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Ion Exchange Distribution Coefficient Tests and Computer Modeling at High Ionic Strength Supporting Technetium Removal Resin Maturation

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EXECUTIVE SUMMARY

The primary treatment of the tank waste at the DOE Hanford site will be done in the Waste Treatment and Immobilization Plant (WTP) that is currently under construction. The baseline plan for this facility is to treat the waste, splitting it into High Level Waste (HLW) and Low Activity Waste (LAW). Both waste streams are then separately vitrified as glass and poured into canisters for disposition. The LAW glass will be disposed onsite in the Integrated Disposal Facility (IDF). There are currently no plans to treat the waste to remove technetium, so its disposition path is the LAW glass. Due to the water solubility properties of pertechnetate and long half-life of ^{99}Tc, effective management of ^{99}Tc is important to the overall success of the Hanford River Protection Project mission. To achieve the full target WTP throughput, additional LAW immobilization capacity is needed, and options are being explored to immobilize the supplemental LAW portion of the tank waste. Removal of ^{99}Tc, followed by off-site disposal, would eliminate a key risk contributor for the IDF Performance Assessment (PA) for supplemental waste forms, and has potential to reduce treatment and disposal costs. Washington River Protection Solutions (WRPS) is developing some conceptual flow sheets for supplemental LAW treatment and disposal that could benefit from technetium removal. One of these flow-sheets will specifically examine removing ^{99}Tc from the LAW feed stream to supplemental immobilization. To enable an informed decision regarding the viability of technetium removal, further maturation of available technologies is being performed.

This report contains results of experimental ion exchange distribution coefficient testing and computer modeling using the resin SuperLig® 639[a] to selectively remove perrhenate from high ionic strength simulated LAW. It is advantageous to operate at higher concentration in order to treat the waste stream without dilution and to minimize the volume of the final wasteform. This work examined the impact of high ionic strength, high density, and high viscosity if higher concentration LAW feed solution is used. Perrhenate (ReO_4^-) has been shown to be a good non-radioactive surrogate for pertechnetate in laboratory testing for this ion exchange resin, and the performance bias is well established. Equilibrium contact testing with 7.8 M [Na^+] average simulant concentrations indicated that the SuperLig® 639 resin average perrhenate distribution coefficient was 368 mL/g at a 100:1 phase ratio. Although this indicates good performance at high ionic strength, an equilibrium test cannot examine the impact of liquid viscosity, which impacts the diffusivity of ions and therefore the loading kinetics. To get an understanding of the effect of diffusivity, modeling was performed, which will be followed up with column tests in the future.

The table below summarizes the modeled performance for a full-size 3-column carousel using 7.8 M HTWOS Average LAW composition. The parameters of the column geometry and flow rates are identical to those used in previous work. The use of 7.8 M [Na^+] solution instead of 5.0 M [Na^+] has a dramatic impact on performance. The breakthrough is approximately 40% earlier at 25 °C, and is ~80% earlier at 45 °C. The primary cause of the decrease is the large increase in viscosity, which impacts diffusivity. These results indicate that it would be possible to run a full scale system at 25 °C, since the loading cycle time would be about 36 hours, and displacement, rinsing, and elution takes about 22 hours. It also indicates that it is not practical to run a full scale system at 45 °C with 7.8 M [Na^+] solution. At 25 °C, although the loading cycle times are shorter, and it will generate ~40% more eluate per unit volume of waste processed, that is almost mostly offset by getting more "waste" through the columns (i.e., same quantity of salt but in less

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[a] SuperLig is a trademark of IBC Advanced Technologies, Inc., American Fork, UT

volume). Overall, the model predicts that the quantity of eluate generated would be only about 10% more per mole of waste sodium processed by operating at 7.8 M [Na^+] instead of 5.0 M.

Temperature (°C)	**Simulant HTWOS Avg Na^+ [M]**	**# Bed Volumes Processed (-)**	**Processed Volume (kgal)**	**Waste Na^+ processed (moles)**
25	**5.0**	207.6	75.2	1.42E6
	7.8	120.1	43.5	1.28E6
45	**5.0**	103.4	37.4	7.07E5
	7.8	20.9	7.6	2.2E5

To reasonably achieve a DF of 100, the system would need to incorporate three ion exchange columns in series. Using two columns would require too short of a loading cycle time to be practical. If future engineering estimates conclude that this system is not adequate, other options to improve performance would be to reduce the resin particle size (although this would impact pressure drop), and/or decrease flow rate.

Testing is planned to confirm the modeling results on this high density liquid. This testing will also examine the resin bed packing, which cannot be predicted from modeling. If the bed does not pack tightly, the liquid will channel and cause early breakthrough of Tc, yielding poor decontamination.

