

Table 10-6. Number of bed volumes required to reach lag column Cs breakthrough and 50% breakthrough during three-column carousel operation for Hot Commissioning Operations cases. 50% breakthrough bed volumes in parentheses.

| Cycle Number | HC_01 Nominal | HC_09 | HC_10 | HC_11 | HC_12 | HC_13 | HC_14 |
|---|---|---|---|---|---|---|---|
| 1 | 206 (142) | 171 (141) | 166 (112) | 134 (91) | 209 (142) | 209 (135) | 198 (137) |
| 2 | 128 ( 80) | 121 (111) | 101 ( 57) | 84 (47) | 131 ( 77) | 132 ( 65) | 124 ( 74) |
| 3 | 131 ( 94) | 124 (124) | 104 ( 70) | 84 (54) | 131 ( 87) | 131 ( 67) | 128 ( 87) |
| 4 | 134 (107) | 124 (124) | 104 ( 77) | 84 (60) | 137 (100) | 131 ( 70) | 131 ( 94) |
| 5 | 138 (111) | 131 (131) | 107 ( 84) | 87 (67) | 135 (104) | 134 ( 77) | 131 ( 97) |
| 6 | 138 (114) | 128 (128) | 107 ( 87) | 88 (67) | 137 (111) | 134 ( 77) | 134 (100) |
| 7 | 138 (114) | 131 (131) | 111 ( 90) | 88 (71) | 141 (114) | 134 ( 81) | 131 (104) |

Table 10-7. Number of bed volumes required to reach lag column Cs breakthrough and 50% breakthrough during three-column carousel operation for Envelope B Operations cases. 50% breakthrough bed volumes in parentheses.

| Cycle Number | EB_01 Nominal | EB_02 |
|---|---|---|
| 1 | 524 (276) | 523 (276) |
| 2 | 276 ( 28) | 272 ( 30) |
| 3 | 277 ( 27) | 278 ( 31) |
| 4 | | 272 ( 30) |
| 5 | | 267 ( 31) |
| 6 | | 281 ( 39) |

Table 10-8. Number of bed volumes required to reach lag column Cs breakthrough and 50% breakthrough during three-column carousel operation for Subsequent Operations cases. 50% breakthrough bed volumes in parentheses.

| Cycle Number | SO_01 Nominal | SO_02 | SO_03 | SO_04 | SO_05 | SO_06 | SO_07 | SO_08 |
|---|---|---|---|---|---|---|---|---|
| 1 | 494 (326) | 635 (386) | 390 (259) | 715 (513) | 684 (512) | 366 (241) | 517 (327) | 509 (319) |
| 2 | 313 (158) | 382 (140) | 245 (124) | 480 (319) | 470 (346) | 228 (118) | 325 (136) | 310 (128) |
| 3 | 319 (171) | 381 (141) | 255 (137) | 494 (353) | 487 (386) | 232 (131) | 323 (138) | 312 (134) |
| 4 | 323 (178) | 386 (147) | 252 (138) | 504 (373) | 497 (403) | 235 (141) | 323 (141) | 316 (141) |
| 5 | 323 (181) | 388 (147) | 255 (144) | 507 (380) | 504 (410) | 238 (148) | 326 (144) | 319 (141) |
| 6 | 326 (185) | 383 (148) | 259 (148) | 511 (383) | 501 (410) | 242 (151) | 326 (146) | 316 (141) |
| 7 | 326 (185) | | 255 (144) | 507 (383) | 504 (413) | 238 (148) | 326 (146) | 319 (141) |

Table 10-9. Number of bed volumes required to reach lag column Cs breakthrough and 50% breakthrough during three-column carousel operation for Subsequent Operations cases. 50% breakthrough bed volumes in parentheses.

| Cycle Number | SO_01 Nominal | SO_09 | SO_10 | SO_11 | SO_12 | SO_13 | SO_14 |
|---|---|---|---|---|---|---|---|
| 1 | 494 (326) | 474 (326) | 448 (323) | 398 (247) | 312 (195) | 297 (193) | 533 (327) |
| 2 | 313 (158) | 306 (178) | 299 (205) | 244 ( 98) | 185 ( 74) | 181 ( 87) | 313 (121) |
| 3 | 319 (171) | 316 (198) | 309 (228) | 242 (101) | 188 ( 80) | 188 (100) | 330 (132) |
| 4 | 323 (178) | 322 (208) | 319 (242) | 249 (107) | 191 ( 84) | 188 (104) | 325 (128) |
| 5 | 323 (181) | 322 (212) | 319 (245) | 245 (107) | 191 ( 84) | 191 (107) | 324 (131) |
| 6 | 326 (185) | 322 (215) | 319 (248) | 249 (111) | 192 ( 88) | 192 (108) | 328 (131) |
| 7 | 326 (185) | 326 (215) | 322 (249) | 245 (107) | 192 ( 88) | 191 (107) | 328 (131) |

Table 10-10. Bed volumes required to reach $^{137}Cs$ loading limits (Prior to Cycling).

| LAW Feed Operations | Isotherm | LLL 75000 Ci | LCO 125000 Ci | TSL 150000 Ci |
|---|---|---|---|---|
| Hot Commissioning | Nominal | NA | NA | NA |
| Envelope B | Nominal | 30 | 50 | 60 |
| Subsequent Operation | Nominal | 235 | 392 | 470 |

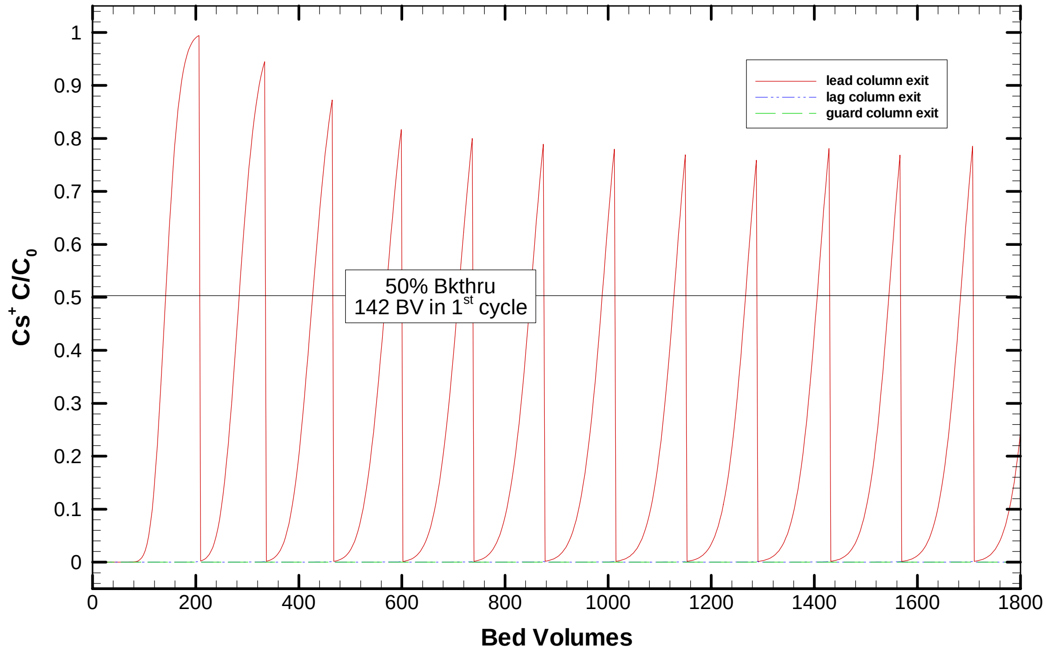


Figure 10-1. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

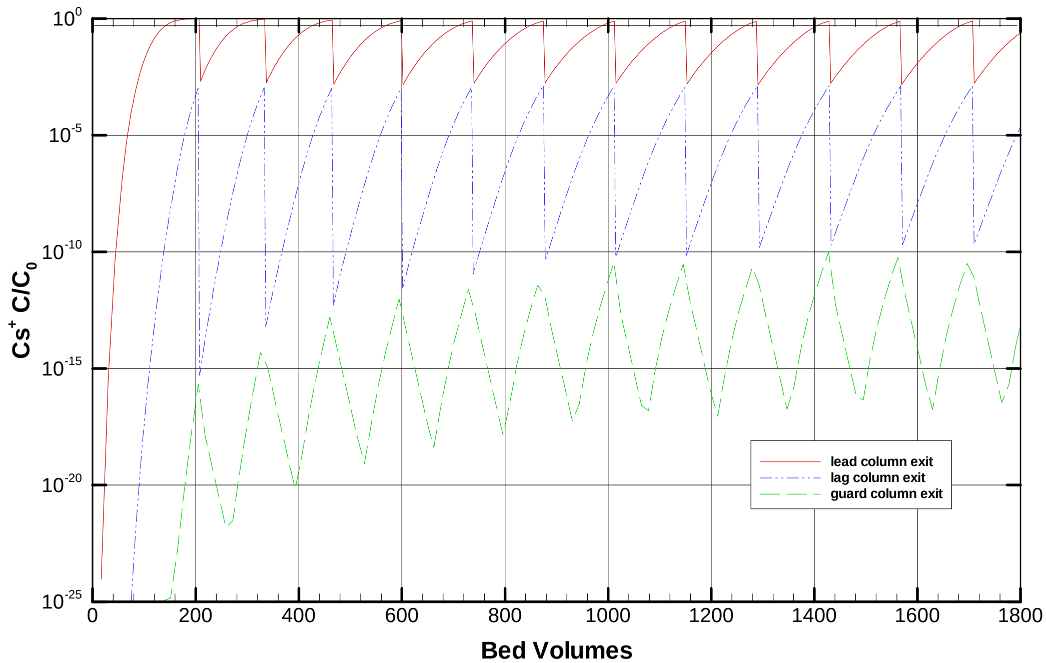


Figure 10-2. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

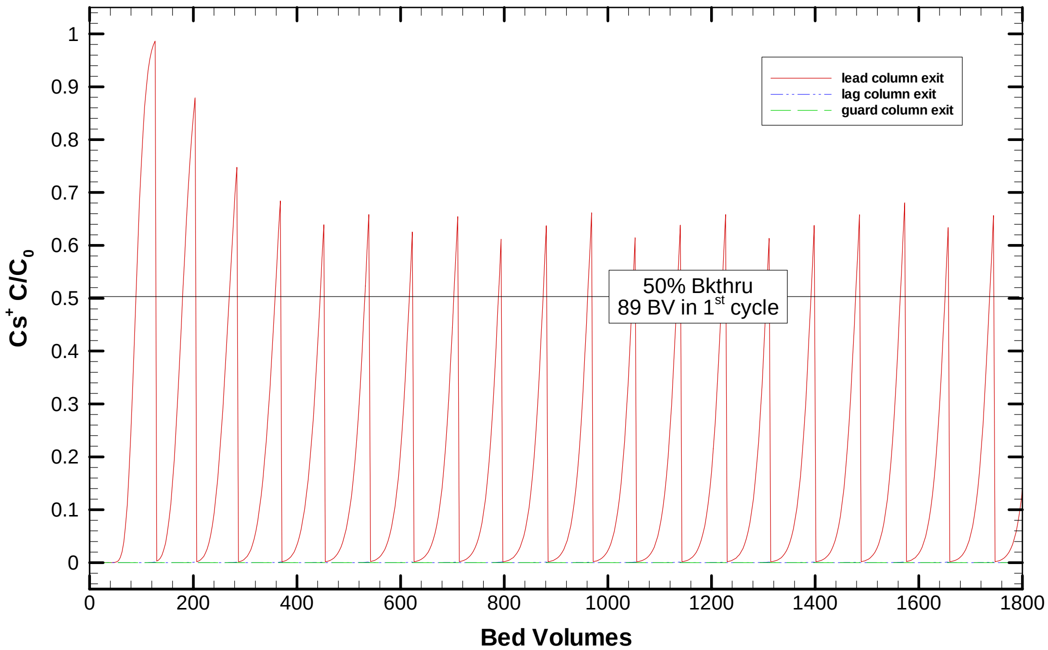


Figure 10-3. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with 0.8 M potassium Hot Commissioning Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

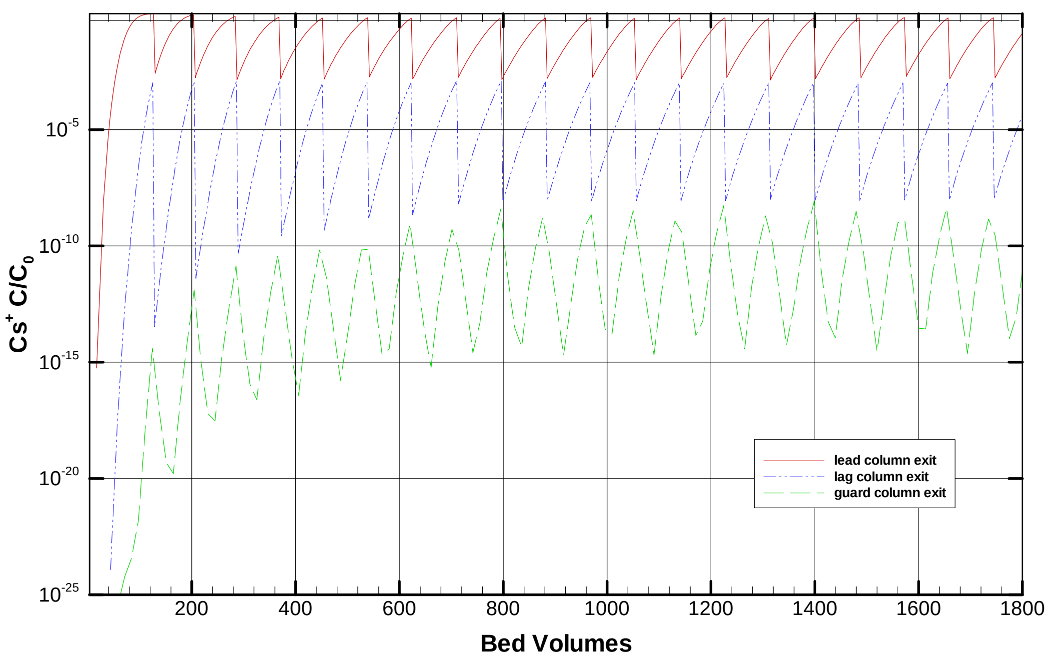


Figure 10-4. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with 0.8 M potassium Hot Commissioning Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

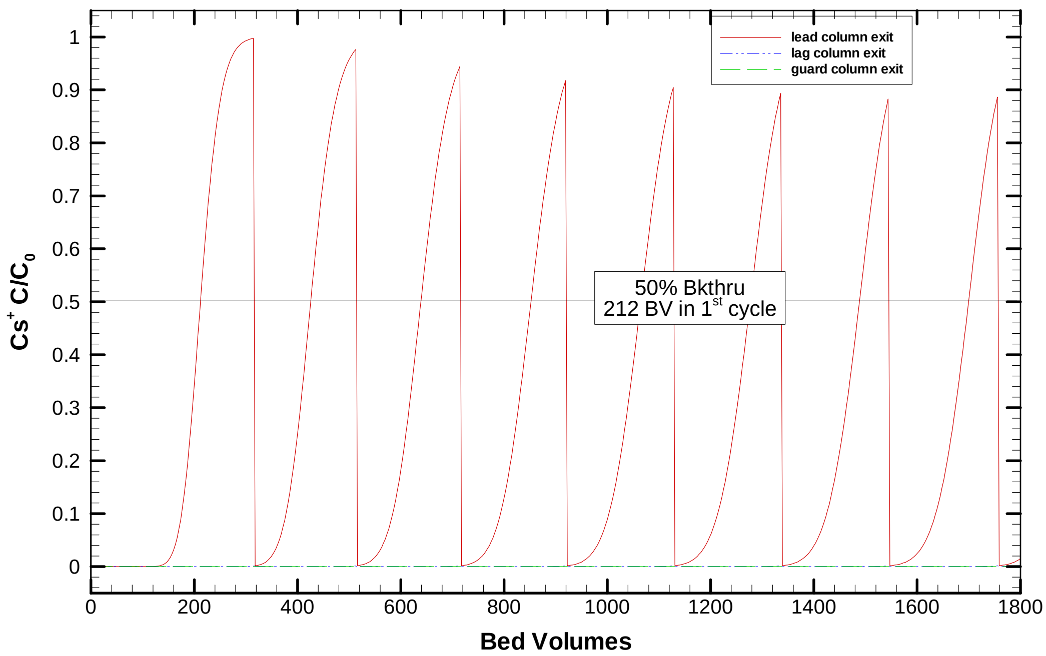


Figure 10-5. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with 0.3 M potassium Hot Commissioning Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

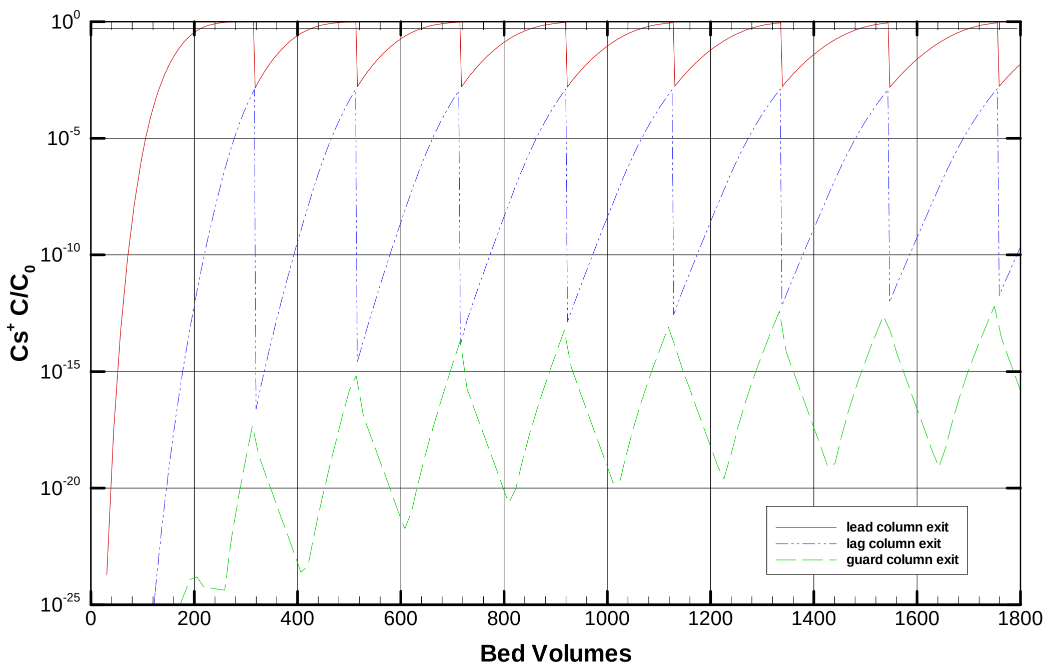


Figure 10-6. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with 0.3 M potassium Hot Commissioning Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

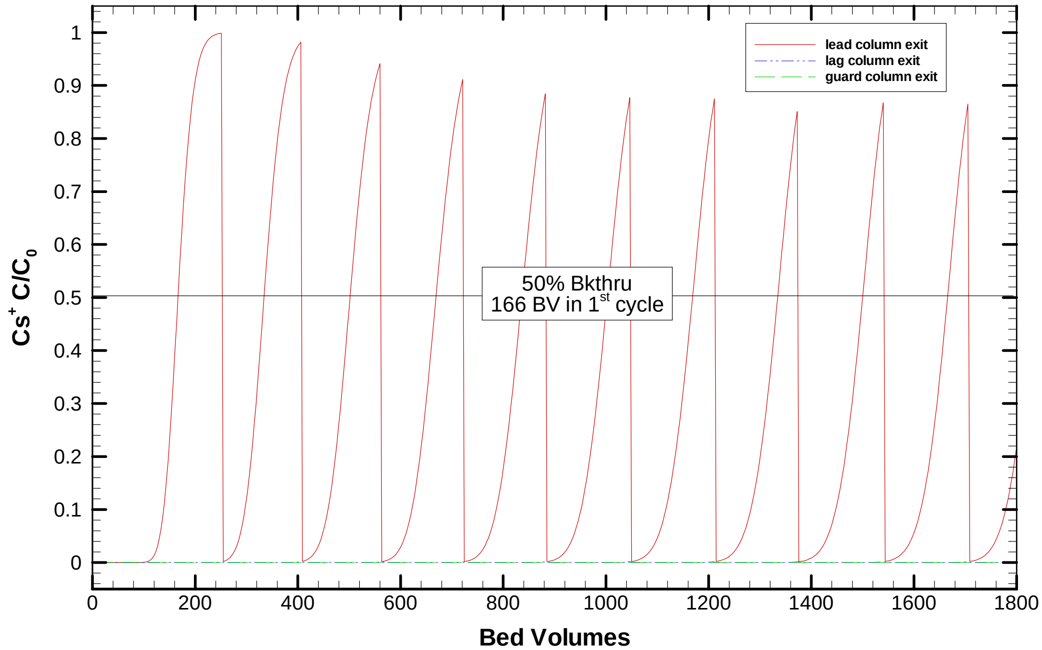


Figure 10-7. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed diluted to 4 M sodium at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

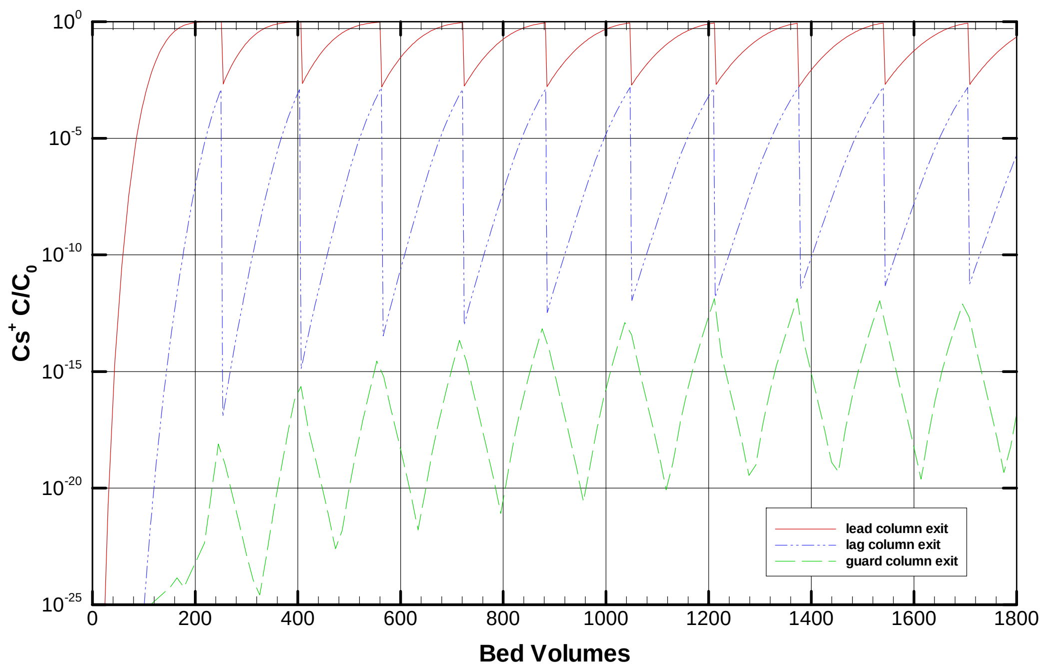


Figure 10-8. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed diluted to 4 M sodium at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

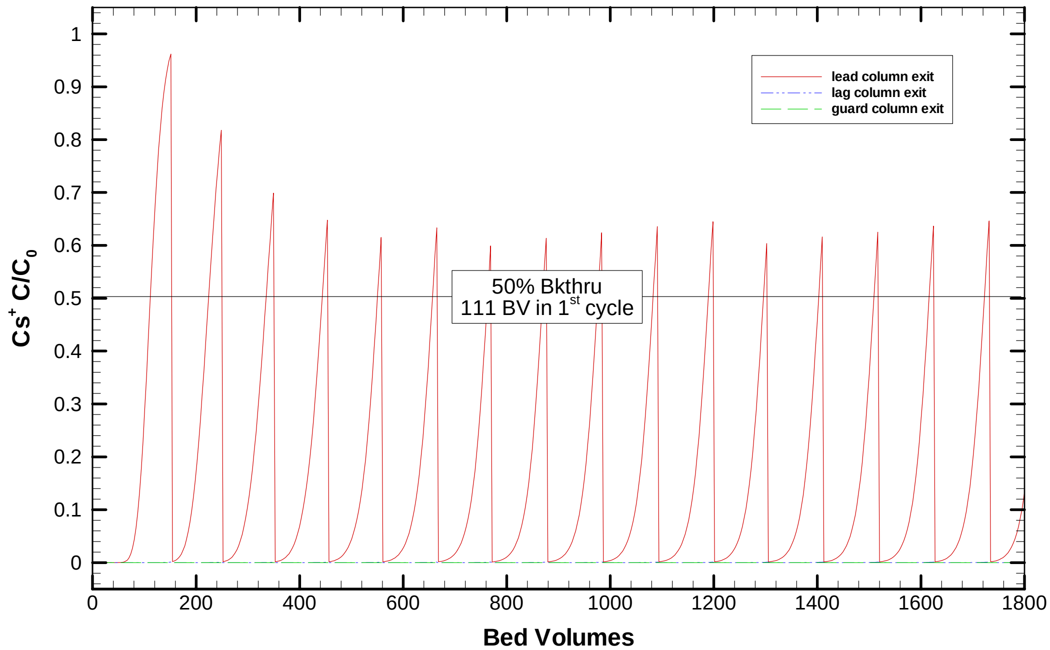


Figure 10-9. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed concentrated to 5.5 M sodium at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

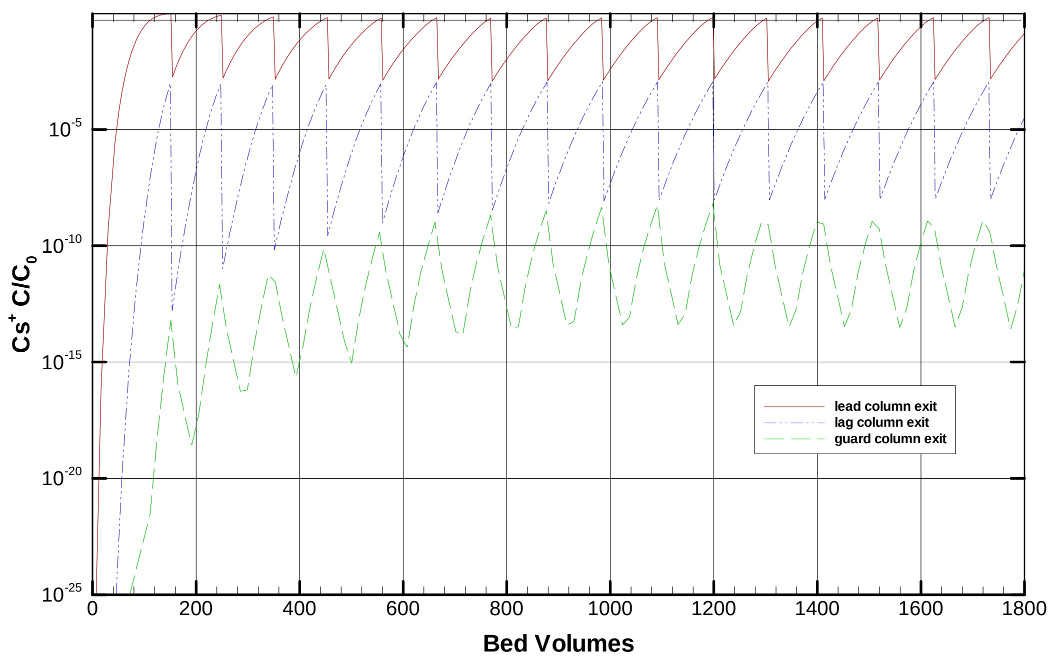


Figure 10-10. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed concentrated to 5.5 M sodium at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

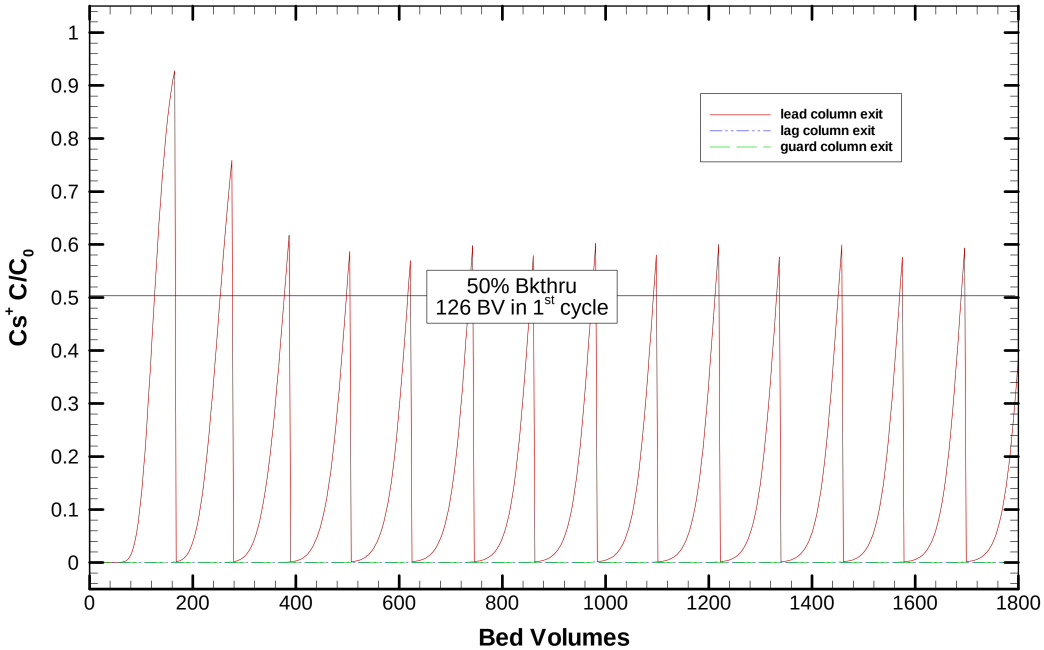


Figure 10-11. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed concentrated to 5 M sodium at a flow rate of 20 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

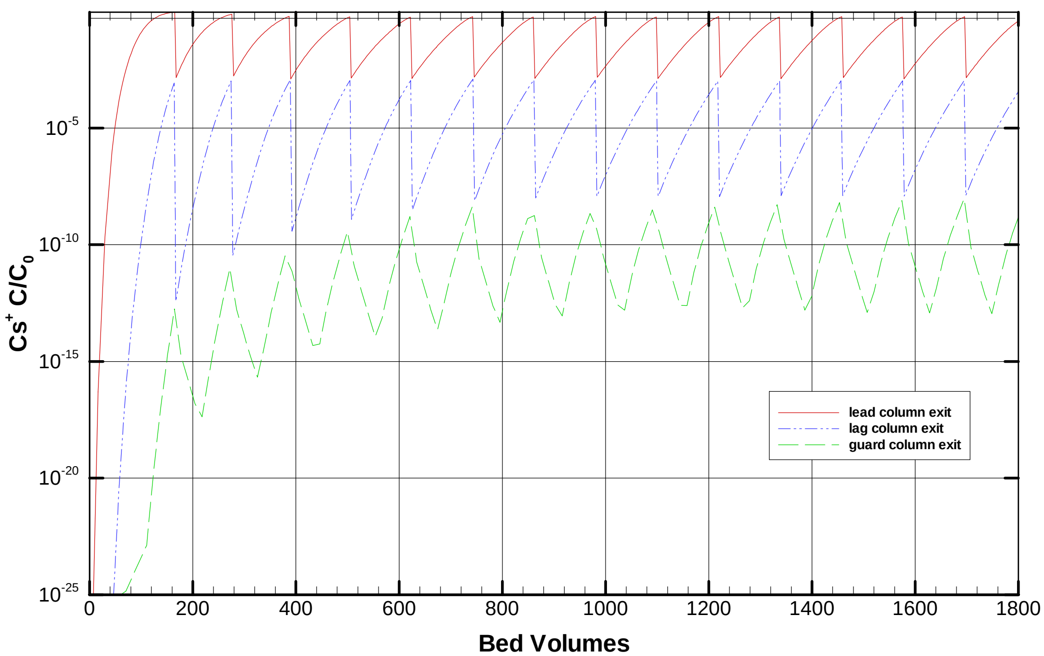


Figure 10-12. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed concentrated to 5 M sodium at a flow rate of 20 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

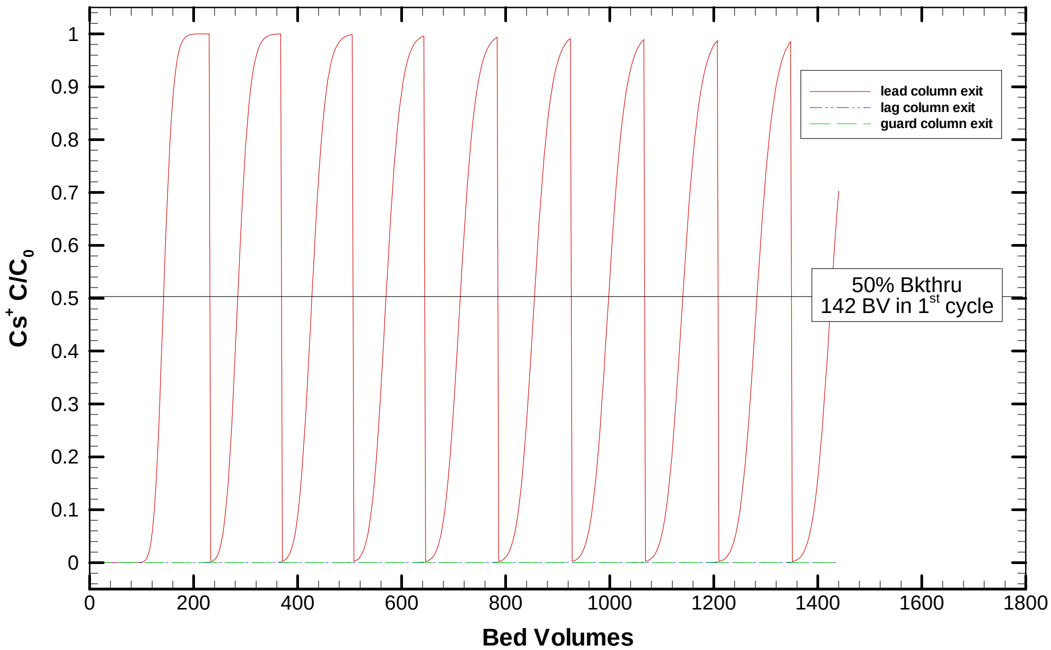


Figure 10-13. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate of 7.2 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

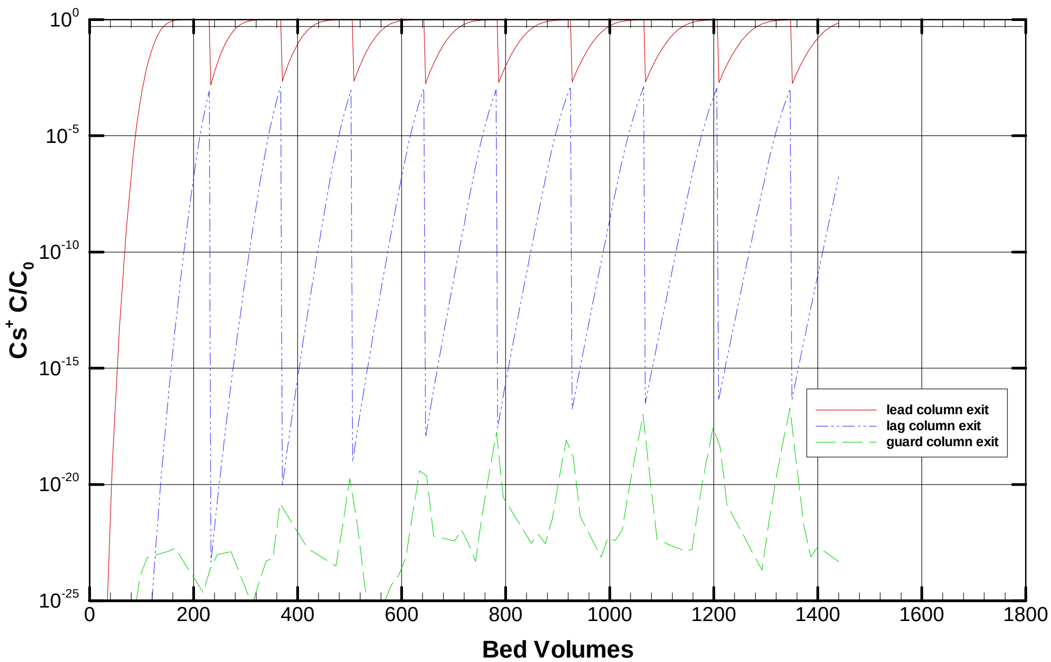


Figure 10-14. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate of 7.2 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

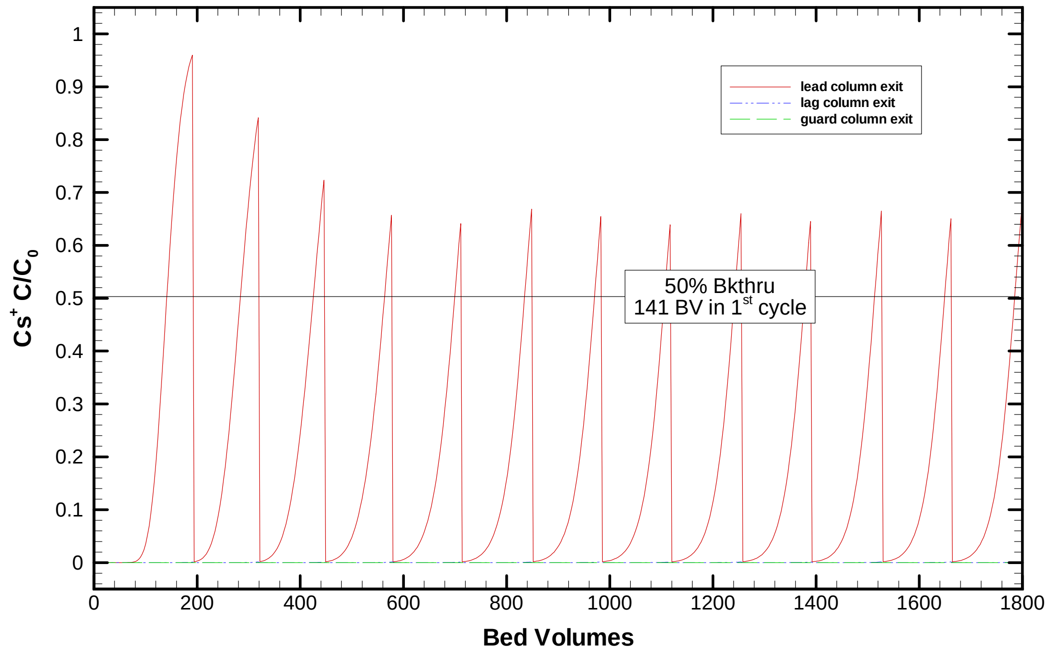


Figure 10-15. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate 20 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

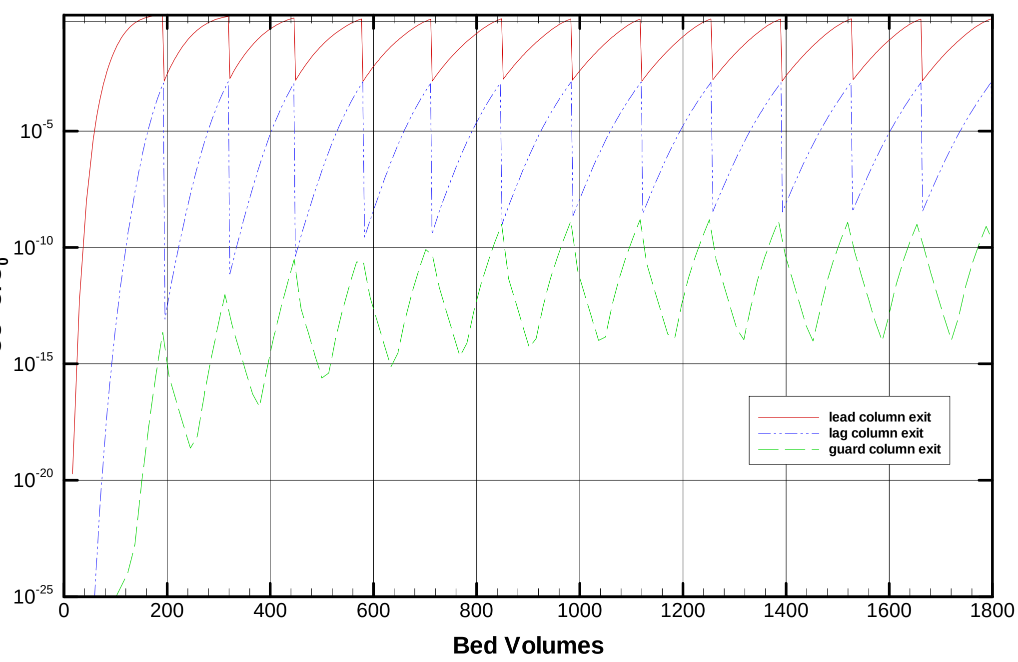


Figure 10-16. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate 20 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

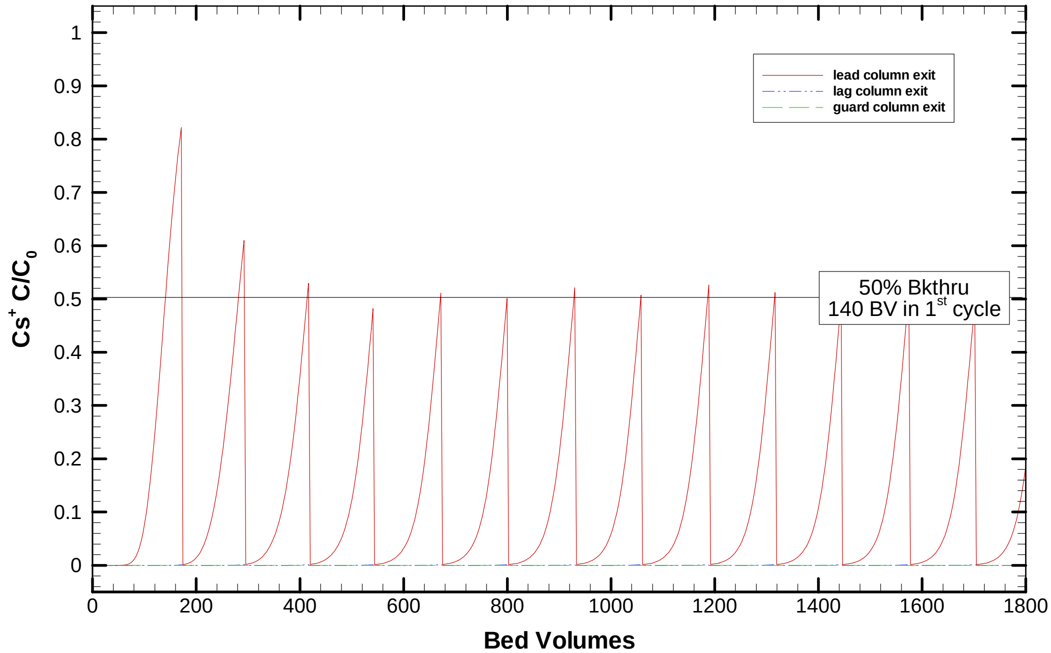


Figure 10-17. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate 30 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

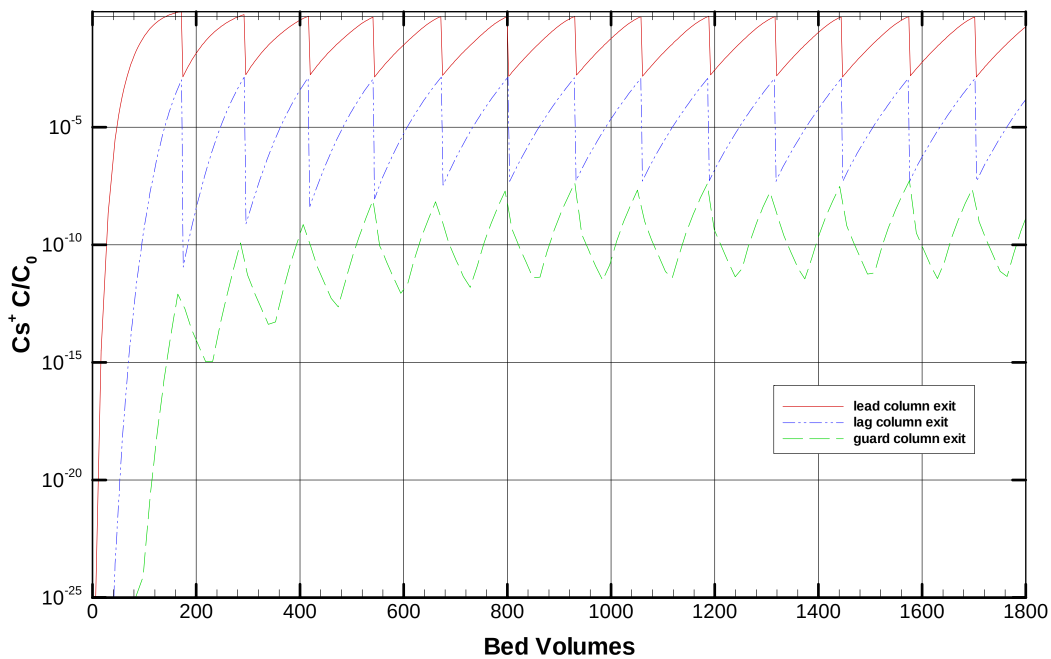


Figure 10-18. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate 30 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

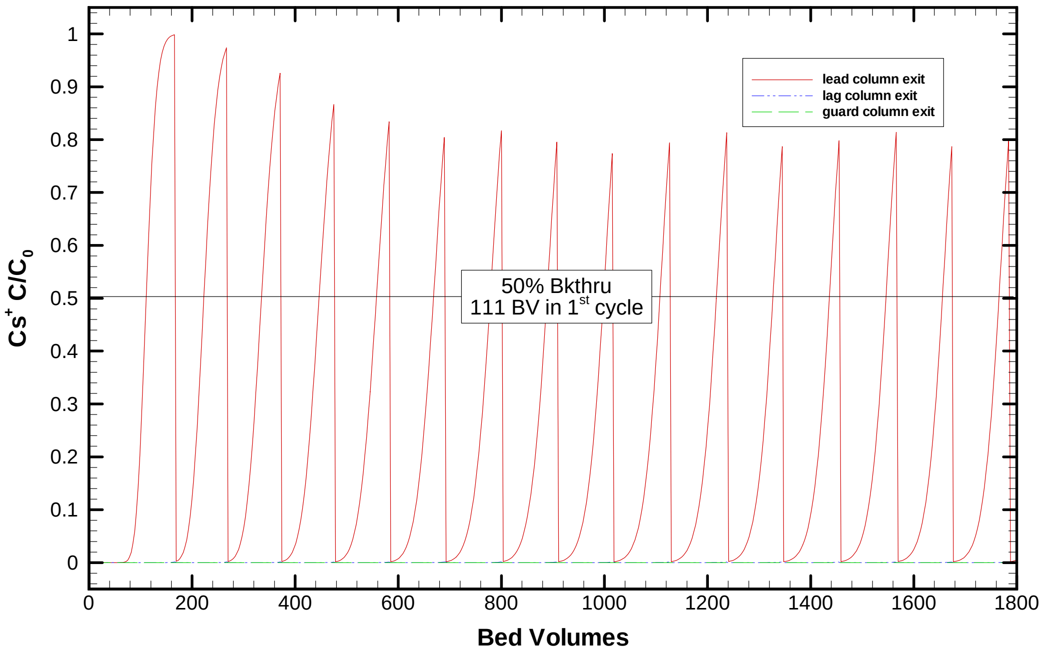


Figure 10-19. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate 15 gpm and a temperature of 35 °C with 460 µm diameter RF spheres.

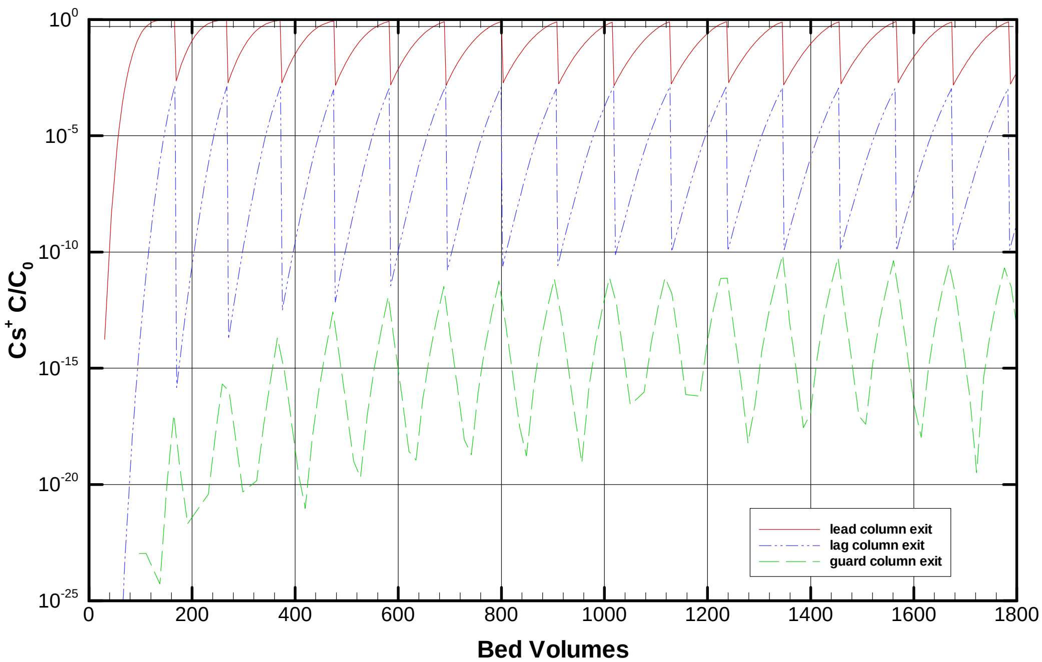


Figure 10-20. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate 15 gpm and a temperature of 35 °C with 460 µm diameter RF spheres.

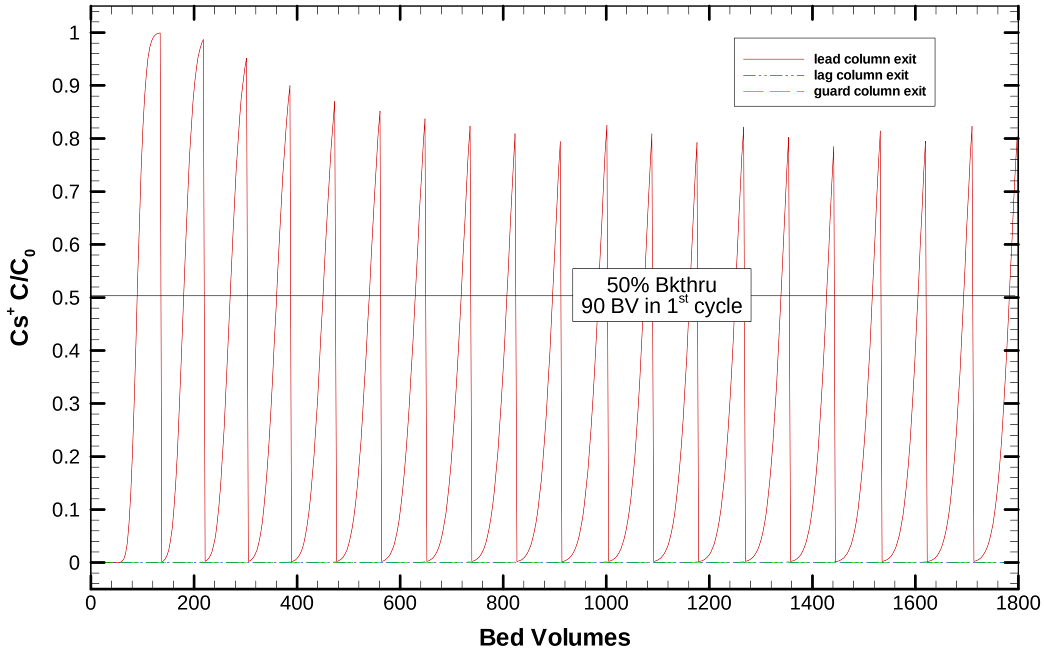


Figure 10-21. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate of 15 gpm and a temperature of 45 °C with 460 μm diameter RF spheres.

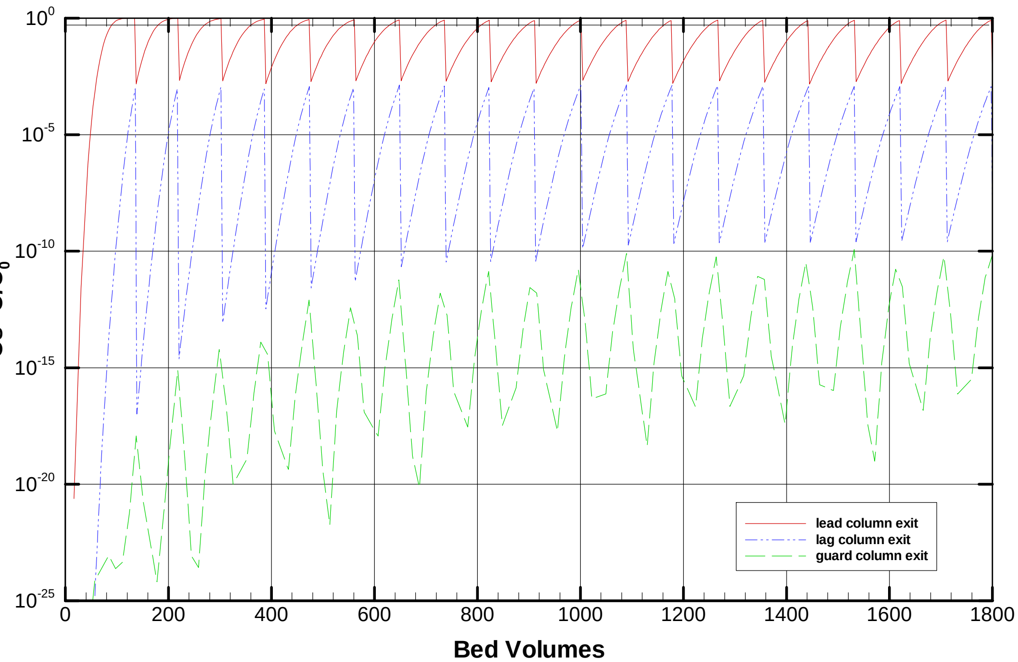


Figure 10-22. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate of 15 gpm and a temperature of 45 °C with 460 μm diameter RF spheres.

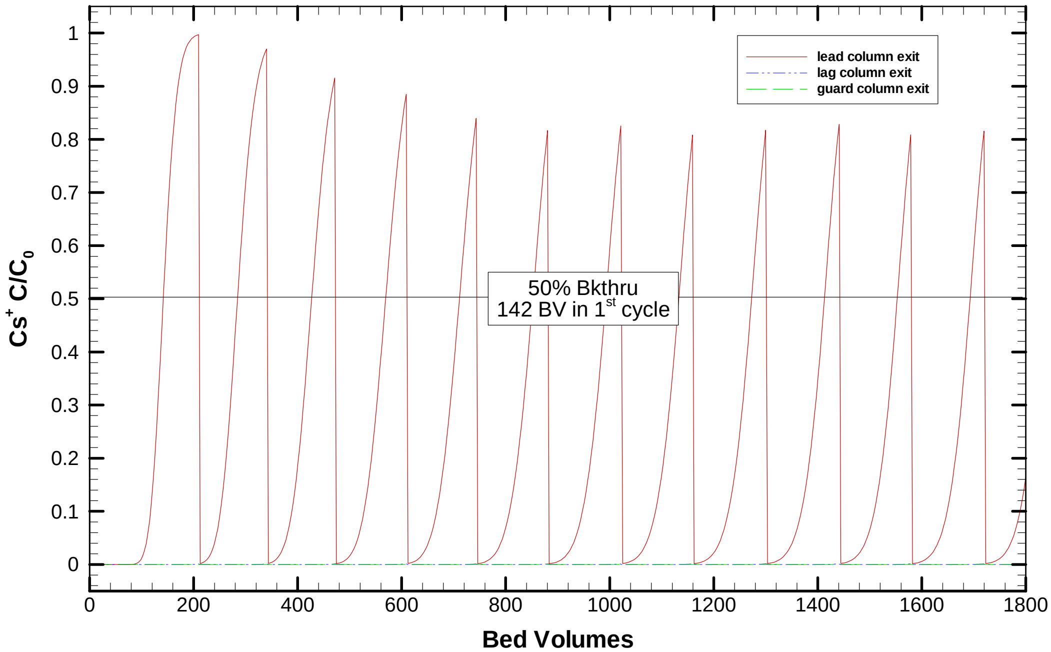


Figure 10-23. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate of 20 gpm and a temperature of 25 °C with 380 μm diameter RF spheres.

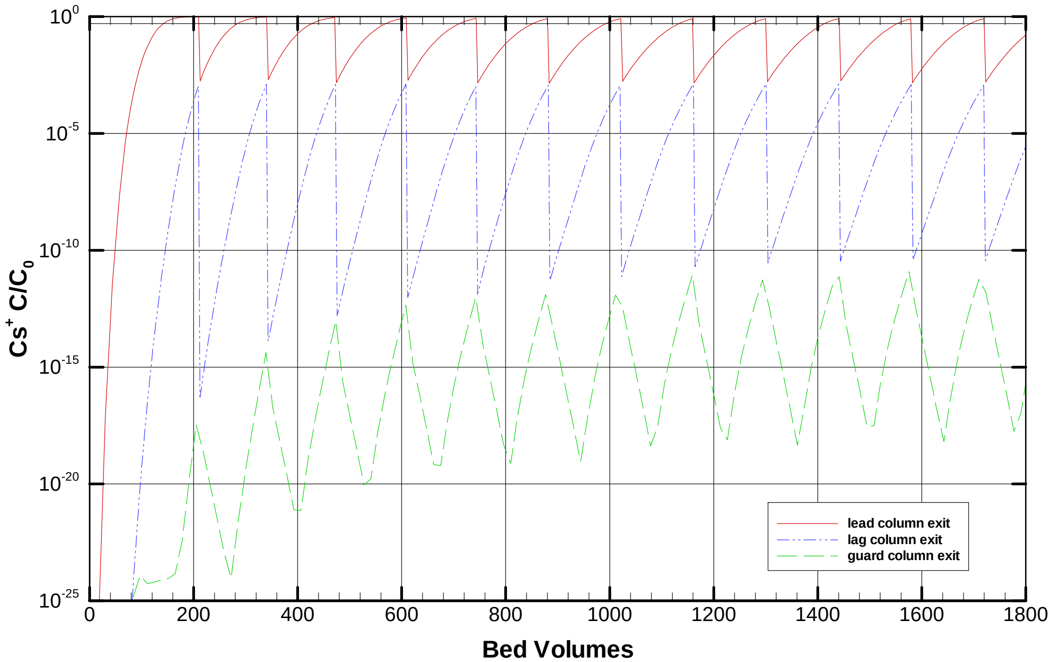


Figure 10-24. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Hot Commissioning Operations feed at a flow rate of 20 gpm and a temperature of 25 °C with 380 μm diameter RF spheres.

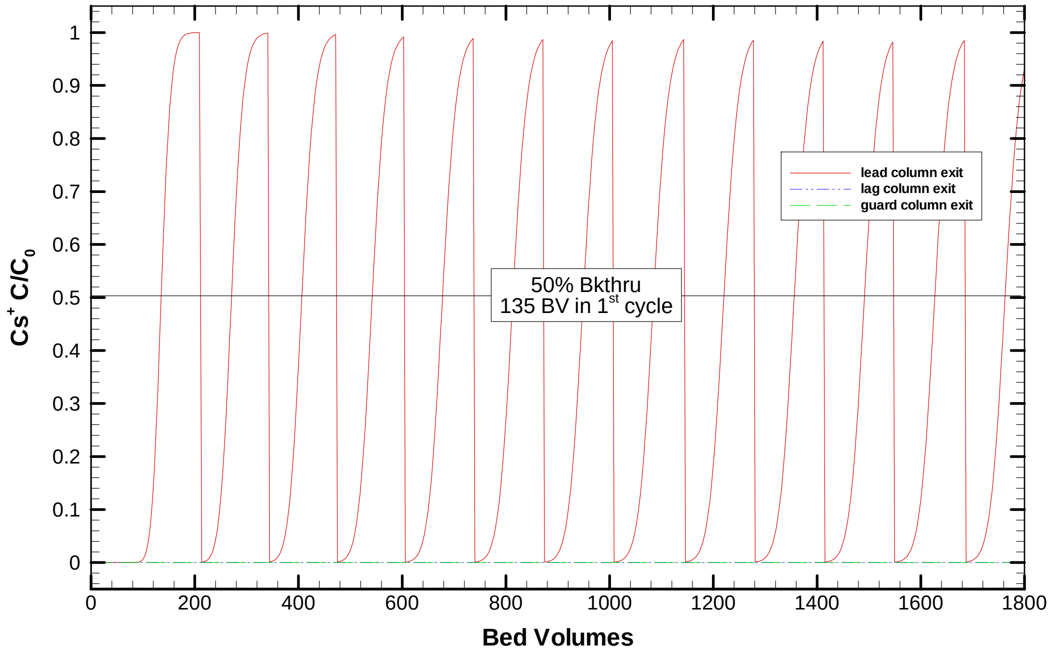


Figure 10-25. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed having twice nominal cesium at a flow rate of 15 gpm and a temperature of 25 °C with 380 μm diameter RF spheres.

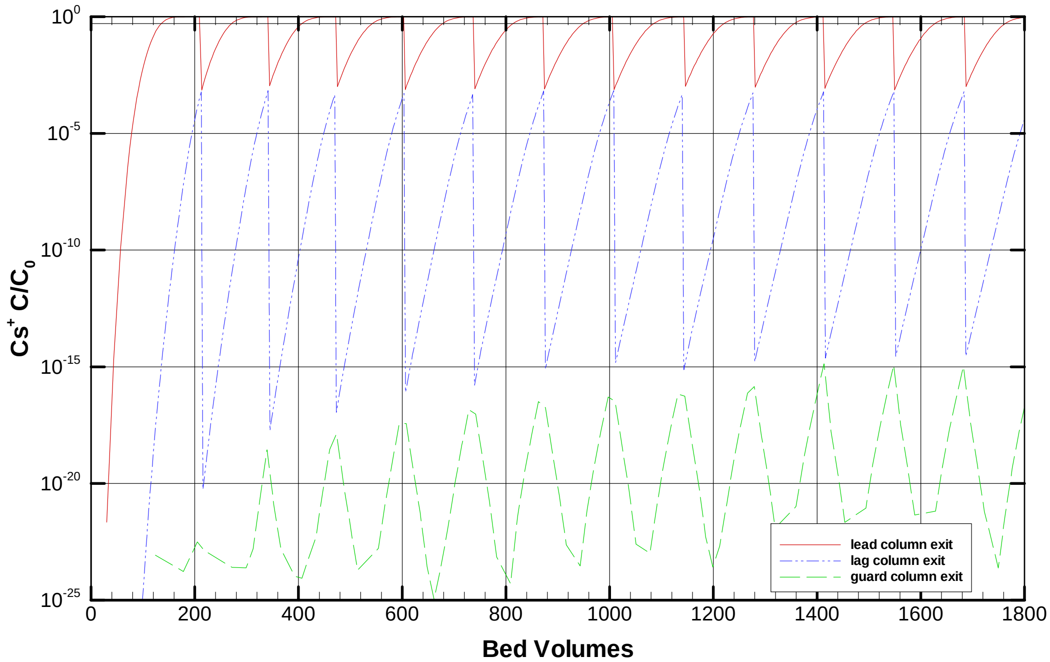


Figure 10-26. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed having twice nominal cesium at a flow rate of 15 gpm and a temperature of 25 °C with 380 μm diameter RF spheres.

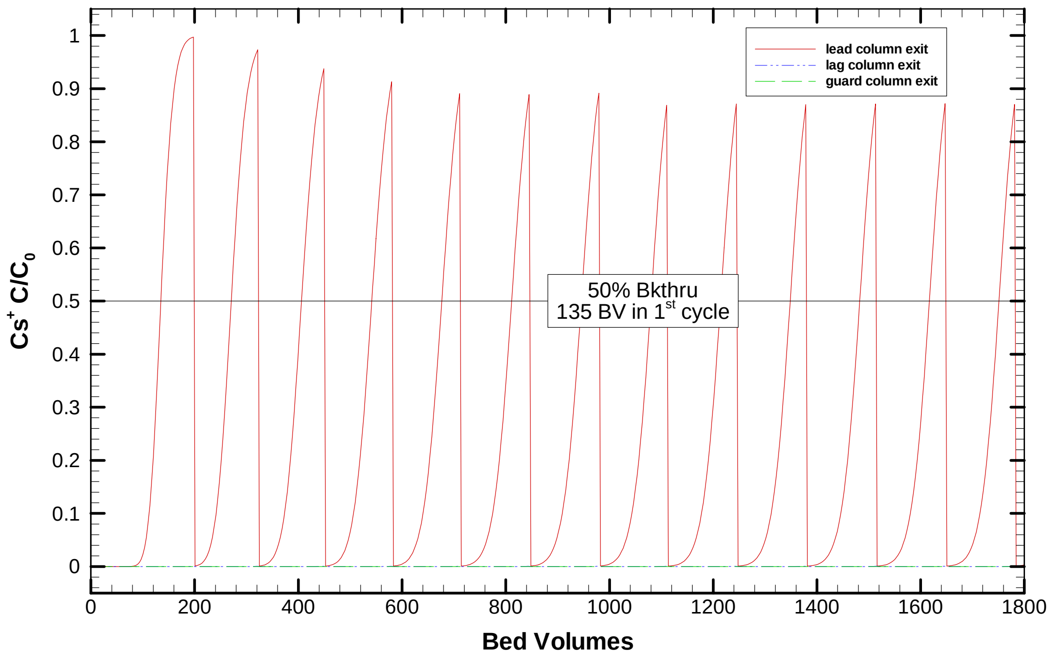


Figure 10-27. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed having twice nominal cesium at a flow rate of 22 gpm and a temperature of 25 °C with 380 µm diameter RF spheres.

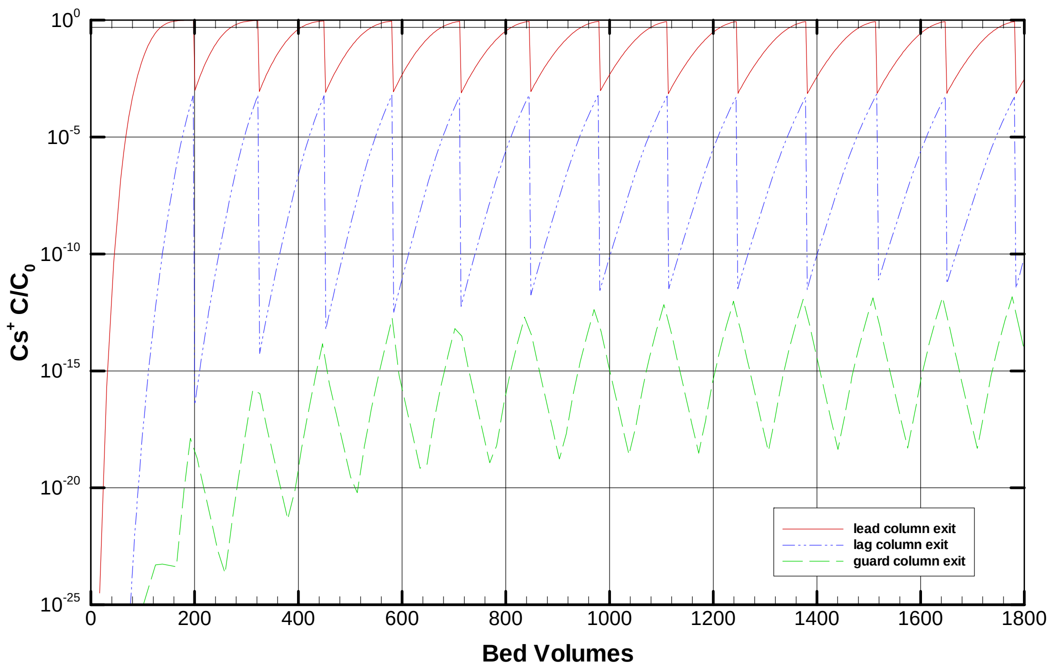


Figure 10-28. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Hot Commissioning Operations feed having twice nominal cesium at a flow rate of 22 gpm and a temperature of 25 °C with 380 µm diameter RF spheres.

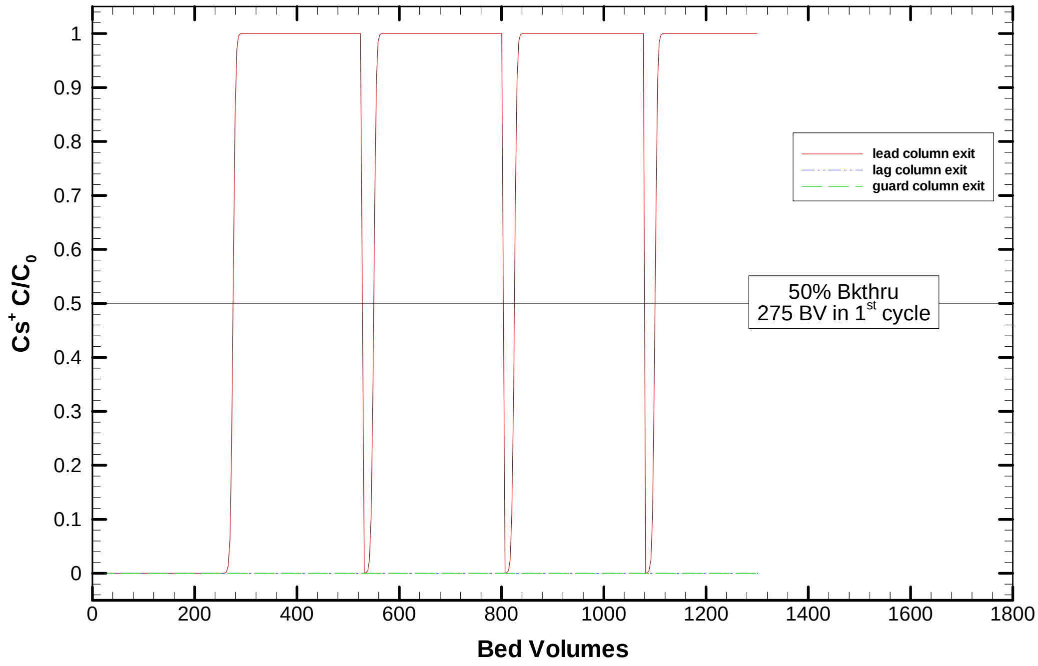


Figure 10-29. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Envelope B Operations feed at a flow rate of 6.5 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

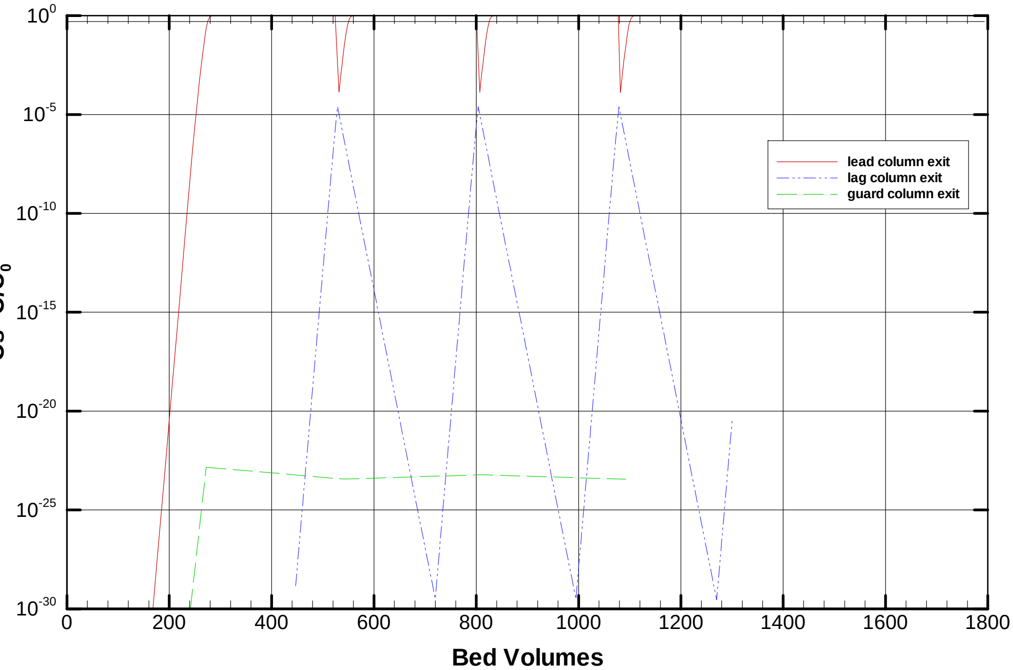


Figure 10-30. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Envelope B Operations feed at a flow rate of 6.5 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

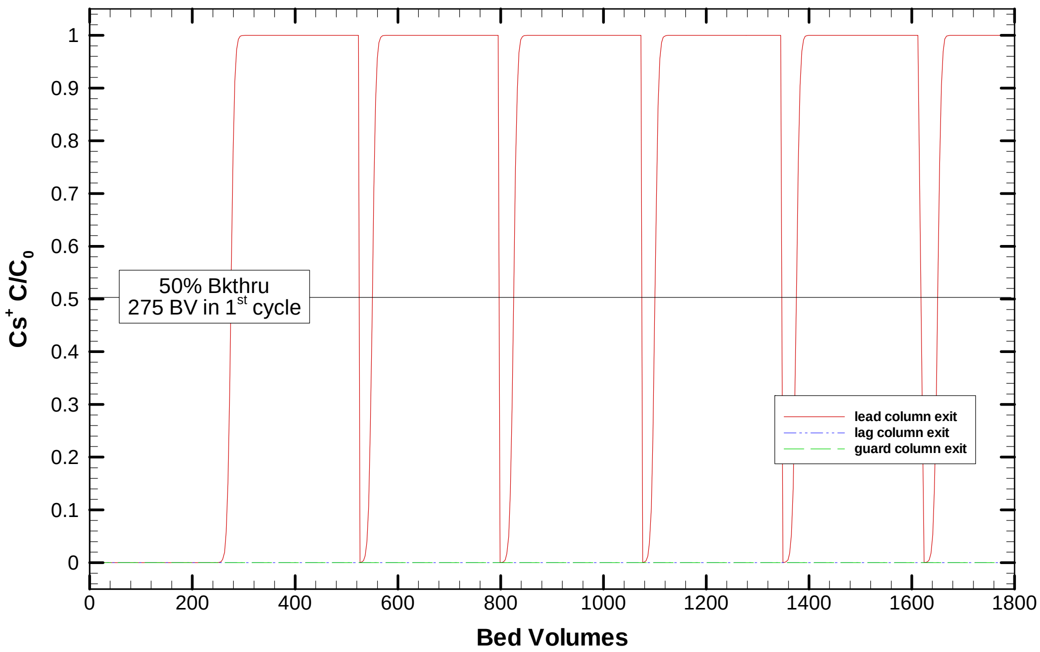


Figure 10-31. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Envelope B Operations feed at a flow rate of 10 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

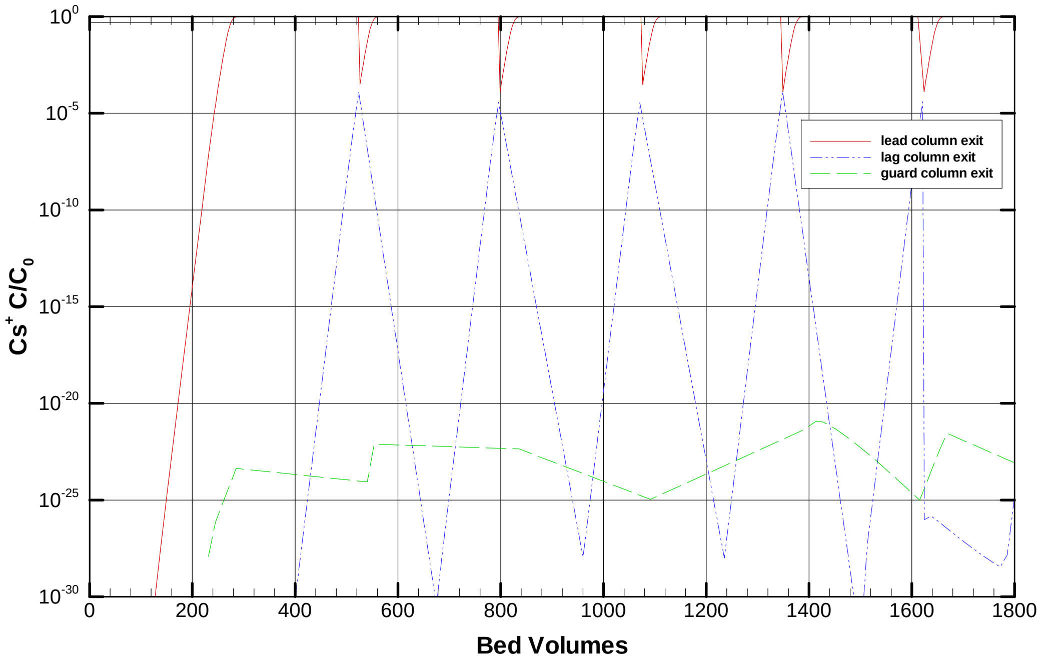


Figure 10-32. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Envelope B Operations feed at a flow rate of 10 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

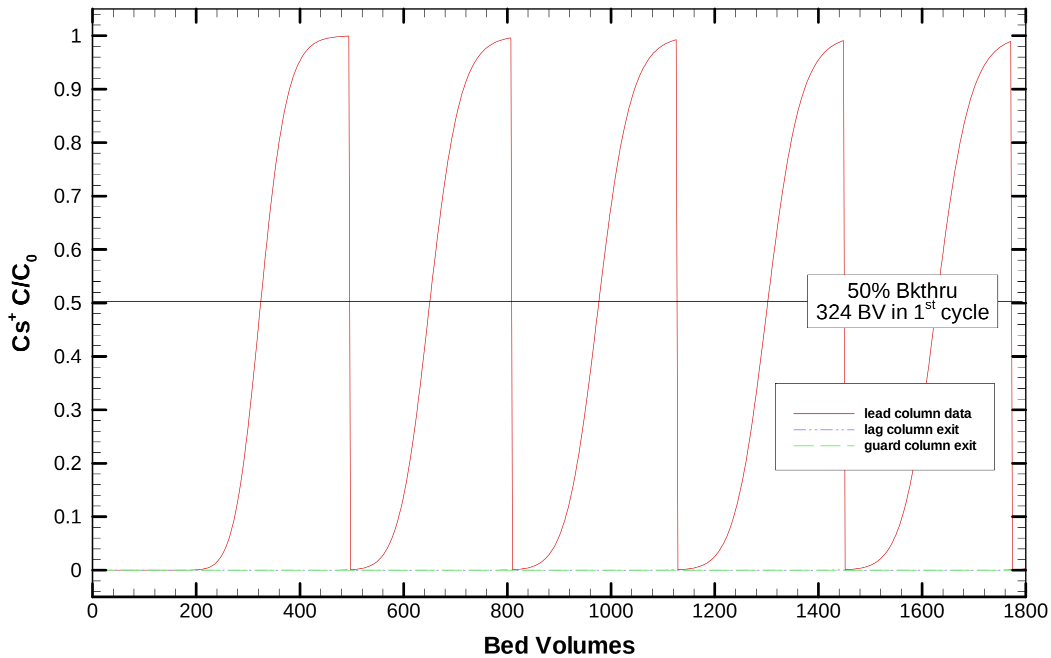


Figure 10-33. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 20 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

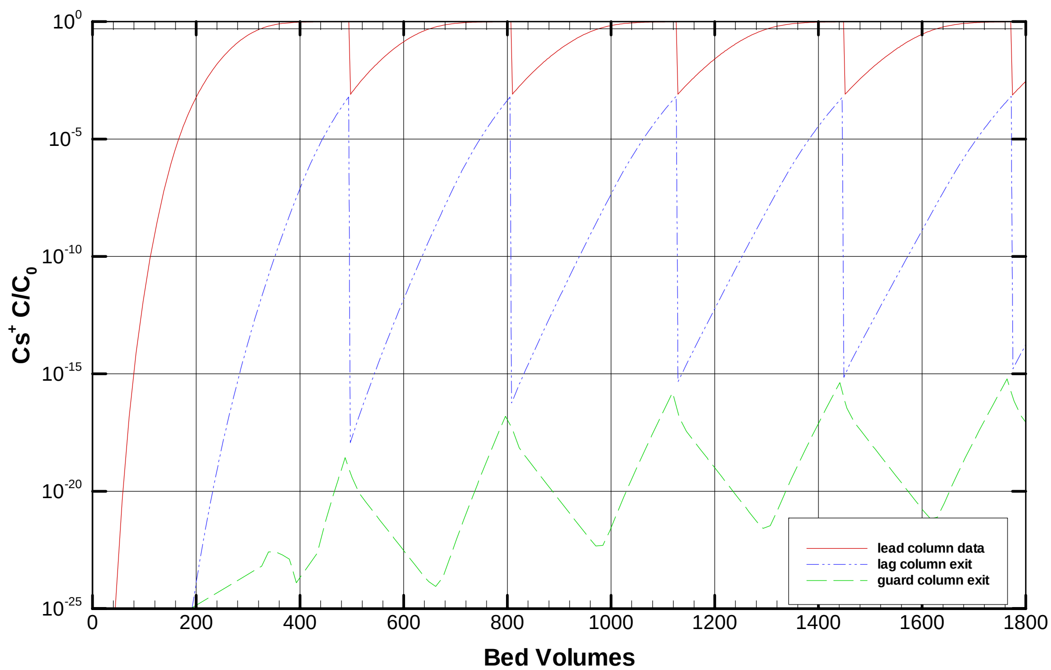


Figure 10-34. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 20 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

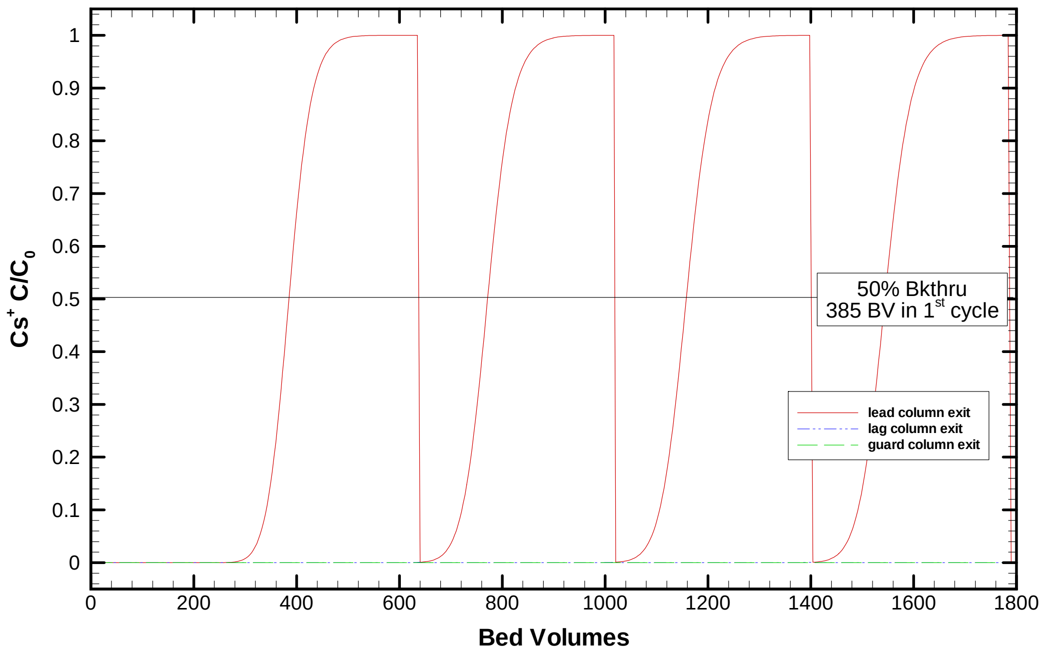


Figure 10-35. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations feed diluted to 4 M sodium at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

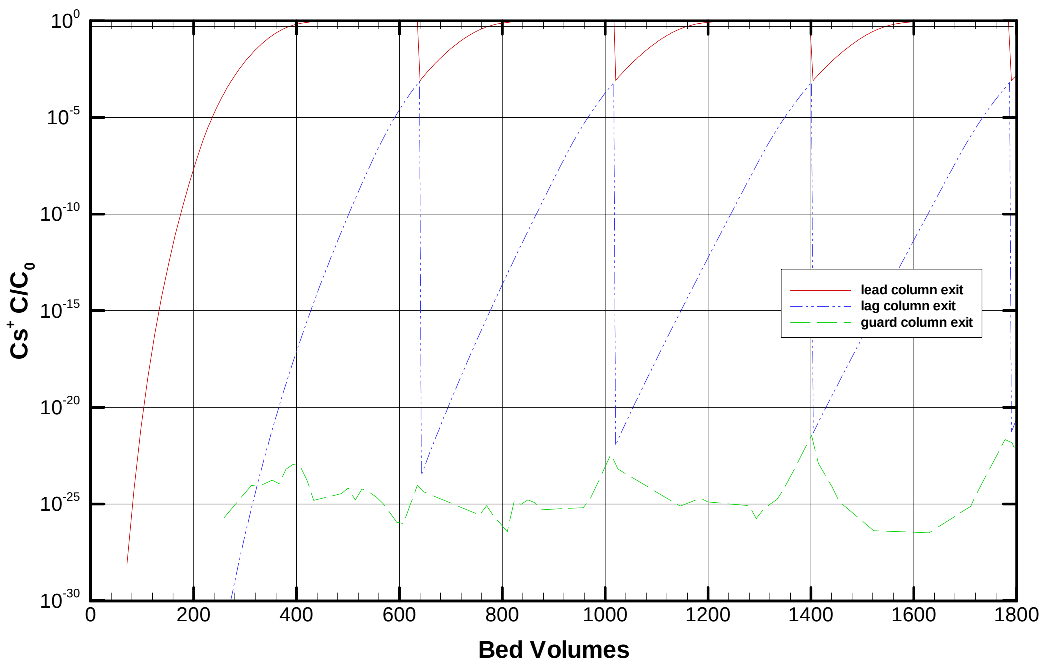


Figure 10-36. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations feed diluted to 4 M sodium at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

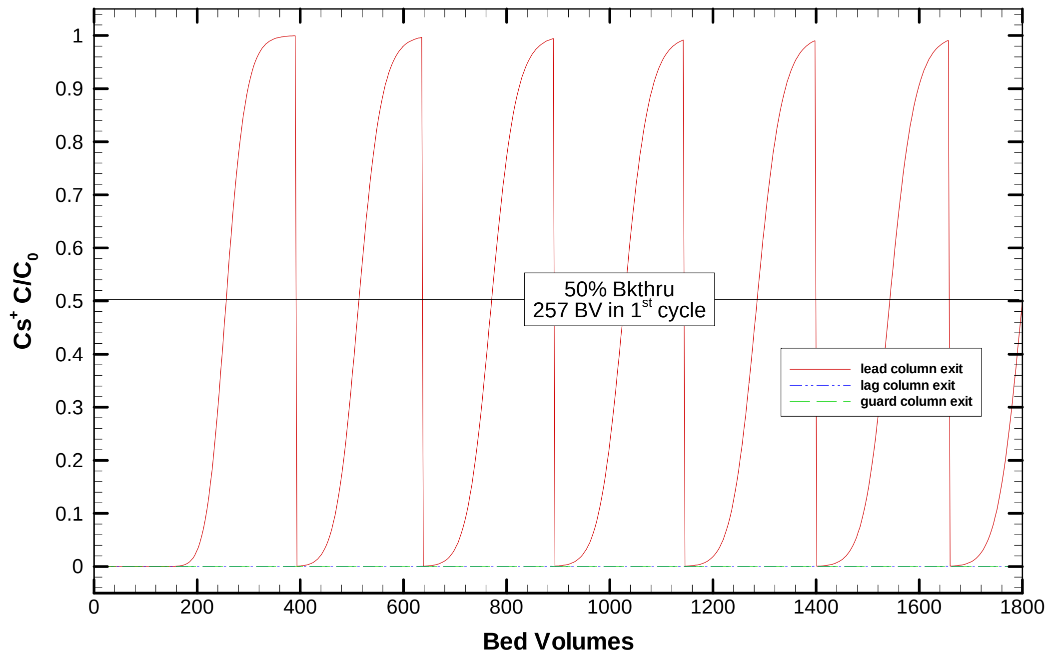


Figure 10-37. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations feed concentrated to 5.5 M sodium at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