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LIST OF ABBREVIATIONS

ASTM	American Society of Testing and Materials
BV	Bed Volumes
°C	Celsius
C	Concentration
DI	Deionized
DOE	U.S. Department of Energy
DST	Double Shell Tank
F	resin dry weight correction Factor
g	Gram
HLW	High Level Waste
hr	Hour
HTWOS	Hanford Tank Waste Operations Simulator
ICP-ES	Inductively Coupled Plasma Emission Spectroscopy
ICP-MS	Inductively Coupled Plasma Mass Spectroscopy
ID	Internal Diameter
IDF	Integrated Disposal Facility
IX	Ion Exchange
K_d	Distribution Coefficient
L	Liter
LAW	Low Activity Waste
M	Molarity
m	meter
mg	milligram
min	minute
mL	milliliter
PA	Performance Assessment
SRNL	Savannah River National Laboratory
SST	Single Shell Tank
V	Volume of liquid (mL)
WRPS	Washington River Protection Solutions
WTP	Waste Treatment and Immobilization Plant

1.0 Introduction

Savannah River National Laboratory (SRNL) is performing studies on behalf of WRPS to support the disposition of tank waste at the DOE Hanford site near Richland, Washington. The primary treatment of the tank waste will be done in the WTP that is currently under construction. The baseline plan for this facility is to treat the waste, splitting it into HLW and LAW. Both waste streams are then separately vitrified as glass and sealed in canisters. The LAW glass is the principal disposition path for the soluble ^{99}Tc, and it will be disposed onsite in the IDF. Because ^{99}Tc has a very long half-life (211,000 years) and is highly mobile [Icenhower, 2008, 2010], it has potential to be a major dose contributor to the PA of the IDF [Mann, 2003], although it is largely retained in the glass wasteform matrix. Due to the water solubility properties of pertechnetate, and the potential for impact to the PA, effective management of ^{99}Tc is important to the overall success of the River Protection Project mission. Options for waste form are being explored to immobilize the LAW portion of the tank waste, as well as to examine the volatility of technetium during the vitrification process. Removal of ^{99}Tc, followed by off-site disposal of technetium from the supplemental LAW flow sheet, would eliminate a key risk contributor for the IDF PA for supplemental waste forms, and has potential to reduce treatment and disposal costs. WRPS is developing some conceptual flow sheets for supplemental LAW treatment and disposal that could benefit from technetium removal. One of these flow-sheets will specifically examine removing ^{99}Tc from the LAW feed stream to supplemental immobilization. To enable an informed decision regarding the viability of technetium removal, further maturation of available technologies is being performed.

Technetium in the tank waste is predominantly found in the tank supernate as pertechnetate (TcO_4^-), although there is also a soluble non-pertechnetate, and some insoluble technetium, which is presumably Tc(IV) oxide. Technology development for ^{99}Tc removal has focused on pertechnetate separations. No methods have been identified that can remove the soluble non-pertechnetate specie(s) unless first destroyed and converted to pertechnetate. The insoluble technetium oxide can be removed by filtration.

This report contains results of experimental ion exchange distribution coefficient testing using the resin SuperLig® 639 to selectively remove perrhenate from simulated supplemental LAW and computer modeling prediction of the ion exchange column performance. SuperLig® 639 is an elutable ion exchange resin available from a vendor. This document summarizes the testing performed to further mature the technical readiness of SuperLig® 639 for treatment of LAW at Hanford, and operation at elevated temperature. The WTP baseline flow-sheet condition for supplemental LAW feed that exits the pretreatment facility is at 7.8 M [Na^+] and is at 45˚C. Removal of pertechnetate from tank waste samples using SuperLig®639 has been demonstrated many times [McCabe, 2013], but the current tests examine removal using new batches of resin and a substantially more concentrated tank waste composition that represents the entire tank waste inventory. The new batches of resin were produced to meet a specification defined as part of this program and manufactured by the vendor [Bruening, 2013]. The simulant formulation was derived from a computer model of the WTP LAW composition that accounts for the tank retrieval schedule, internal recycle streams, and composition changes due to pretreatment processing, and mathematical averaging. This composition (Table 1-1) was based on Hanford Tank Waste Operations Simulator (HTWOS) model, and adjusted to create an entirely soluble aqueous simulant [Russell, PNNL-22352, 2013]. Chromate was left out of the formulation because it is a minor component that is not needed for effective prediction of performance, and would have made the simulant characteristically hazardous for chromium. Although the formulation shown below indicates the average is 0.05 M [K^+], this was not the amount actually added in the simulant preparation. Only 0.02 M [K^+] was used in the initial formulation so that it could be spiked in at higher concentrations to examine its impact. Since potassium nitrate was used for the spike, a small increase in nitrate also accompanied its addition, but this is insignificant compared to the total nitrate in the simulant. In the current tests, perrhenate (ReO_4^-) is used as a non-radioactive substitute for pertechnetate. This has been shown to be a good substitute, once adjusted for the measured bias in performance [Hamm, 2013]. Actual analytical measurements of the simulant components are in Attachment A.