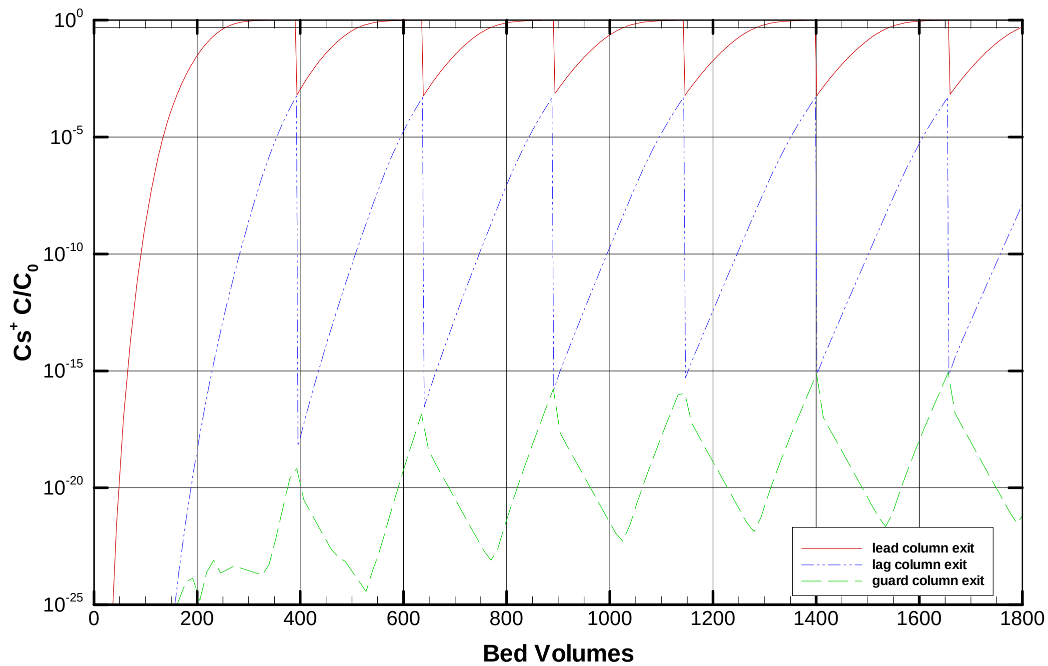


Figure 10-38. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations feed concentrated to 5.5 M sodium at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

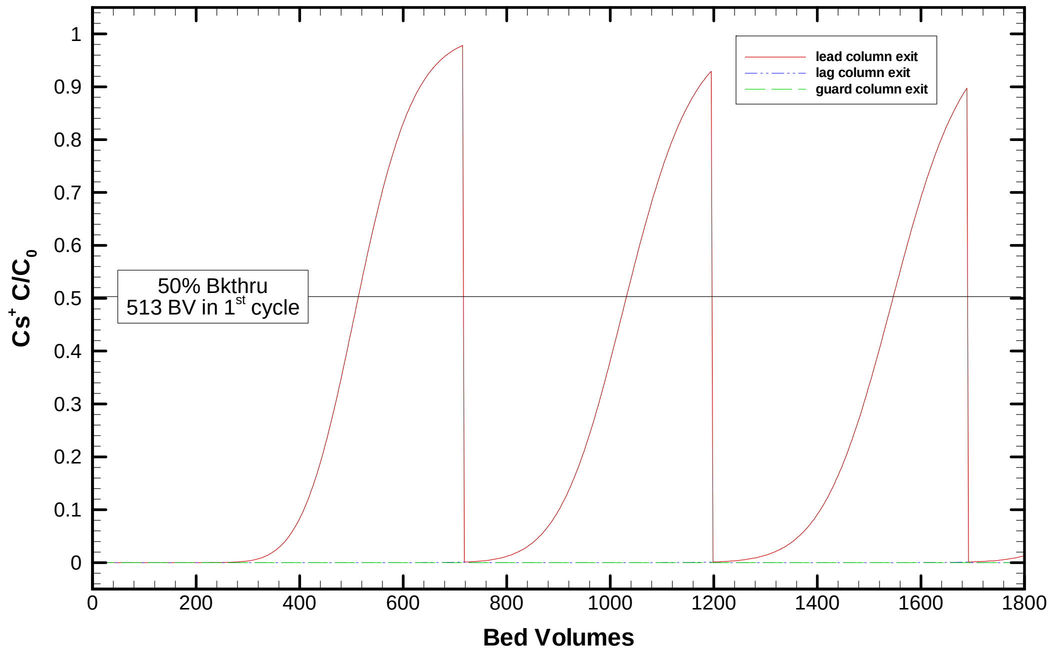


Figure 10-39. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations caustic leach feed (50% Na from NaOH) at a flow rate of 30 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

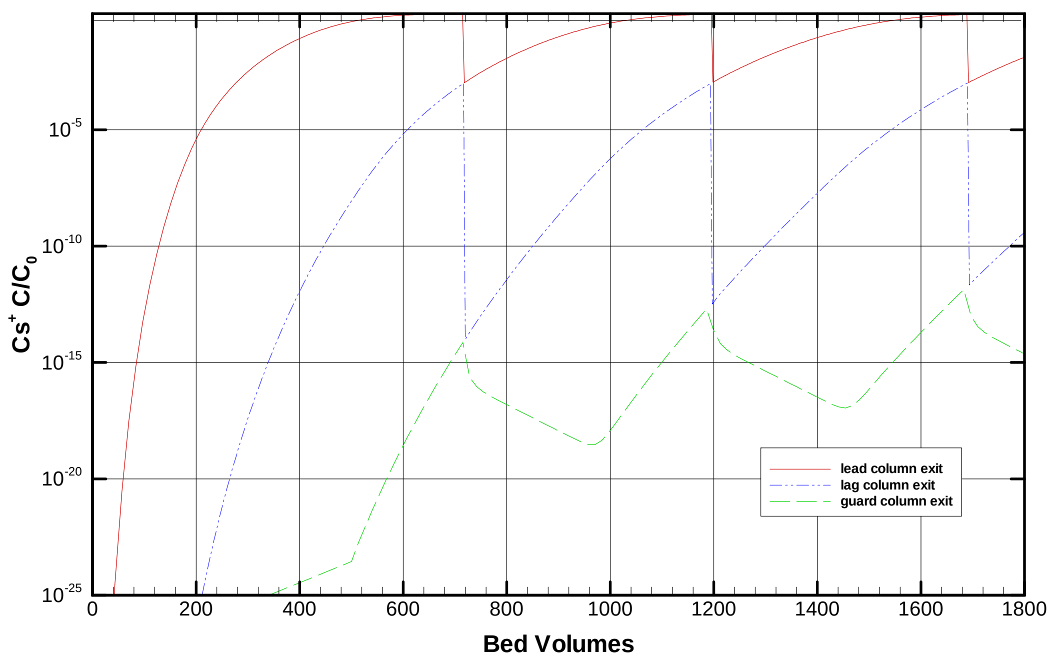


Figure 10-40. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations caustic leach feed (50% Na from NaOH) at a flow rate of 30 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

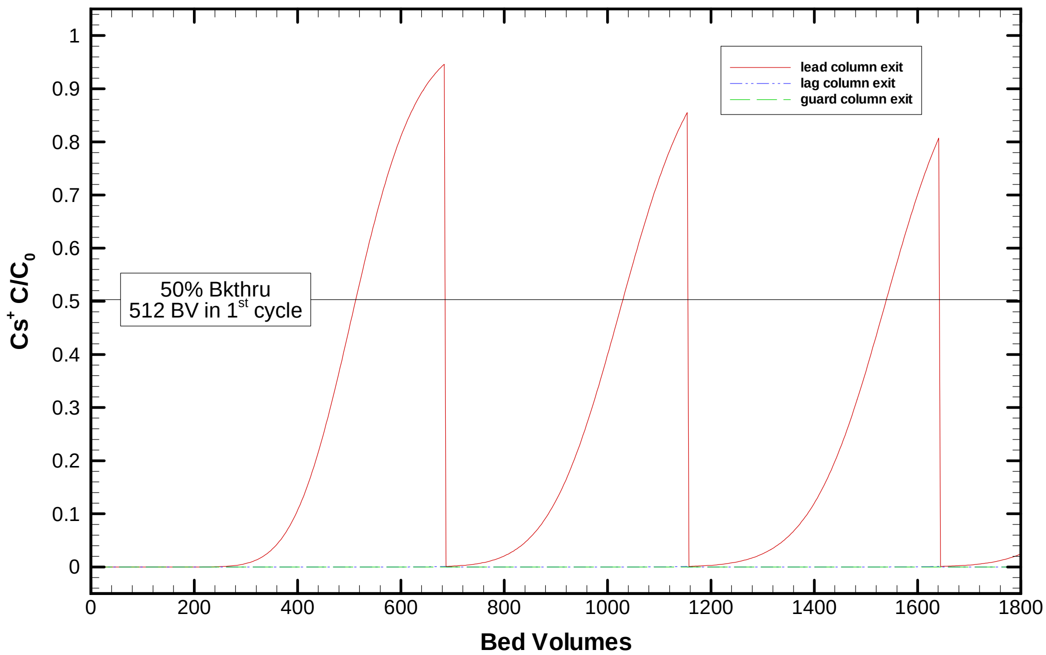


Figure 10-41. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations caustic leach feed (50% Na from NaOH) at a flow rate of 35 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

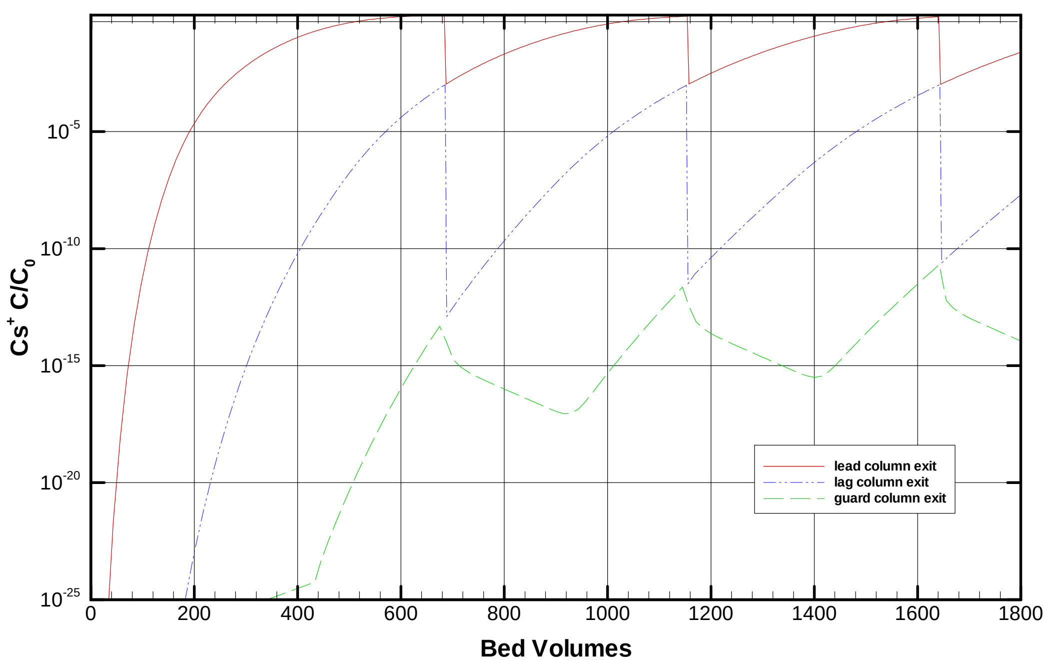


Figure 10-42. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations caustic leach feed (50% Na from NaOH) at a flow rate of 35 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

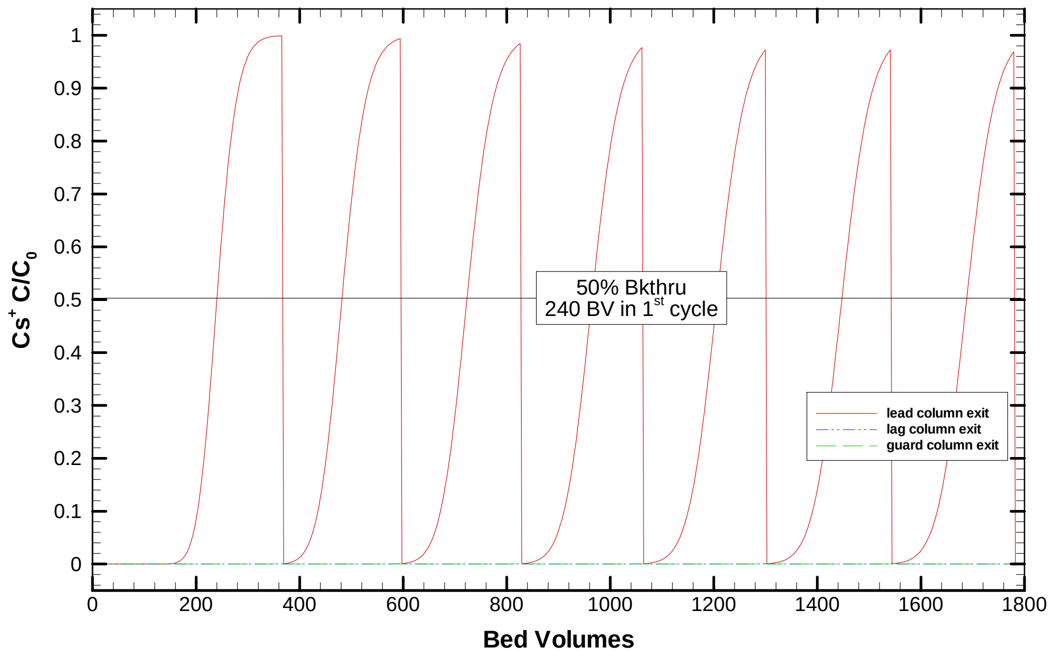


Figure 10-43. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations caustic leach feed (20% Na from NaOH) at a flow rate of 24 gpm and a temperature of 45 °C with 460 µm diameter RF spheres.

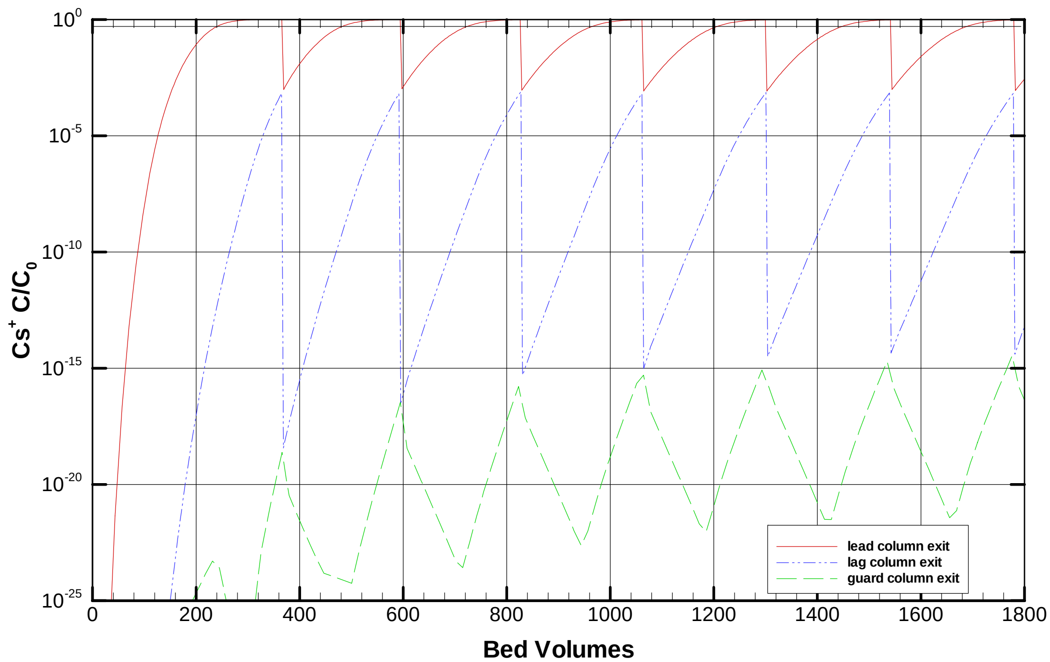


Figure 10-44. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with Subsequent Operations caustic leach feed (20% Na from NaOH) at a flow rate of 24 gpm and a temperature of 45 °C with 460 µm diameter RF spheres.

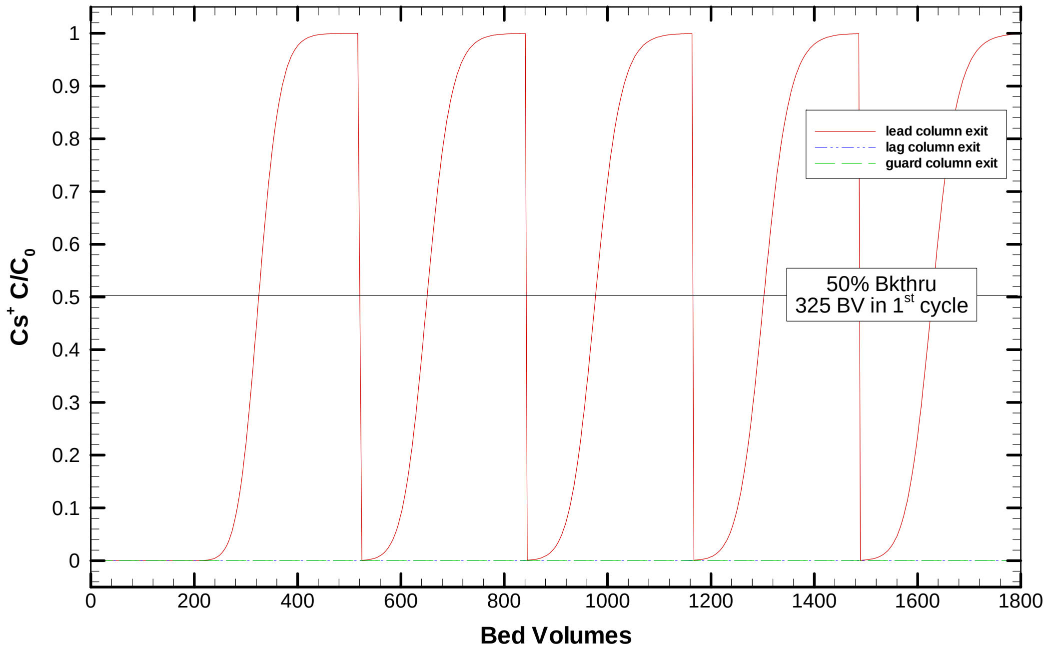


Figure 10-45. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

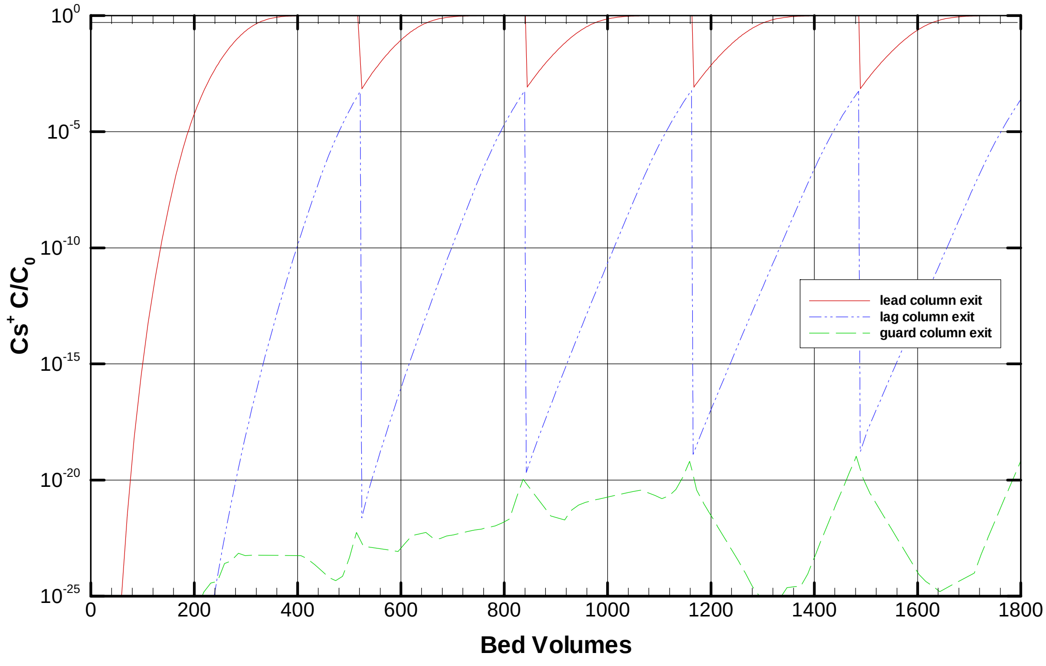


Figure 10-46. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

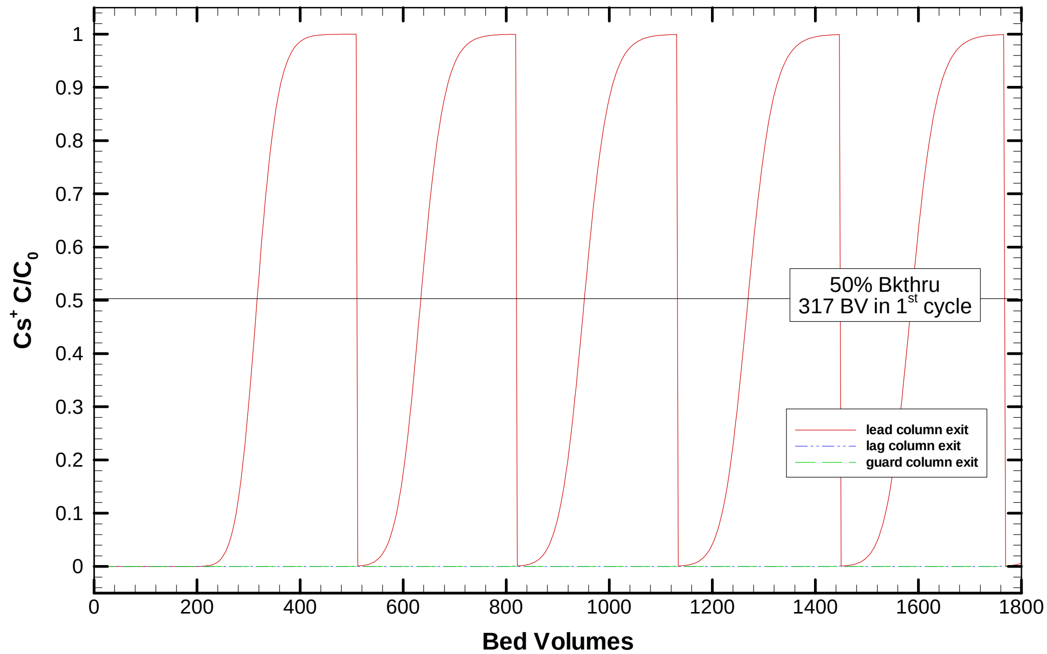


Figure 10-47. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with 0.6 M free hydroxide Subsequent Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

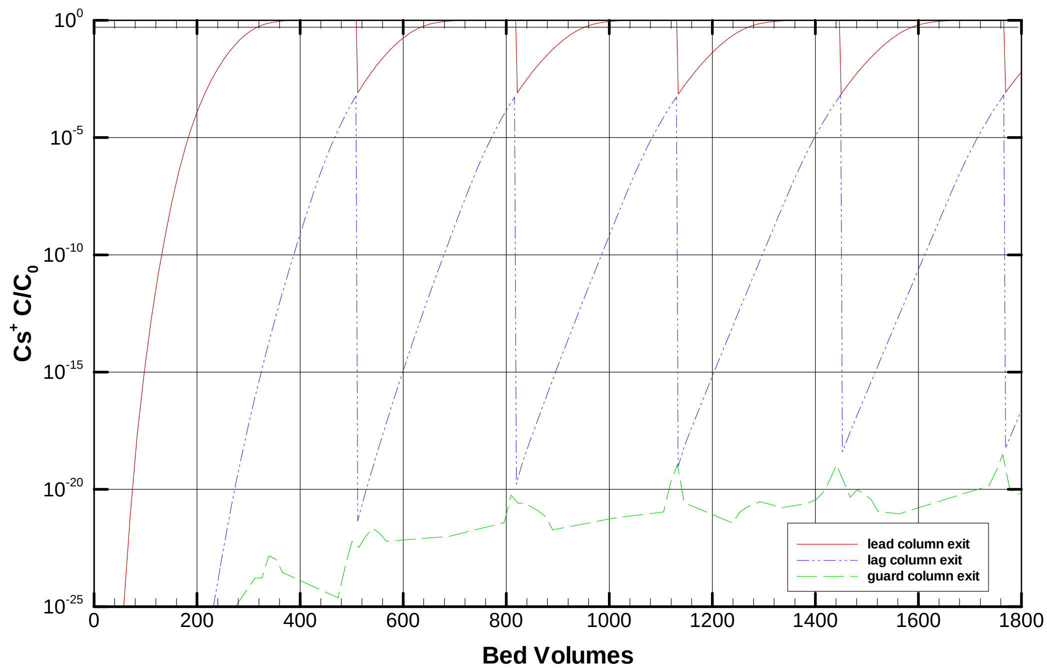


Figure 10-48. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with 0.6 M free hydroxide Subsequent Operations feed at a flow rate of 15 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

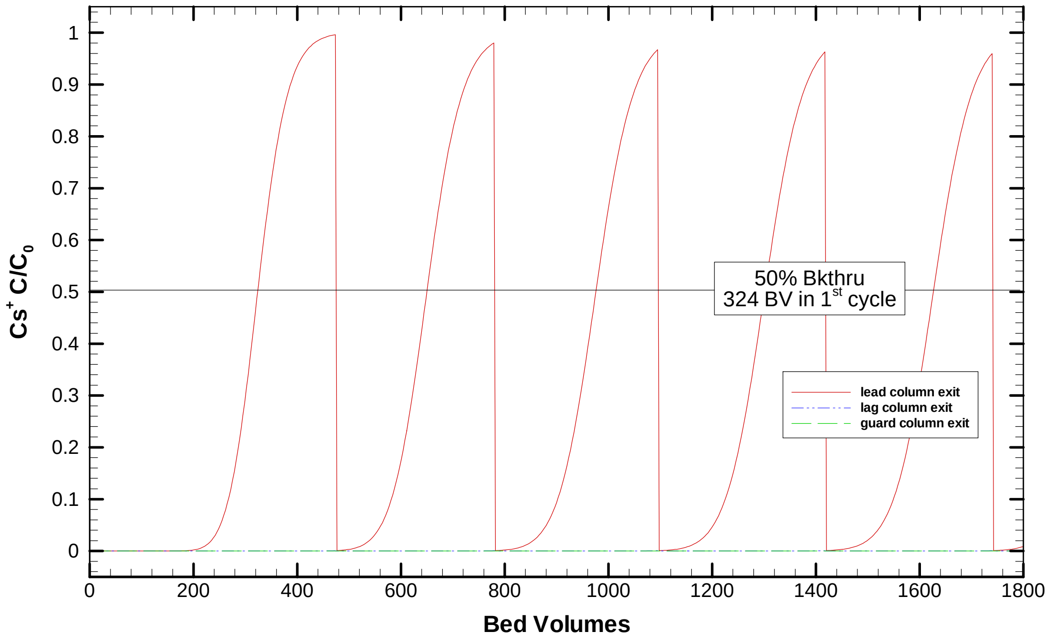


Figure 10-49. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 24 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

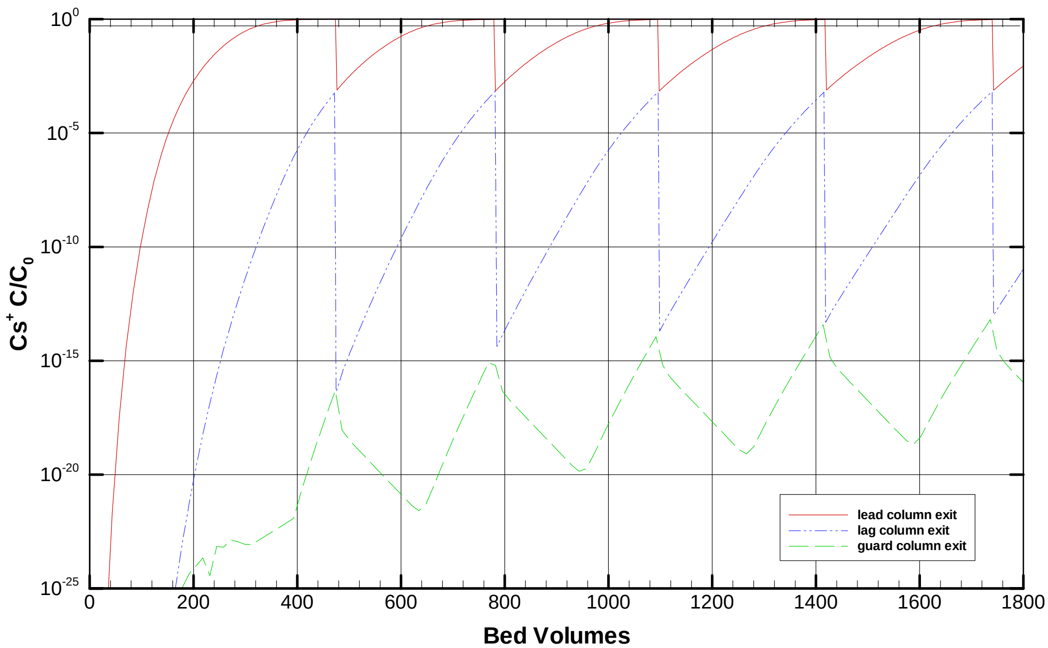


Figure 10-50. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 24 gpm and a temperature of 25 °C with 460 µm diameter RF spheres.

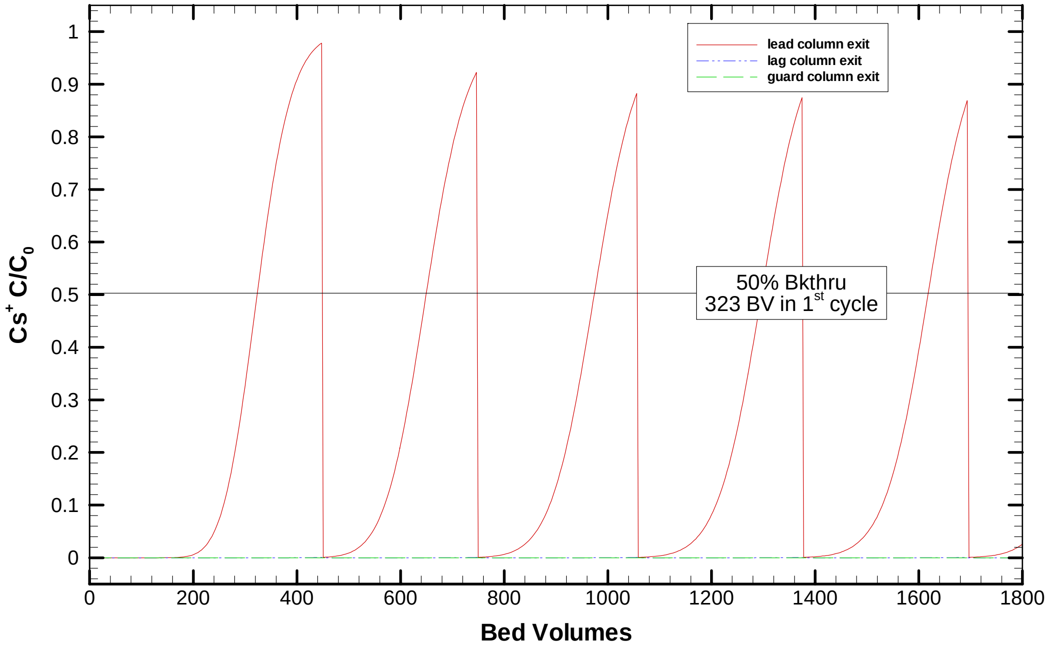


Figure 10-51. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 30 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

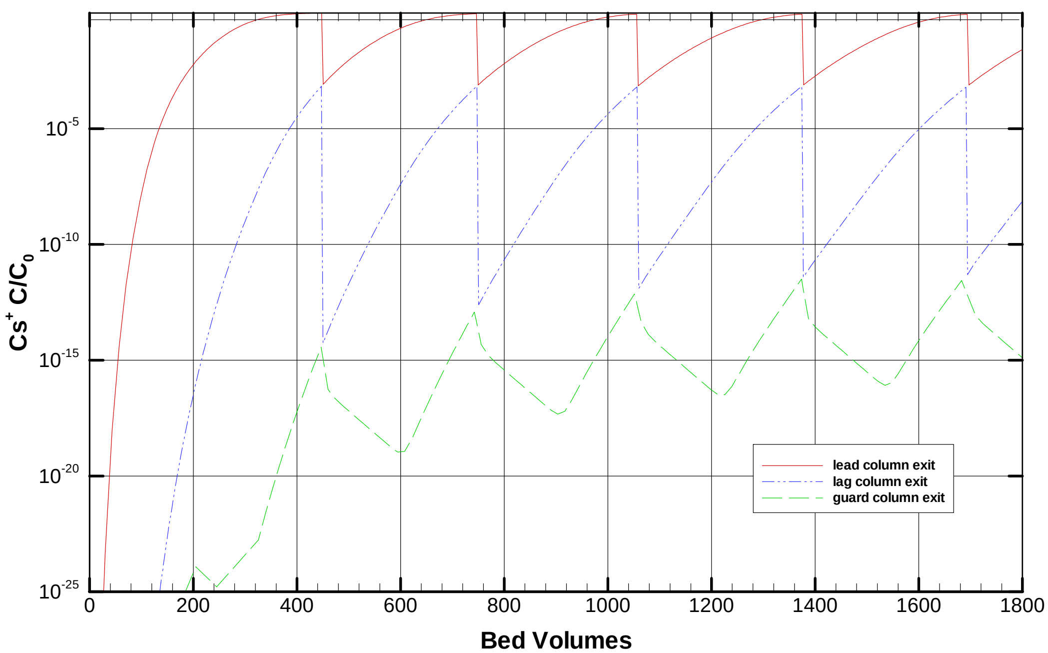


Figure 10-52. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 30 gpm and a temperature of 25 °C with 460 μm diameter RF spheres.

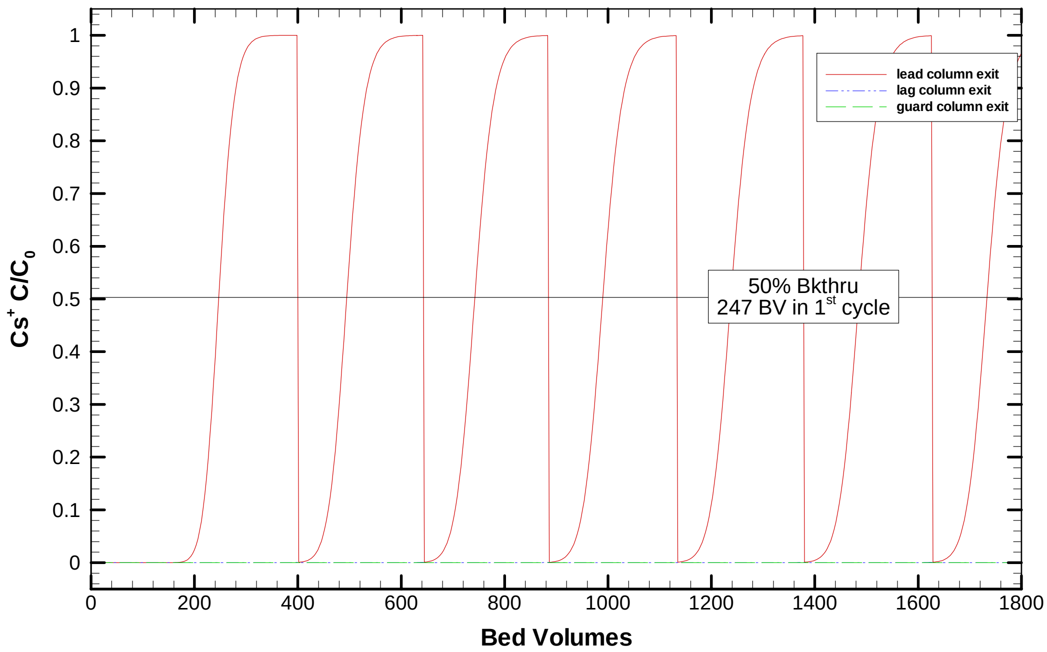


Figure 10-53. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 15 gpm and a temperature of 35 °C with 460 µm diameter RF spheres.

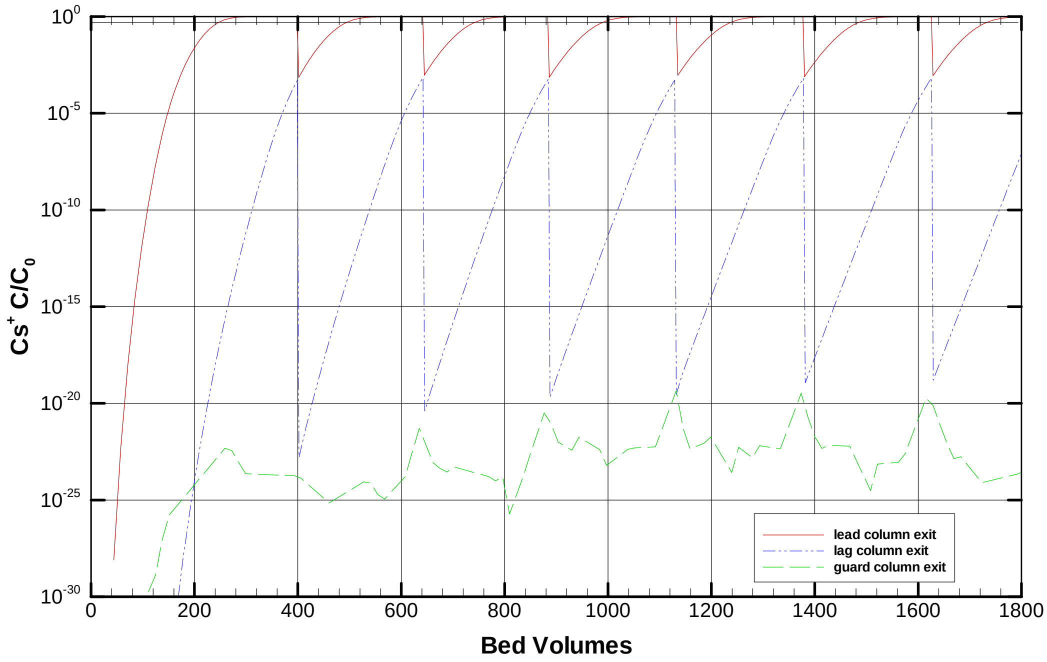


Figure 10-54. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 15 gpm and a temperature of 35 °C with 460 µm diameter RF spheres.

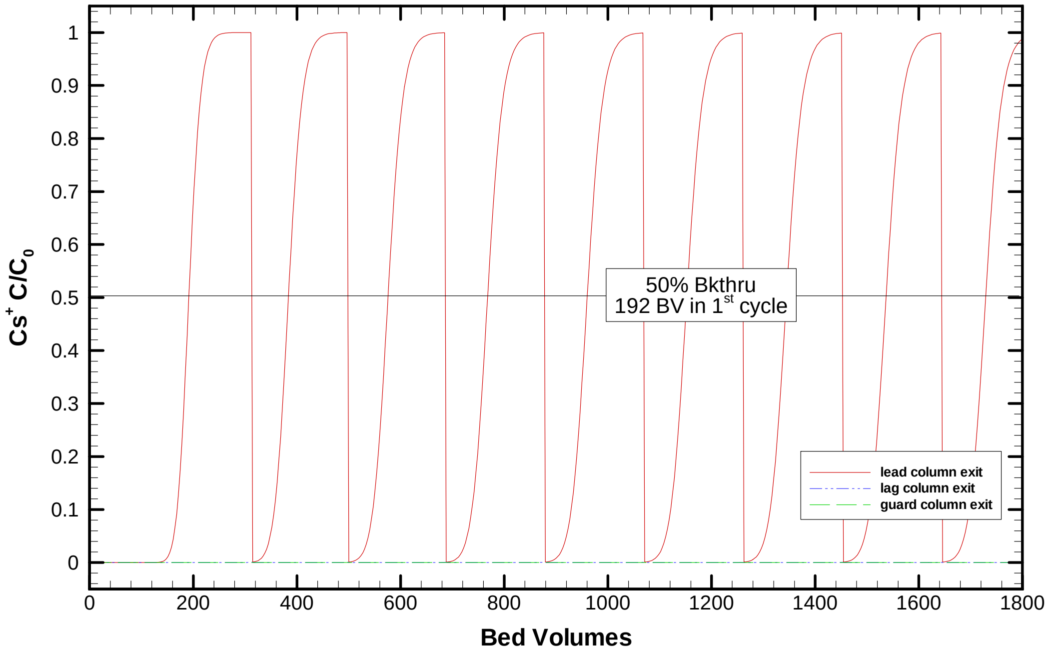


Figure 10-55. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 15 gpm and a temperature of 45 °C with 460 µm diameter RF spheres.

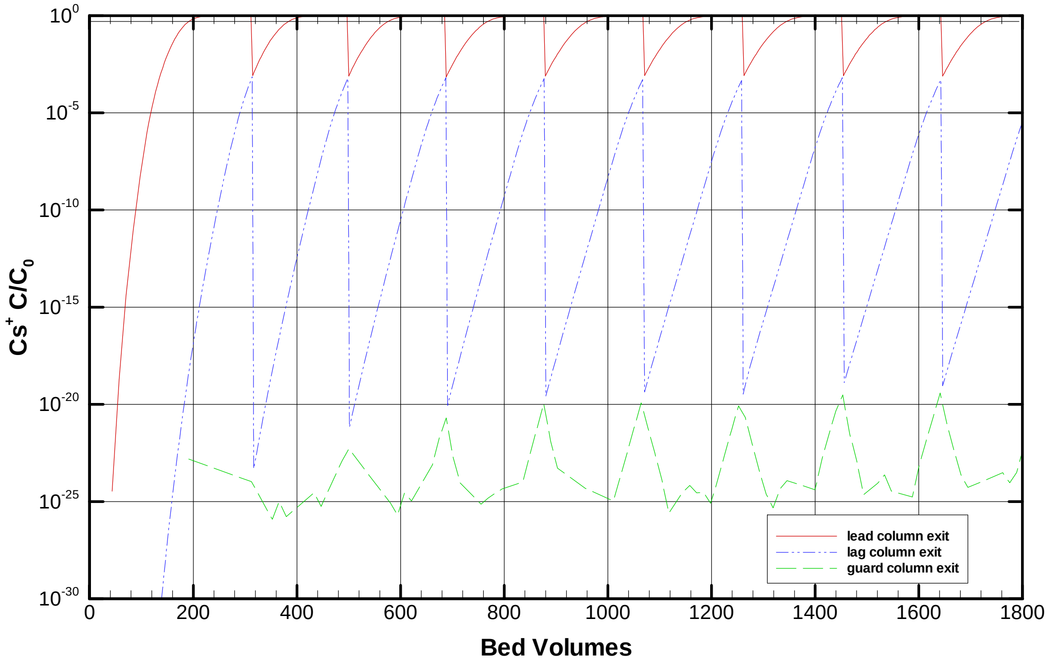


Figure 10-56. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 15 gpm and a temperature of 45 °C with 460 µm diameter RF spheres.

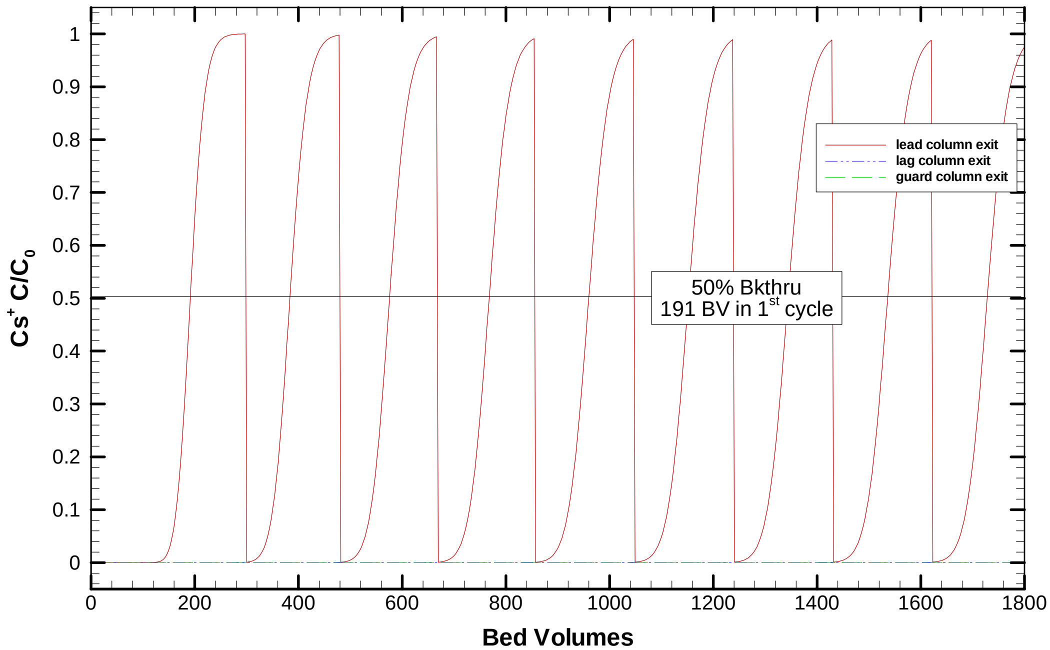


Figure 10-57. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 20 gpm and a temperature of 45 °C with 460 µm diameter RF spheres.

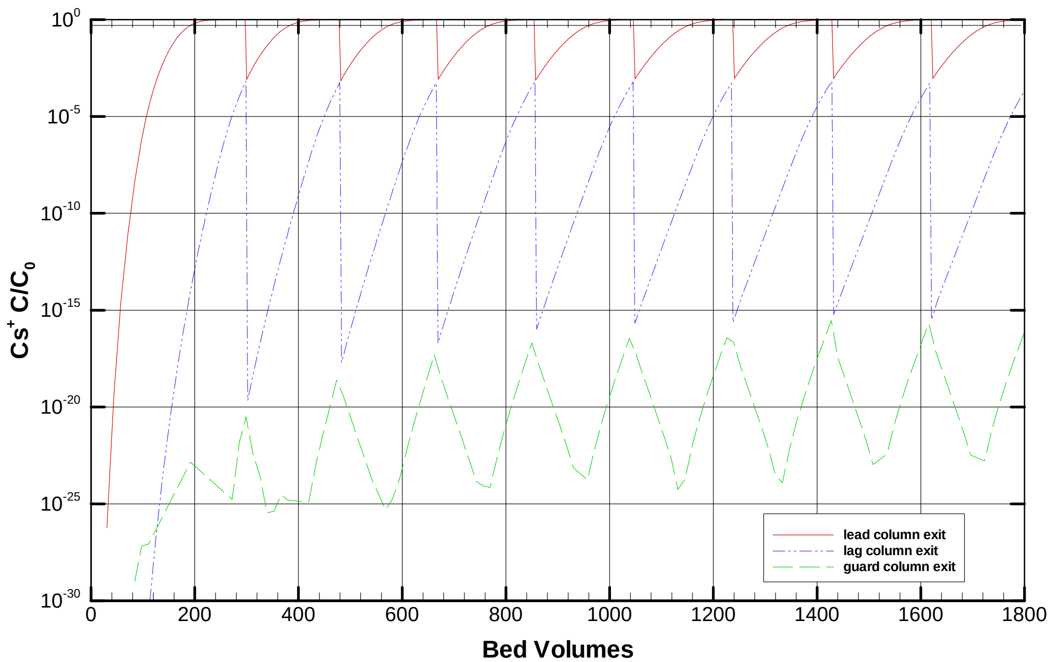


Figure 10-58. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 20 gpm and a temperature of 45 °C with 460 µm diameter RF spheres.

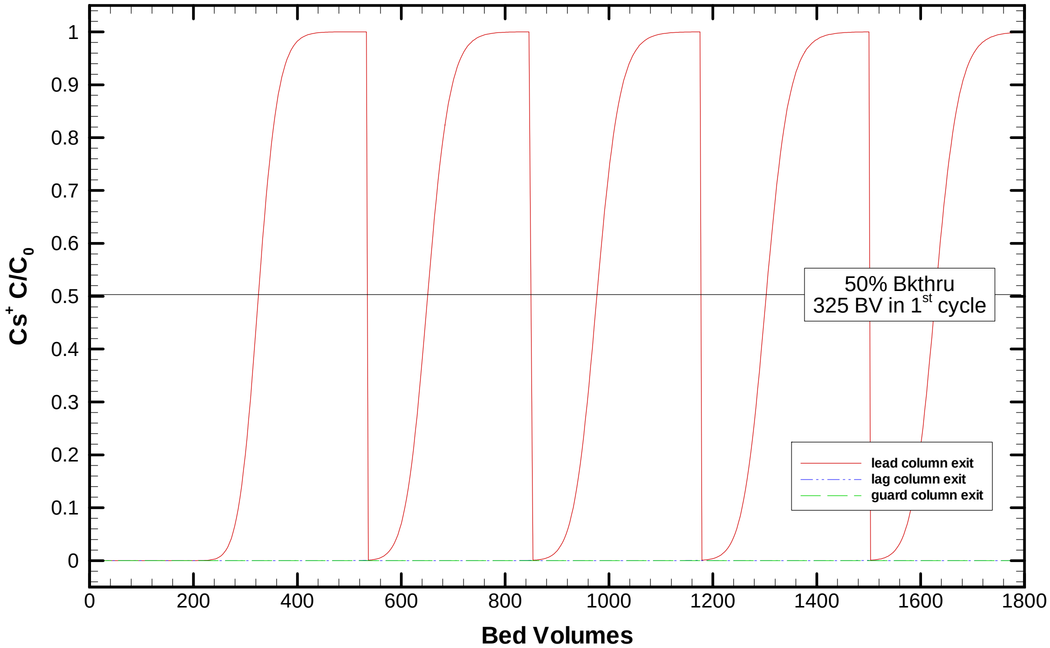


Figure 10-59. Linear plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 20 gpm and a temperature of 25 °C with 380 µm diameter RF spheres.

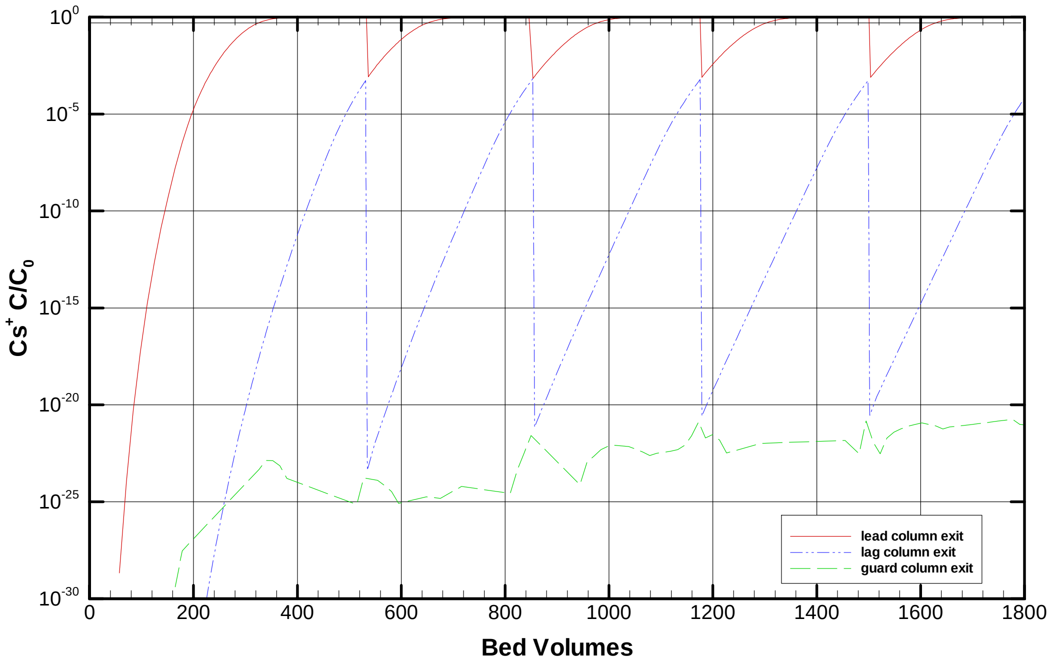


Figure 10-60. Log plot of VERSE-LC cesium breakthrough predictions for full-scale three column carousel with nominal Subsequent Operations feed at a flow rate of 20 gpm and a temperature of 25 °C with 380 µm diameter RF spheres.

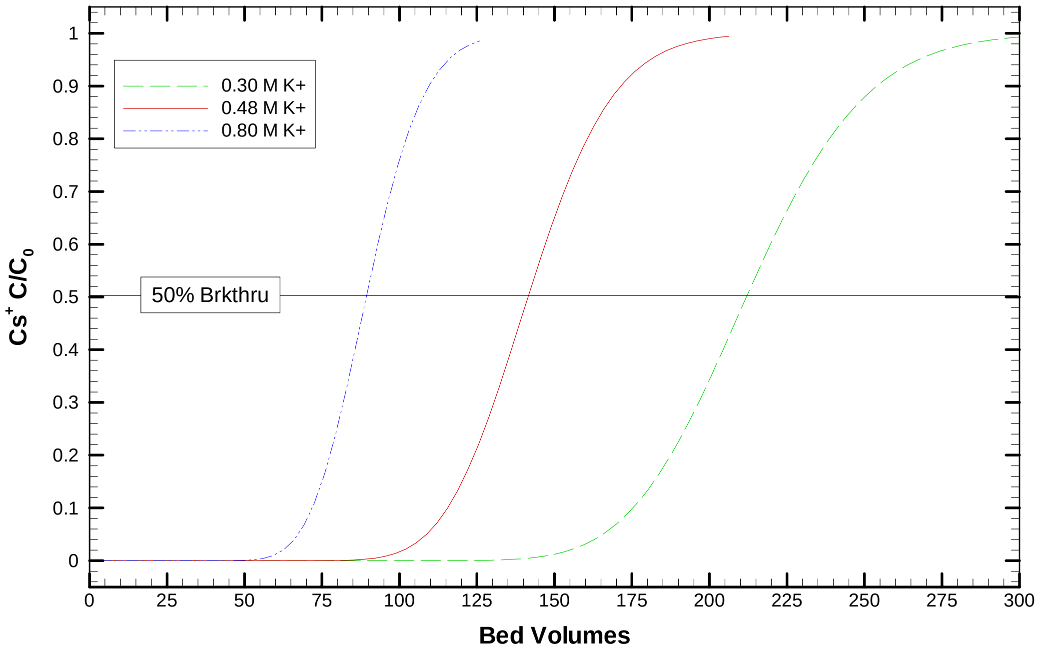


Figure 10-61. VERSE-LC cesium breakthrough prediction for the lead column with Hot Commissioning Operations feed. The impact on breakthrough with variation in potassium concentration is shown for the first cycle.

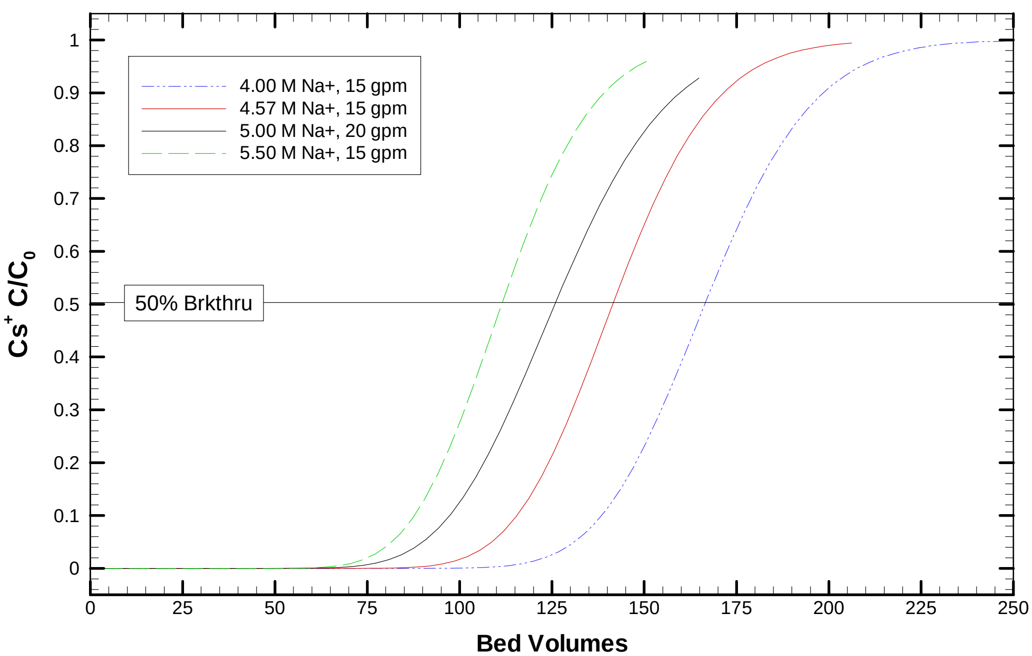


Figure 10-62. VERSE-LC cesium breakthrough prediction for the lead column with Hot Commissioning Operations feed. The impact on breakthrough with variation in sodium concentration is shown for the first cycle.

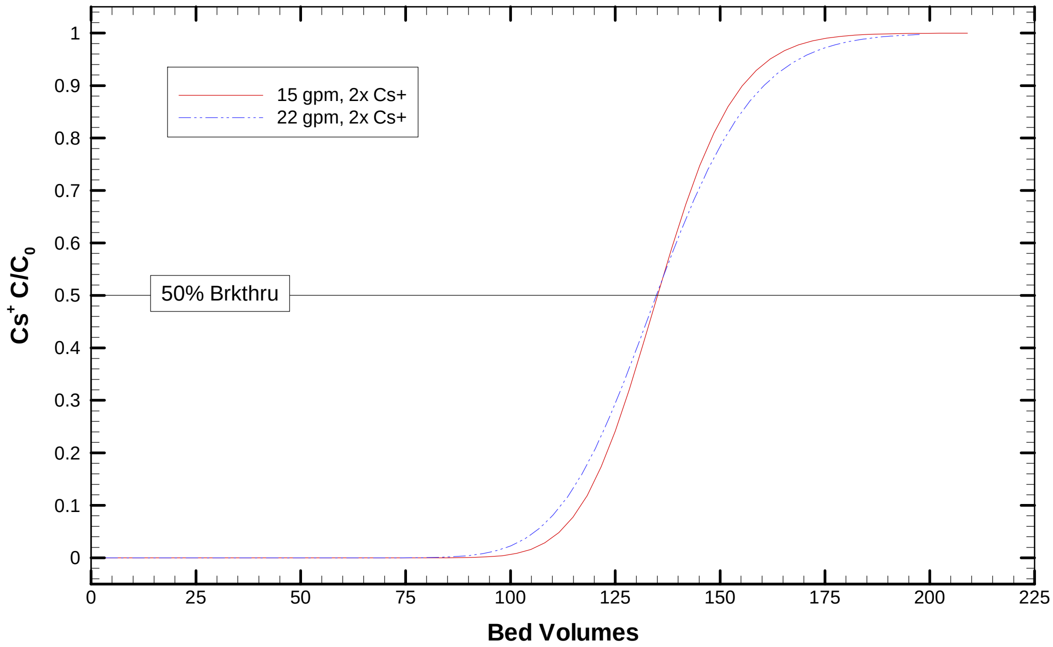


Figure 10-63. Linear plot of VERSE-LC cesium breakthrough prediction for the lead column with Hot Commissioning Operations feed. The impact on breakthrough with variation in liquid flow rate at twice nominal cesium concentration is shown for the first cycle.

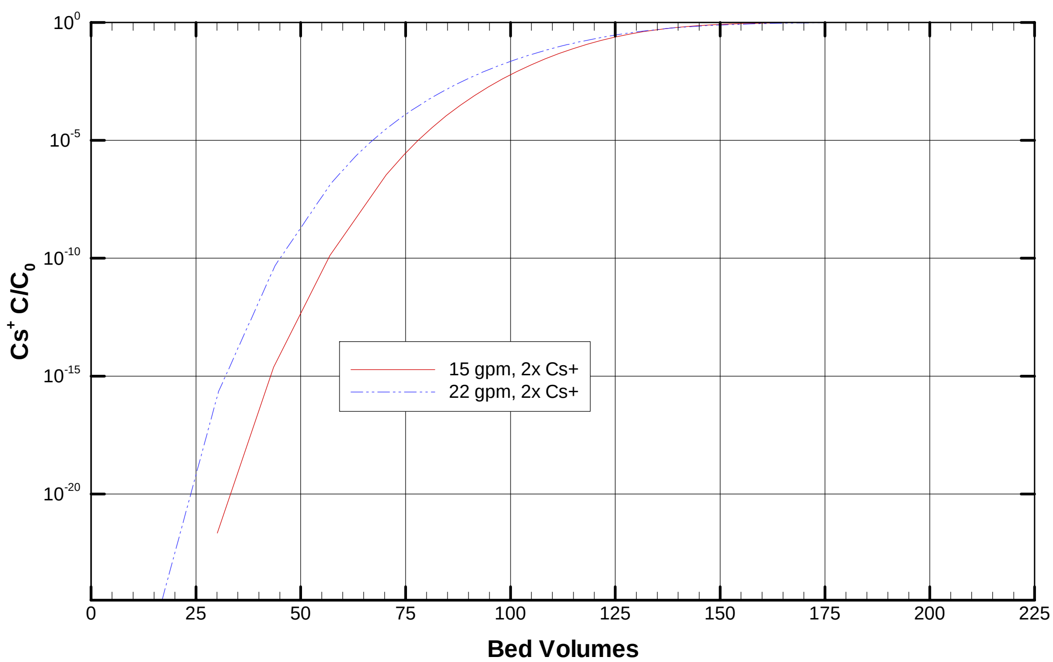


Figure 10-64. Log plot of VERSE-LC cesium breakthrough prediction for the lead column with Hot Commissioning Operations feed. The impact on breakthrough with variation in liquid flow rate at twice nominal cesium concentration is shown for the first cycle.

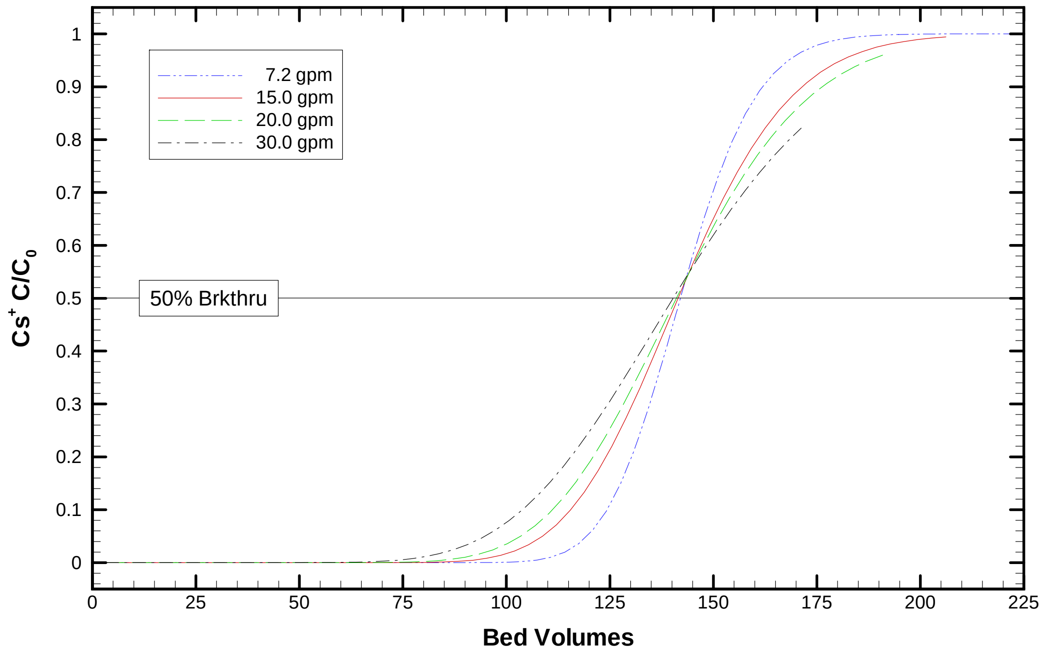


Figure 10-65. Linear plot of VERSE-LC cesium breakthrough prediction for the lead column with Hot Commissioning Operations feed. The impact on breakthrough with nominal feed and variation in liquid flow rate is shown for the first cycle.

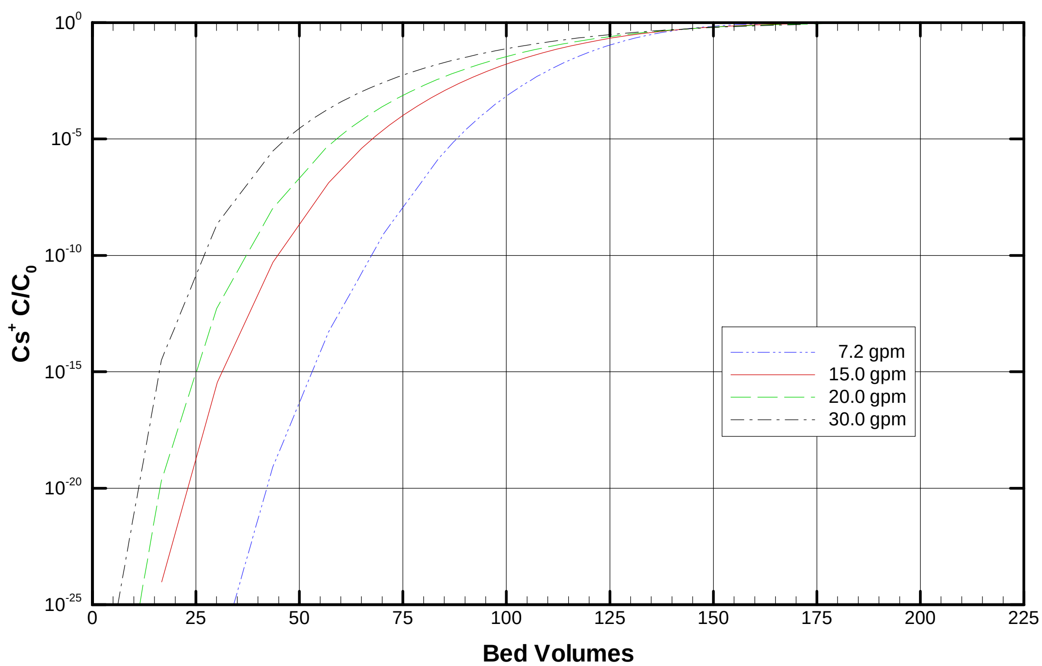


Figure 10-66. Log plot of VERSE-LC cesium breakthrough prediction for the lead column with Hot Commissioning Operations feed. The impact on breakthrough with nominal feed and variation in liquid flow rate is shown for the first cycle.

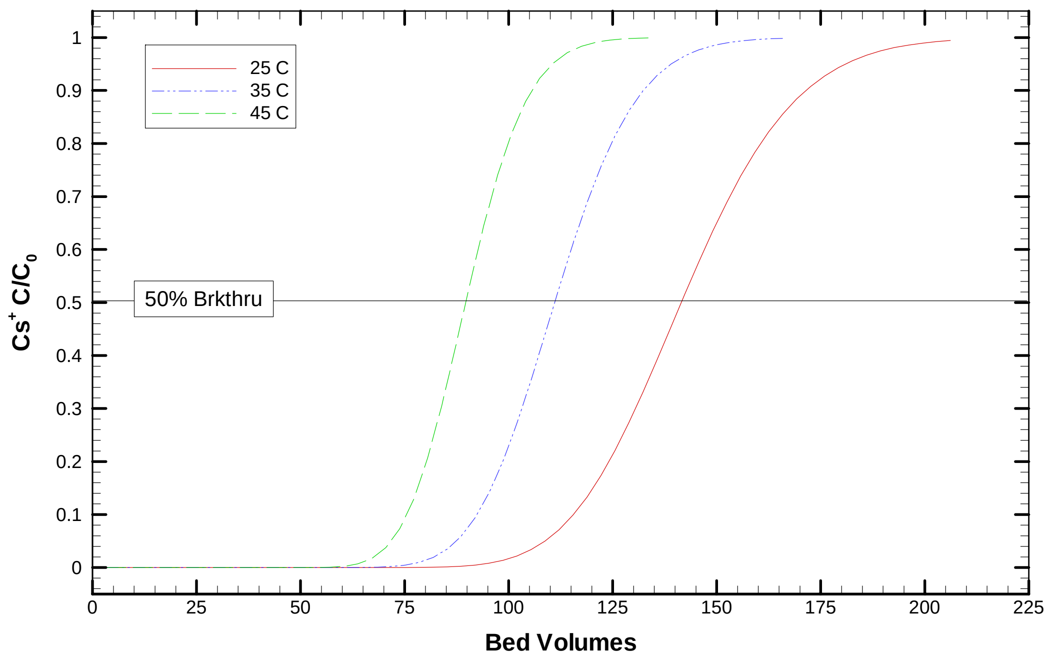


Figure 10-67. VERSE-LC cesium breakthrough prediction for the lead column with Hot Commissioning Operations feed. The impact on breakthrough with nominal feed and variation in temperature is shown for the first cycle.

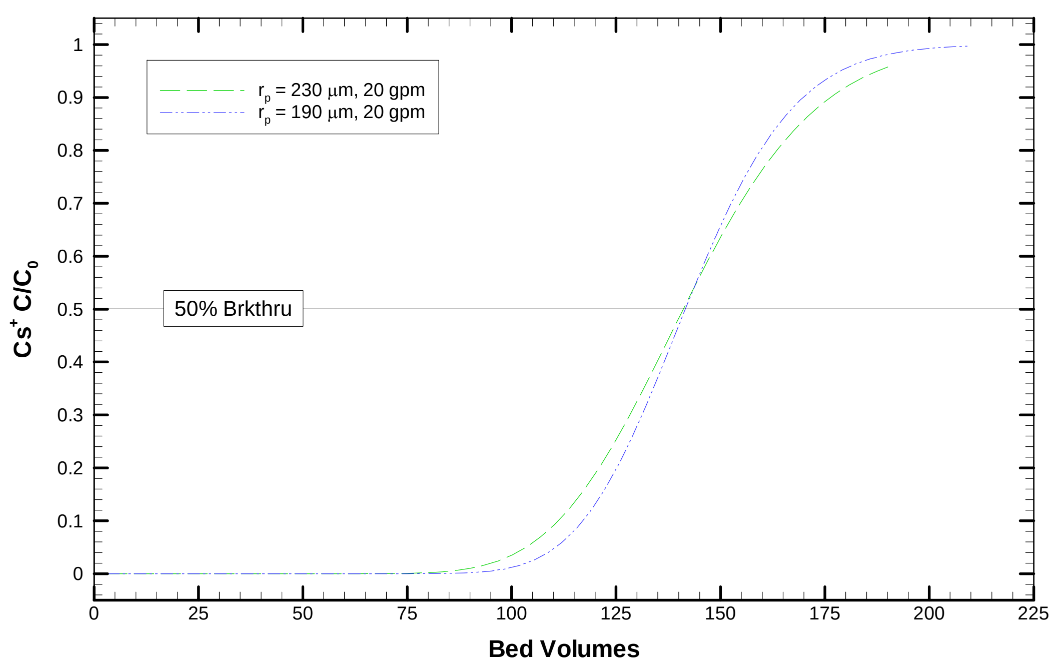


Figure 10-68. VERSE-LC cesium breakthrough prediction for the lead column with Hot Commissioning Operations feed. The impact on breakthrough with nominal feed and variation in RF particle radius is shown for the first cycle.

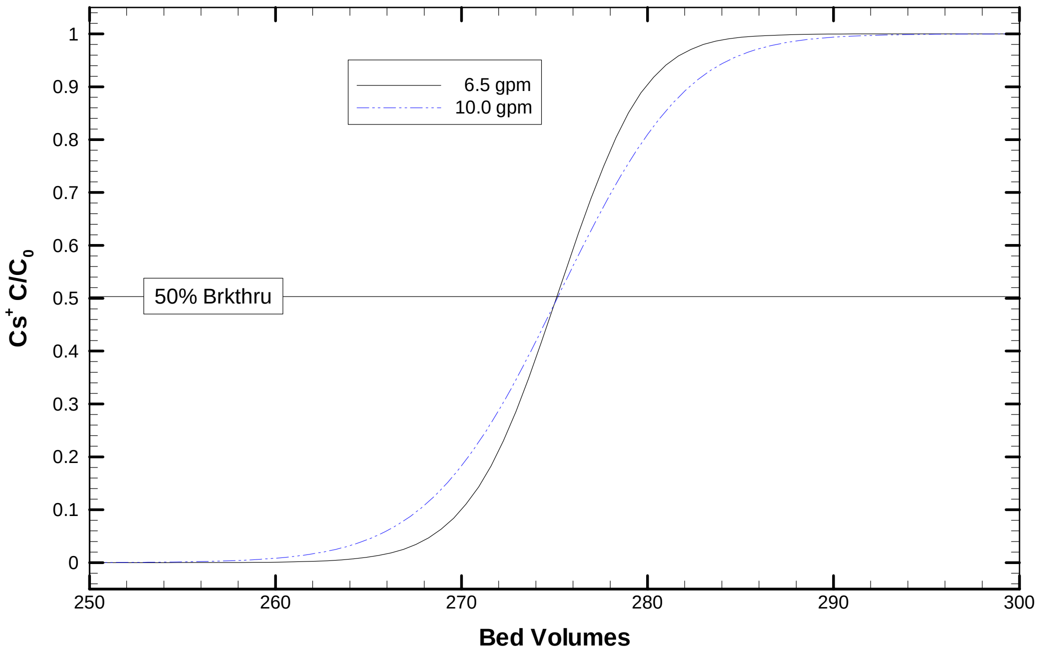


Figure 10-69. Linear plot of VERSE-LC cesium breakthrough prediction for the lead column with Envelope B feed. The impact on breakthrough with variation in liquid flow rate is shown for the first cycle.

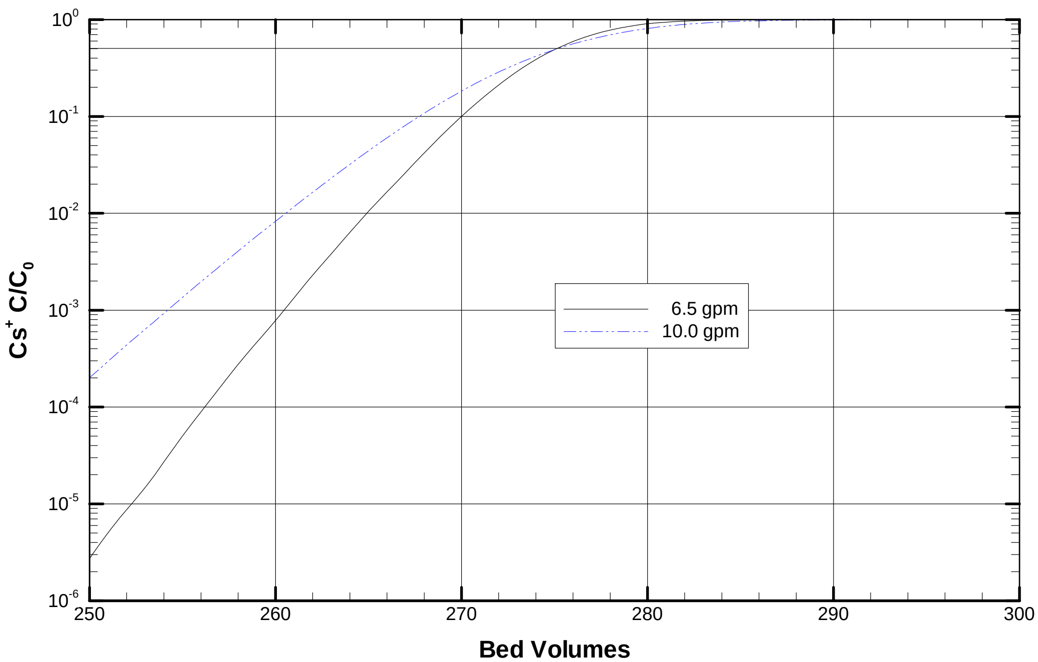


Figure 10-70. Log plot of VERSE-LC cesium breakthrough prediction for the lead column with Envelope B feed. The impact on breakthrough with variation in liquid flow rate is shown for the first cycle.

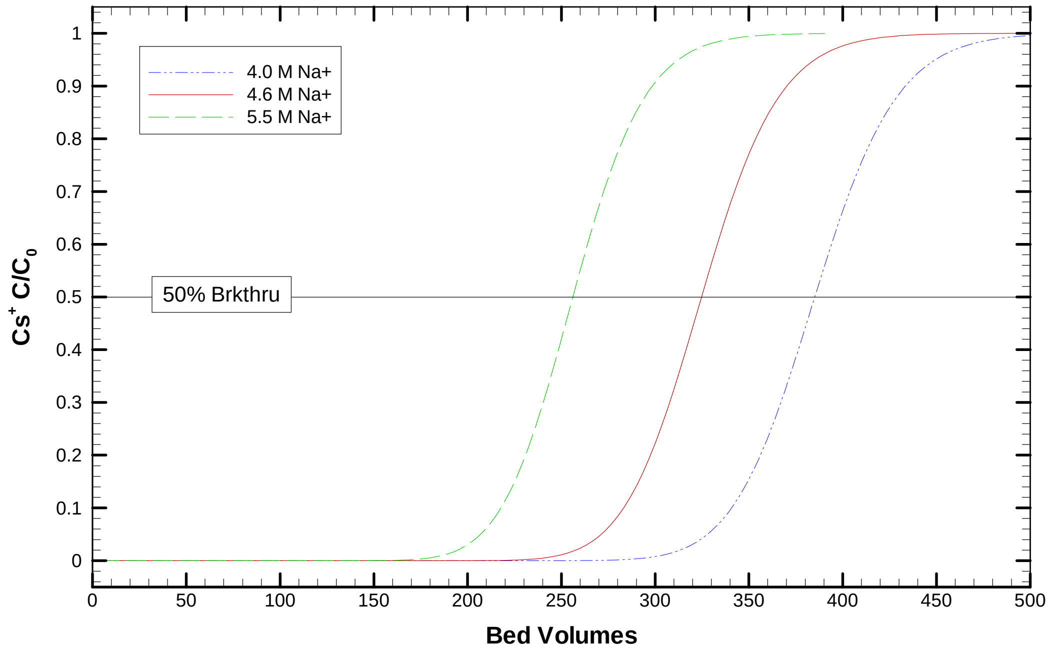


Figure 10-71. VERSE-LC cesium breakthrough prediction for the lead column with Subsequent Operations feed. The impact on breakthrough with variation in sodium concentration is shown for the first cycle.

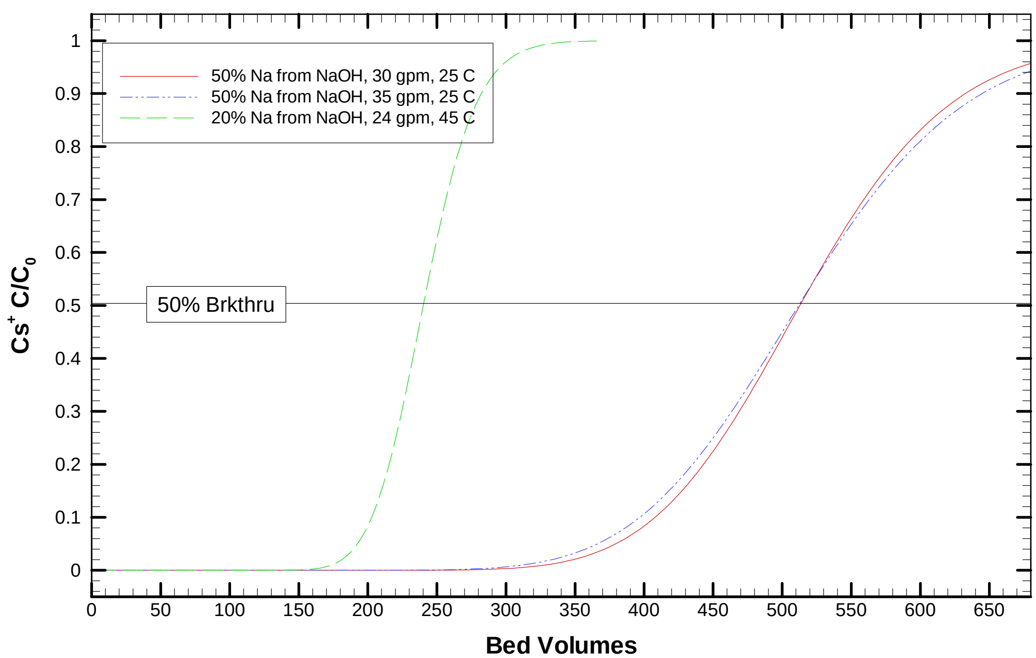


Figure 10-72. VERSE-LC cesium breakthrough prediction for the lead column with Subsequent Operations feed. The impact on breakthrough with variation in caustic leach case is shown for the first cycle.

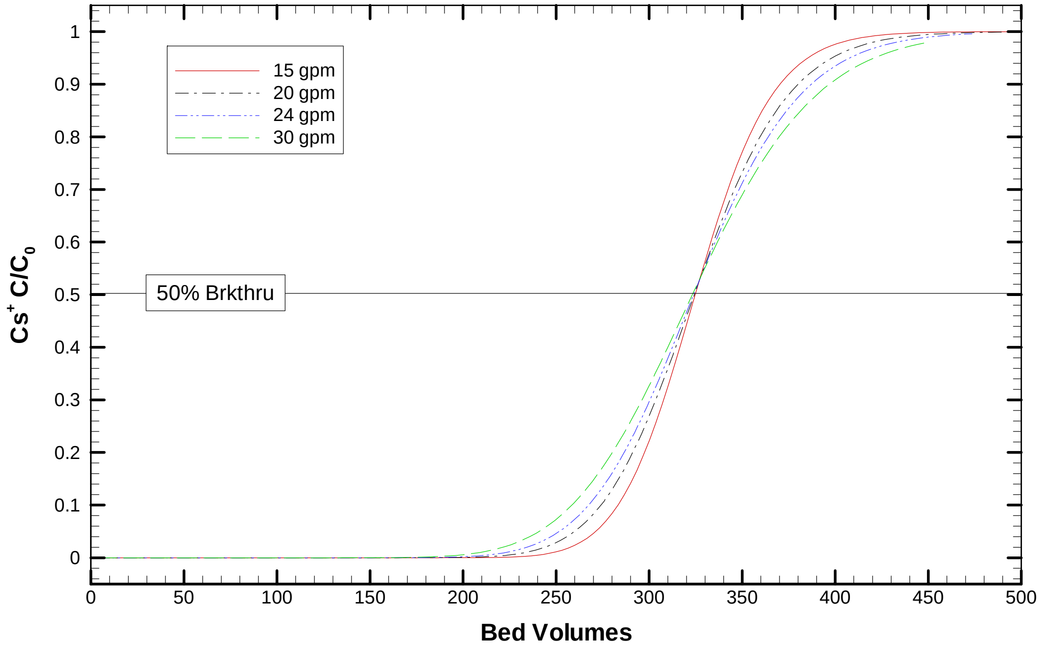


Figure 10-73. Linear plot of VERSE-LC cesium breakthrough prediction for the lead column with Subsequent Operations feed. The impact on breakthrough with variation in liquid flow rate is shown for the first cycle.

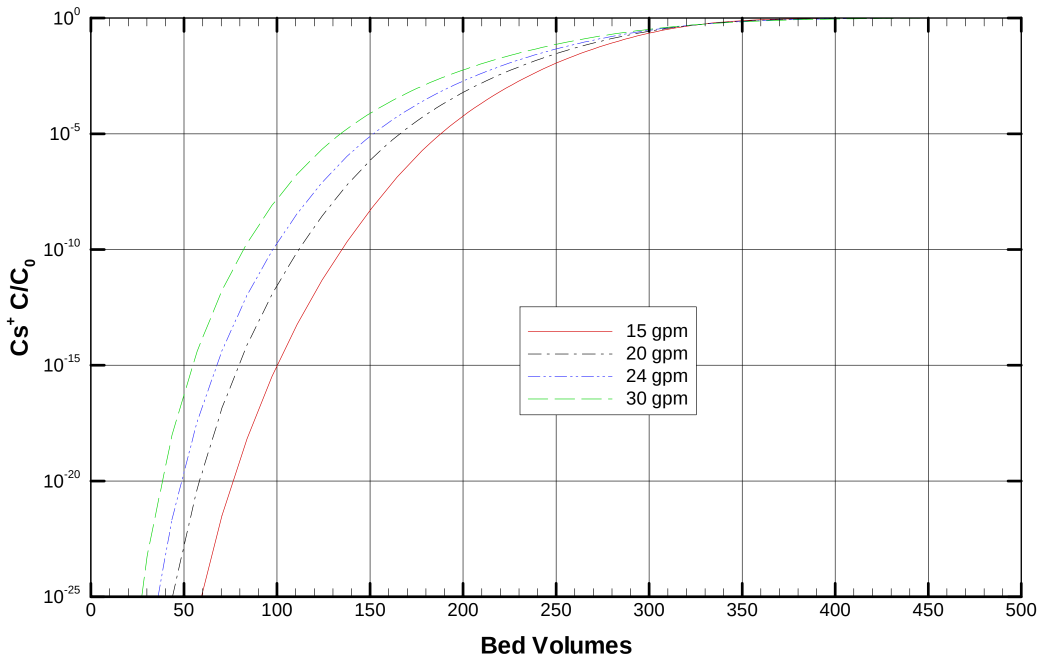


Figure 10-74. Log plot of VERSE-LC cesium breakthrough prediction for the lead column with Subsequent Operations feed. The impact on breakthrough with variation in liquid flow rate is shown for the first cycle.

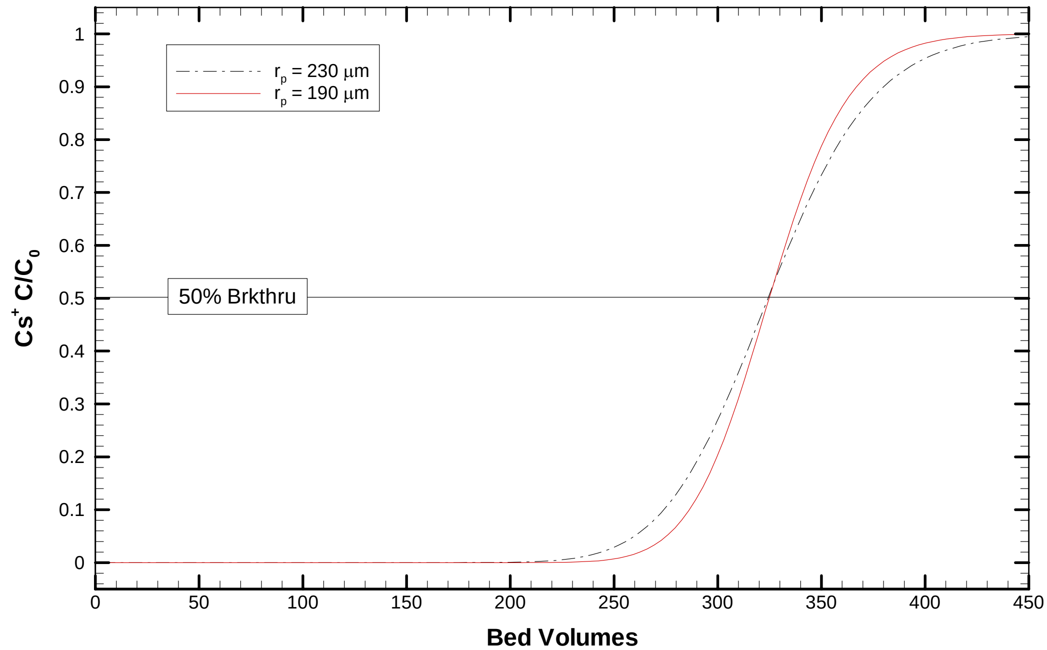


Figure 10-75. VERSE-LC cesium breakthrough prediction for the lead column with Subsequent Operations feed. The impact on breakthrough with variation in RF particle radius is shown for the first cycle at a flow rate of 20 gpm and temperature of 25 °C.

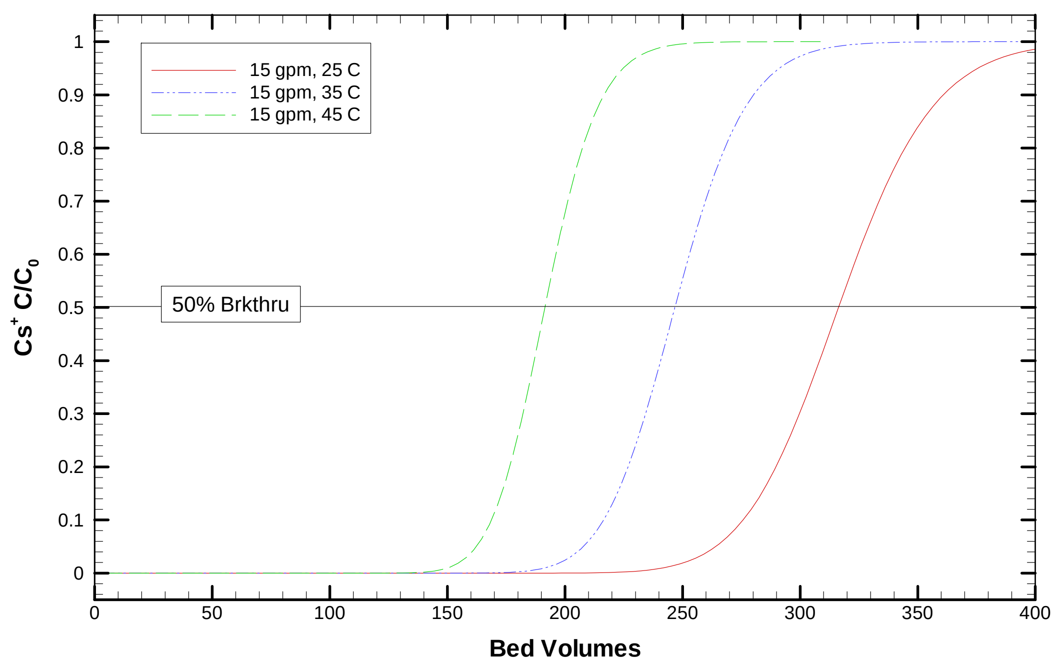


Figure 10-76. VERSE-LC cesium breakthrough prediction for the lead column with Subsequent Operations feed. The impact on breakthrough with variation in temperature at a liquid flow rate of 15 gpm is shown for the first cycle.