Table 1-1. HTWOS Average 7.8 M Simulant Target Molar Composition

Ion	**Molarity (M)**
NO_3^-	2.53
OH^-	2.43
SO_4^{-2}	0.13
$Al(OH)_4^-$	0.48
NO_2^-	0.88
CO_3^{-2}	0.43
K^+	0.051
Acetate	0.060
F^-	0.049
PO_4^{-3}	0.076
Cl^-	0.066
ReO_4^-	5.23E-05
Total [Na+]	7.8

The test matrix used is shown below:

Table 1-2. Resin batch contact test matrix

T (°C)	Simulant	[K] (M)	[Re] (M)	Resin batch
25	average	0.05	5.2E-05	May, 2013
35	average	0.05	5.2E-05	May, 2013
45	average	0.05	5.2E-05	May, 2013
25	K modified	0.02	5.2E-05	May, 2013
25	K modified	0.15	5.2E-05	May, 2013
25	K modified	0.25	5.2E-05	May, 2013
25	K modified	0.25	5.2E-05	July, 2013
25	average	0.05	1.5E-04	July, 2013
25	1st recontact	0.05	NA	May, 2013
25	2nd recontact	0.05	NA	May, 2013

2.0 Experimental Procedure

2.1 Ion Exchange Resin

The resin for batch contacts and in the ion exchange columns was SuperLig® 639 resin from lot # 130611SS2-56, manufactured by IBC Advanced Technologies, Inc., in American Fork, Utah in May, 2013 [Bruening, 2013]. Additional tests were also performed using the second batch of resin from lot # 130718SS2-60 manufactured in July, 2013. The resin lots were stored as received (dry) at room temperature in a laboratory since receipt. No preconditioning of the resin was performed.

2.2 Simulant Feed Composition

HTWOS 7.8M Average [Na^+] Mass Based Simulant aliquots were spiked with various amounts of potassium nitrate and sodium perrhenate to test the impact on loading. Perrhenate was adjusted by adding 0.04 M sodium perrhenate solution to simulant. Typical additions were 25, 50, or 75 microliters to a 20 mL sample. Solid potassium nitrate was added to boost the initial 0.02 M potassium concentration in the simulant to 0.05, 0.15, or 0.25 M as needed. Detailed simulant information can be found in Appendix A. Detailed analytical analysis results can also be found in Electronic Laboratory Notebook T7692-00085 experiment 02. Analysis of the simulant was performed to confirm the composition (Appendix A).

2.3 Batch Contact Tests

The Distribution Coefficient (K_d) batch contacts were performed by weighing out approximately 0.20 g of resin in a poly bottle, then adding approximately 20 mL of the simulant as measured by weight. Solution weight was converted to volume using a solution density of 1.322 g/mL +/- 0.6% RSD. Solution density had been measured in triplicate for the average simulant. The bottles were agitated in a shaker oven at 25, 35, or 45 °C +/- 1 °C for 48 hours. At the end of shaking, the samples were filtered to remove the resin. Liquid filtrates were analyzed for Re concentration by Inductively Coupled Plasma Emission Spectroscopy (ICP-ES) or Inductively Coupled Plasma Mass Spectroscopy (ICP-MS). Initial simulant samples that had not been contacted with resin were also analyzed.

The F-factor (moisture content) of this resin batch was reported as <0.2 wt % in the acceptance report, so mass contributions from adsorbed water were ignored in the calculations.

2.4 Quality Assurance

Requirements for performing reviews of technical reports and the extent of review are established in manual E7 2.60. SRNL documents the extent and type of review in WSRC-IM-2002-00011, Rev. 2. Completion of this work fulfills the requirements of Distribution Coefficient measurements and modeling described in Task 3.9 of the Task Technical and Quality Assurance Plan for Technetium Ion Exchange Resin Manufacturing Maturation, SRNL-RP-2012-00708, Revision 3. (IEWO M0SRV00074 Revision 9, Deliverable 12).