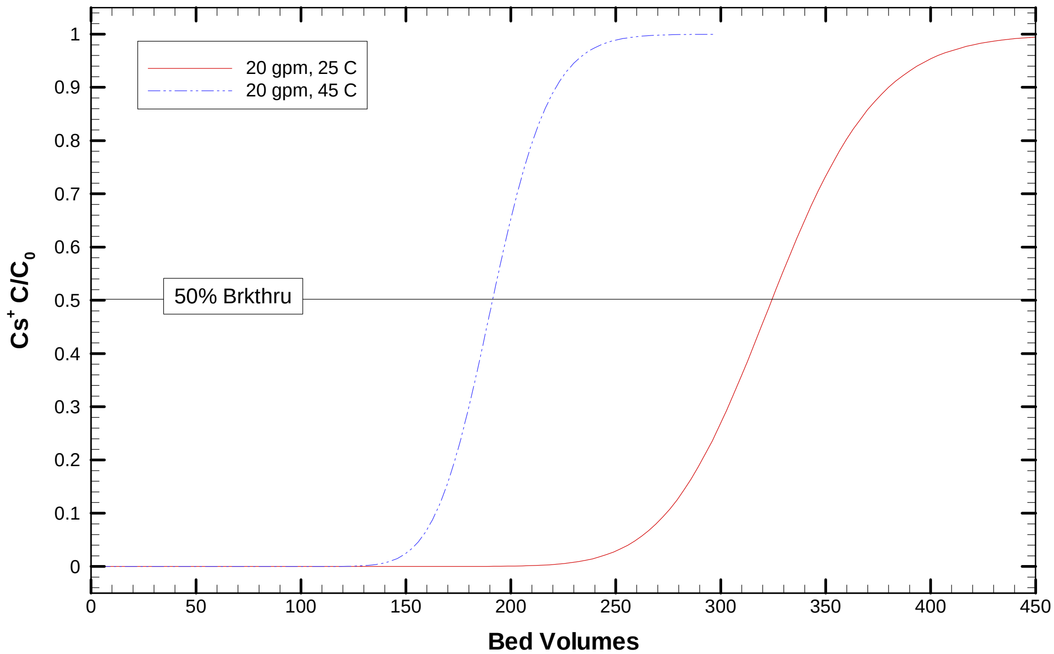


Figure 10-77. VERSE-LC cesium breakthrough prediction for the lead column with Subsequent Operations feed. The impact on breakthrough with variation in temperature at a liquid flow rate of 20 gpm is shown for the first cycle.

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# 12.0 Appendix A

Table A-1. Comparison of $Cs^+$ $K_d$ from detailed thermodynamic equilibrium model versus data for the spherical RF-641 resin at 25°C (RMS = 0.194).

| Simulant | Data Point | $K_d$ observed (g/ml) | $K_d$ model (g/ml) | Error (%) |
|---|---|---|---|---|
| S01 | H-A | 1.15E+02 | 9.16E+01 | -20.35 |
| | H-B | 1.29E+02 | 9.15E+01 | -29.09 |
| | H-C | 1.18E+02 | 9.14E+01 | -22.58 |
| | L-A | 4.59E+02 | 4.67E+02 | 1.74 |
| | L-B | 4.57E+02 | 4.67E+02 | 2.12 |
| | L-C | 4.61E+02 | 4.67E+02 | 1.24 |
| | M-A | 3.71E+02 | 4.34E+02 | 16.90 |
| | M-B | 3.80E+02 | 4.34E+02 | 14.29 |
| | M-C | 3.71E+02 | 4.35E+02 | 17.03 |
| | MH-A | 2.73E+02 | 2.96E+02 | 8.64 |
| | MH-B | 2.98E+02 | 2.97E+02 | -0.47 |
| | MH-C | 2.59E+02 | 2.97E+02 | 14.68 |
| S03 | H-A | 1.21E+02 | 9.07E+01 | -25.00 |
| | H-B | 1.20E+02 | 9.08E+01 | -24.53 |
| | L-A | 4.93E+02 | 4.70E+02 | -4.74 |
| | L-B | 5.07E+02 | 4.69E+02 | -7.37 |
| | M-A | 3.86E+02 | 4.36E+02 | 13.09 |
| | M-B | 3.97E+02 | 4.37E+02 | 9.85 |
| | MH-A | 2.56E+02 | 3.02E+02 | 17.94 |
| | MH-B | 2.31E+02 | 3.03E+02 | 30.85 |
| S04 | H-A | 9.72E+01 | 8.62E+01 | -11.31 |
| | H-B | 1.04E+02 | 8.63E+01 | -17.32 |
| | L-A | 4.31E+02 | 4.37E+02 | 1.24 |
| | L-B | 4.14E+02 | 4.37E+02 | 5.64 |
| S05 | H-A | 1.34E+02 | 9.28E+01 | -30.85 |
| | H-B | 1.36E+02 | 9.28E+01 | -31.99 |
| | L-A | 5.74E+02 | 4.89E+02 | -14.84 |
| | L-B | 5.43E+02 | 4.89E+02 | -9.94 |
| S06 | H-A | 1.90E+02 | 2.78E+02 | 46.62 |
| | H-B | 2.04E+02 | 2.80E+02 | 37.27 |
| | L-A | 5.85E+03 | 6.03E+03 | 3.10 |
| | L-B | 5.45E+03 | 6.03E+03 | 10.51 |
| S07 | H-A | 2.82E+02 | 2.90E+02 | 2.62 |
| | H-B | 2.71E+02 | 2.92E+02 | 7.55 |
| | L-A | 8.72E+03 | 8.55E+03 | -1.98 |
| | L-B | 8.32E+03 | 8.55E+03 | 2.83 |
| S08 | H-A | 9.36E+01 | 8.67E+01 | -7.29 |
| | H-B | 9.73E+01 | 8.75E+01 | -10.05 |
| | L-A | 4.58E+02 | 4.28E+02 | -6.62 |
| | L-B | 4.83E+02 | 4.28E+02 | -11.34 |
| S09 | H-A | 9.06E+01 | 8.01E+01 | -11.51 |
| | H-B | 8.53E+01 | 8.01E+01 | -6.07 |
| | L-A | 4.31E+02 | 3.94E+02 | -8.59 |
| | L-B | 5.20E+02 | 3.93E+02 | -24.44 |
| S10 | H-A | 3.48E+02 | 3.14E+02 | -9.97 |
| | H-B | 3.93E+02 | 3.16E+02 | -19.57 |
| | L-A | 1.22E+04 | 1.25E+04 | 2.05 |
| | L-B | 1.26E+04 | 1.25E+04 | -1.27 |
| S11 | H-A | 2.18E+02 | 2.03E+02 | -6.88 |
| | H-B | 1.78E+02 | 2.03E+02 | 14.59 |
| | L-A | 7.88E+03 | 9.44E+03 | 19.72 |
| | L-AR | 8.47E+03 | 9.44E+03 | 11.46 |
| | L-B | 8.45E+03 | 9.44E+03 | 11.75 |
| S12 | H-A | 1.78E+02 | 1.84E+02 | 3.44 |
| | H-B | 1.56E+02 | 1.85E+02 | 18.78 |
| | L-A | 6.28E+03 | 7.13E+03 | 13.60 |
| | L-AR | 6.28E+03 | 7.13E+03 | 13.51 |
| | L-B | 6.17E+03 | 7.13E+03 | 15.65 |
| S13 | H-A | 1.40E+02 | 1.48E+02 | 6.05 |
| | H-B | 1.27E+02 | 1.48E+02 | 17.03 |
| | L-A | 4.94E+03 | 5.07E+03 | 2.66 |
| | L-B | 5.19E+03 | 5.07E+03 | -2.35 |
| S16 | VLA | 1.84E+04 | 9.65E+03 | -47.71 |
| | VL-B | 1.73E+04 | 9.65E+03 | -44.10 |
| | VL-BR | 1.54E+04 | 9.65E+03 | -37.56 |
| S17 | VLA | 1.52E+04 | 9.66E+03 | -36.52 |
| | VL-B | 1.54E+04 | 9.66E+03 | -37.36 |
| S18 | VLA | 1.33E+04 | 9.68E+03 | -27.43 |
| | VL-B | 1.34E+04 | 9.68E+03 | -27.62 |

Table A-2. Comparison of $Cs^+$ loading from detailed thermodynamic equilibrium model versus data for the spherical RF-641 resin in $H^+$ form at 25°C (RMS = 0.054).

| Simulant | Data Point | Q observed (mmol/g) | Q model (mmol/g) | Error (%) |
|---|---|---|---|---|
| S01 | H-A | 4.95E-01 | 4.44E-01 | -10.35 |
| | H-B | 5.22E-01 | 4.44E-01 | -14.85 |
| | H-C | 5.02E-01 | 4.44E-01 | -11.52 |
| | L-A | 3.55E-03 | 3.56E-03 | 0.30 |
| | L-B | 3.54E-03 | 3.56E-03 | 0.36 |
| | L-C | 3.54E-03 | 3.56E-03 | 0.34 |
| | M-A | 1.95E-02 | 2.01E-02 | 3.03 |
| | M-B | 1.97E-02 | 2.02E-02 | 2.58 |
| | M-C | 1.94E-02 | 2.00E-02 | 3.04 |
| | MH-A | 1.14E-01 | 1.16E-01 | 2.10 |
| | MH-B | 1.16E-01 | 1.16E-01 | -0.11 |
| | MH-C | 1.12E-01 | 1.16E-01 | 3.56 |
| S03 | H-A | 5.12E-01 | 4.47E-01 | -12.81 |
| | H-B | 5.10E-01 | 4.46E-01 | -12.55 |
| | L-A | 3.76E-03 | 3.73E-03 | -0.79 |
| | L-B | 3.82E-03 | 3.77E-03 | -1.25 |
| | M-A | 1.98E-02 | 2.03E-02 | 2.34 |
| | M-B | 1.99E-02 | 2.02E-02 | 1.76 |
| | MH-A | 1.07E-01 | 1.12E-01 | 4.30 |
| | MH-B | 1.04E-01 | 1.11E-01 | 7.38 |
| S04 | H-A | 4.70E-01 | 4.43E-01 | -5.91 |
| | H-B | 4.86E-01 | 4.42E-01 | -9.03 |
| | L-A | 3.64E-03 | 3.66E-03 | 0.79 |
| | L-B | 3.63E-03 | 3.64E-03 | 0.36 |
| S05 | H-A | 5.34E-01 | 4.51E-01 | -15.51 |
| | H-B | 5.38E-01 | 4.51E-01 | -16.08 |
| | L-A | 3.84E-03 | 3.74E-03 | -2.40 |
| | L-B | 3.80E-03 | 3.74E-03 | -1.60 |
| S06 | H-A | 5.97E-01 | 6.68E-01 | 11.79 |
| | H-B | 6.10E-01 | 6.67E-01 | 9.37 |
| | L-A | 4.45E-03 | 4.46E-03 | 0.05 |
| | L-B | 4.47E-03 | 4.47E-03 | 0.16 |
| S07 | H-A | 6.84E-01 | 6.88E-01 | 0.64 |
| | H-B | 6.75E-01 | 6.88E-01 | 1.84 |
| | L-A | 4.50E-03 | 4.50E-03 | -0.02 |
| | L-B | 4.49E-03 | 4.49E-03 | 0.03 |
| S08 | H-A | 4.50E-01 | 4.33E-01 | -3.82 |
| | H-B | 4.54E-01 | 4.31E-01 | -5.20 |
| | L-A | 3.81E-03 | 3.77E-03 | -1.19 |
| | L-B | 3.84E-03 | 3.76E-03 | -2.04 |
| S09 | H-A | 4.45E-01 | 4.18E-01 | -6.20 |
| | H-B | 4.32E-01 | 4.18E-01 | -3.27 |
| | L-A | 3.62E-03 | 3.56E-03 | -1.65 |
| | L-B | 3.85E-03 | 3.66E-03 | -4.83 |
| S10 | H-A | 7.19E-01 | 7.03E-01 | -2.30 |
| | H-B | 7.35E-01 | 7.02E-01 | -4.48 |
| | L-A | 4.47E-03 | 4.47E-03 | 0.02 |
| | L-B | 4.47E-03 | 4.47E-03 | -0.01 |
| S11 | H-A | 7.26E-01 | 7.10E-01 | -2.25 |
| | H-B | 6.78E-01 | 7.10E-01 | 4.74 |
| | L-A | 4.76E-03 | 4.77E-03 | 0.20 |
| | L-AR | 4.77E-03 | 4.77E-03 | 0.11 |
| | L-B | 4.77E-03 | 4.77E-03 | 0.12 |
| S12 | H-A | 6.89E-01 | 6.97E-01 | 1.19 |
| | H-B | 6.54E-01 | 6.97E-01 | 6.47 |
| | L-A | 4.46E-03 | 4.47E-03 | 0.18 |
| | L-AR | 4.46E-03 | 4.47E-03 | 0.18 |
| | L-B | 4.45E-03 | 4.46E-03 | 0.21 |
| S13 | H-A | 6.20E-01 | 6.35E-01 | 2.40 |
| | H-B | 5.95E-01 | 6.35E-01 | 6.76 |
| | L-A | 4.40E-03 | 4.40E-03 | 0.04 |
| | L-B | 4.39E-03 | 4.39E-03 | -0.05 |
| S16 | VLA | 8.09E-05 | 8.05E-05 | -0.48 |
| | VL-B | 8.05E-05 | 8.02E-05 | -0.44 |
| | VL-BR | 8.06E-05 | 8.02E-05 | -0.51 |
| S17 | VLA | 8.10E-05 | 8.07E-05 | -0.37 |
| | VL-B | 8.05E-05 | 8.01E-05 | -0.38 |
| S18 | VLA | 8.25E-05 | 8.22E-05 | -0.28 |
| | VL-B | 8.20E-05 | 8.18E-05 | -0.28 |

Table A-3. Comparison of $Cs^+$ liquid concentration from detailed thermodynamic equilibrium model versus data for the spherical RF-641 resin at 25°C (RMS = 0.225).

| Simulant | Data Point | c observed [M] | c model [M] | Error (%) |
|---|---|---|---|---|
| S01 | H-A | 4.30E-03 | 4.84E-03 | 12.56 |
| | H-B | 4.04E-03 | 4.86E-03 | 20.09 |
| | H-C | 4.25E-03 | 4.86E-03 | 14.29 |
| | L-A | 7.73E-06 | 7.62E-06 | -1.42 |
| | L-B | 7.75E-06 | 7.61E-06 | -1.72 |
| | L-C | 7.68E-06 | 7.62E-06 | -0.89 |
| | M-A | 5.25E-05 | 4.63E-05 | -11.86 |
| | M-B | 5.19E-05 | 4.66E-05 | -10.25 |
| | M-C | 5.23E-05 | 4.61E-05 | -11.95 |
| | MH-A | 4.18E-04 | 3.93E-04 | -6.02 |
| | MH-B | 3.89E-04 | 3.90E-04 | 0.36 |
| | MH-C | 4.34E-04 | 3.92E-04 | -9.70 |
| S03 | H-A | 4.23E-03 | 4.92E-03 | 16.26 |
| | H-B | 4.24E-03 | 4.91E-03 | 15.87 |
| | L-A | 7.61E-06 | 7.93E-06 | 4.15 |
| | L-B | 7.54E-06 | 8.03E-06 | 6.61 |
| | M-A | 5.13E-05 | 4.64E-05 | -9.51 |
| | M-B | 5.00E-05 | 4.64E-05 | -7.37 |
| | MH-A | 4.18E-04 | 3.69E-04 | -11.56 |
| | MH-B | 4.49E-04 | 3.68E-04 | -17.94 |
| S04 | H-A | 4.84E-03 | 5.13E-03 | 6.09 |
| | H-B | 4.66E-03 | 5.13E-03 | 10.02 |
| | L-A | 8.43E-06 | 8.39E-06 | -0.44 |
| | L-B | 8.78E-06 | 8.34E-06 | -5.00 |
| S05 | H-A | 3.98E-03 | 4.86E-03 | 22.18 |
| | H-B | 3.94E-03 | 4.86E-03 | 23.39 |
| | L-A | 6.68E-06 | 7.66E-06 | 14.62 |
| | L-B | 7.00E-06 | 7.65E-06 | 9.26 |
| S06 | H-A | 3.14E-03 | 2.40E-03 | -23.76 |
| | H-B | 2.99E-03 | 2.38E-03 | -20.33 |
| | L-A | 7.62E-07 | 7.39E-07 | -2.97 |
| | L-B | 8.19E-07 | 7.42E-07 | -9.36 |
| S07 | H-A | 2.42E-03 | 2.38E-03 | -1.93 |
| | H-B | 2.49E-03 | 2.36E-03 | -5.31 |
| | L-A | 5.16E-07 | 5.26E-07 | 2.00 |
| | L-B | 5.40E-07 | 5.25E-07 | -2.72 |
| S08 | H-A | 4.81E-03 | 4.99E-03 | 3.74 |
| | H-B | 4.67E-03 | 4.92E-03 | 5.40 |
| | L-A | 8.32E-06 | 8.80E-06 | 5.81 |
| | L-B | 7.95E-06 | 8.79E-06 | 10.50 |
| S09 | H-A | 4.92E-03 | 5.21E-03 | 6.00 |
| | H-B | 5.06E-03 | 5.21E-03 | 2.99 |
| | L-A | 8.40E-06 | 9.04E-06 | 7.60 |
| | L-B | 7.40E-06 | 9.32E-06 | 25.95 |
| S10 | H-A | 2.06E-03 | 2.24E-03 | 8.52 |
| | H-B | 1.87E-03 | 2.22E-03 | 18.75 |
| | L-A | 3.65E-07 | 3.58E-07 | -1.99 |
| | L-B | 3.54E-07 | 3.58E-07 | 1.28 |
| S11 | H-A | 3.34E-03 | 3.50E-03 | 4.98 |
| | H-B | 3.82E-03 | 3.49E-03 | -8.60 |
| | L-A | 6.04E-07 | 5.05E-07 | -16.31 |
| | L-AR | 5.63E-07 | 5.05E-07 | -10.18 |
| | L-B | 5.65E-07 | 5.06E-07 | -10.41 |
| S12 | H-A | 3.87E-03 | 3.78E-03 | -2.18 |
| | H-B | 4.20E-03 | 3.76E-03 | -10.37 |
| | L-A | 7.11E-07 | 6.27E-07 | -11.81 |
| | L-AR | 7.10E-07 | 6.27E-07 | -11.74 |
| | L-B | 7.21E-07 | 6.25E-07 | -13.36 |
| S13 | H-A | 4.44E-03 | 4.28E-03 | -3.44 |
| | H-B | 4.69E-03 | 4.28E-03 | -8.78 |
| | L-A | 8.90E-07 | 8.68E-07 | -2.55 |
| | L-B | 8.45E-07 | 8.65E-07 | 2.35 |
| S16 | VLA | 4.39E-09 | 8.35E-09 | 90.31 |
| | VL-B | 4.67E-09 | 8.31E-09 | 78.10 |
| | VL-BR | 5.22E-09 | 8.31E-09 | 59.33 |
| S17 | VLA | 5.32E-09 | 8.35E-09 | 56.95 |
| | VL-B | 5.22E-09 | 8.30E-09 | 59.04 |
| S18 | VLA | 6.18E-09 | 8.49E-09 | 37.41 |
| | VL-B | 6.13E-09 | 8.45E-09 | 37.78 |

Table A-4. Comparison of $Cs^+$ $K_d$ from detailed thermodynamic equilibrium model versus data for the spherical RF-641 resin at 45°C (RMS = 0.348).

| Simulant | Data Point | $K_d$ observed (g/ml) | $K_d$ model (g/ml) | Error (%) |
|---|---|---|---|---|
| S01 | H-A | 9.08E+01 | 8.46E+01 | -6.75 |
| | H-B | 9.14E+01 | 8.45E+01 | -7.48 |
| | L-A | 2.73E+02 | 4.00E+02 | 46.39 |
| | L-B | 2.59E+02 | 4.00E+02 | 54.73 |
| | M-A | 2.24E+02 | 3.73E+02 | 66.22 |
| | M-B | 2.34E+02 | 3.73E+02 | 59.36 |
| | MH-A | 1.77E+02 | 2.58E+02 | 45.89 |
| | MH-B | 1.77E+02 | 2.58E+02 | 46.31 |
| S03 | H-A | 9.38E+01 | 8.38E+01 | -10.69 |
| | H-B | 9.68E+01 | 8.43E+01 | -12.96 |
| | L-A | 2.85E+02 | 4.03E+02 | 41.28 |
| | L-B | 2.91E+02 | 4.03E+02 | 38.18 |
| | M-A | 2.44E+02 | 3.75E+02 | 53.76 |
| | M-B | 2.45E+02 | 3.75E+02 | 52.91 |
| | MH-A | 1.69E+02 | 2.64E+02 | 56.30 |
| | MH-B | 1.66E+02 | 2.64E+02 | 59.45 |
| S04 | H-A | 8.74E+01 | 8.03E+01 | -8.11 |
| | H-B | 8.46E+01 | 8.06E+01 | -4.76 |
| | L-A | 3.02E+02 | 3.87E+02 | 28.22 |
| | L-B | 2.40E+02 | 3.86E+02 | 60.76 |
| S05 | H-A | 1.15E+02 | 8.32E+01 | -27.52 |
| | H-B | 1.11E+02 | 8.34E+01 | -24.97 |
| | L-A | 3.64E+02 | 4.06E+02 | 11.63 |
| | L-B | 3.52E+02 | 4.06E+02 | 15.49 |
| S06 | H-A | 1.56E+02 | 2.21E+02 | 42.31 |
| | H-B | 1.50E+02 | 2.22E+02 | 47.97 |
| | L-A | 2.52E+03 | 3.54E+03 | 40.69 |
| | L-B | 2.68E+03 | 3.54E+03 | 31.88 |
| S07 | H-A | 2.07E+02 | 2.36E+02 | 14.40 |
| | H-B | 2.12E+02 | 2.37E+02 | 11.41 |
| | L-A | 3.82E+03 | 5.13E+03 | 34.49 |
| | L-B | 3.65E+03 | 5.13E+03 | 40.64 |
| S08 | H-A | 8.43E+01 | 7.92E+01 | -6.13 |
| | H-B | 9.80E+01 | 7.92E+01 | -19.13 |
| | L-A | 3.14E+02 | 3.64E+02 | 15.95 |
| | L-B | 3.25E+02 | 3.64E+02 | 12.04 |
| S09 | H-A | 7.74E+01 | 7.26E+01 | -6.20 |
| | H-B | 8.32E+01 | 7.27E+01 | -12.64 |
| | L-A | 3.34E+02 | 3.34E+02 | -0.11 |
| | L-B | 2.95E+02 | 3.34E+02 | 13.31 |
| S10 | H-A | 3.01E+02 | 2.62E+02 | -13.11 |
| | H-B | 2.75E+02 | 2.61E+02 | -4.83 |
| | L-A | 6.25E+03 | 7.69E+03 | 22.94 |
| | L-B | 6.36E+03 | 7.69E+03 | 20.94 |
| S11 | H-A | 1.84E+02 | 1.84E+02 | 0.00 |
| | H-B | 1.88E+02 | 1.84E+02 | -1.87 |
| | L-A | 4.30E+03 | 6.48E+03 | 50.68 |
| | L-B | 4.15E+03 | 6.48E+03 | 56.05 |
| S12 | H-A | 1.44E+02 | 1.67E+02 | 16.54 |
| | H-B | 1.56E+02 | 1.67E+02 | 7.03 |
| | L-A | 3.43E+03 | 4.96E+03 | 44.49 |
| | L-B | 3.11E+03 | 4.96E+03 | 59.74 |
| S13 | H-A | 1.07E+02 | 1.36E+02 | 27.20 |
| | H-B | 1.08E+02 | 1.36E+02 | 26.10 |
| | L-A | 2.85E+03 | 3.58E+03 | 25.37 |
| | L-B | 2.41E+03 | 3.58E+03 | 48.59 |

Table A-5. Comparison of $Cs^+$ loading from detailed thermodynamic equilibrium model versus data for the spherical RF-641 resin in $H^+$ form at 45°C (RMS = 0.078).

| Simulant | Data Point | Q observed (mmol/g) | Q model (mmol/g) | Error (%) |
|---|---|---|---|---|
| S01 | H-A | 4.41E-01 | 4.26E-01 | -3.56 |
| | H-B | 4.43E-01 | 4.26E-01 | -3.95 |
| | L-A | 3.16E-03 | 3.44E-03 | 8.90 |
| | L-B | 3.11E-03 | 3.44E-03 | 10.49 |
| | M-A | 1.72E-02 | 1.95E-02 | 13.42 |
| | M-B | 1.73E-02 | 1.94E-02 | 11.97 |
| | MH-A | 9.97E-02 | 1.12E-01 | 12.34 |
| | MH-B | 9.94E-02 | 1.12E-01 | 12.41 |
| S03 | H-A | 4.54E-01 | 4.28E-01 | -5.69 |
| | H-B | 4.59E-01 | 4.27E-01 | -6.84 |
| | L-A | 3.36E-03 | 3.62E-03 | 7.83 |
| | L-B | 3.39E-03 | 3.64E-03 | 7.27 |
| | M-A | 1.78E-02 | 1.97E-02 | 10.85 |
| | M-B | 1.79E-02 | 1.98E-02 | 10.73 |
| | MH-A | 9.33E-02 | 1.07E-01 | 14.85 |
| | MH-B | 9.26E-02 | 1.07E-01 | 15.68 |
| S04 | H-A | 4.51E-01 | 4.31E-01 | -4.44 |
| | H-B | 4.42E-01 | 4.31E-01 | -2.60 |
| | L-A | 3.60E-03 | 3.67E-03 | 1.89 |
| | L-B | 3.26E-03 | 3.81E-03 | 16.68 |
| S05 | H-A | 5.09E-01 | 4.33E-01 | -14.83 |
| | H-B | 5.00E-01 | 4.33E-01 | -13.40 |
| | L-A | 3.63E-03 | 3.71E-03 | 2.23 |
| | L-B | 3.61E-03 | 3.71E-03 | 2.97 |
| S06 | H-A | 5.67E-01 | 6.40E-01 | 12.90 |
| | H-B | 5.58E-01 | 6.40E-01 | 14.57 |
| | L-A | 4.52E-03 | 4.57E-03 | 1.07 |
| | L-B | 4.51E-03 | 4.55E-03 | 0.84 |
| S07 | H-A | 6.40E-01 | 6.67E-01 | 4.19 |
| | H-B | 6.46E-01 | 6.67E-01 | 3.32 |
| | L-A | 4.58E-03 | 4.61E-03 | 0.63 |
| | L-B | 4.56E-03 | 4.59E-03 | 0.74 |
| S08 | H-A | 4.31E-01 | 4.16E-01 | -3.39 |
| | H-B | 4.65E-01 | 4.16E-01 | -10.55 |
| | L-A | 3.64E-03 | 3.76E-03 | 3.36 |
| | L-B | 3.66E-03 | 3.75E-03 | 2.53 |
| S09 | H-A | 4.17E-01 | 4.03E-01 | -3.55 |
| | H-B | 4.34E-01 | 4.02E-01 | -7.24 |
| | L-A | 3.55E-03 | 3.55E-03 | -0.03 |
| | L-B | 3.45E-03 | 3.55E-03 | 2.99 |
| S10 | H-A | 7.12E-01 | 6.87E-01 | -3.55 |
| | H-B | 6.96E-01 | 6.87E-01 | -1.32 |
| | L-A | 4.69E-03 | 4.71E-03 | 0.28 |
| | L-B | 4.72E-03 | 4.74E-03 | 0.25 |
| S11 | H-A | 6.98E-01 | 6.98E-01 | 0.01 |
| | H-B | 7.02E-01 | 6.98E-01 | -0.65 |
| | L-A | 4.83E-03 | 4.87E-03 | 0.78 |
| | L-B | 4.84E-03 | 4.88E-03 | 0.86 |
| S12 | H-A | 6.43E-01 | 6.83E-01 | 6.19 |
| | H-B | 6.66E-01 | 6.83E-01 | 2.64 |
| | L-A | 4.54E-03 | 4.58E-03 | 0.89 |
| | L-B | 4.51E-03 | 4.56E-03 | 1.19 |
| S13 | H-A | 5.58E-01 | 6.22E-01 | 11.52 |
| | H-B | 5.60E-01 | 6.22E-01 | 11.11 |
| | L-A | 4.47E-03 | 4.50E-03 | 0.70 |
| | L-B | 4.42E-03 | 4.48E-03 | 1.33 |

Table A-6. Comparison of $Cs^+$ liquid concentration from detailed thermodynamic equilibrium model versus data for the spherical RF-641 resin at 45°C (RMS = 0.198).

| Simulant | Data Point | c observed [M] | c model [M] | Error (%) |
|---|---|---|---|---|
| S01 | H-A | 4.86E-03 | 5.03E-03 | 3.42 |
| | H-B | 4.85E-03 | 5.04E-03 | 3.81 |
| | L-A | 1.16E-05 | 8.61E-06 | -25.61 |
| | L-B | 1.20E-05 | 8.60E-06 | -28.59 |
| | M-A | 7.66E-05 | 5.22E-05 | -31.77 |
| | M-B | 7.40E-05 | 5.20E-05 | -29.74 |
| | MH-A | 5.64E-04 | 4.34E-04 | -23.00 |
| | MH-B | 5.63E-04 | 4.32E-04 | -23.17 |
| S03 | H-A | 4.84E-03 | 5.11E-03 | 5.60 |
| | H-B | 4.74E-03 | 5.07E-03 | 7.03 |
| | L-A | 1.18E-05 | 9.00E-06 | -23.68 |
| | L-B | 1.16E-05 | 9.03E-06 | -22.37 |
| | M-A | 7.29E-05 | 5.26E-05 | -27.91 |
| | M-B | 7.29E-05 | 5.28E-05 | -27.59 |
| | MH-A | 5.52E-04 | 4.06E-04 | -26.52 |
| | MH-B | 5.60E-04 | 4.06E-04 | -27.45 |
| S04 | H-A | 5.17E-03 | 5.37E-03 | 3.99 |
| | H-B | 5.22E-03 | 5.34E-03 | 2.28 |
| | L-A | 1.19E-05 | 9.47E-06 | -20.54 |
| | L-B | 1.36E-05 | 9.87E-06 | -27.42 |
| S05 | H-A | 4.43E-03 | 5.21E-03 | 17.51 |
| | H-B | 4.50E-03 | 5.19E-03 | 15.41 |
| | L-A | 9.97E-06 | 9.13E-06 | -8.42 |
| | L-B | 1.02E-05 | 9.13E-06 | -10.84 |
| S06 | H-A | 3.64E-03 | 2.89E-03 | -20.67 |
| | H-B | 3.72E-03 | 2.88E-03 | -22.57 |
| | L-A | 1.80E-06 | 1.29E-06 | -28.16 |
| | L-B | 1.68E-06 | 1.29E-06 | -23.54 |
| S07 | H-A | 3.10E-03 | 2.82E-03 | -8.92 |
| | H-B | 3.04E-03 | 2.82E-03 | -7.27 |
| | L-A | 1.20E-06 | 8.98E-07 | -25.18 |
| | L-B | 1.25E-06 | 8.95E-07 | -28.37 |
| S08 | H-A | 5.11E-03 | 5.25E-03 | 2.92 |
| | H-B | 4.74E-03 | 5.25E-03 | 10.61 |
| | L-A | 1.16E-05 | 1.03E-05 | -10.86 |
| | L-B | 1.13E-05 | 1.03E-05 | -8.49 |
| S09 | H-A | 5.39E-03 | 5.54E-03 | 2.82 |
| | H-B | 5.22E-03 | 5.54E-03 | 6.18 |
| | L-A | 1.06E-05 | 1.06E-05 | 0.08 |
| | L-B | 1.17E-05 | 1.06E-05 | -9.11 |
| S10 | H-A | 2.36E-03 | 2.62E-03 | 11.00 |
| | H-B | 2.53E-03 | 2.63E-03 | 3.69 |
| | L-A | 7.50E-07 | 6.12E-07 | -18.44 |
| | L-B | 7.43E-07 | 6.16E-07 | -17.10 |
| S11 | H-A | 3.80E-03 | 3.80E-03 | 0.01 |
| | H-B | 3.74E-03 | 3.79E-03 | 1.24 |
| | L-A | 1.12E-06 | 7.52E-07 | -33.12 |
| | L-B | 1.17E-06 | 7.53E-07 | -35.37 |
| S12 | H-A | 4.48E-03 | 4.08E-03 | -8.88 |
| | H-B | 4.27E-03 | 4.09E-03 | -4.10 |
| | L-A | 1.32E-06 | 9.23E-07 | -30.17 |
| | L-B | 1.45E-06 | 9.20E-07 | -36.65 |
| S13 | H-A | 5.21E-03 | 4.57E-03 | -12.32 |
| | H-B | 5.21E-03 | 4.59E-03 | -11.89 |
| | L-A | 1.57E-06 | 1.26E-06 | -19.68 |
| | L-B | 1.84E-06 | 1.25E-06 | -31.81 |

# 13.0 Appendix B

Table B-1. Model calculated equilibrium liquid compositions for batch contact experiments at 25 C.

| Simulant | Data Point | $K^+$ [M] | $Na^+$ [M] | $Cs^+$ [M] | $Rb^+$ [M] | $OH^-$ [M] |
|---|---|---|---|---|---|---|
| S01 | H-A | 6.47807E-01 | 4.99691E+00 | 4.82320E-03 | 5.33376E-05 | 1.87003E+00 |
| | H-B | 6.48024E-01 | 4.99692E+00 | 4.83579E-03 | 5.33629E-05 | 1.87028E+00 |
| | H-C | 6.48094E-01 | 4.99693E+00 | 4.83987E-03 | 5.33711E-05 | 1.87036E+00 |
| | L-A | 6.44005E-01 | 4.99666E+00 | 1.15157E-05 | 4.54393E-05 | 1.87065E+00 |
| | L-B | 6.43892E-01 | 4.99665E+00 | 1.14996E-05 | 4.54197E-05 | 1.87053E+00 |
| | L-C | 6.43917E-01 | 4.99665E+00 | 1.15031E-05 | 4.54240E-05 | 1.87055E+00 |
| | M-A | 6.43708E-01 | 4.99664E+00 | 6.69790E-05 | 4.55943E-05 | 1.87017E+00 |
| | M-B | 6.44170E-01 | 4.99667E+00 | 6.73684E-05 | 4.56748E-05 | 1.87067E+00 |
| | M-C | 6.43391E-01 | 4.99662E+00 | 6.67148E-05 | 4.55393E-05 | 1.86983E+00 |
| | MH-A | 6.44789E-01 | 4.99671E+00 | 4.69031E-04 | 4.70858E-05 | 1.87037E+00 |
| | MH-B | 6.44368E-01 | 4.99668E+00 | 4.66435E-04 | 4.70123E-05 | 1.86992E+00 |
| | MH-C | 6.44643E-01 | 4.99670E+00 | 4.68128E-04 | 4.70603E-05 | 1.87021E+00 |
| S02 | H-A | 6.51421E-01 | 4.99602E+00 | 4.88242E-03 | 4.38605E-05 | 1.87478E+00 |
| | H-B | 6.51513E-01 | 4.99602E+00 | 4.88770E-03 | 4.38690E-05 | 1.87489E+00 |
| | L-A | 6.47390E-01 | 4.99577E+00 | 1.20337E-05 | 3.77253E-05 | 1.87509E+00 |
| | L-B | 6.47243E-01 | 4.99576E+00 | 1.20121E-05 | 3.77052E-05 | 1.87494E+00 |
| | M-A | 6.47440E-01 | 4.99577E+00 | 8.41044E-05 | 3.79322E-05 | 1.87495E+00 |
| | M-B | 6.46924E-01 | 4.99574E+00 | 8.35731E-05 | 3.78613E-05 | 1.87440E+00 |
| | MH-A | 6.48569E-01 | 4.99584E+00 | 4.75841E-04 | 3.90353E-05 | 1.87528E+00 |
| | MH-B | 6.47979E-01 | 4.99581E+00 | 4.72234E-04 | 3.89542E-05 | 1.87465E+00 |
| S03 | H-A | 6.48290E-01 | 4.99786E+00 | 4.90037E-03 | 0.00000E+00 | 1.87085E+00 |
| | H-B | 6.48143E-01 | 4.99785E+00 | 4.89172E-03 | 0.00000E+00 | 1.87069E+00 |
| | L-A | 6.43133E-01 | 4.99752E+00 | 1.20267E-05 | 0.00000E+00 | 1.87002E+00 |
| | L-B | 6.44078E-01 | 4.99758E+00 | 1.21685E-05 | 0.00000E+00 | 1.87103E+00 |
| | M-A | 6.43585E-01 | 4.99755E+00 | 6.73954E-05 | 0.00000E+00 | 1.87035E+00 |
| | M-B | 6.43451E-01 | 4.99754E+00 | 6.72826E-05 | 0.00000E+00 | 1.87020E+00 |
| | MH-A | 6.44957E-01 | 4.99764E+00 | 4.44760E-04 | 0.00000E+00 | 1.87091E+00 |
| | MH-B | 6.44750E-01 | 4.99762E+00 | 4.43546E-04 | 0.00000E+00 | 1.87069E+00 |
| S04 | H-A | 6.48798E-01 | 5.99500E+00 | 5.11050E-03 | 5.34746E-05 | 1.86897E+00 |
| | H-B | 6.48701E-01 | 5.99499E+00 | 5.10470E-03 | 5.34636E-05 | 1.86886E+00 |
| | L-A | 6.44462E-01 | 5.99460E+00 | 1.26047E-05 | 4.56977E-05 | 1.86892E+00 |
| | L-B | 6.44007E-01 | 5.99456E+00 | 1.25342E-05 | 4.56193E-05 | 1.86842E+00 |
| S05 | H-A | 6.46265E-01 | 3.99836E+00 | 4.84614E-03 | 5.33070E-05 | 1.86882E+00 |
| | H-B | 6.46244E-01 | 3.99836E+00 | 4.84492E-03 | 5.33045E-05 | 1.86880E+00 |
| | L-A | 6.41803E-01 | 3.99816E+00 | 1.16370E-05 | 4.49424E-05 | 1.86894E+00 |
| | L-B | 6.41649E-01 | 3.99815E+00 | 1.16151E-05 | 4.49157E-05 | 1.86877E+00 |
| S06 | H-A | 0.00000E+00 | 5.93705E+00 | 2.79453E-03 | 4.72087E-05 | 1.87000E+00 |
| | H-B | 0.00000E+00 | 5.93687E+00 | 2.77853E-03 | 4.71338E-05 | 1.86981E+00 |
| | L-A | 0.00000E+00 | 5.92987E+00 | 1.15883E-06 | 1.15195E-05 | 1.86943E+00 |
| | L-B | 0.00000E+00 | 5.93017E+00 | 1.16370E-06 | 1.15604E-05 | 1.86973E+00 |
| S07 | H-A | 0.00000E+00 | 4.93277E+00 | 2.87598E-03 | 4.74458E-05 | 1.86906E+00 |
| | H-B | 0.00000E+00 | 4.93253E+00 | 2.85334E-03 | 4.73439E-05 | 1.86880E+00 |
| | L-A | 0.00000E+00 | 4.92581E+00 | 8.26406E-07 | 8.75941E-06 | 1.86882E+00 |
| | L-B | 0.00000E+00 | 4.92565E+00 | 8.24557E-07 | 8.74201E-06 | 1.86866E+00 |
| S08 | H-A | 6.49918E-01 | 4.99649E+00 | 4.96551E-03 | 5.11772E-05 | 7.30924E-01 |
| | H-B | 6.48811E-01 | 4.99639E+00 | 4.90073E-03 | 5.09977E-05 | 7.29650E-01 |
| | L-A | 6.44730E-01 | 4.99602E+00 | 1.31927E-05 | 4.11217E-05 | 7.29781E-01 |
| | L-B | 6.44607E-01 | 4.99601E+00 | 1.31727E-05 | 4.10957E-05 | 7.29647E-01 |
| S09 | H-A | 6.51938E-01 | 4.99420E+00 | 5.20015E-03 | 4.98810E-05 | 1.31116E-01 |
| | H-B | 6.51925E-01 | 4.99420E+00 | 5.19937E-03 | 4.98786E-05 | 1.31101E-01 |
| | L-A | 6.47954E-01 | 4.99379E+00 | 1.34749E-05 | 3.89769E-05 | 1.31150E-01 |
| | L-B | 6.50034E-01 | 4.99401E+00 | 1.38370E-05 | 3.94707E-05 | 1.33456E-01 |
| S10 | H-A | 0.00000E+00 | 3.94044E+00 | 2.81832E-03 | 4.72204E-05 | 1.87059E+00 |
| | H-B | 0.00000E+00 | 3.94026E+00 | 2.80026E-03 | 4.71371E-05 | 1.87039E+00 |
| | L-A | 0.00000E+00 | 3.93164E+00 | 5.63247E-07 | 6.18996E-06 | 1.86859E+00 |
| | L-B | 0.00000E+00 | 3.93164E+00 | 5.63309E-07 | 6.19060E-06 | 1.86860E+00 |
| S11 | H-A | 0.00000E+00 | 4.93839E+00 | 4.09989E-03 | 0.00000E+00 | 1.93175E+00 |
| | H-B | 0.00000E+00 | 4.93829E+00 | 4.08902E-03 | 0.00000E+00 | 1.93163E+00 |
| | L-A | 0.00000E+00 | 4.93130E+00 | 8.04234E-07 | 0.00000E+00 | 1.93125E+00 |
| | L-B | 0.00000E+00 | 4.93135E+00 | 8.04836E-07 | 0.00000E+00 | 1.93130E+00 |
| S12 | H-A | 0.00000E+00 | 4.93859E+00 | 4.34357E-03 | 0.00000E+00 | 9.32019E-01 |
| | H-B | 0.00000E+00 | 4.93838E+00 | 4.32254E-03 | 0.00000E+00 | 9.31790E-01 |
| | L-A | 0.00000E+00 | 4.93208E+00 | 9.96653E-07 | 0.00000E+00 | 9.32031E-01 |
| | L-B | 0.00000E+00 | 4.93189E+00 | 9.93992E-07 | 0.00000E+00 | 9.31847E-01 |
| S13 | H-A | 0.00000E+00 | 4.94398E+00 | 4.82062E-03 | 0.00000E+00 | 3.80232E-02 |
| | H-B | 0.00000E+00 | 4.94393E+00 | 4.81535E-03 | 0.00000E+00 | 3.79657E-02 |
| | L-A | 0.00000E+00 | 4.93808E+00 | 1.38405E-06 | 0.00000E+00 | 3.80310E-02 |
| | L-B | 0.00000E+00 | 4.93787E+00 | 1.37961E-06 | 0.00000E+00 | 3.78275E-02 |
| S16 | VLA | 0.00000E+00 | 4.93148E+00 | 1.31776E-08 | 0.00000E+00 | 1.93148E+00 |
| | VL-B | 0.00000E+00 | 4.93119E+00 | 1.31236E-08 | 0.00000E+00 | 1.93119E+00 |
| S17 | VLA | 0.00000E+00 | 4.93224E+00 | 1.74248E-08 | 0.00000E+00 | 9.32238E-01 |
| | VL-B | 0.00000E+00 | 4.93178E+00 | 1.73096E-08 | 0.00000E+00 | 9.31779E-01 |
| S18 | VLA | 0.00000E+00 | 4.93813E+00 | 2.48504E-08 | 0.00000E+00 | 3.81273E-02 |
| | VL-B | 0.00000E+00 | 4.93782E+00 | 2.47316E-08 | 0.00000E+00 | 3.78221E-02 |

Table B-2. Model calculated equilibrium liquid compositions for batch contact experiments at 45 C.

| Simulant | Data Point | $K^+$ [M] | $Na^+$ [M] | $Cs^+$ [M] | $Rb^+$ [M] | $OH^-$ [M] |
|---|---|---|---|---|---|---|
| S01 | H-A | 6.4837E-01 | 4.9962E+00 | 4.7924E-03 | 5.3304E-05 | 1.8699E+00 |
| | H-B | 6.4853E-01 | 4.9962E+00 | 4.8018E-03 | 5.3323E-05 | 1.8701E+00 |
| | L-A | 6.4428E-01 | 4.9959E+00 | 1.1288E-05 | 4.5225E-05 | 1.8702E+00 |
| | L-B | 6.4420E-01 | 4.9959E+00 | 1.1277E-05 | 4.5211E-05 | 1.8701E+00 |
| | M-A | 6.4423E-01 | 4.9959E+00 | 6.5862E-05 | 4.5425E-05 | 1.8700E+00 |
| | M-B | 6.4391E-01 | 4.9959E+00 | 6.5598E-05 | 4.5369E-05 | 1.8696E+00 |
| | MH-A | 6.4525E-01 | 4.9960E+00 | 4.6142E-04 | 4.6928E-05 | 1.8701E+00 |
| | MH-B | 6.4500E-01 | 4.9960E+00 | 4.5987E-04 | 4.6883E-05 | 1.8698E+00 |
| S02 | H-A | 6.5180E-01 | 4.9954E+00 | 4.8374E-03 | 4.3811E-05 | 1.8745E+00 |
| | H-B | 6.5193E-01 | 4.9954E+00 | 4.8451E-03 | 4.3824E-05 | 1.8747E+00 |
| | L-A | 6.4764E-01 | 4.9951E+00 | 1.1753E-05 | 3.7513E-05 | 1.8747E+00 |
| | L-B | 6.4775E-01 | 4.9951E+00 | 1.1769E-05 | 3.7528E-05 | 1.8748E+00 |
| | M-A | 6.4773E-01 | 4.9951E+00 | 8.2210E-05 | 3.7730E-05 | 1.8746E+00 |
| | M-B | 6.4756E-01 | 4.9951E+00 | 8.2034E-05 | 3.7706E-05 | 1.8744E+00 |
| | MH-A | 6.4838E-01 | 4.9952E+00 | 4.6283E-04 | 3.8787E-05 | 1.8744E+00 |
| | MH-B | 6.4869E-01 | 4.9952E+00 | 4.6472E-04 | 3.8831E-05 | 1.8747E+00 |
| S03 | H-A | 6.4899E-01 | 4.9972E+00 | 4.8784E-03 | 0.0000E+00 | 1.8709E+00 |
| | H-B | 6.4820E-01 | 4.9971E+00 | 4.8313E-03 | 0.0000E+00 | 1.8700E+00 |
| | L-A | 6.4383E-01 | 4.9968E+00 | 1.1853E-05 | 0.0000E+00 | 1.8700E+00 |
| | L-B | 6.4411E-01 | 4.9968E+00 | 1.1894E-05 | 0.0000E+00 | 1.8703E+00 |
| | M-A | 6.4433E-01 | 4.9968E+00 | 6.6475E-05 | 0.0000E+00 | 1.8704E+00 |
| | M-B | 6.4465E-01 | 4.9969E+00 | 6.6741E-05 | 0.0000E+00 | 1.8707E+00 |
| | MH-A | 6.4501E-01 | 4.9969E+00 | 4.3518E-04 | 0.0000E+00 | 1.8702E+00 |
| | MH-B | 6.4502E-01 | 4.9969E+00 | 4.3527E-04 | 0.0000E+00 | 1.8702E+00 |
| S04 | H-A | 6.5176E-01 | 5.9939E+00 | 5.1288E-03 | 5.3533E-05 | 1.8708E+00 |
| | H-B | 6.5126E-01 | 5.9938E+00 | 5.0968E-03 | 5.3473E-05 | 1.8702E+00 |
| | L-A | 6.4767E-01 | 5.9934E+00 | 1.2278E-05 | 4.5394E-05 | 1.8709E+00 |
| | L-B | 6.5057E-01 | 5.9938E+00 | 1.2758E-05 | 4.5929E-05 | 1.8742E+00 |
| S05 | H-A | 6.4873E-01 | 3.9982E+00 | 4.9906E-03 | 5.3617E-05 | 1.8712E+00 |
| | H-B | 6.4838E-01 | 3.9982E+00 | 4.9699E-03 | 5.3578E-05 | 1.8709E+00 |
| | L-A | 6.4404E-01 | 3.9979E+00 | 1.2035E-05 | 4.5478E-05 | 1.8709E+00 |
| | L-B | 6.4408E-01 | 3.9979E+00 | 1.2041E-05 | 4.5486E-05 | 1.8710E+00 |
| S06 | H-A | 0.0000E+00 | 5.9389E+00 | 3.0198E-03 | 4.8242E-05 | 1.8721E+00 |
| | H-B | 0.0000E+00 | 5.9388E+00 | 3.0069E-03 | 4.8189E-05 | 1.8720E+00 |
| | L-A | 0.0000E+00 | 5.9324E+00 | 1.3862E-06 | 1.3378E-05 | 1.8720E+00 |
| | L-B | 0.0000E+00 | 5.9322E+00 | 1.3814E-06 | 1.3341E-05 | 1.8717E+00 |
| S07 | H-A | 0.0000E+00 | 4.9348E+00 | 3.1013E-03 | 4.8446E-05 | 1.8713E+00 |
| | H-B | 0.0000E+00 | 4.9347E+00 | 3.0975E-03 | 4.8431E-05 | 1.8712E+00 |
| | L-A | 0.0000E+00 | 4.9280E+00 | 9.6461E-07 | 1.0054E-05 | 1.8710E+00 |
| | L-B | 0.0000E+00 | 4.9277E+00 | 9.6124E-07 | 1.0023E-05 | 1.8708E+00 |
| S08 | H-A | 6.5238E-01 | 4.9955E+00 | 5.0124E-03 | 5.1298E-05 | 7.3239E-01 |
| | H-B | 6.5227E-01 | 4.9954E+00 | 5.0057E-03 | 5.1280E-05 | 7.3227E-01 |
| | L-A | 6.4835E-01 | 4.9950E+00 | 1.3355E-05 | 4.1323E-05 | 7.3238E-01 |
| | L-B | 6.4814E-01 | 4.9950E+00 | 1.3318E-05 | 4.1276E-05 | 7.3215E-01 |
| S09 | H-A | 6.5567E-01 | 4.9930E+00 | 5.3065E-03 | 5.0158E-05 | 1.3370E-01 |
| | H-B | 6.5561E-01 | 4.9929E+00 | 5.3029E-03 | 5.0147E-05 | 1.3364E-01 |
| | L-A | 6.5187E-01 | 4.9925E+00 | 1.3636E-05 | 3.9116E-05 | 1.3372E-01 |
| | L-B | 6.5178E-01 | 4.9924E+00 | 1.3621E-05 | 3.9095E-05 | 1.3363E-01 |
| S10 | H-A | 0.0000E+00 | 3.9423E+00 | 3.0249E-03 | 4.8167E-05 | 1.8727E+00 |
| | H-B | 0.0000E+00 | 3.9424E+00 | 3.0300E-03 | 4.8188E-05 | 1.8727E+00 |
| | L-A | 0.0000E+00 | 3.9356E+00 | 6.5721E-07 | 7.1533E-06 | 1.8726E+00 |
| | L-B | 0.0000E+00 | 3.9361E+00 | 6.6148E-07 | 7.1956E-06 | 1.8730E+00 |
| S11 | H-A | 0.0000E+00 | 4.9399E+00 | 4.2515E-03 | 0.0000E+00 | 1.9334E+00 |
| | H-B | 0.0000E+00 | 4.9398E+00 | 4.2425E-03 | 0.0000E+00 | 1.9333E+00 |
| | L-A | 0.0000E+00 | 4.9330E+00 | 8.1915E-07 | 0.0000E+00 | 1.9330E+00 |
| | L-B | 0.0000E+00 | 4.9331E+00 | 8.2023E-07 | 0.0000E+00 | 1.9331E+00 |
| S12 | H-A | 0.0000E+00 | 4.9400E+00 | 4.4800E-03 | 0.0000E+00 | 9.3354E-01 |
| | H-B | 0.0000E+00 | 4.9401E+00 | 4.4916E-03 | 0.0000E+00 | 9.3367E-01 |
| | L-A | 0.0000E+00 | 4.9341E+00 | 1.0063E-06 | 0.0000E+00 | 9.3407E-01 |
| | L-B | 0.0000E+00 | 4.9339E+00 | 1.0026E-06 | 0.0000E+00 | 9.3382E-01 |
| S13 | H-A | 0.0000E+00 | 4.9452E+00 | 4.9330E-03 | 0.0000E+00 | 3.9315E-02 |
| | H-B | 0.0000E+00 | 4.9454E+00 | 4.9557E-03 | 0.0000E+00 | 3.9560E-02 |
| | L-A | 0.0000E+00 | 4.9398E+00 | 1.3799E-06 | 0.0000E+00 | 3.9746E-02 |
| | L-B | 0.0000E+00 | 4.9395E+00 | 1.3726E-06 | 0.0000E+00 | 3.9419E-02 |

Table B-3. Model calculated equilibrium liquid compositions for batch contact experiments at 15 C.

| Simulant | Data Point | $K^+$ [M] | $Na^+$ [M] | $Cs^+$ [M] | $Rb^+$ [M] | $OH^-$ [M] |
|---|---|---|---|---|---|---|
| S02 | H-A | 6.5446E-01 | 4.9964E+00 | 5.0453E-03 | 4.4106E-05 | 1.8784E+00 |
| | H-B | 6.5433E-01 | 4.9964E+00 | 5.0371E-03 | 4.4093E-05 | 1.8782E+00 |
| | L-A | 6.5035E-01 | 4.9962E+00 | 1.2327E-05 | 3.7975E-05 | 1.8785E+00 |
| | L-B | 6.5022E-01 | 4.9962E+00 | 1.2307E-05 | 3.7957E-05 | 1.8783E+00 |
| | M-A | 6.5030E-01 | 4.9962E+00 | 8.6097E-05 | 3.8173E-05 | 1.8782E+00 |
| | M-B | 6.5015E-01 | 4.9962E+00 | 8.5927E-05 | 3.8151E-05 | 1.8781E+00 |
| | MH-A | 6.5145E-01 | 4.9963E+00 | 4.8875E-04 | 3.9300E-05 | 1.8786E+00 |
| | MH-B | 6.5109E-01 | 4.9962E+00 | 4.8641E-04 | 3.9249E-05 | 1.8782E+00 |
| | L-24 | 6.5018E-01 | 4.9962E+00 | 1.2301E-05 | 3.7951E-05 | 1.8783E+00 |
| | L-48 | 6.5003E-01 | 4.9962E+00 | 1.2277E-05 | 3.7930E-05 | 1.8781E+00 |
| | L-48R | 6.5008E-01 | 4.9962E+00 | 1.2286E-05 | 3.7938E-05 | 1.8782E+00 |

# 14. Appendix C

VERSE-LC input and output files for the particle kinetics rig and laboratory-scale test columns are provided in this appendix. The input and output files for each case are listed below. A datafile.yio file was required for each of the models for the SRNL particle kinetics experiments, but not for the column experiments. In this appendix, the datafile.yio files are listed after their corresponding datafile.

## C.1 SRNL Particle Kinetics Experiment at 15 °C

### C.1.1 VERSE-LC Datafile

```
SRNL Kinetics Rig - AP-101S, 15C, Batch 641 RF
Particle radius = volume mean radius, Dp = Dinf/3
1, 2, 1, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                           isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNYN                           input-only,perfusable,feed-equil,datafile.yio
M                               comp-conc units
0.4974, 1.75, 30.0, 60.0        Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
228.5, 0.420, 0.6579,  0.0      part-rad(um), bed-void, part-void, sorb-cap()
0.0d-4                          initial concentrations (M)
S                               COMMAND - conc step change
1, 0.0, 5.7259d-4, 1, 0.0       spec id, time(min), conc(M), freq, dt(min)
R                               COMMAND - Total recycle
0.0001, 9000.0, 1, 0.0          start time(min), duration(min), freq, wait time(min)
V                               COMMAND - viscosity/density change
0.03935, 1.255                  fluid viscosity(poise), density(g/cm^3)
h                               COMMAND - effluent history dump
0, 0.02, 0.02, 0.01, 0.01       unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
1, 0.02, 0.02, 0.01, 0.01       unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
2, 0.02, 0.02, 0.01, 0.01       unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
3, 0.02, 0.02, 0.01, 0.01       unit op#, ptscale(1-4) filtering
-                               end of commands
8640.0, 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
1.0690d-4                       part-pore diffusivities(cm^2/min)tau = 3
3.2069d-4                       Brownian diffusivities(cm^2/min)
0.2912                          Freundlich/Langmuir Hybrid a    (moles/L B.V.) 110%
1.0                             Freundlich/Langmuir Hybrid b    (1/M)
0.9862                          Freundlich/Langmuir Hybrid Ma   (-)
0.8575                          Freundlich/Langmuir Hybrid Mb   (-)
2.9558d-3                       Freundlich/Langmuir Hybrid beta (-)
```

### C.1.2 VERSE-LC Datafile.yio

```
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
5.7259d-4, 0.0000
5.7259d-4, 0.0000
```

### C.1.3 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: AP-101S-15C
SRNL Kinetics Rig - AP-101S, 15C, Batch 641 RF
Particle radius = volume mean radius, Dp = Dinf/3
Begin Run:  07:24:43 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:  2  particle: 1
Collocation points - axial:  1  particle: 6 => Number of eqns:    42
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? Y   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
===============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        =   8640.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =       .49740 cm          D              =      1.75000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =      1.19639 mL
F              =     30.00000 mL/min      Uo (linear)    =     29.69655 cm/min
R              =    228.50000 microns     L/R            =     21.76805
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     76.14880 1/cm        Time/BV        =       .01675 min
Vol CSTRs      =     60.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .27643E+01
Dp  [cm2/min]  =  .10690E-03
Doo [cm2/min]  =  .32069E-03
kf  [cm/min]   =  .22060E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .30298E+00
Sc(i)          =  .58663E+04
Peb(i)         =  .53436E+01
Bi(i)          =  .71673E+02
Nf(i)          =  .66992E+00
Np(i)          =  .22561E-02
Pep(i)         =  .96484E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .29120E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98620E+00
Iso. Const. 4  =  .85750E+00
Iso. Const. 5  =  .29558E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5726E-03 M
     Execute   1 times, every .0000     mins.
  2: Full Recycle from .1000E-03 min to 9000.     min.
     Execute   1 times, every .0000     mins.
  3: User set viscosity to .3935E-01 poise and density to 1.255     g/cm3
  4: Monitor conc. history at stream  0.  Filename = AP-101S-15C.h01
     Output density adjustments:
     .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
     .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
  5: Monitor conc. history at stream  1.  Filename = AP-101S-15C.h02
     Output density adjustments:
     .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
     .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
  6: Monitor conc. history at stream  2.  Filename = AP-101S-15C.h03
     Output density adjustments:
     .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
     .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
  7: Monitor conc. history at stream  3.  Filename = AP-101S-15C.h04
     Output density adjustments:
     .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
     .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
===============================================================================
VERSE-LC finished in ***** steps.  Average step size .1675E-01 minutes
End run:  07:26:27 on 05-04-2007
Integrated Areas in History Files:
AP-101S-15C.h01           2.71209
AP-101S-15C.h02           2.71261
AP-101S-15C.h03           2.71157
AP-101S-15C.h04           2.71209
```

## C.2 SRNL Particle Kinetics Experiment at 25 °C

### C.2.1 VERSE-LC Datafile

```
SRNL Kinetics Rig - AP-101S, 25C, Batch 641 RF
Particle radius = volume mean radius, Dp = Dinf
1, 2, 1, 6                       ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNYN                            input-only,perfusable,feed-equil,datafile.yio
M                                comp-conc units
0.5094, 1.75, 30.0, 60.0         Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
241.5, 0.420, 0.6579,  0.0       part-rad(um), bed-void, part-void, sorb-cap() 228.5
```

```
0.0d-4                          initial concentrations (M)
S                               COMMAND - conc step change
1, 0.0, 5.9102d-4, 1, 0.0       spec id, time(min), conc(M), freq, dt(min)
R                               COMMAND - Total recycle
0.0001, 9000.0, 1, 0.0          start time(min), duration(min), freq, wait time(min)
V                               COMMAND - viscosity/density change
0.02967, 1.249                  fluid viscosity(poise), density(g/cm^3)
h                               COMMAND - effluent history dump
0, 0.02, 0.02, 0.01, 0.01       unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
1, 0.02, 0.02, 0.01, 0.01       unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
2, 0.02, 0.02, 0.01, 0.01       unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
3, 0.02, 0.02, 0.01, 0.01       unit op#, ptscale(1-4) filtering
-                               end of commands
8640.0, 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
1.2034d-4                       part-pore diffusivities(cm^2/min) tau = 3
3.6103d-4                       Brownian diffusivities(cm^2/min)
0.2964                          Freundlich/Langmuir Hybrid a    (moles/L B.V.) 110%
1.0                             Freundlich/Langmuir Hybrid b    (1/M)
0.9890                          Freundlich/Langmuir Hybrid Ma   (-)
0.8575                          Freundlich/Langmuir Hybrid Mb   (-)
2.9558d-3                       Freundlich/Langmuir Hybrid beta (-)
```

### C.2.2 VERSE-LC Datafile.yio

```
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
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0.0000,    0.0000
0.0000,    0.0000
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0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
5.9102d-4, 0.0000
5.9102d-4, 0.0000
```

### C.2.3 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: AP-101S-25C
SRNL Kinetics Rig - AP-101S, 25C, Batch 641 RF
Particle radius = volume mean radius, Dp = Dinf
Begin Run:  07:12:16 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:  2  particle: 1
Collocation points - axial:  1  particle: 6 => Number of eqns:    42
Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
Use Profile File? Y   Generate Profile File? N
Axial dispersion correlation:   Chung & Wen (1968)
Film mass transfer correlation: Wilson & Geankoplis (1966)
===============================================================================
SYSTEM PARAMETERS (at initial conditions):

t(stop)        =   8640.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =       .50940 cm          D              =      1.75000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =      1.22525 mL
F              =     30.00000 mL/min      Uo (linear)    =     29.69655 cm/min
R              =    241.50000 microns     L/R            =     21.09317
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     72.04969 1/cm        Time/BV        =       .01715 min
```

```
 Vol CSTRs      =     60.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .29064E+01
 Dp  [cm2/min]  =  .12034E-03
 Doo [cm2/min]  =  .36103E-03
 kf  [cm/min]   =  .23009E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .42266E+00
 Sc(i)          =  .39479E+04
 Peb(i)         =  .52049E+01
 Bi(i)          =  .70184E+02
 Nf(i)          =  .67706E+00
 Np(i)          =  .23286E-02
 Pep(i)         =  .90584E+04

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .29640E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .98900E+00
 Iso. Const. 4  =  .85750E+00
 Iso. Const. 5  =  .29558E-02
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units         M
 ===============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .5910E-03 M
      Execute   1 times, every .0000     mins.
   2: Full Recycle from .1000E-03 min to 9000.     min.
      Execute   1 times, every .0000     mins.
   3: User set viscosity to .2967E-01 poise and density to 1.249     g/cm3
   4: Monitor conc. history at stream  0.  Filename = AP-101S-25C.h01
      Output density adjustments:
      .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
      .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
   5: Monitor conc. history at stream  1.  Filename = AP-101S-25C.h02
      Output density adjustments:
      .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
      .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
   6: Monitor conc. history at stream  2.  Filename = AP-101S-25C.h03
      Output density adjustments:
      .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
      .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
   7: Monitor conc. history at stream  3.  Filename = AP-101S-25C.h04
      Output density adjustments:
      .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
      .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
 ===============================================================================
 VERSE-LC finished in ***** steps.  Average step size .1715E-01 minutes
 End run:  07:13:59 on 05-04-2007
 Integrated Areas in History Files:
 AP-101S-25C.h01           2.78250
 AP-101S-25C.h02           2.78304
 AP-101S-25C.h03           2.78196
 AP-101S-25C.h04           2.78250
```

## C.3 SRNL Particle Kinetics Experiment at 45 °C

### C.3.1 VERSE-LC Datafile

```
SRNL Kinetics Rig - AP-101S, 41C, Batch 641 RF
Particle radius = volume mean radius, Dp = Dinf/3
1, 2, 1, 6                        ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNYN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
0.5402, 1.75, 30.0, 60.0          Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
228.5, 0.420, 0.6579,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
0.0d-4                            initial concentrations (M)
S                                 COMMAND - conc step change
1, 0.0, 5.6732d-4, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
R                                 COMMAND - Total recycle
0.0001, 9000.0, 1, 0.0            start time(min), duration(min), freq, wait time(min)
V                                 COMMAND - viscosity/density change
0.02057, 1.238                    fluid viscosity(poise), density(g/cm^3)
h                                 COMMAND - effluent history dump
0, 0.02, 0.02, 0.01, 0.01         unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
1, 0.02, 0.02, 0.01, 0.01         unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
2, 0.02, 0.02, 0.01, 0.01         unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
3, 0.02, 0.02, 0.01, 0.01         unit op#, ptscale(1-4) filtering
-                                 end of commands
8640.0, 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
1.9249d-4                         part-pore diffusivities(cm^2/min) tau = 3
5.7747d-4                         Brownian diffusivities(cm^2/min)
0.3050                            Freundlich/Langmuir Hybrid a    (moles/L B.V.) 110%
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9933                            Freundlich/Langmuir Hybrid Ma   (-)
0.8404                            Freundlich/Langmuir Hybrid Mb   (-)
```

```
4.43995d-3                     Freundlich/Langmuir Hybrid beta (-)
```

### C.3.2 VERSE-LC Datafile.yio

```
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
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0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
0.0000,    0.0000
5.6732d-4, 0.0000
5.6732d-4, 0.0000
```

### C.3.3 VERSE-LC Datafile.run

```
===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: AP-101S-45C
 SRNL Kinetics Rig - AP-101S, 41C, Batch 641 RF
 Particle radius = volume mean radius, Dp = Dinf/3
 Begin Run:  07:32:34 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:  2  particle: 1
 Collocation points - axial:  1  particle: 6 => Number of eqns:    42
 Inlet species at equilib.? N   Perfusable sorbent? N   Feed profile only? N
 Use Profile File? Y   Generate Profile File? N
 Axial dispersion correlation:   Chung & Wen (1968)
 Film mass transfer correlation: Wilson & Geankoplis (1966)
 ===============================================================================
 SYSTEM PARAMETERS (at initial conditions):

 t(stop)        =   8640.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =       .54020 cm          D              =      1.75000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =      1.29933 mL
 F              =     30.00000 mL/min      Uo (linear)    =     29.69655 cm/min
 R              =    228.50000 microns     L/R            =     23.64114
 Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
 Spec. Area     =     76.14880 1/cm        Time/BV        =       .01819 min
 Vol CSTRs      =     60.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .27350E+01
 Dp  [cm2/min]  =  .19249E-03
 Doo [cm2/min]  =  .57747E-03
 kf  [cm/min]   =  .32652E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .57175E+00
 Sc(i)          =  .17264E+04
 Peb(i)         =  .58656E+01
 Bi(i)          =  .58915E+02
 Nf(i)          =  .10769E+01
 Np(i)          =  .44121E-02
 Pep(i)         =  .53583E+04

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .30500E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .99330E+00
 Iso. Const. 4  =  .84040E+00
 Iso. Const. 5  =  .44399E-02
 Init. Conc.    =  .00000E+00
```

```
 Conc. at eqb.  =  .00000E+00
 Conc. units          M
 ==============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .5673E-03 M
      Execute   1 times, every .0000     mins.
   2: Full Recycle from .1000E-03 min to 9000.     min.
      Execute   1 times, every .0000     mins.
   3: User set viscosity to .2057E-01 poise and density to 1.238     g/cm3
   4: Monitor conc. history at stream  0.  Filename = AP-101S-45C.h01
      Output density adjustments:
      .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
      .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
   5: Monitor conc. history at stream  1.  Filename = AP-101S-45C.h02
      Output density adjustments:
      .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
      .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
   6: Monitor conc. history at stream  2.  Filename = AP-101S-45C.h03
      Output density adjustments:
      .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
      .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
   7: Monitor conc. history at stream  3.  Filename = AP-101S-45C.h04
      Output density adjustments:
      .20E-01*default abs conc delta,      .20E-01*default rel conc delta,
      .10E-01*default force w/ conc delta, .10E-01*default force w/o conc delta
 ==============================================================================
 VERSE-LC finished in ***** steps.  Average step size .1819E-01 minutes
 End run:  07:34:07 on 05-04-2007
 Integrated Areas in History Files:
 AP-101S-45C.h01           3.02690
 AP-101S-45C.h02           3.02733
 AP-101S-45C.h03           3.02646
 AP-101S-45C.h04           3.02690
```

## C.4 PNWD Column AP-101 Actual Waste

### C.4.1 VERSE-LC Datafile

```
PNNL Lead Column Run - AP-101 Actual DF, 26.5C, Batch 641 RF lead/lag column
1 component (Cs) isotherm (AP-101 Actual Waste)
1, 100, 3, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,datafile.yio
M                                comp-conc units
12.45, 1.5, 0.5298, 11.0         Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
228.5, 0.420, 0.6579,  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, 4.484d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02954, 1.255                   fluid viscosity(poise), density(g/cm^3)
m                                COMMAND - subcolumns
50, 100, 0, 1, 4.9328d+8, 0.0, 50000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5           unit op#, ptscale(1-4) filtering
D
-1, 10000., 1, 0.0
-                                end of commands
10000.0, 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
1.3787d-4                        part-pore diffusivities(cm^2/min) (tau = 3)
4.1361d-4                        Brownian diffusivities(cm^2/min)
0.27562                          Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                              Freundlich/Langmuir Hybrid b    (1/M)
0.9896                           Freundlich/Langmuir Hybrid Ma   (-)
0.8550                           Freundlich/Langmuir Hybrid Mb   (-)
3.13171d-3                       Freundlich/Langmuir Hybrid beta (-)
```

### C.4.2 VERSE-LC Datafile.run

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: PNNL-26.5C
 PNNL Lead Column Run - AP-101 Actual DF, 26.5C, Batch 641 RF lead/lag colum
 1 component (Cs) isotherm (AP-101 Actual Waste)
 Begin Run:  08:00:34 on 05-04-2007   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)        =  10000.00000 min        dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
 Total Length   =     12.45000 cm         D              =      1.50000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =     22.00097 mL
 F              =       .52980 mL/min     Uo (linear)    =       .71382 cm/min
 R              =    228.50000 microns    L/R            =    544.85777
 Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
```

```
 Spec. Area     =     76.14880 1/cm        Time/BV        =      8.72065 min
 Vol CSTRs      =     11.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .68101E-01
 Dp  [cm2/min]  =  .13787E-03
 Doo [cm2/min]  =  .41361E-03
 kf  [cm/min]   =  .75435E-01
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .97015E-02
 Sc(i)          =  .34145E+04
 Peb(i)         =  .65250E+02
 Bi(i)          =  .19003E+02
 Nf(i)          =  .11927E+03
 Np(i)          =  .15150E+01
 Pep(i)         =  .17982E+03

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .27562E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .98960E+00
 Iso. Const. 4  =  .85500E+00
 Iso. Const. 5  =  .31317E-02
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units        M
 ==============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .4484E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .2954E-01 poise and density to 1.255     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .5000E+05 min.
      When comp.  1 reaches .4933E+09 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  2.  Filename = PNNL-26.5C.h01
      Output density adjustments:
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .50    *default force w/ conc delta, .50    *default force w/o conc delta
   5: Monitor conc. history at stream  4.  Filename = PNNL-26.5C.h02
      Output density adjustments:
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .50    *default force w/ conc delta, .50    *default force w/o conc delta
   6: Dump full profile file at  .1000E+05 min
      Execute   1 times, every .0000     mins.
 ==============================================================================
 VERSE-LC finished in  1154 steps.  Average step size 8.666     minutes
 End run:  08:00:49 on 05-04-2007
 Integrated Areas in History Files:
 PNNL-26.5C.h01             .361032
 PNNL-26.5C.h02             .273663
```

## C.5 PNWD Column AP-101 Simulant

### C.5.1 VERSE-LC Datafile

```
PNNL Lead Column Run - AP-101FR Simulant, 19C, Batch 641 RF lead/lag column
1 component (Cs) isotherm (AP-101FR Simulant)
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
12.45, 1.5, 0.5372, 11.0        Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
228.5, 0.420, 0.6579,  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, 4.379d-5, 1, 0.0        spec id, time(min), conc(M), freq, dt(min)
V                               COMMAND - viscosity/density change
0.03486, 1.253                  fluid viscosity(poise), density(g/cm^3)
m                               COMMAND - subcolumns
50, 100, 0, 1, 4.4092d+8, 0.0, 50000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                               COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5          unit op#, ptscale(1-4) filtering
h                               COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5          unit op#, ptscale(1-4) filtering
D
-1, 10000., 1, 0.0
-                               end of commands
10000.0, 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
1.2003d-4                       part-pore diffusivities(cm^2/min) (tau = 3)
3.6008d-4                       Brownian diffusivities(cm^2/min)
0.27145                         Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                             Freundlich/Langmuir Hybrid b    (1/M)
0.9874                          Freundlich/Langmuir Hybrid Ma   (-)
0.8630                          Freundlich/Langmuir Hybrid Mb   (-)
2.55278d-3                      Freundlich/Langmuir Hybrid beta (-)
```

### C.5.2 VERSE-LC Datafile.run

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: PNNL-19C
```

```
PNNL Lead Column Run - AP-101FR Simulant, 19C, Batch 641 RF lead/lag column
1 component (Cs) isotherm (AP-101FR Simulant)
Begin Run:  08:00:49 on 05-04-2007   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)        =  10000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =     12.45000 cm         D              =      1.50000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =     22.00097 mL
F              =       .53720 mL/min     Uo (linear)    =       .72379 cm/min
R              =    228.50000 microns    L/R            =    544.85777
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     76.14880 1/cm       Time/BV        =      8.60053 min
Vol CSTRs      =     11.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .69081E-01
Dp  [cm2/min]  =  .12003E-03
Doo [cm2/min]  =  .36008E-03
kf  [cm/min]   =  .69096E-01
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .83225E-02
Sc(i)          =  .46358E+04
Peb(i)         =  .65222E+02
Bi(i)          =  .19994E+02
Nf(i)          =  .10774E+03
Np(i)          =  .13008E+01
Pep(i)         =  .20944E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .27145E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98740E+00
Iso. Const. 4  =  .86300E+00
Iso. Const. 5  =  .25528E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .4379E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .3486E-01 poise and density to 1.253     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .5000E+05 min.
     When comp.  1 reaches .4409E+09 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = PNNL-19C.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = PNNL-19C.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Dump full profile file at  .1000E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in  1170 steps.  Average step size 8.547     minutes
End run:  08:01:05 on 05-04-2007
Integrated Areas in History Files:
PNNL-19C.h01              .334956
PNNL-19C.h02              .232011
```

## C.6 SRNL Column AP-101 Simulant

### C.6.1 VERSE-LC Datafile

```
SRNL Column Run - AP-101S, 45C, Batch 641 RF
1 component (Cs) isotherm (AP-101FR Simulant)
1, 50, 3, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNA                           isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                           input-only,perfusable,feed-equil,datafile.yio
M                               comp-conc units
5.6840, 1.574, 0.2396, 13.1     Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
228.5, 0.420, 0.6579,  0.0      part-rad(um), bed-void, part-void, sorb-cap()
0.0d-4                          initial concentrations (M)
S                               COMMAND - conc step change
1, 0.0, 4.5070d-5, 1, 0.0       spec id, time(min), conc(M), freq, dt(min)
V                               COMMAND - viscosity/density change
0.01904, 1.236                  fluid viscosity(poise), density(g/cm^3)
h                               COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5          unit op#, ptscale(1-4) filtering
D
-1, 10000., 1, 0.0
-                               end of commands
10000.0, 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
2.0683d-4                        part-pore diffusivities(cm^2/min) (tau = 3)
6.2049d-4                        Brownian diffusivities(cm^2/min)
0.28225                          Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                              Freundlich/Langmuir Hybrid b    (1/M)
0.9933                           Freundlich/Langmuir Hybrid Ma   (-)
0.8404                           Freundlich/Langmuir Hybrid Mb   (-)
4.43995d-3                       Freundlich/Langmuir Hybrid beta (-)
```

### C.6.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: SRNL-45C
 SRNL Column Run - AP-101S, 45C, Batch 641 RF
 1 component (Cs) isotherm (AP-101FR Simulant)
 Begin Run:  08:47:37 on 05-04-2007   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)        =  10000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =      5.68400 cm          D              =      1.57400 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     11.05996 mL
 F              =       .23960 mL/min      Uo (linear)    =       .29318 cm/min
 R              =    228.50000 microns     L/R            =    248.75274
 Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
 Spec. Area     =     76.14880 1/cm        Time/BV        =     19.38724 min
 Vol CSTRs      =     13.10000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .28004E-01
 Dp  [cm2/min]  =  .20683E-03
 Doo [cm2/min]  =  .62049E-03
 kf  [cm/min]   =  .73483E-01
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .60884E-02
 Sc(i)          =  .14896E+04
 Peb(i)         =  .59508E+02
 Bi(i)          =  .12340E+02
 Nf(i)          =  .25829E+03
 Np(i)          =  .50526E+01
 Pep(i)         =  .49232E+02

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .28225E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .99330E+00
 Iso. Const. 4  =  .84040E+00
 Iso. Const. 5  =  .44399E-02
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units          M
 ===============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .4507E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .1904E-01 poise and density to 1.236     g/cm3
   3: Monitor conc. history at stream  2.  Filename = SRNL-45C.h01
      Output density adjustments:
      1.0    *default abs conc delta,      1.0    *default rel conc delta,
      .50    *default force w/ conc delta, .50    *default force w/o conc delta
   4: Dump full profile file at  .1000E+05 min
      Execute   1 times, every .0000     mins.
 ===============================================================================
 VERSE-LC finished in   521 steps.  Average step size 19.19     minutes
 End run:  08:47:41 on 05-04-2007
 Integrated Areas in History Files:
 SRNL-45C.h01               .311895
```

## C.7 PNWD Column AN-102

### C.7.1 VERSE-LC Datafile

```
PNNL Lead Column Run - AN-102 Actual DF, 26.5C, Batch 641 RF lead/lag column
1 component (Cs) isotherm (AN-102 Actual DF)
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
M                                comp-conc units
12.45, 1.5, 0.5298, 11.0         Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
228.5, 0.420, 0.6579,  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, 5.967d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.02289, 1.230                   fluid viscosity(poise), density(g/cm^3)
```

```
m                                 COMMAND - subcolumns
50, 100, 0, 1, 5.9134d+8, 0.0, 50000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
4, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
D
-1, 10000., 1, 0.0
-                                 end of commands
10000.0, 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
1.6771d-4                         part-pore diffusivities(cm^2/min) tau = 3
5.0314d-4                         Brownian diffusivities(cm^2/min)
0.23902                           Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9718                            Freundlich/Langmuir Hybrid Ma   (-)
0.9120                            Freundlich/Langmuir Hybrid Mb   (-)
3.33496d-4                        Freundlich/Langmuir Hybrid beta (-)
```

### C.7.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: WTP-RPT-135-1
PNNL Lead Column Run - AN-102 Actual DF, 26.5C, Batch 641 RF lead/lag colum
1 component (Cs) isotherm (AN-102 Actual DF)
Begin Run:  08:15:26 on 05-04-2007   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)        =  10000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =     12.45000 cm          D              =      1.50000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     22.00097 mL
F              =       .52980 mL/min      Uo (linear)    =       .71382 cm/min
R              =    228.50000 microns     L/R            =    544.85777
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     76.14880 1/cm        Time/BV        =      8.72065 min
Vol CSTRs      =     11.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .68053E-01
Dp  [cm2/min]  =  .16771E-03
Doo [cm2/min]  =  .50314E-03
kf  [cm/min]   =  .85962E-01
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .12271E-01
Sc(i)          =  .22192E+04
Peb(i)         =  .65296E+02
Bi(i)          =  .17802E+02
Nf(i)          =  .13592E+03
Np(i)          =  .18429E+01
Pep(i)         =  .14783E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .23902E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97180E+00
Iso. Const. 4  =  .91200E+00
Iso. Const. 5  =  .33350E-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 .5967E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2289E-01 poise and density to 1.230     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .5000E+05 min.
     When comp.  1 reaches .5913E+09 M      at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = WTP-RPT-135-1.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = WTP-RPT-135-1.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  6: Dump full profile file at  .1000E+05 min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in  1151 steps.  Average step size 8.688     minutes
End run:  08:15:42 on 05-04-2007
Integrated Areas in History Files:
WTP-RPT-135-1.h01          .465137E-02
WTP-RPT-135-1.h02          .102811E-08
```

## C.8 PNWD Column AZ-102

### C.8.1 VERSE-LC Datafile

```
PNNL Column Run - AZ-102S, 22C, Batch ??? RF
1 component (Cs) isotherm model: (1-Cs) (AZ-102S Simulant)
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
6.3025, 2.0, 0.495, 19.8          Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
228.5, 0.420, 0.6579,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
0.0, 0.0                          initial concentrations (M)
S                                 COMMAND - conc step change (Cs+)
1, 0.0, 3.928d-4, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.03336, 1.239                    fluid viscosity(poise), density(g/cm^3)
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
D
-1, 10000., 1, 0.0
-                                 end of commands
15000.0, 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
1.0000d0                          size exclusion factor
3.2723d-4                         part-pore diffusivities(cm^2/min) Tau = 3
9.8170d-4                         Brownian diffusivities(cm^2/min)
0.345                             Freundlich/Langmuir Hybrid a    (moles/L B.V.) rhob=0.2563
1.0                              Freundlich/Langmuir Hybrid b    (1/M)           C_T=0.6717
0.9761                          Freundlich/Langmuir Hybrid Ma   (-)
0.8942                          Freundlich/Langmuir Hybrid Mb   (-)
8.1347E-04                        Freundlich/Langmuir Hybrid beta (-)
```

### C.8.2 VERSE-LC Datafile.run

```
==============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
==============================================================================
Input file: AZ-102S-22C
PNNL Column Run - AZ-102S, 22C, Batch ??? RF
1 component (Cs) isotherm model: (1-Cs) (AZ-102S Simulant)
Begin Run:  14:13:17 on 05-07-2007   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)        =  15000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =      6.30250 cm          D              =      2.00000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     19.79989 mL
F              =       .49500 mL/min      Uo (linear)    =       .37515 cm/min
R              =    228.50000 microns     L/R            =    275.82057
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     76.14880 1/cm        Time/BV        =     16.79990 min
Vol CSTRs      =     19.80000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .35857E-01
Dp  [cm2/min]  =  .32723E-03
Doo [cm2/min]  =  .98170E-03
kf  [cm/min]   =  .10832E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .44572E-02
Sc(i)          =  .16456E+04
Peb(i)         =  .65940E+02
Bi(i)          =  .11497E+02
Nf(i)          =  .32993E+03
Np(i)          =  .69270E+01
Pep(i)         =  .39818E+02

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .34500E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97610E+00
Iso. Const. 4  =  .89420E+00
Iso. Const. 5  =  .81347E-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 .3928E-03 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .3336E-01 poise and density to 1.239     g/cm3
  3: Monitor conc. history at stream  2.  Filename = AZ-102S-22C.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  .1000E+05 min
```

```
      Execute   1 times, every .0000     mins.
 ================================================================================
 VERSE-LC finished in   907 steps.  Average step size 16.54     minutes
 End run:  14:13:25 on 05-07-2007
 Integrated Areas in History Files:
 AZ-102S-22C.h01            2.04934
```

## C.9 SRNL Column AN-107

### C.9.1 VERSE-LC Datafile

```
SRNL Column Run - AN-107, 25C, Batch 641 RF
1 component (Cs) isotherm (AN-107 Simulant)
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
M                                 comp-conc units
5.551, 1.571, 0.2457, 10.76       Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
228.5, 0.420, 0.6579,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
0.0d-4                            initial concentrations (M)
S                                 COMMAND - conc step change
1, 0.0, 6.937d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.03020, 1.274                    fluid viscosity(poise), density(g/cm^3)
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5            unit op#, ptscale(1-4) filtering
D
-1, 10000., 1, 0.0
-                                 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
1.2034d-4                         part-pore diffusivities(cm^2/min) Tau = 3
3.6103d-4                         Brownian diffusivities(cm^2/min)
0.24938                           Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9721                            Freundlich/Langmuir Hybrid Ma   (-)
0.9060                            Freundlich/Langmuir Hybrid Mb   (-)
4.31382d-4                        Freundlich/Langmuir Hybrid beta (-)
```

### C.9.2 VERSE-LC Datafile.run

```
 ================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ================================================================================
 Input file: AN-107-25C
 SRNL Column Run - AN-107, 25C, Batch 641 RF
 1 component (Cs) isotherm (AN-107 Simulant)
 Begin Run:  10:01:37 on 05-04-2007   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)        =  30000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =      5.55100 cm          D              =      1.57100 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =     10.76003 mL
 F              =       .24570 mL/min      Uo (linear)    =       .30180 cm/min
 R              =    228.50000 microns     L/R            =    242.93217
 Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
 Spec. Area     =     76.14880 1/cm        Time/BV        =     18.39321 min
 Vol CSTRs      =     11.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .28850E-01
 Dp  [cm2/min]  =  .12034E-03
 Doo [cm2/min]  =  .36103E-03
 kf  [cm/min]   =  .51711E-01
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .40728E-02
 Sc(i)          =  .39395E+04
 Peb(i)         =  .58068E+02
 Bi(i)          =  .14924E+02
 Nf(i)          =  .17245E+03
 Np(i)          =  .27890E+01
 Pep(i)         =  .87102E+02

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .24938E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .97210E+00
 Iso. Const. 4  =  .90600E+00
 Iso. Const. 5  =  .43138E-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 .6937E-04 M
```

```
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .3020E-01 poise and density to 1.274     g/cm3
  3: Monitor conc. history at stream  2.  Filename = AN-107-25C.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .50    *default force w/ conc delta, .50    *default force w/o conc delta
  4: Dump full profile file at  .1000E+05 min
     Execute   1 times, every .0000     mins.
================================================================================
VERSE-LC finished in  1636 steps.  Average step size 18.34     minutes
End run:  10:01:47 on 05-04-2007
Integrated Areas in History Files:
AN-107-25C.h01             .440983
```

# 15. Appendix D

VERSE-LC input and output files for the thirty full-scale facility simulations are provided in this appendix. The case studies use three nominal LAW feed compositions to represent Hot Commissioning, Envelope B, and Subsequent Operations with variations about the nominal compositions to test sensitivity.

## D.1 Hot Commissioning Operations HC_01 (Nominal Isotherm)

### D.1.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: None
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.025032, 1.2181                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.6451d-4                         part-pore diffusivities(cm^2/min)
4.9353d-4                         Brownian diffusivities(cm^2/min)
0.2632                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9850                            Freundlich/Langmuir Hybrid Ma   (-)
0.8695                            Freundlich/Langmuir Hybrid Mb   (-)
2.076d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.1.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: HC_01
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: None
Begin Run:  16:07:42 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max      =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.       =       .10000E-03
Total Length   =    478.71000 cm          D               =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.       =6813677.17928 mL
F              =  56781.20000 mL/min      Uo (linear)     =      9.49831 cm/min
R              =    230.00000 microns     L/R             =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity   =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV         =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89775E+00
Dp  [cm2/min]  =  .16451E-03
Doo [cm2/min]  =  .49353E-03
kf  [cm/min]   =  .20022E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .14883E+00
Sc(i)          =  .24983E+04
Peb(i)         =  .16883E+04
Bi(i)          =  .42549E+02
Nf(i)          =  .60588E+03
Np(i)          =  .34372E+01
Pep(i)         =  .20185E+04

Isotherm       =  Freundlich/Langmuir Hybrid
```

```
 Iso. Const. 1  =  .26320E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .98500E+00
 Iso. Const. 4  =  .86950E+00
 Iso. Const. 5  =  .20760E-02
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units          M
 ===============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .2740E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .2503E-01 poise and density to 1.218     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3700E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = HC_01.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = HC_01.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = HC_01.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = HC_01.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = 8264.     min
 Conc. Carousel caused bed shift at t = .1340E+05 min
 Conc. Carousel caused bed shift at t = .1867E+05 min
 Conc. Carousel caused bed shift at t = .2405E+05 min
 Conc. Carousel caused bed shift at t = .2949E+05 min
 Conc. Carousel caused bed shift at t = .3499E+05 min
 Conc. Carousel caused bed shift at t = .4051E+05 min
 Conc. Carousel caused bed shift at t = .4604E+05 min
 Conc. Carousel caused bed shift at t = .5160E+05 min
 Conc. Carousel caused bed shift at t = .5716E+05 min
 Conc. Carousel caused bed shift at t = .6272E+05 min
 Conc. Carousel caused bed shift at t = .6830E+05 min
 Conc. Carousel caused bed shift at t = .7386E+05 min
 Conc. Carousel caused bed shift at t = .7942E+05 min
 Conc. Carousel caused bed shift at t = .8500E+05 min
 Conc. Carousel caused bed shift at t = .9056E+05 min
 Conc. Carousel caused bed shift at t = .9612E+05 min
 Conc. Carousel caused bed shift at t = .1017E+06 min
 Conc. Carousel caused bed shift at t = .1073E+06 min
 Conc. Carousel caused bed shift at t = .1128E+06 min
 Conc. Carousel caused bed shift at t = .1184E+06 min
 VERSE-LC finished in  7801 steps.  Average step size 15.38     minutes
 End run:  16:22:18 on 05-04-2007
 Integrated Areas in History Files:
 HC_01.h01                 3.28800
 HC_01.h02                 .761388
 HC_01.h03                 .353545E-03
 HC_01.h04                 .172087E-10
```

## D.2 Hot Commissioning Operations HC_02

### D.2.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: high K+
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.025832, 1.2354                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.5791d-4                         part-pore diffusivities(cm^2/min)
4.7373d-4                         Brownian diffusivities(cm^2/min)
0.2717                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
```

```
0.9900                            Freundlich/Langmuir Hybrid Ma   (-)
0.8527                            Freundlich/Langmuir Hybrid Mb   (-)
3.281d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.2.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: HC_02
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: high K+
Begin Run:  16:22:19 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  56781.20000 mL/min      Uo (linear)    =      9.49831 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89791E+00
Dp  [cm2/min]  =  .15791E-03
Doo [cm2/min]  =  .47373E-03
kf  [cm/min]   =  .19483E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .14627E+00
Sc(i)          =  .26483E+04
Peb(i)         =  .16880E+04
Bi(i)          =  .43134E+02
Nf(i)          =  .58957E+03
Np(i)          =  .32993E+01
Pep(i)         =  .21028E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .27170E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .99000E+00
Iso. Const. 4  =  .85270E+00
Iso. Const. 5  =  .32810E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2740E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2583E-01 poise and density to 1.235     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_02.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_02.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_02.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_02.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = 5054.     min
Conc. Carousel caused bed shift at t = 8225.     min
Conc. Carousel caused bed shift at t = .1148E+05 min
Conc. Carousel caused bed shift at t = .1480E+05 min
Conc. Carousel caused bed shift at t = .1817E+05 min
Conc. Carousel caused bed shift at t = .2157E+05 min
Conc. Carousel caused bed shift at t = .2500E+05 min
Conc. Carousel caused bed shift at t = .2844E+05 min
Conc. Carousel caused bed shift at t = .3188E+05 min
Conc. Carousel caused bed shift at t = .3532E+05 min
Conc. Carousel caused bed shift at t = .3878E+05 min
Conc. Carousel caused bed shift at t = .4222E+05 min
Conc. Carousel caused bed shift at t = .4568E+05 min
Conc. Carousel caused bed shift at t = .4912E+05 min
Conc. Carousel caused bed shift at t = .5256E+05 min
Conc. Carousel caused bed shift at t = .5601E+05 min
```

```
Conc. Carousel caused bed shift at t = .5945E+05 min
Conc. Carousel caused bed shift at t = .6291E+05 min
Conc. Carousel caused bed shift at t = .6635E+05 min
Conc. Carousel caused bed shift at t = .6979E+05 min
Conc. Carousel caused bed shift at t = .7325E+05 min
Conc. Carousel caused bed shift at t = .7669E+05 min
Conc. Carousel caused bed shift at t = .8013E+05 min
Conc. Carousel caused bed shift at t = .8359E+05 min
Conc. Carousel caused bed shift at t = .8703E+05 min
Conc. Carousel caused bed shift at t = .9049E+05 min
Conc. Carousel caused bed shift at t = .9393E+05 min
Conc. Carousel caused bed shift at t = .9737E+05 min
Conc. Carousel caused bed shift at t = .1008E+06 min
Conc. Carousel caused bed shift at t = .1043E+06 min
Conc. Carousel caused bed shift at t = .1077E+06 min
Conc. Carousel caused bed shift at t = .1112E+06 min
Conc. Carousel caused bed shift at t = .1146E+06 min
Conc. Carousel caused bed shift at t = .1181E+06 min
VERSE-LC finished in  8238 steps.  Average step size 14.57     minutes
End run:  16:44:34 on 05-04-2007
Integrated Areas in History Files:
HC_02.h01                  3.28800
HC_02.h02                  .558418
HC_02.h03                  .447376E-03
HC_02.h04                  .164496E-08
```

## D.3 Hot Commissioning Operations HC_03

### D.3.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: low K+
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.024612, 1.2084                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.6832d-4                         part-pore diffusivities(cm^2/min)
5.0495d-4                         Brownian diffusivities(cm^2/min)
0.2561                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9808                            Freundlich/Langmuir Hybrid Ma   (-)
0.8816                            Freundlich/Langmuir Hybrid Mb   (-)
1.383d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.3.2 VERSE-LC Datafile.run

```
============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
============================================================================
Input file: HC_03
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: low K+
Begin Run:  16:44:34 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  56781.20000 mL/min      Uo (linear)    =      9.49831 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89767E+00
```

```
 Dp  [cm2/min]  =  .16832E-03
 Doo [cm2/min]  =  .50495E-03
 kf  [cm/min]   =  .20330E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .15016E+00
 Sc(i)          =  .24201E+04
 Peb(i)         =  .16884E+04
 Bi(i)          =  .42225E+02
 Nf(i)          =  .61520E+03
 Np(i)          =  .35168E+01
 Pep(i)         =  .19728E+04

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .25610E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .98080E+00
 Iso. Const. 4  =  .88160E+00
 Iso. Const. 5  =  .13830E-02
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units          M
 ===============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .2740E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .2461E-01 poise and density to 1.208     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3700E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = HC_03.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = HC_03.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = HC_03.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = HC_03.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = .1270E+05 min
 Conc. Carousel caused bed shift at t = .2054E+05 min
 Conc. Carousel caused bed shift at t = .2861E+05 min
 Conc. Carousel caused bed shift at t = .3682E+05 min
 Conc. Carousel caused bed shift at t = .4510E+05 min
 Conc. Carousel caused bed shift at t = .5343E+05 min
 Conc. Carousel caused bed shift at t = .6181E+05 min
 Conc. Carousel caused bed shift at t = .7022E+05 min
 Conc. Carousel caused bed shift at t = .7864E+05 min
 Conc. Carousel caused bed shift at t = .8708E+05 min
 Conc. Carousel caused bed shift at t = .9552E+05 min
 Conc. Carousel caused bed shift at t = .1040E+06 min
 Conc. Carousel caused bed shift at t = .1124E+06 min
 VERSE-LC finished in  7544 steps.  Average step size 15.91     minutes
 End run:  16:54:41 on 05-04-2007
 Integrated Areas in History Files:
 HC_03.h01                 3.28800
 HC_03.h02                 1.00791
 HC_03.h03                 .275137E-03
 HC_03.h04                 .133231E-12
```

## D.4 Hot Commissioning Operations HC_04

### D.4.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: diluted to 4 M Na+
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.4000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.021357, 1.1923                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.9282d-4                         part-pore diffusivities(cm^2/min)
5.7847d-4                         Brownian diffusivities(cm^2/min)
0.2599                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9833                            Freundlich/Langmuir Hybrid Ma   (-)
0.8744                            Freundlich/Langmuir Hybrid Mb   (-)
1.778d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.4.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: HC_04
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: diluted to 4 M Na+
Begin Run:  16:54:41 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm         D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
F              =  56781.20000 mL/min     Uo (linear)    =      9.49831 cm/min
R              =    230.00000 microns    L/R            =  20813.47826
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm       Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89643E+00
Dp  [cm2/min]  =  .19282E-03
Doo [cm2/min]  =  .57847E-03
kf  [cm/min]   =  .22258E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .17074E+00
Sc(i)          =  .18579E+04
Peb(i)         =  .16908E+04
Bi(i)          =  .40356E+02
Nf(i)          =  .67355E+03
Np(i)          =  .40287E+01
Pep(i)         =  .17221E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .25990E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98330E+00
Iso. Const. 4  =  .87440E+00
Iso. Const. 5  =  .17780E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units         M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2400E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2136E-01 poise and density to 1.192     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_04.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_04.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_04.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_04.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = .1008E+05 min
Conc. Carousel caused bed shift at t = .1623E+05 min
Conc. Carousel caused bed shift at t = .2252E+05 min
Conc. Carousel caused bed shift at t = .2893E+05 min
Conc. Carousel caused bed shift at t = .3538E+05 min
Conc. Carousel caused bed shift at t = .4190E+05 min
Conc. Carousel caused bed shift at t = .4845E+05 min
Conc. Carousel caused bed shift at t = .5502E+05 min
Conc. Carousel caused bed shift at t = .6161E+05 min
```

```
 Conc. Carousel caused bed shift at t = .6821E+05 min
 Conc. Carousel caused bed shift at t = .7481E+05 min
 Conc. Carousel caused bed shift at t = .8142E+05 min
 Conc. Carousel caused bed shift at t = .8805E+05 min
 Conc. Carousel caused bed shift at t = .9466E+05 min
 Conc. Carousel caused bed shift at t = .1013E+06 min
 Conc. Carousel caused bed shift at t = .1079E+06 min
 Conc. Carousel caused bed shift at t = .1145E+06 min
 VERSE-LC finished in  7620 steps.  Average step size 15.75     minutes
 End run:  17:06:02 on 05-04-2007
 Integrated Areas in History Files:
 HC_04.h01                 2.88000
 HC_04.h02                 .842529
 HC_04.h03                 .293310E-03
 HC_04.h04                 .354014E-12
```

## D.5 Hot Commissioning Operations HC_05

### D.5.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: concentrated to 5.5 M Na+
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 3.3000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.032938, 1.2598                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.2502d-4                         part-pore diffusivities(cm^2/min)
3.7507d-4                         Brownian diffusivities(cm^2/min)
0.2679                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9875                            Freundlich/Langmuir Hybrid Ma   (-)
0.8615                            Freundlich/Langmuir Hybrid Mb   (-)
2.607d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.5.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: HC_05
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: concentrated to 5.5
 Begin Run:  17:06:02 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm          D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
 F              =  56781.20000 mL/min      Uo (linear)    =      9.49831 cm/min
 R              =    230.00000 microns     L/R            =  20813.47826
 Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
 Spec. Area     =     75.65217 1/cm        Time/BV        =     16.79984 min
 Vol CSTRs      =1892706.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .89987E+00
 Dp  [cm2/min]  =  .12502E-03
 Doo [cm2/min]  =  .37507E-03
 kf  [cm/min]   =  .16674E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .11698E+00
 Sc(i)          =  .41825E+04
 Peb(i)         =  .16843E+04
 Bi(i)          =  .46627E+02
```

```
 Nf(i)         =  .50457E+03
 Np(i)         =  .26121E+01
 Pep(i)        =  .26560E+04

 Isotherm      =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .26790E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .98750E+00
 Iso. Const. 4  =  .86150E+00
 Iso. Const. 5  =  .26070E-02
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units          M
 ===============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .3300E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .3294E-01 poise and density to 1.260     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3700E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = HC_05.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = HC_05.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = HC_05.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = HC_05.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = 6062.     min
 Conc. Carousel caused bed shift at t = 9963.     min
 Conc. Carousel caused bed shift at t = .1403E+05 min
 Conc. Carousel caused bed shift at t = .1815E+05 min
 Conc. Carousel caused bed shift at t = .2237E+05 min
 Conc. Carousel caused bed shift at t = .2659E+05 min
 Conc. Carousel caused bed shift at t = .3085E+05 min
 Conc. Carousel caused bed shift at t = .3513E+05 min
 Conc. Carousel caused bed shift at t = .3939E+05 min
 Conc. Carousel caused bed shift at t = .4367E+05 min
 Conc. Carousel caused bed shift at t = .4793E+05 min
 Conc. Carousel caused bed shift at t = .5219E+05 min
 Conc. Carousel caused bed shift at t = .5647E+05 min
 Conc. Carousel caused bed shift at t = .6073E+05 min
 Conc. Carousel caused bed shift at t = .6500E+05 min
 Conc. Carousel caused bed shift at t = .6926E+05 min
 Conc. Carousel caused bed shift at t = .7352E+05 min
 Conc. Carousel caused bed shift at t = .7780E+05 min
 Conc. Carousel caused bed shift at t = .8206E+05 min
 Conc. Carousel caused bed shift at t = .8632E+05 min
 Conc. Carousel caused bed shift at t = .9060E+05 min
 Conc. Carousel caused bed shift at t = .9486E+05 min
 Conc. Carousel caused bed shift at t = .9912E+05 min
 Conc. Carousel caused bed shift at t = .1034E+06 min
 Conc. Carousel caused bed shift at t = .1077E+06 min
 Conc. Carousel caused bed shift at t = .1119E+06 min
 Conc. Carousel caused bed shift at t = .1162E+06 min
 VERSE-LC finished in  8213 steps.  Average step size 14.61     minutes
 End run:  17:27:19 on 05-04-2007
 Integrated Areas in History Files:
 HC_05.h01                3.96000
 HC_05.h02                .632253
 HC_05.h03                .434950E-03
 HC_05.h04                .130068E-08
```

## D.6 Hot Commissioning Operations HC_06

### D.6.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: concentrated to 5 M Na, 20 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 75708.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 3.0000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.028368, 1.2375                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
```

```
h                                      COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
-                                end of commands
120000.0, 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
1.0                              size exclusion factor
1.4516d-4                        part-pore diffusivities(cm^2/min)
4.3549d-4                        Brownian diffusivities(cm^2/min)
0.2654                           Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                              Freundlich/Langmuir Hybrid b    (1/M)
0.9862                           Freundlich/Langmuir Hybrid Ma   (-)
0.8658                           Freundlich/Langmuir Hybrid Mb   (-)
2.314d-3                        Freundlich/Langmuir Hybrid beta (-)
```

### D.6.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: HC_06
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: concentrated to 5 M
Begin Run:  17:27:19 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm         D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  75708.20000 mL/min      Uo (linear)    =     12.66440 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     12.59989 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .11947E+01
Dp  [cm2/min]  =  .14516E-03
Doo [cm2/min]  =  .43549E-03
kf  [cm/min]   =  .20274E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .17789E+00
Sc(i)          =  .31583E+04
Peb(i)         =  .16915E+04
Bi(i)          =  .48827E+02
Nf(i)          =  .46012E+03
Np(i)          =  .22747E+01
Pep(i)         =  .30500E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26540E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98620E+00
Iso. Const. 4  =  .86580E+00
Iso. Const. 5  =  .23140E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .3000E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2837E-01 poise and density to 1.238     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_06.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_06.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_06.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_06.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = 5009.     min
Conc. Carousel caused bed shift at t = 8282.     min
Conc. Carousel caused bed shift at t = .1169E+05 min
Conc. Carousel caused bed shift at t = .1519E+05 min
Conc. Carousel caused bed shift at t = .1872E+05 min
```

```
 Conc. Carousel caused bed shift at t = .2229E+05 min
 Conc. Carousel caused bed shift at t = .2586E+05 min
 Conc. Carousel caused bed shift at t = .2944E+05 min
 Conc. Carousel caused bed shift at t = .3302E+05 min
 Conc. Carousel caused bed shift at t = .3660E+05 min
 Conc. Carousel caused bed shift at t = .4017E+05 min
 Conc. Carousel caused bed shift at t = .4375E+05 min
 Conc. Carousel caused bed shift at t = .4734E+05 min
 Conc. Carousel caused bed shift at t = .5091E+05 min
 Conc. Carousel caused bed shift at t = .5448E+05 min
 Conc. Carousel caused bed shift at t = .5807E+05 min
 Conc. Carousel caused bed shift at t = .6164E+05 min
 Conc. Carousel caused bed shift at t = .6522E+05 min
 Conc. Carousel caused bed shift at t = .6879E+05 min
 Conc. Carousel caused bed shift at t = .7238E+05 min
 Conc. Carousel caused bed shift at t = .7595E+05 min
 Conc. Carousel caused bed shift at t = .7952E+05 min
 Conc. Carousel caused bed shift at t = .8311E+05 min
 Conc. Carousel caused bed shift at t = .8668E+05 min
 Conc. Carousel caused bed shift at t = .9026E+05 min
 Conc. Carousel caused bed shift at t = .9383E+05 min
 Conc. Carousel caused bed shift at t = .9742E+05 min
 Conc. Carousel caused bed shift at t = .1010E+06 min
 Conc. Carousel caused bed shift at t = .1046E+06 min
 Conc. Carousel caused bed shift at t = .1082E+06 min
 Conc. Carousel caused bed shift at t = .1117E+06 min
 Conc. Carousel caused bed shift at t = .1153E+06 min
 Conc. Carousel caused bed shift at t = .1189E+06 min
 VERSE-LC finished in 10968 steps.  Average step size 10.94     minutes
 End run:  17:56:29 on 05-04-2007
 Integrated Areas in History Files:
 HC_06.h01                 3.60000
 HC_06.h02                 .535064
 HC_06.h03                 .460904E-03
 HC_06.h04                 .244265E-08
```

## D.7 Hot Commissioning Operations HC_07

### D.7.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 7.2 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 27255.0, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.025032, 1.2181                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.6451d-4                         part-pore diffusivities(cm^2/min)
4.9353d-4                         Brownian diffusivities(cm^2/min)
0.2632                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9850                            Freundlich/Langmuir Hybrid Ma   (-)
0.8695                            Freundlich/Langmuir Hybrid Mb   (-)
2.076d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.7.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: HC_07
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 7.2 gpm
 Begin Run:  17:56:29 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min        dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm         D              =    134.62000 cm
```

```
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  27255.00000 mL/min      Uo (linear)    =      4.55919 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     34.99963 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .43370E+00
Dp  [cm2/min]  =  .16451E-03
Doo [cm2/min]  =  .49353E-03
kf  [cm/min]   =  .15677E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .71438E-01
Sc(i)          =  .24983E+04
Peb(i)         =  .16775E+04
Bi(i)          =  .33315E+02
Nf(i)          =  .98832E+03
Np(i)          =  .71608E+01
Pep(i)         =  .96887E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26320E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98500E+00
Iso. Const. 4  =  .86950E+00
Iso. Const. 5  =  .20760E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units           M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2740E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2503E-01 poise and density to 1.218     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_07.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_07.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_07.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_07.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = .1938E+05 min
Conc. Carousel caused bed shift at t = .3064E+05 min
Conc. Carousel caused bed shift at t = .4208E+05 min
Conc. Carousel caused bed shift at t = .5369E+05 min
Conc. Carousel caused bed shift at t = .6532E+05 min
Conc. Carousel caused bed shift at t = .7707E+05 min
Conc. Carousel caused bed shift at t = .8882E+05 min
Conc. Carousel caused bed shift at t = .1006E+06 min
Conc. Carousel caused bed shift at t = .1124E+06 min
VERSE-LC finished in  3574 steps.  Average step size 33.58     minutes
End run:  18:00:05 on 05-04-2007
Integrated Areas in History Files:
HC_07.h01                 3.28800
HC_07.h02                 1.55019
HC_07.h03                 .181523E-03
HC_07.h04                 .906865E-18
```

## D.8 Hot Commissioning Operations HC_08

### D.8.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 20 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 75708.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.025032, 1.2181                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
```

```
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.6451d-4                         part-pore diffusivities(cm^2/min)
4.9353d-4                         Brownian diffusivities(cm^2/min)
0.2632                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9850                            Freundlich/Langmuir Hybrid Ma   (-)
0.8695                            Freundlich/Langmuir Hybrid Mb   (-)
2.076d-3                          Freundlich/Langmuir Hybrid beta (-)
```

## D.8.2 VERSE-LC Datafile.run

```
=============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
=============================================================================
Input file: HC_08
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 20 gpm
Begin Run:  18:00:05 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  75708.20000 mL/min      Uo (linear)    =     12.66440 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     12.59989 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .11932E+01
Dp  [cm2/min]  =  .16451E-03
Doo [cm2/min]  =  .49353E-03
kf  [cm/min]   =  .22037E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .19844E+00
Sc(i)          =  .24983E+04
Peb(i)         =  .16937E+04
Bi(i)          =  .46831E+02
Nf(i)          =  .50015E+03
Np(i)          =  .25779E+01
Pep(i)         =  .26913E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26320E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98500E+00
Iso. Const. 4  =  .86950E+00
Iso. Const. 5  =  .20760E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
=============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2740E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2503E-01 poise and density to 1.218     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_08.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_08.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_08.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_08.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
=============================================================================
Conc. Carousel caused bed shift at t = 5815.     min
Conc. Carousel caused bed shift at t = 9564.     min
Conc. Carousel caused bed shift at t = .1344E+05 min
```

```
 Conc. Carousel caused bed shift at t = .1739E+05 min
 Conc. Carousel caused bed shift at t = .2140E+05 min
 Conc. Carousel caused bed shift at t = .2545E+05 min
 Conc. Carousel caused bed shift at t = .2952E+05 min
 Conc. Carousel caused bed shift at t = .3359E+05 min
 Conc. Carousel caused bed shift at t = .3767E+05 min
 Conc. Carousel caused bed shift at t = .4175E+05 min
 Conc. Carousel caused bed shift at t = .4582E+05 min
 Conc. Carousel caused bed shift at t = .4989E+05 min
 Conc. Carousel caused bed shift at t = .5397E+05 min
 Conc. Carousel caused bed shift at t = .5804E+05 min
 Conc. Carousel caused bed shift at t = .6212E+05 min
 Conc. Carousel caused bed shift at t = .6619E+05 min
 Conc. Carousel caused bed shift at t = .7027E+05 min
 Conc. Carousel caused bed shift at t = .7434E+05 min
 Conc. Carousel caused bed shift at t = .7842E+05 min
 Conc. Carousel caused bed shift at t = .8249E+05 min
 Conc. Carousel caused bed shift at t = .8656E+05 min
 Conc. Carousel caused bed shift at t = .9064E+05 min
 Conc. Carousel caused bed shift at t = .9471E+05 min
 Conc. Carousel caused bed shift at t = .9879E+05 min
 Conc. Carousel caused bed shift at t = .1029E+06 min
 Conc. Carousel caused bed shift at t = .1069E+06 min
 Conc. Carousel caused bed shift at t = .1110E+06 min
 Conc. Carousel caused bed shift at t = .1151E+06 min
 Conc. Carousel caused bed shift at t = .1192E+06 min
 VERSE-LC finished in 10527 steps.  Average step size 11.40     minutes
 End run:  18:21:43 on 05-04-2007
 Integrated Areas in History Files:
 HC_08.h01                  3.28800
 HC_08.h02                  .573997
 HC_08.h03                  .422171E-03
 HC_08.h04                  .504752E-09
```

## D.9 Hot Commissioning Operations HC_09

### D.9.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 30 gpm
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,datafile.yio
M                                comp-conc units
478.71, 134.62, 113562.4, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0        part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentration (M)
S                                COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0        spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.025032, 1.2181                 fluid viscosity(poise), density(g/cm^3)
m                                      COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6    elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                      COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
h                                      COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
h                                      COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
h                                      COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
-                                end of commands
120000.0, 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
1.0                              size exclusion factor
1.6451d-4                        part-pore diffusivities(cm^2/min)
4.9353d-4                        Brownian diffusivities(cm^2/min)
0.2632                           Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                              Freundlich/Langmuir Hybrid b    (1/M)
0.9850                           Freundlich/Langmuir Hybrid Ma   (-)
0.8695                           Freundlich/Langmuir Hybrid Mb   (-)
2.076d-3                         Freundlich/Langmuir Hybrid beta (-)
```

### D.9.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: HC_09
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 30 gpm
 Begin Run:  18:21:43 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min        dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm         D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
 F              = 113562.40000 mL/min      Uo (linear)    =     18.99661 cm/min
```

```
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =      8.39992 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .17803E+01
Dp  [cm2/min]  =  .16451E-03
Doo [cm2/min]  =  .49353E-03
kf  [cm/min]   =  .25226E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .29766E+00
Sc(i)          =  .24983E+04
Peb(i)         =  .17026E+04
Bi(i)          =  .53608E+02
Nf(i)          =  .38168E+03
Np(i)          =  .17186E+01
Pep(i)         =  .40369E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26320E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98500E+00
Iso. Const. 4  =  .86950E+00
Iso. Const. 5  =  .20760E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
==============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2740E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2503E-01 poise and density to 1.218     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_09.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_09.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_09.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_09.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
==============================================================================
Conc. Carousel caused bed shift at t = 3483.     min
Conc. Carousel caused bed shift at t = 5850.     min
Conc. Carousel caused bed shift at t = 8337.     min
Conc. Carousel caused bed shift at t = .1088E+05 min
Conc. Carousel caused bed shift at t = .1345E+05 min
Conc. Carousel caused bed shift at t = .1603E+05 min
Conc. Carousel caused bed shift at t = .1861E+05 min
Conc. Carousel caused bed shift at t = .2119E+05 min
Conc. Carousel caused bed shift at t = .2377E+05 min
Conc. Carousel caused bed shift at t = .2635E+05 min
Conc. Carousel caused bed shift at t = .2893E+05 min
Conc. Carousel caused bed shift at t = .3151E+05 min
Conc. Carousel caused bed shift at t = .3409E+05 min
Conc. Carousel caused bed shift at t = .3667E+05 min
Conc. Carousel caused bed shift at t = .3925E+05 min
Conc. Carousel caused bed shift at t = .4183E+05 min
Conc. Carousel caused bed shift at t = .4441E+05 min
Conc. Carousel caused bed shift at t = .4699E+05 min
Conc. Carousel caused bed shift at t = .4957E+05 min
Conc. Carousel caused bed shift at t = .5215E+05 min
Conc. Carousel caused bed shift at t = .5473E+05 min
Conc. Carousel caused bed shift at t = .5731E+05 min
Conc. Carousel caused bed shift at t = .5989E+05 min
Conc. Carousel caused bed shift at t = .6247E+05 min
Conc. Carousel caused bed shift at t = .6505E+05 min
Conc. Carousel caused bed shift at t = .6763E+05 min
Conc. Carousel caused bed shift at t = .7021E+05 min
Conc. Carousel caused bed shift at t = .7278E+05 min
Conc. Carousel caused bed shift at t = .7536E+05 min
Conc. Carousel caused bed shift at t = .7794E+05 min
Conc. Carousel caused bed shift at t = .8052E+05 min
Conc. Carousel caused bed shift at t = .8310E+05 min
Conc. Carousel caused bed shift at t = .8568E+05 min
Conc. Carousel caused bed shift at t = .8826E+05 min
Conc. Carousel caused bed shift at t = .9084E+05 min
Conc. Carousel caused bed shift at t = .9342E+05 min
Conc. Carousel caused bed shift at t = .9600E+05 min
Conc. Carousel caused bed shift at t = .9858E+05 min
Conc. Carousel caused bed shift at t = .1012E+06 min
Conc. Carousel caused bed shift at t = .1037E+06 min
Conc. Carousel caused bed shift at t = .1063E+06 min
Conc. Carousel caused bed shift at t = .1089E+06 min
Conc. Carousel caused bed shift at t = .1115E+06 min
Conc. Carousel caused bed shift at t = .1141E+06 min
```

```
 Conc. Carousel caused bed shift at t = .1166E+06 min
 Conc. Carousel caused bed shift at t = .1192E+06 min
 VERSE-LC finished in 16145 steps.  Average step size 7.433     minutes
 End run:  19:00:43 on 05-04-2007
 Integrated Areas in History Files:
 HC_09.h01                 3.28800
 HC_09.h02                 .408959
 HC_09.h03                 .519773E-03
 HC_09.h04                 .121809E-07
```

## D.10 Hot Commissioning Operations HC_10

### D.10.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 35 C
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.019702, 1.2113                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
2.0500d-4                         part-pore diffusivities(cm^2/min)
6.1499d-4                         Brownian diffusivities(cm^2/min)
0.2678                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9877                            Freundlich/Langmuir Hybrid Ma   (-)
0.8609                            Freundlich/Langmuir Hybrid Mb   (-)
2.646d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.10.2 VERSE-LC Datafile.run

```
 ==============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ==============================================================================
 Input file: HC_10
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 35 C
 Begin Run:  19:00:43 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min        dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm         D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
 F              =  56781.20000 mL/min     Uo (linear)    =      9.49831 cm/min
 R              =    230.00000 microns    L/R            =  20813.47826
 Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
 Spec. Area     =     75.65217 1/cm       Time/BV        =     16.79984 min
 Vol CSTRs      =1892706.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .89545E+00
 Dp  [cm2/min]  =  .20500E-03
 Doo [cm2/min]  =  .61499E-03
 kf  [cm/min]   =  .23185E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .18804E+00
 Sc(i)          =  .15869E+04
 Peb(i)         =  .16926E+04
 Bi(i)          =  .39539E+02
 Nf(i)          =  .70161E+03
 Np(i)          =  .42831E+01
 Pep(i)         =  .16198E+04

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .26780E+00
```

```
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .98770E+00
 Iso. Const. 4  =  .86090E+00
 Iso. Const. 5  =  .26460E-02
 Init. Conc.    =  .00000E+00
 Conc. at eqb.  =  .00000E+00
 Conc. units          M
 ===============================================================================
 COMMAND LIST:
   1: Step conc. of component 1 at .0000     min to .2740E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .1970E-01 poise and density to 1.211     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3700E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = HC_10.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = HC_10.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = HC_10.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = HC_10.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = 6669.     min
 Conc. Carousel caused bed shift at t = .1071E+05 min
 Conc. Carousel caused bed shift at t = .1488E+05 min
 Conc. Carousel caused bed shift at t = .1910E+05 min
 Conc. Carousel caused bed shift at t = .2337E+05 min
 Conc. Carousel caused bed shift at t = .2768E+05 min
 Conc. Carousel caused bed shift at t = .3202E+05 min
 Conc. Carousel caused bed shift at t = .3636E+05 min
 Conc. Carousel caused bed shift at t = .4073E+05 min
 Conc. Carousel caused bed shift at t = .4510E+05 min
 Conc. Carousel caused bed shift at t = .4949E+05 min
 Conc. Carousel caused bed shift at t = .5387E+05 min
 Conc. Carousel caused bed shift at t = .5826E+05 min
 Conc. Carousel caused bed shift at t = .6264E+05 min
 Conc. Carousel caused bed shift at t = .6703E+05 min
 Conc. Carousel caused bed shift at t = .7142E+05 min
 Conc. Carousel caused bed shift at t = .7580E+05 min
 Conc. Carousel caused bed shift at t = .8019E+05 min
 Conc. Carousel caused bed shift at t = .8457E+05 min
 Conc. Carousel caused bed shift at t = .8896E+05 min
 Conc. Carousel caused bed shift at t = .9334E+05 min
 Conc. Carousel caused bed shift at t = .9773E+05 min
 Conc. Carousel caused bed shift at t = .1021E+06 min
 Conc. Carousel caused bed shift at t = .1065E+06 min
 Conc. Carousel caused bed shift at t = .1109E+06 min
 Conc. Carousel caused bed shift at t = .1153E+06 min
 Conc. Carousel caused bed shift at t = .1197E+06 min
 VERSE-LC finished in  7930 steps.  Average step size 15.13     minutes
 End run:  19:17:10 on 05-04-2007
 Integrated Areas in History Files:
 HC_10.h01                3.28800
 HC_10.h02                .804114
 HC_10.h03                .356423E-03
 HC_10.h04                .138345E-10
```

## D.11 Hot Commissioning Operations HC_11

### D.11.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 45 C
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.016135, 1.2050                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
```

```
1.0                                size exclusion factor
2.4629d-4                          part-pore diffusivities(cm^2/min)
7.3888d-4                          Brownian diffusivities(cm^2/min)
0.2720                             Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                                Freundlich/Langmuir Hybrid b    (1/M)
0.9900                             Freundlich/Langmuir Hybrid Ma   (-)
0.8525                             Freundlich/Langmuir Hybrid Mb   (-)
3.282d-3                           Freundlich/Langmuir Hybrid beta (-)
```

## D.11.2 VERSE-LC Datafile.run

```
================================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
================================================================================
Input file: HC_11
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 45 C
Begin Run:  19:17:10 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  56781.20000 mL/min      Uo (linear)    =      9.49831 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89335E+00
Dp  [cm2/min]  =  .24629E-03
Doo [cm2/min]  =  .73888E-03
kf  [cm/min]   =  .26203E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .22841E+00
Sc(i)          =  .10873E+04
Peb(i)         =  .16966E+04
Bi(i)          =  .37194E+02
Nf(i)          =  .79292E+03
Np(i)          =  .51458E+01
Pep(i)         =  .13482E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .27200E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .99000E+00
Iso. Const. 4  =  .85250E+00
Iso. Const. 5  =  .32820E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
================================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2740E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1614E-01 poise and density to 1.205     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_11.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_11.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_11.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_11.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
================================================================================
Conc. Carousel caused bed shift at t = 5490.     min
Conc. Carousel caused bed shift at t = 8775.     min
Conc. Carousel caused bed shift at t = .1213E+05 min
Conc. Carousel caused bed shift at t = .1554E+05 min
Conc. Carousel caused bed shift at t = .1899E+05 min
Conc. Carousel caused bed shift at t = .2246E+05 min
Conc. Carousel caused bed shift at t = .2594E+05 min
Conc. Carousel caused bed shift at t = .2946E+05 min
Conc. Carousel caused bed shift at t = .3298E+05 min
Conc. Carousel caused bed shift at t = .3651E+05 min
Conc. Carousel caused bed shift at t = .4004E+05 min
```

```
Conc. Carousel caused bed shift at t = .4358E+05 min
Conc. Carousel caused bed shift at t = .4713E+05 min
Conc. Carousel caused bed shift at t = .5068E+05 min
Conc. Carousel caused bed shift at t = .5421E+05 min
Conc. Carousel caused bed shift at t = .5776E+05 min
Conc. Carousel caused bed shift at t = .6131E+05 min
Conc. Carousel caused bed shift at t = .6486E+05 min
Conc. Carousel caused bed shift at t = .6841E+05 min
Conc. Carousel caused bed shift at t = .7196E+05 min
Conc. Carousel caused bed shift at t = .7551E+05 min
Conc. Carousel caused bed shift at t = .7904E+05 min
Conc. Carousel caused bed shift at t = .8259E+05 min
Conc. Carousel caused bed shift at t = .8614E+05 min
Conc. Carousel caused bed shift at t = .8969E+05 min
Conc. Carousel caused bed shift at t = .9324E+05 min
Conc. Carousel caused bed shift at t = .9679E+05 min
Conc. Carousel caused bed shift at t = .1003E+06 min
Conc. Carousel caused bed shift at t = .1039E+06 min
Conc. Carousel caused bed shift at t = .1074E+06 min
Conc. Carousel caused bed shift at t = .1110E+06 min
Conc. Carousel caused bed shift at t = .1145E+06 min
Conc. Carousel caused bed shift at t = .1181E+06 min
VERSE-LC finished in  8000 steps.  Average step size 15.00     minutes
End run:  19:34:29 on 05-04-2007
Integrated Areas in History Files:
HC_11.h01                  3.28800
HC_11.h02                  .808342
HC_11.h03                  .358490E-03
HC_11.h04                  .184196E-10
```

## D.12 Hot Commissioning Operations HC_12

### D.12.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 20 gpm, 380 um
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 75708.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
190.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.7400d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.025032, 1.2181                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.6451d-4                         part-pore diffusivities(cm^2/min)
4.9353d-4                         Brownian diffusivities(cm^2/min)
0.2632                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9850                            Freundlich/Langmuir Hybrid Ma   (-)
0.8695                            Freundlich/Langmuir Hybrid Mb   (-)
2.076d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.12.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: HC_12
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 20 gpm, 380 um
Begin Run:  19:34:29 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm         D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
F              =  75708.20000 mL/min     Uo (linear)    =     12.66440 cm/min
R              =    190.00000 microns    L/R            =  25195.26316
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     91.57895 1/cm       Time/BV        =     12.59989 min
Vol CSTRs      =1892706.00000 mL
```

```
Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .98781E+00
Dp  [cm2/min]  =  .16451E-03
Doo [cm2/min]  =  .49353E-03
kf  [cm/min]   =  .25031E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .16393E+00
Sc(i)          =  .24983E+04
Peb(i)         =  .20458E+04
Bi(i)          =  .43942E+02
Nf(i)          =  .68768E+03
Np(i)          =  .37776E+01
Pep(i)         =  .22232E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26320E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98500E+00
Iso. Const. 4  =  .86950E+00
Iso. Const. 5  =  .20760E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .2740E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2503E-01 poise and density to 1.218     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_12.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_12.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_12.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_12.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = 6321.     min
Conc. Carousel caused bed shift at t = .1021E+05 min
Conc. Carousel caused bed shift at t = .1420E+05 min
Conc. Carousel caused bed shift at t = .1826E+05 min
Conc. Carousel caused bed shift at t = .2237E+05 min
Conc. Carousel caused bed shift at t = .2650E+05 min
Conc. Carousel caused bed shift at t = .3066E+05 min
Conc. Carousel caused bed shift at t = .3484E+05 min
Conc. Carousel caused bed shift at t = .3903E+05 min
Conc. Carousel caused bed shift at t = .4323E+05 min
Conc. Carousel caused bed shift at t = .4742E+05 min
Conc. Carousel caused bed shift at t = .5162E+05 min
Conc. Carousel caused bed shift at t = .5583E+05 min
Conc. Carousel caused bed shift at t = .6002E+05 min
Conc. Carousel caused bed shift at t = .6423E+05 min
Conc. Carousel caused bed shift at t = .6843E+05 min
Conc. Carousel caused bed shift at t = .7264E+05 min
Conc. Carousel caused bed shift at t = .7683E+05 min
Conc. Carousel caused bed shift at t = .8104E+05 min
Conc. Carousel caused bed shift at t = .8524E+05 min
Conc. Carousel caused bed shift at t = .8944E+05 min
Conc. Carousel caused bed shift at t = .9364E+05 min
Conc. Carousel caused bed shift at t = .9784E+05 min
Conc. Carousel caused bed shift at t = .1021E+06 min
Conc. Carousel caused bed shift at t = .1062E+06 min
Conc. Carousel caused bed shift at t = .1104E+06 min
Conc. Carousel caused bed shift at t = .1146E+06 min
Conc. Carousel caused bed shift at t = .1189E+06 min
VERSE-LC finished in 10351 steps.  Average step size 11.59     minutes
End run:  19:52:54 on 05-04-2007
Integrated Areas in History Files:
HC_12.h01                 3.28800
HC_12.h02                 .826409
HC_12.h03                 .337870E-03
HC_12.h04                 .409936E-11
```

## D.13 Hot Commissioning Operations HC_13

### D.13.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 2X Cs+, 380 um
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
```

```
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
190.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.5000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.025032, 1.2181                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.6451d-4                         part-pore diffusivities(cm^2/min)
4.9353d-4                         Brownian diffusivities(cm^2/min)
0.2632                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9850                            Freundlich/Langmuir Hybrid Ma   (-)
0.8695                            Freundlich/Langmuir Hybrid Mb   (-)
2.076d-3                          Freundlich/Langmuir Hybrid beta (-)
```

## D.13.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: HC_13
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 2X Cs+, 380 um
Begin Run:  19:52:54 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  56781.20000 mL/min      Uo (linear)    =      9.49831 cm/min
R              =    190.00000 microns     L/R            =  25195.26316
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     91.57895 1/cm        Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .74302E+00
Dp  [cm2/min]  =  .16451E-03
Doo [cm2/min]  =  .49353E-03
kf  [cm/min]   =  .22742E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .12295E+00
Sc(i)          =  .24983E+04
Peb(i)         =  .20398E+04
Bi(i)          =  .39924E+02
Nf(i)          =  .83307E+03
Np(i)          =  .50367E+01
Pep(i)         =  .16674E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26320E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98500E+00
Iso. Const. 4  =  .86950E+00
Iso. Const. 5  =  .20760E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5500E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2503E-01 poise and density to 1.218     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_13.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_13.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
```

```
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = HC_13.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = HC_13.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = 8528.     min
 Conc. Carousel caused bed shift at t = .1365E+05 min
 Conc. Carousel caused bed shift at t = .1890E+05 min
 Conc. Carousel caused bed shift at t = .2421E+05 min
 Conc. Carousel caused bed shift at t = .2956E+05 min
 Conc. Carousel caused bed shift at t = .3493E+05 min
 Conc. Carousel caused bed shift at t = .4032E+05 min
 Conc. Carousel caused bed shift at t = .4571E+05 min
 Conc. Carousel caused bed shift at t = .5113E+05 min
 Conc. Carousel caused bed shift at t = .5654E+05 min
 Conc. Carousel caused bed shift at t = .6197E+05 min
 Conc. Carousel caused bed shift at t = .6738E+05 min
 Conc. Carousel caused bed shift at t = .7281E+05 min
 Conc. Carousel caused bed shift at t = .7822E+05 min
 Conc. Carousel caused bed shift at t = .8365E+05 min
 Conc. Carousel caused bed shift at t = .8906E+05 min
 Conc. Carousel caused bed shift at t = .9449E+05 min
 Conc. Carousel caused bed shift at t = .9992E+05 min
 Conc. Carousel caused bed shift at t = .1053E+06 min
 Conc. Carousel caused bed shift at t = .1108E+06 min
 Conc. Carousel caused bed shift at t = .1162E+06 min
 VERSE-LC finished in  7504 steps.  Average step size 15.99     minutes
 End run:  20:01:30 on 05-04-2007
 Integrated Areas in History Files:
 HC_13.h01                 6.60000
 HC_13.h02                 2.79467
 HC_13.h03                 .218839E-03
 HC_13.h04                 .273655E-15
```

## D.14 Hot Commissioning Operations HC_14

### D.14.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 2X Cs+, 380 um, 22 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 83279.1, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
190.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.5000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.025032, 1.2181                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.70d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.6451d-4                         part-pore diffusivities(cm^2/min)
4.9353d-4                         Brownian diffusivities(cm^2/min)
0.2632                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9850                            Freundlich/Langmuir Hybrid Ma   (-)
0.8695                            Freundlich/Langmuir Hybrid Mb   (-)
2.076d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.14.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: HC_14
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Hot Commissioning, CT: Nominal, Sensitivity: 2X Cs+, 380 um, 22 g
 Begin Run:  20:01:30 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm         D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
F              =  83279.10000 mL/min     Uo (linear)    =     13.93085 cm/min
R              =    190.00000 microns    L/R            =  25195.26316
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     91.57895 1/cm       Time/BV        =     11.45443 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .10854E+01
Dp  [cm2/min]  =  .16451E-03
Doo [cm2/min]  =  .49353E-03
kf  [cm/min]   =  .25839E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .18032E+00
Sc(i)          =  .24983E+04
Peb(i)         =  .20480E+04
Bi(i)          =  .45360E+02
Nf(i)          =  .64535E+03
Np(i)          =  .34341E+01
Pep(i)         =  .24456E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .26320E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98500E+00
Iso. Const. 4  =  .86950E+00
Iso. Const. 5  =  .20760E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units         M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5500E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2503E-01 poise and density to 1.218     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3700E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = HC_14.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = HC_14.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = HC_14.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = HC_14.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = 5410.     min
Conc. Carousel caused bed shift at t = 8806.     min
Conc. Carousel caused bed shift at t = .1229E+05 min
Conc. Carousel caused bed shift at t = .1585E+05 min
Conc. Carousel caused bed shift at t = .1945E+05 min
Conc. Carousel caused bed shift at t = .2307E+05 min
Conc. Carousel caused bed shift at t = .2671E+05 min
Conc. Carousel caused bed shift at t = .3035E+05 min
Conc. Carousel caused bed shift at t = .3400E+05 min
Conc. Carousel caused bed shift at t = .3767E+05 min
Conc. Carousel caused bed shift at t = .4133E+05 min
Conc. Carousel caused bed shift at t = .4498E+05 min
Conc. Carousel caused bed shift at t = .4865E+05 min
Conc. Carousel caused bed shift at t = .5231E+05 min
Conc. Carousel caused bed shift at t = .5598E+05 min
Conc. Carousel caused bed shift at t = .5963E+05 min
Conc. Carousel caused bed shift at t = .6329E+05 min
Conc. Carousel caused bed shift at t = .6696E+05 min
Conc. Carousel caused bed shift at t = .7061E+05 min
Conc. Carousel caused bed shift at t = .7427E+05 min
Conc. Carousel caused bed shift at t = .7794E+05 min
Conc. Carousel caused bed shift at t = .8159E+05 min
Conc. Carousel caused bed shift at t = .8526E+05 min
Conc. Carousel caused bed shift at t = .8892E+05 min
Conc. Carousel caused bed shift at t = .9258E+05 min
Conc. Carousel caused bed shift at t = .9624E+05 min
Conc. Carousel caused bed shift at t = .9990E+05 min
Conc. Carousel caused bed shift at t = .1036E+06 min
Conc. Carousel caused bed shift at t = .1072E+06 min
Conc. Carousel caused bed shift at t = .1109E+06 min
Conc. Carousel caused bed shift at t = .1145E+06 min
Conc. Carousel caused bed shift at t = .1182E+06 min
VERSE-LC finished in 11507 steps.  Average step size 10.43     minutes
End run:  20:23:40 on 05-04-2007
Integrated Areas in History Files:
HC_14.h01                  6.60000
HC_14.h02                  1.77388
HC_14.h03                   .306984E-03
HC_14.h04                   .118791E-11
```

## D.15 Envelope B Operations EB_01

### D.15.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Envelope B, CT: Nominal, Sensitivity: None
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 24605.2, 1892706. Length(cm), Diam(cm), Q-flow(ml/min), CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.8300d-4, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.019695, 1.1822                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
2.0291d-4                         part-pore diffusivities(cm^2/min)
6.0872d-4                         Brownian diffusivities(cm^2/min)
0.2401                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9727                            Freundlich/Langmuir Hybrid Ma   (-)
0.9042                            Freundlich/Langmuir Hybrid Mb   (-)
4.783d-4                          Freundlich/Langmuir Hybrid beta (-)
```

### D.15.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: EB_01
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Envelope B, CT: Nominal, Sensitivity: None
Begin Run:  15:46:40 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max      =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.       =       .10000E-03
Total Length   =    478.71000 cm          D               =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.       =6813677.17928 mL
F              =  24605.20000 mL/min      Uo (linear)     =      4.11594 cm/min
R              =    230.00000 microns     L/R             =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity   =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV         =     38.76883 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .39122E+00
Dp  [cm2/min]  =  .20291E-03
Doo [cm2/min]  =  .60872E-03
kf  [cm/min]   =  .17426E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .79554E-01
Sc(i)          =  .16421E+04
Peb(i)         =  .16788E+04
Bi(i)          =  .30023E+02
Nf(i)          =  .12169E+04
Np(i)          =  .97834E+01
Pep(i)         =  .70914E+03

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .24010E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97270E+00
Iso. Const. 4  =  .90420E+00
Iso. Const. 5  =  .47830E-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 .2830E-03 M
```

```
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .1970E-01 poise and density to 1.182     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3400E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = EB_01.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = EB_01.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = EB_01.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = EB_01.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = .4909E+05 min
 Conc. Carousel caused bed shift at t = .7448E+05 min
 Conc. Carousel caused bed shift at t = .9986E+05 min
 VERSE-LC finished in  3446 steps.  Average step size 34.82     minutes
 End run:  15:55:06 on 05-04-2007
 Integrated Areas in History Files:
 EB_01.h01                  33.9600
 EB_01.h02                  25.3449
 EB_01.h03                  .184202E-04
 EB_01.h04                 -.483223E-21
```

## D.16 Envelope B Operations EB_02

### D.16.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Envelope B, CT: Nominal, Sensitivity: 10 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 37854.1, 1892706. Length(cm), Diam(cm), Q-flow(ml/min), CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 2.8300d-4, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.019695, 1.1822                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
2.0291d-4                         part-pore diffusivities(cm^2/min)
6.0872d-4                         Brownian diffusivities(cm^2/min)
0.2401                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9727                            Freundlich/Langmuir Hybrid Ma   (-)
0.9042                            Freundlich/Langmuir Hybrid Mb   (-)
4.783d-4                          Freundlich/Langmuir Hybrid beta (-)
```

### D.16.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: EB_02
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Envelope B, CT: Nominal, Sensitivity: 10 gpm
 Begin Run:  15:55:06 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min        dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm         D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
 F              =  37854.10000 mL/min     Uo (linear)    =      6.33220 cm/min
 R              =    230.00000 microns    L/R            =  20813.47826
```

```
Bed Void frac. =       .42000           Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm      Time/BV        =     25.19978 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .59966E+00
Dp  [cm2/min]  =  .20291E-03
Doo [cm2/min]  =  .60872E-03
kf  [cm/min]   =  .20116E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .12239E+00
Sc(i)          =  .16421E+04
Peb(i)         =  .16850E+04
Bi(i)          =  .34659E+02
Nf(i)          =  .91310E+03
Np(i)          =  .63592E+01
Pep(i)         =  .10910E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .24010E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97270E+00
Iso. Const. 4  =  .90420E+00
Iso. Const. 5  =  .47830E-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 .2830E-03 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1970E-01 poise and density to 1.182     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = EB_02.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = EB_02.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = EB_02.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = EB_02.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = .3143E+05 min
Conc. Carousel caused bed shift at t = .4793E+05 min
Conc. Carousel caused bed shift at t = .6443E+05 min
Conc. Carousel caused bed shift at t = .8094E+05 min
Conc. Carousel caused bed shift at t = .9744E+05 min
Conc. Carousel caused bed shift at t = .1139E+06 min
VERSE-LC finished in  5308 steps.  Average step size 22.61     minutes
End run:  16:07:42 on 05-04-2007
Integrated Areas in History Files:
EB_02.h01                 33.9600
EB_02.h02                 26.6149
EB_02.h03                 .309535E-04
EB_02.h04                -.140696E-21
```

## D.17 Subsequent Operations SO_01

### D.17.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 20 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 75708.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.019791, 1.2178                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.9021d-4                         part-pore diffusivities(cm^2/min)
5.7062d-4                         Brownian diffusivities(cm^2/min)
0.2458                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9761                            Freundlich/Langmuir Hybrid Ma   (-)
0.8941                            Freundlich/Langmuir Hybrid Mb   (-)
8.174d-4                         Freundlich/Langmuir Hybrid beta (-)
```

## D.17.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: SO_01
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 20 gpm
Begin Run:  20:23:40 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  75708.20000 mL/min      Uo (linear)    =     12.66440 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     12.59989 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .11897E+01
Dp  [cm2/min]  =  .19021E-03
Doo [cm2/min]  =  .57062E-03
kf  [cm/min]   =  .24276E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .25093E+00
Sc(i)          =  .17088E+04
Peb(i)         =  .16986E+04
Bi(i)          =  .44619E+02
Nf(i)          =  .55096E+03
Np(i)          =  .29806E+01
Pep(i)         =  .23277E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .24580E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97610E+00
Iso. Const. 4  =  .89410E+00
Iso. Const. 5  =  .81740E-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 .5000E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1979E-01 poise and density to 1.218     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_01.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = SO_01.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = SO_01.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = SO_01.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = .1485E+05 min
Conc. Carousel caused bed shift at t = .2420E+05 min
Conc. Carousel caused bed shift at t = .3377E+05 min
Conc. Carousel caused bed shift at t = .4345E+05 min
Conc. Carousel caused bed shift at t = .5316E+05 min
Conc. Carousel caused bed shift at t = .6291E+05 min
Conc. Carousel caused bed shift at t = .7268E+05 min
Conc. Carousel caused bed shift at t = .8244E+05 min
Conc. Carousel caused bed shift at t = .9221E+05 min
```

```
Conc. Carousel caused bed shift at t = .1020E+06 min
Conc. Carousel caused bed shift at t = .1117E+06 min
VERSE-LC finished in  9774 steps.  Average step size 12.28     minutes
End run:  20:31:11 on 05-04-2007
Integrated Areas in History Files:
SO_01.h01                  6.00000
SO_01.h02                  2.55304
SO_01.h03                  .187135E-03
SO_01.h04                  .272651E-15
```

## D.18 Subsequent Operations SO_02

### D.18.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: diluted to 4 M Na+, 15 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 4.3800d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.017332, 1.1908                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
2.1719d-4                         part-pore diffusivities(cm^2/min)
6.5156d-4                         Brownian diffusivities(cm^2/min)
0.2423                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9749                            Freundlich/Langmuir Hybrid Ma   (-)
0.8976                            Freundlich/Langmuir Hybrid Mb   (-)
6.877d-4                          Freundlich/Langmuir Hybrid beta (-)
```

### D.18.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: SO_02
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: diluted to 4 M Na
Begin Run:  20:31:11 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm         D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
F              =  56781.20000 mL/min     Uo (linear)    =      9.49831 cm/min
R              =    230.00000 microns    L/R            =  20813.47826
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm       Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89428E+00
Dp  [cm2/min]  =  .21719E-03
Doo [cm2/min]  =  .65156E-03
kf  [cm/min]   =  .24096E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .21013E+00
Sc(i)          =  .13403E+04
Peb(i)         =  .16948E+04
Bi(i)          =  .38785E+02
Nf(i)          =  .72915E+03
Np(i)          =  .45378E+01
Pep(i)         =  .15289E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .24230E+00
```

```
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .97490E+00
 Iso. Const. 4  =  .89760E+00
 Iso. Const. 5  =  .68770E-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 .4380E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .1733E-01 poise and density to 1.191     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3400E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = SO_02.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = SO_02.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = SO_02.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = SO_02.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = .2558E+05 min
 Conc. Carousel caused bed shift at t = .4077E+05 min
 Conc. Carousel caused bed shift at t = .5614E+05 min
 Conc. Carousel caused bed shift at t = .7156E+05 min
 Conc. Carousel caused bed shift at t = .8700E+05 min
 Conc. Carousel caused bed shift at t = .1024E+06 min
 Conc. Carousel caused bed shift at t = .1179E+06 min
 VERSE-LC finished in  7346 steps.  Average step size 16.34     minutes
 End run:  20:36:47 on 05-04-2007
 Integrated Areas in History Files:
 SO_02.h01                5.25600
 SO_02.h02                3.00860
 SO_02.h03                .128958E-03
 SO_02.h04                .839688E-22
```

## D.19 Subsequent Operations SO_03

### D.19.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: concentrated to 5.5 M Na+, 15 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 6.0200d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.024496, 1.2575                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.5367d-4                         part-pore diffusivities(cm^2/min)
4.6101d-4                         Brownian diffusivities(cm^2/min)
0.2504                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9781                            Freundlich/Langmuir Hybrid Ma   (-)
0.8889                            Freundlich/Langmuir Hybrid Mb   (-)
1.034d-3                         Freundlich/Langmuir Hybrid beta (-)
```

### D.19.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: SO_03
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: concentrated to 5
 Begin Run:  20:36:47 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
```

```
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  56781.20000 mL/min      Uo (linear)    =      9.49831 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89725E+00
Dp  [cm2/min]  =  .15367E-03
Doo [cm2/min]  =  .46101E-03
kf  [cm/min]   =  .19133E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .15701E+00
Sc(i)          =  .25353E+04
Peb(i)         =  .16892E+04
Bi(i)          =  .43527E+02
Nf(i)          =  .57897E+03
Np(i)          =  .32107E+01
Pep(i)         =  .21609E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .25040E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97810E+00
Iso. Const. 4  =  .88890E+00
Iso. Const. 5  =  .10340E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
==============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .6020E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2450E-01 poise and density to 1.258     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_03.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = SO_03.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = SO_03.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = SO_03.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
==============================================================================
Conc. Carousel caused bed shift at t = .1570E+05 min
Conc. Carousel caused bed shift at t = .2554E+05 min
Conc. Carousel caused bed shift at t = .3562E+05 min
Conc. Carousel caused bed shift at t = .4580E+05 min
Conc. Carousel caused bed shift at t = .5603E+05 min
Conc. Carousel caused bed shift at t = .6629E+05 min
Conc. Carousel caused bed shift at t = .7657E+05 min
Conc. Carousel caused bed shift at t = .8684E+05 min
Conc. Carousel caused bed shift at t = .9714E+05 min
Conc. Carousel caused bed shift at t = .1074E+06 min
Conc. Carousel caused bed shift at t = .1177E+06 min
VERSE-LC finished in  7445 steps.  Average step size 16.12     minutes
End run:  20:44:18 on 05-04-2007
Integrated Areas in History Files:
SO_03.h01                 7.22400
SO_03.h02                 3.09762
SO_03.h03                  .192530E-03
SO_03.h04                  .198045E-15
```

## D.20 Subsequent Operations SO_04

### D.20.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 50% caustic leach, 30 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
```

```
478.71, 134.62, 113562.4, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 3.3300d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.023203, 1.1971                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.8194d-4                         part-pore diffusivities(cm^2/min)
5.4582d-4                         Brownian diffusivities(cm^2/min)
0.2426                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9733                            Freundlich/Langmuir Hybrid Ma   (-)
0.9024                            Freundlich/Langmuir Hybrid Mb   (-)
5.281d-4                          Freundlich/Langmuir Hybrid beta (-)
```

## D.20.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: SO_04
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 50% caustic leach
Begin Run:  20:44:18 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              = 113562.40000 mL/min      Uo (linear)    =     18.99661 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =      8.39992 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .17788E+01
Dp  [cm2/min]  =  .18194E-03
Doo [cm2/min]  =  .54582E-03
kf  [cm/min]   =  .26978E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .31559E+00
Sc(i)          =  .21307E+04
Peb(i)         =  .17041E+04
Bi(i)          =  .51839E+02
Nf(i)          =  .40819E+03
Np(i)          =  .19007E+01
Pep(i)         =  .36502E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .24260E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97330E+00
Iso. Const. 4  =  .90240E+00
Iso. Const. 5  =  .52810E-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 .3330E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .2320E-01 poise and density to 1.197     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_04.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = SO_04.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
```

```
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = SO_04.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = SO_04.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = .1435E+05 min
 Conc. Carousel caused bed shift at t = .2391E+05 min
 Conc. Carousel caused bed shift at t = .3380E+05 min
 Conc. Carousel caused bed shift at t = .4387E+05 min
 Conc. Carousel caused bed shift at t = .5402E+05 min
 Conc. Carousel caused bed shift at t = .6421E+05 min
 Conc. Carousel caused bed shift at t = .7441E+05 min
 Conc. Carousel caused bed shift at t = .8461E+05 min
 Conc. Carousel caused bed shift at t = .9482E+05 min
 Conc. Carousel caused bed shift at t = .1050E+06 min
 Conc. Carousel caused bed shift at t = .1152E+06 min
 VERSE-LC finished in 14737 steps.  Average step size 8.143     minutes
 End run:  20:57:11 on 05-04-2007
 Integrated Areas in History Files:
 SO_04.h01                3.99600
 SO_04.h02                1.08456
 SO_04.h03                .272077E-03
 SO_04.h04                .154393E-11
```

## D.21 Subsequent Operations SO_05

### D.21.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 50% caustic leach, 35 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 132489.4, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 3.3300d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.023203, 1.1971                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.8194d-4                         part-pore diffusivities(cm^2/min)
5.4582d-4                         Brownian diffusivities(cm^2/min)
0.2426                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9733                            Freundlich/Langmuir Hybrid Ma   (-)
0.9024                            Freundlich/Langmuir Hybrid Mb   (-)
5.281d-4                          Freundlich/Langmuir Hybrid beta (-)
```

### D.21.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: SO_05
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 50% caustic leach
 Begin Run:  20:57:11 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm          D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
 F              = 132489.40000 mL/min      Uo (linear)    =     22.16271 cm/min
 R              =    230.00000 microns     L/R            =  20813.47826
 Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
 Spec. Area     =     75.65217 1/cm        Time/BV        =      7.19993 min
 Vol CSTRs      =1892706.00000 mL
```

```
 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .20704E+01
 Dp  [cm2/min]  =  .18194E-03
 Doo [cm2/min]  =  .54582E-03
 kf  [cm/min]   =  .28401E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .36818E+00
 Sc(i)          =  .21307E+04
 Peb(i)         =  .17081E+04
 Bi(i)          =  .54572E+02
 Nf(i)          =  .36832E+03
 Np(i)          =  .16291E+01
 Pep(i)         =  .42586E+04

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .24260E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .97330E+00
 Iso. Const. 4  =  .90240E+00
 Iso. Const. 5  =  .52810E-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 .3330E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .2320E-01 poise and density to 1.197     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3400E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = SO_05.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = SO_05.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = SO_05.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = SO_05.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ==============================================================================
 Conc. Carousel caused bed shift at t = .1176E+05 min
 Conc. Carousel caused bed shift at t = .1980E+05 min
 Conc. Carousel caused bed shift at t = .2817E+05 min
 Conc. Carousel caused bed shift at t = .3669E+05 min
 Conc. Carousel caused bed shift at t = .4529E+05 min
 Conc. Carousel caused bed shift at t = .5391E+05 min
 Conc. Carousel caused bed shift at t = .6253E+05 min
 Conc. Carousel caused bed shift at t = .7116E+05 min
 Conc. Carousel caused bed shift at t = .7978E+05 min
 Conc. Carousel caused bed shift at t = .8840E+05 min
 Conc. Carousel caused bed shift at t = .9702E+05 min
 Conc. Carousel caused bed shift at t = .1056E+06 min
 Conc. Carousel caused bed shift at t = .1143E+06 min
 VERSE-LC finished in 17224 steps.  Average step size 6.967     minutes
 End run:  21:12:41 on 05-04-2007
 Integrated Areas in History Files:
 SO_05.h01                3.99600
 SO_05.h02                .879295
 SO_05.h03                .305909E-03
 SO_05.h04                .185990E-10
```

## D.22 Subsequent Operations SO_06

### D.22.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 20% caustic leach, 24 gpm, 45 C
1, 150, 4, 6                       ncomp, nelem, ncol-bed, ncol-part
FCWNA                              isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                              input-only,perfusable,feed-equil,datafile.yio
M                                  comp-conc units
478.71, 134.62, 90849.9, 1892706.  Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0          part-rad(um), bed-void, part-void, sorb-cap()
0.0                                initial concentration (M)
S                                  COMMAND - conc step change
1, 0.0, 4.1700d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                  COMMAND - viscosity/density change
0.014066, 1.1948                   fluid viscosity(poise), density(g/cm^3)
m                                        COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6      elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                        COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016              unit op#, ptscale(1-4) filtering
h                                        COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016              unit op#, ptscale(1-4) filtering
h                                        COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016              unit op#, ptscale(1-4) filtering
h                                        COMMAND - effluent history dump
```

```
6, 2.0, 50, 4.033d-4, 0.016          unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
2.7623d-4                         part-pore diffusivities(cm^2/min)
8.2870d-4                         Brownian diffusivities(cm^2/min)
0.2529                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9792                            Freundlich/Langmuir Hybrid Ma   (-)
0.8859                            Freundlich/Langmuir Hybrid Mb   (-)
1.168d-3                          Freundlich/Langmuir Hybrid beta (-)
```

## D.22.2 VERSE-LC Datafile.run

```
==============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
==============================================================================
Input file: SO_06
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 20% caustic leach
Begin Run:  21:12:41 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm         D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  90849.90000 mL/min     Uo (linear)    =     15.19729 cm/min
R              =    230.00000 microns    L/R            =  20813.47826
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm       Time/BV        =     10.49990 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .14169E+01
Dp  [cm2/min]  =  .27623E-03
Doo [cm2/min]  =  .82870E-03
kf  [cm/min]   =  .33083E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .41567E+00
Sc(i)          =  .85237E+03
Peb(i)         =  .17115E+04
Bi(i)          =  .41870E+02
Nf(i)          =  .62570E+03
Np(i)          =  .36071E+01
Pep(i)         =  .19234E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .25290E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97920E+00
Iso. Const. 4  =  .88590E+00
Iso. Const. 5  =  .11680E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
==============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .4170E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1407E-01 poise and density to 1.195     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_06.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = SO_06.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = SO_06.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = SO_06.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
==============================================================================
Conc. Carousel caused bed shift at t = 9182.     min
Conc. Carousel caused bed shift at t = .1486E+05 min
Conc. Carousel caused bed shift at t = .2069E+05 min
Conc. Carousel caused bed shift at t = .2660E+05 min
Conc. Carousel caused bed shift at t = .3256E+05 min
Conc. Carousel caused bed shift at t = .3854E+05 min
```

```
 Conc. Carousel caused bed shift at t = .4454E+05 min
 Conc. Carousel caused bed shift at t = .5055E+05 min
 Conc. Carousel caused bed shift at t = .5657E+05 min
 Conc. Carousel caused bed shift at t = .6259E+05 min
 Conc. Carousel caused bed shift at t = .6860E+05 min
 Conc. Carousel caused bed shift at t = .7463E+05 min
 Conc. Carousel caused bed shift at t = .8065E+05 min
 Conc. Carousel caused bed shift at t = .8668E+05 min
 Conc. Carousel caused bed shift at t = .9270E+05 min
 Conc. Carousel caused bed shift at t = .9872E+05 min
 Conc. Carousel caused bed shift at t = .1048E+06 min
 Conc. Carousel caused bed shift at t = .1108E+06 min
 Conc. Carousel caused bed shift at t = .1168E+06 min
 VERSE-LC finished in 11910 steps.  Average step size 10.08     minutes
 End run:  21:25:25 on 05-04-2007
 Integrated Areas in History Files:
 SO_06.h01                 5.00400
 SO_06.h02                 1.90724
 SO_06.h03                 .215579E-03
 SO_06.h04                 .129482E-14
```

## D.23 Subsequent Operations SO_07

### D.23.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: none
1, 150, 4, 6                     ncomp, nelem, ncol-bed, ncol-part
FCWNA                            isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                            input-only,perfusable,feed-equil,datafile.yio
M                                comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0        part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentration (M)
S                                COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0        spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.019791, 1.2178                 fluid viscosity(poise), density(g/cm^3)
m                                      COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6    elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                      COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
h                                      COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
h                                      COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
h                                      COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016            unit op#, ptscale(1-4) filtering
-                                end of commands
120000.0, 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
1.0                              size exclusion factor
1.9021d-4                        part-pore diffusivities(cm^2/min)
5.7062d-4                        Brownian diffusivities(cm^2/min)
0.2458                           Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                              Freundlich/Langmuir Hybrid b    (1/M)
0.9761                           Freundlich/Langmuir Hybrid Ma   (-)
0.8941                           Freundlich/Langmuir Hybrid Mb   (-)
8.174d-4                        Freundlich/Langmuir Hybrid beta (-)
```

### D.23.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: SO_07
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: none
 Begin Run:  21:25:25 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm          D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
 F              =  56781.20000 mL/min      Uo (linear)    =      9.49831 cm/min
 R              =    230.00000 microns     L/R            =  20813.47826
 Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
 Spec. Area     =     75.65217 1/cm        Time/BV        =     16.79984 min
 Vol CSTRs      =1892706.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .89545E+00
 Dp  [cm2/min]  =  .19021E-03
 Doo [cm2/min]  =  .57062E-03
 kf  [cm/min]   =  .22056E+00
 Ds  [cm2/min]  =  .00000E+00
```

```
 Dimensionless Groups:
 Re             =  .18820E+00
 Sc(i)          =  .17088E+04
 Peb(i)         =  .16926E+04
 Bi(i)          =  .40539E+02
 Nf(i)          =  .66744E+03
 Np(i)          =  .39741E+01
 Pep(i)         =  .17457E+04

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .24580E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .97610E+00
 Iso. Const. 4  =  .89410E+00
 Iso. Const. 5  =  .81740E-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 .5000E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .1979E-01 poise and density to 1.218     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3400E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = SO_07.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = SO_07.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = SO_07.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = SO_07.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ============================================================================
 Conc. Carousel caused bed shift at t = .2096E+05 min
 Conc. Carousel caused bed shift at t = .3366E+05 min
 Conc. Carousel caused bed shift at t = .4656E+05 min
 Conc. Carousel caused bed shift at t = .5955E+05 min
 Conc. Carousel caused bed shift at t = .7256E+05 min
 Conc. Carousel caused bed shift at t = .8558E+05 min
 Conc. Carousel caused bed shift at t = .9862E+05 min
 Conc. Carousel caused bed shift at t = .1117E+06 min
 VERSE-LC finished in  7373 steps.  Average step size 16.28     minutes
 End run:  21:31:20 on 05-04-2007
 Integrated Areas in History Files:
 SO_07.h01                 6.00000
 SO_07.h02                 3.12341
 SO_07.h03                 .142369E-03
 SO_07.h04                 .390010E-19
```

## D.24 Subsequent Operations SO_08

### D.24.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 75% OH-
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.019274, 1.2206                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.9124d-4                         part-pore diffusivities(cm^2/min)
5.7371d-4                         Brownian diffusivities(cm^2/min)
0.2449                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9763                            Freundlich/Langmuir Hybrid Ma   (-)
0.8936                            Freundlich/Langmuir Hybrid Mb   (-)
8.366d-4                          Freundlich/Langmuir Hybrid beta (-)
```

## D.24.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: SO_08
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 75% OH-
Begin Run:  21:31:20 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm         D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
F              =  56781.20000 mL/min     Uo (linear)    =      9.49831 cm/min
R              =    230.00000 microns    L/R            =  20813.47826
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm       Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89515E+00
Dp  [cm2/min]  =  .19124E-03
Doo [cm2/min]  =  .57371E-03
kf  [cm/min]   =  .22136E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .19369E+00
Sc(i)          =  .16514E+04
Peb(i)         =  .16932E+04
Bi(i)          =  .40466E+02
Nf(i)          =  .66985E+03
Np(i)          =  .39957E+01
Pep(i)         =  .17363E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .24490E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97630E+00
Iso. Const. 4  =  .89360E+00
Iso. Const. 5  =  .83660E-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 .5000E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1927E-01 poise and density to 1.221     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_08.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = SO_08.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = SO_08.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = SO_08.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = .2040E+05 min
Conc. Carousel caused bed shift at t = .3277E+05 min
Conc. Carousel caused bed shift at t = .4533E+05 min
Conc. Carousel caused bed shift at t = .5798E+05 min
Conc. Carousel caused bed shift at t = .7064E+05 min
Conc. Carousel caused bed shift at t = .8334E+05 min
Conc. Carousel caused bed shift at t = .9604E+05 min
Conc. Carousel caused bed shift at t = .1087E+06 min
VERSE-LC finished in  7373 steps.  Average step size 16.28     minutes
End run:  21:37:17 on 05-04-2007
Integrated Areas in History Files:
SO_08.h01                  6.00000
SO_08.h02                  3.17955
SO_08.h03                  .141490E-03
SO_08.h04                  .479823E-19
```

## D.25 Subsequent Operations SO_09

### D.25.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 24 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 90849.9, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.019791, 1.2178                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.9021d-4                         part-pore diffusivities(cm^2/min)
5.7062d-4                         Brownian diffusivities(cm^2/min)
0.2458                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9761                            Freundlich/Langmuir Hybrid Ma   (-)
0.8941                            Freundlich/Langmuir Hybrid Mb   (-)
8.174d-4                         Freundlich/Langmuir Hybrid beta (-)
```

### D.25.2 VERSE-LC Datafile.run

```
================================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
================================================================================
Input file: SO_09
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 24 gpm
Begin Run:  21:37:17 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  90849.90000 mL/min      Uo (linear)    =     15.19729 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     10.49990 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .14240E+01
Dp  [cm2/min]  =  .19021E-03
Doo [cm2/min]  =  .57062E-03
kf  [cm/min]   =  .25797E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .30111E+00
Sc(i)          =  .17088E+04
Peb(i)         =  .17029E+04
Bi(i)          =  .47414E+02
Nf(i)          =  .48790E+03
Np(i)          =  .24838E+01
Pep(i)         =  .27932E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .24580E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97610E+00
Iso. Const. 4  =  .89410E+00
Iso. Const. 5  =  .81740E-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 .5000E-04 M
```

```
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .1979E-01 poise and density to 1.218     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3400E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = SO_09.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = SO_09.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = SO_09.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = SO_09.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = .1187E+05 min
 Conc. Carousel caused bed shift at t = .1954E+05 min
 Conc. Carousel caused bed shift at t = .2743E+05 min
 Conc. Carousel caused bed shift at t = .3544E+05 min
 Conc. Carousel caused bed shift at t = .4351E+05 min
 Conc. Carousel caused bed shift at t = .5160E+05 min
 Conc. Carousel caused bed shift at t = .5971E+05 min
 Conc. Carousel caused bed shift at t = .6782E+05 min
 Conc. Carousel caused bed shift at t = .7593E+05 min
 Conc. Carousel caused bed shift at t = .8405E+05 min
 Conc. Carousel caused bed shift at t = .9217E+05 min
 Conc. Carousel caused bed shift at t = .1003E+06 min
 Conc. Carousel caused bed shift at t = .1084E+06 min
 Conc. Carousel caused bed shift at t = .1165E+06 min
 VERSE-LC finished in 11808 steps.  Average step size 10.16     minutes
 End run:  21:48:04 on 05-04-2007
 Integrated Areas in History Files:
 SO_09.h01                  6.00000
 SO_09.h02                  2.05837
 SO_09.h03                  .231775E-03
 SO_09.h04                  .269931E-13
```

## D.26 Subsequent Operations SO_10

### D.26.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 30 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 113562.4, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.019791, 1.2178                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.9021d-4                         part-pore diffusivities(cm^2/min)
5.7062d-4                         Brownian diffusivities(cm^2/min)
0.2458                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9761                            Freundlich/Langmuir Hybrid Ma   (-)
0.8941                            Freundlich/Langmuir Hybrid Mb   (-)
8.174d-4                          Freundlich/Langmuir Hybrid beta (-)
```

### D.26.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: SO_10
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 30 gpm
 Begin Run:  21:48:04 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm          D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
 F              = 113562.40000 mL/min      Uo (linear)    =     18.99661 cm/min
 R              =    230.00000 microns     L/R            =  20813.47826
 Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
 Spec. Area     =     75.65217 1/cm        Time/BV        =      8.39992 min
 Vol CSTRs      =1892706.00000 mL

 Component no.  =      1
 Ke  [-]        =  .10000E+01
 Eb  [cm2/min]  =  .17740E+01
 Dp  [cm2/min]  =  .19021E-03
 Doo [cm2/min]  =  .57062E-03
 kf  [cm/min]   =  .27789E+00
 Ds  [cm2/min]  =  .00000E+00

 Dimensionless Groups:
 Re             =  .37639E+00
 Sc(i)          =  .17088E+04
 Peb(i)         =  .17087E+04
 Bi(i)          =  .51076E+02
 Nf(i)          =  .42046E+03
 Np(i)          =  .19871E+01
 Pep(i)         =  .34915E+04

 Isotherm       =  Freundlich/Langmuir Hybrid
 Iso. Const. 1  =  .24580E+00
 Iso. Const. 2  =  .10000E+01
 Iso. Const. 3  =  .97610E+00
 Iso. Const. 4  =  .89410E+00
 Iso. Const. 5  =  .81740E-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 .5000E-04 M
      Execute   1 times, every .0000     mins.
   2: User set viscosity to .1979E-01 poise and density to 1.218     g/cm3
   3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
      When comp.  1 reaches .3400E-07 M     at end of node 100,
      shift  50 axial elements out the feed end
   4: Monitor conc. history at stream  0.  Filename = SO_10.h01
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = SO_10.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = SO_10.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = SO_10.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ===============================================================================
 Conc. Carousel caused bed shift at t = 8951.     min
 Conc. Carousel caused bed shift at t = .1495E+05 min
 Conc. Carousel caused bed shift at t = .2116E+05 min
 Conc. Carousel caused bed shift at t = .2749E+05 min
 Conc. Carousel caused bed shift at t = .3387E+05 min
 Conc. Carousel caused bed shift at t = .4028E+05 min
 Conc. Carousel caused bed shift at t = .4671E+05 min
 Conc. Carousel caused bed shift at t = .5312E+05 min
 Conc. Carousel caused bed shift at t = .5954E+05 min
 Conc. Carousel caused bed shift at t = .6596E+05 min
 Conc. Carousel caused bed shift at t = .7238E+05 min
 Conc. Carousel caused bed shift at t = .7881E+05 min
 Conc. Carousel caused bed shift at t = .8523E+05 min
 Conc. Carousel caused bed shift at t = .9164E+05 min
 Conc. Carousel caused bed shift at t = .9806E+05 min
 Conc. Carousel caused bed shift at t = .1045E+06 min
 Conc. Carousel caused bed shift at t = .1109E+06 min
 Conc. Carousel caused bed shift at t = .1173E+06 min
 VERSE-LC finished in 14878 steps.  Average step size 8.066     minutes
 End run:  22:03:40 on 05-04-2007
 Integrated Areas in History Files:
 SO_10.h01                 6.00000
 SO_10.h02                 1.52225
 SO_10.h03                 .282255E-03
 SO_10.h04                 .219731E-11
```

## D.27 Subsequent Operations SO_11

### D.27.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 35 C
```

```
1, 150, 4, 6                        ncomp, nelem, ncol-bed, ncol-part
FCWNA                               isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                               input-only,perfusable,feed-equil,datafile.yio
M                                   comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0           part-rad(um), bed-void, part-void, sorb-cap()
0.0                                 initial concentration (M)
S                                   COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                   COMMAND - viscosity/density change
0.015961, 1.2106                    fluid viscosity(poise), density(g/cm^3)
m                                         COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6       elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                         COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016               unit op#, ptscale(1-4) filtering
h                                         COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016               unit op#, ptscale(1-4) filtering
h                                         COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016               unit op#, ptscale(1-4) filtering
h                                         COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016               unit op#, ptscale(1-4) filtering
-                                   end of commands
120000.0, 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
1.0                                 size exclusion factor
2.3090d-4                           part-pore diffusivities(cm^2/min)
6.9269d-4                           Brownian diffusivities(cm^2/min)
0.2502                              Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                                 Freundlich/Langmuir Hybrid b    (1/M)
0.9786                              Freundlich/Langmuir Hybrid Ma   (-)
0.8874                              Freundlich/Langmuir Hybrid Mb   (-)
1.104d-3                            Freundlich/Langmuir Hybrid beta (-)
```

## D.27.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: SO_11
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 35 C
Begin Run:  22:03:40 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min        dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm         D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
F              =  56781.20000 mL/min     Uo (linear)    =      9.49831 cm/min
R              =    230.00000 microns    L/R            =  20813.47826
Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm       Time/BV        =     16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89317E+00
Dp  [cm2/min]  =  .23090E-03
Doo [cm2/min]  =  .69269E-03
kf  [cm/min]   =  .25099E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .23198E+00
Sc(i)          =  .11420E+04
Peb(i)         =  .16969E+04
Bi(i)          =  .38002E+02
Nf(i)          =  .75952E+03
Np(i)          =  .48243E+01
Pep(i)         =  .14381E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .25020E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97860E+00
Iso. Const. 4  =  .88740E+00
Iso. Const. 5  =  .11040E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5000E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1596E-01 poise and density to 1.211     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_11.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
```

```
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   5: Monitor conc. history at stream  2.  Filename = SO_11.h02
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   6: Monitor conc. history at stream  4.  Filename = SO_11.h03
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
   7: Monitor conc. history at stream  6.  Filename = SO_11.h04
      Output density adjustments:
      2.0    *default abs conc delta,      50.    *default rel conc delta,
      .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
 ================================================================================
 Conc. Carousel caused bed shift at t = .1606E+05 min
 Conc. Carousel caused bed shift at t = .2568E+05 min
 Conc. Carousel caused bed shift at t = .3544E+05 min
 Conc. Carousel caused bed shift at t = .4528E+05 min
 Conc. Carousel caused bed shift at t = .5515E+05 min
 Conc. Carousel caused bed shift at t = .6504E+05 min
 Conc. Carousel caused bed shift at t = .7495E+05 min
 Conc. Carousel caused bed shift at t = .8485E+05 min
 Conc. Carousel caused bed shift at t = .9476E+05 min
 Conc. Carousel caused bed shift at t = .1047E+06 min
 Conc. Carousel caused bed shift at t = .1146E+06 min
 VERSE-LC finished in  7337 steps.  Average step size 16.36     minutes
 End run:  22:08:53 on 05-04-2007
 Integrated Areas in History Files:
 SO_11.h01                  6.00000
 SO_11.h02                  3.18391
 SO_11.h03                  .146947E-03
 SO_11.h04                  .126966E-19
```

## D.28 Subsequent Operations SO_12

### D.28.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 45 C
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 56781.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.013232, 1.2034                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
2.7362d-4                         part-pore diffusivities(cm^2/min)
8.2087d-4                         Brownian diffusivities(cm^2/min)
0.2545                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9812                            Freundlich/Langmuir Hybrid Ma   (-)
0.8804                            Freundlich/Langmuir Hybrid Mb   (-)
1.445d-3                          Freundlich/Langmuir Hybrid beta (-)
```

### D.28.2 VERSE-LC Datafile.run

```
 ================================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ================================================================================
 Input file: SO_12
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 45 C
 Begin Run:  22:08:53 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min         dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm          D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
 F              =  56781.20000 mL/min      Uo (linear)    =      9.49831 cm/min
 R              =    230.00000 microns     L/R            =  20813.47826
```

```
Bed Void frac. =       .42000            Pcl. Porosity  =      .65790
Spec. Area     =     75.65217 1/cm       Time/BV        =    16.79984 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .89102E+00
Dp  [cm2/min]  =  .27362E-03
Doo [cm2/min]  =  .82087E-03
kf  [cm/min]   =  .28107E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .27815E+00
Sc(i)          =  .80370E+03
Peb(i)         =  .17010E+04
Bi(i)          =  .35912E+02
Nf(i)          =  .85054E+03
Np(i)          =  .57169E+01
Pep(i)         =  .12136E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .25450E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98120E+00
Iso. Const. 4  =  .88040E+00
Iso. Const. 5  =  .14450E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
==============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5000E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1323E-01 poise and density to 1.203     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_12.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = SO_12.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = SO_12.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = SO_12.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
==============================================================================
Conc. Carousel caused bed shift at t = .1255E+05 min
Conc. Carousel caused bed shift at t = .1996E+05 min
Conc. Carousel caused bed shift at t = .2752E+05 min
Conc. Carousel caused bed shift at t = .3513E+05 min
Conc. Carousel caused bed shift at t = .4279E+05 min
Conc. Carousel caused bed shift at t = .5044E+05 min
Conc. Carousel caused bed shift at t = .5812E+05 min
Conc. Carousel caused bed shift at t = .6580E+05 min
Conc. Carousel caused bed shift at t = .7349E+05 min
Conc. Carousel caused bed shift at t = .8117E+05 min
Conc. Carousel caused bed shift at t = .8885E+05 min
Conc. Carousel caused bed shift at t = .9655E+05 min
Conc. Carousel caused bed shift at t = .1042E+06 min
Conc. Carousel caused bed shift at t = .1119E+06 min
Conc. Carousel caused bed shift at t = .1196E+06 min
VERSE-LC finished in  7345 steps.  Average step size 16.34     minutes
End run:  22:14:26 on 05-04-2007
Integrated Areas in History Files:
SO_12.h01                 6.00000
SO_12.h02                 3.27362
SO_12.h03                 .155898E-03
SO_12.h04                 .103926E-19
```

## D.29 Subsequent Operations SO_13

### D.29.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 45 C, 20 gpm
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 75708.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
230.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.013232, 1.2034                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
```

```
0, 2.0, 50, 4.033d-4, 0.016           unit op#, ptscale(1-4) filtering
h                                     COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016           unit op#, ptscale(1-4) filtering
h                                     COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016           unit op#, ptscale(1-4) filtering
h                                     COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016           unit op#, ptscale(1-4) filtering
-                               end of commands
120000.0, 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
1.0                             size exclusion factor
2.7362d-4                       part-pore diffusivities(cm^2/min)
8.2087d-4                       Brownian diffusivities(cm^2/min)
0.2545                          Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                             Freundlich/Langmuir Hybrid b    (1/M)
0.9812                          Freundlich/Langmuir Hybrid Ma   (-)
0.8804                          Freundlich/Langmuir Hybrid Mb   (-)
1.445d-3                        Freundlich/Langmuir Hybrid beta (-)
```

## D.29.2 VERSE-LC Datafile.run

```
===============================================================================
VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
===============================================================================
Input file: SO_13
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 45 C, 20 gpm
Begin Run:  22:14:26 on 05-04-2007   running under Windows 95/8
Finite elements    - axial:150  particle: 1
Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
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)        = 120000.00000 min         dtheta max     =      1.00000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =    478.71000 cm          D              =    134.62000 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =6813677.17928 mL
F              =  75708.20000 mL/min      Uo (linear)    =     12.66440 cm/min
R              =    230.00000 microns     L/R            =  20813.47826
Bed Void frac. =       .42000             Pcl. Porosity  =       .65790
Spec. Area     =     75.65217 1/cm        Time/BV        =     12.59989 min
Vol CSTRs      =1892706.00000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .11830E+01
Dp  [cm2/min]  =  .27362E-03
Doo [cm2/min]  =  .82087E-03
kf  [cm/min]   =  .30936E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .37087E+00
Sc(i)          =  .80370E+03
Peb(i)         =  .17083E+04
Bi(i)          =  .39526E+02
Nf(i)          =  .70211E+03
Np(i)          =  .42876E+01
Pep(i)         =  .16181E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .25450E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .98120E+00
Iso. Const. 4  =  .88040E+00
Iso. Const. 5  =  .14450E-02
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5000E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1323E-01 poise and density to 1.203     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_13.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = SO_13.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = SO_13.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = SO_13.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
```

```
 Conc. Carousel caused bed shift at t = 8962.     min
 Conc. Carousel caused bed shift at t = .1444E+05 min
 Conc. Carousel caused bed shift at t = .2003E+05 min
 Conc. Carousel caused bed shift at t = .2570E+05 min
 Conc. Carousel caused bed shift at t = .3139E+05 min
 Conc. Carousel caused bed shift at t = .3712E+05 min
 Conc. Carousel caused bed shift at t = .4286E+05 min
 Conc. Carousel caused bed shift at t = .4862E+05 min
 Conc. Carousel caused bed shift at t = .5436E+05 min
 Conc. Carousel caused bed shift at t = .6012E+05 min
 Conc. Carousel caused bed shift at t = .6588E+05 min
 Conc. Carousel caused bed shift at t = .7164E+05 min
 Conc. Carousel caused bed shift at t = .7740E+05 min
 Conc. Carousel caused bed shift at t = .8316E+05 min
 Conc. Carousel caused bed shift at t = .8892E+05 min
 Conc. Carousel caused bed shift at t = .9468E+05 min
 Conc. Carousel caused bed shift at t = .1005E+06 min
 Conc. Carousel caused bed shift at t = .1062E+06 min
 Conc. Carousel caused bed shift at t = .1120E+06 min
 Conc. Carousel caused bed shift at t = .1177E+06 min
 VERSE-LC finished in  9876 steps.  Average step size 12.15     minutes
 End run:  22:23:57 on 05-04-2007
 Integrated Areas in History Files:
 SO_13.h01                  6.00000
 SO_13.h02                  2.57260
 SO_13.h03                  .196554E-03
 SO_13.h04                  .882546E-16
```

## D.30 Subsequent Operations SO_14

### D.30.1 VERSE-LC Datafile

```
RF 3-column carousel, single component Cs isotherm, Criterion: lag
LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 20 C, 380 um
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col
NNNNN                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
478.71, 134.62, 75708.2, 1892706. Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
190.0, 0.420, 0.6579, 0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentration (M)
S                                 COMMAND - conc step change
1, 0.0, 5.0000d-5, 1, 0.0         spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.019791, 1.2178                  fluid viscosity(poise), density(g/cm^3)
m                                       COMMAND - subcolumns
50, 100, 0, 1, 3.40d-8, 0.0, 1.0d+6     elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                       COMMAND - effluent history dump
0, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
2, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
4, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
h                                       COMMAND - effluent history dump
6, 2.0, 50, 4.033d-4, 0.016             unit op#, ptscale(1-4) filtering
-                                 end of commands
120000.0, 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
1.0                               size exclusion factor
1.9021d-4                         part-pore diffusivities(cm^2/min)
5.7062d-4                         Brownian diffusivities(cm^2/min)
0.2458                            Freundlich/Langmuir Hybrid a (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
0.9761                            Freundlich/Langmuir Hybrid Ma   (-)
0.8941                            Freundlich/Langmuir Hybrid Mb   (-)
8.174d-4                         Freundlich/Langmuir Hybrid beta (-)
```

### D.30.2 VERSE-LC Datafile.run

```
 ===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: SO_14
 RF 3-column carousel, single component Cs isotherm, Criterion: lag
 LAW feed: Subsequent Operation, CT: Nominal, Sensitivity: 20 C, 380 um
 Begin Run:  22:23:57 on 05-04-2007   running under Windows 95/8
 Finite elements    - axial:150  particle: 1
 Collocation points - axial:  4  particle: 6 => Number of eqns:  6028
 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)        = 120000.00000 min        dtheta max     =      1.00000 BV
 abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
 Total Length   =    478.71000 cm         D              =    134.62000 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.     =6813677.17928 mL
 F              =  75708.20000 mL/min     Uo (linear)    =     12.66440 cm/min
 R              =    190.00000 microns    L/R            =  25195.26316
 Bed Void frac. =       .42000            Pcl. Porosity  =       .65790
 Spec. Area     =     91.57895 1/cm       Time/BV        =     12.59989 min
 Vol CSTRs      =1892706.00000 mL

 Component no.  =      1
```

```
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .98516E+00
Dp  [cm2/min]  =  .19021E-03
Doo [cm2/min]  =  .57062E-03
kf  [cm/min]   =  .27574E+00
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .20729E+00
Sc(i)          =  .17088E+04
Peb(i)         =  .20513E+04
Bi(i)          =  .41866E+02
Nf(i)          =  .75755E+03
Np(i)          =  .43677E+01
Pep(i)         =  .19228E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .24580E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .97610E+00
Iso. Const. 4  =  .89410E+00
Iso. Const. 5  =  .81740E-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 .5000E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .1979E-01 poise and density to 1.218     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+07 min.
     When comp.  1 reaches .3400E-07 M     at end of node 100,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  0.  Filename = SO_14.h01
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  5: Monitor conc. history at stream  2.  Filename = SO_14.h02
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  6: Monitor conc. history at stream  4.  Filename = SO_14.h03
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
  7: Monitor conc. history at stream  6.  Filename = SO_14.h04
     Output density adjustments:
     2.0    *default abs conc delta,      50.    *default rel conc delta,
     .40E-03*default force w/ conc delta, .16E-01*default force w/o conc delta
===============================================================================
Conc. Carousel caused bed shift at t = .1603E+05 min
Conc. Carousel caused bed shift at t = .2560E+05 min
Conc. Carousel caused bed shift at t = .3532E+05 min
Conc. Carousel caused bed shift at t = .4506E+05 min
Conc. Carousel caused bed shift at t = .5483E+05 min
Conc. Carousel caused bed shift at t = .6461E+05 min
Conc. Carousel caused bed shift at t = .7438E+05 min
Conc. Carousel caused bed shift at t = .8416E+05 min
Conc. Carousel caused bed shift at t = .9394E+05 min
Conc. Carousel caused bed shift at t = .1037E+06 min
Conc. Carousel caused bed shift at t = .1135E+06 min
VERSE-LC finished in  9753 steps.  Average step size 12.30     minutes
End run:  22:30:35 on 05-04-2007
Integrated Areas in History Files:
SO_14.h01                 6.00000
SO_14.h02                 3.41819
SO_14.h03                 .135171E-03
SO_14.h04                 .655328E-21
```