3.0 Results and Discussion

3.1 Batch Contacts

Batch contacts were performed with fresh subsamples of the same batch of resin as the column tests. Initial conditions and results for the Re batch contacts are shown in Tables 3-1 through 3-8. Equation 1 provides distribution coefficients:

$$K_d = [(C_0/C_f)-1][V/(M*F)] \quad \text{(Eqn. 1)}$$

where

C_0 = initial concentration
C_f = final concentration
V = Volume of liquid (mL)
M = mass of resin (g)
F = resin dry weight correction factor (F = 1 due to <0.2 wt% moisture as measured by vendor)

Most tests involved the May 2013 IBC resin lot #130611SS2-56. NOTE that rows with blue shading are batch contacts with the second resin (July 2013, IBC Lot #130718SS2-60).

Potassium and initial rhenium concentrations were often calculated using known weights of added reagents and known weights of simulant (converted to volume with the average density above). Tables 3-2 and 3-4 have measured potassium concentrations displayed. Because the product liquid from the first test was used as the starting liquid for the subsequent test, the initial rhenium concentrations for Table 3-3 are the measured values from the product liquid from the prior test because of the sequential nature of that test.

Tables 3-1 to 3-4 provide the batch test conditions and data taken at 25 °C. Tests 5, 6, 9, and 10 below used resin beads from the second of the IBC resin batches. The K_d values were relatively high because perrhenate sorption by the resin is favored by lower temperature. In addition, this set shows significantly better performance for the IBC July 2013 resin batch (lot 130718SS2-60) compared with the May lot (#130611SS2-56). The magnitude of resin lot-to-lot variability is important information, though the May lot performance is in line with past work and is acceptable.

Table 3-1. Batch Contact Initial Conditions at 25 °C

Test	Solution Volume, mL	Resin Mass, g	Phase Ratio, mL/g	Initial Re, mg/L
1 – 25C	20.10	0.2013	99.8	9.24
2 – 25C	19.25	0.2028	94.9	9.24
3 – 25C	22.44	0.2018	111.	8.48
4 – 25C	22.51	0.2018	111.	8.50
5 – 25C	20.08	0.2020	99.4	9.99
6 – 25C	20.08	0.2000	100.4	9.99
7 – 25C	20.10	0.2018	99.6	9.25
8 – 25C	20.13	0.2017	99.8	9.25
9 – 25C	20.09	0.1981	101.	26.52
10 – 25C	14.88	0.1518	98.0	26.52

Table 3-2. Batch Contact Results at 25 °C:

Test	Potassium, M	NO_3^-, M	Final Re, mg/L	Loading, mmol/g	Batch Kd, mL/g
1 – 25C	0.021	2.53	2.80	3.45E-03	229.1
2 – 25C	0.020	2.53	2.74	3.31E-03	224.8
3 – 25C	0.174	2.66	2.63	3.49E-03	247.1
4 – 25C	0.173	2.66	2.65	3.50E-03	246.4
5 – 25C	0.265	2.76	2.21	4.15E-03	349.7
6 – 25C	0.266	2.76	2.25	4.17E-03	346.0
7 – 25C	0.266	2.76	2.65	3.53E-03	247.4
8 – 25C	0.267	2.76	2.65	3.54E-03	248.9
9 – 25C	0.049	2.56	5.67	1.14E-02	373.4
10 – 25C	0.048	2.56	5.63	1.10E-02	363.5

Tables 3-3 and 3-4 are initial conditions and results from a sequential set of batch contacts. Liquid from Recontact1 was both sampled for analyses and used as the initial solution for Recontact2, where it was mixed with fresh resin. Likewise, the end point solution from batch Recontact2 was the starting point for Recontact3 with another sample of fresh resin. Note that the initial Re concentration in this series was 9.30 mg/L, then final concentrations were initial concentrations for the next batch as shown.

Table 3-3. Recontact Batch Contact Initial Conditions at 25 °C

Test	Solution Volume, mL	Resin Mass, g	Phase Ratio, mL/g	Initial Re, mg/L
Recontact1	50.43	0.5013	100.6	9.30
Recontact2	41.36	0.4111	100.6	2.86
Recontact3	30.48	0.3028	100.6	0.93

Table 3-4. Recontact Batch Contact Results at 25 °C:

Test	Potassium, M	NO_3^-, M	Final Re, mg/L	Loading, mmol/g	Batch Kd, mL/g
Recontact1	0.049	2.56	2.86	3.48E-03	226.5
Recontact2	0.049	2.56	0.93	1.04E-03	208.8
Recontact3	0.049	2.56	0.26	3.61E-04	256.7

Tables 3-5 and 3-6 provide the conditions and results for 35 °C batch contacts. Loadings are lower relative to testing at 25 °C. In this dataset, only test 10 used the IBC July 2013 lot resin. The better performance of the test 10 resin is apparent relative to the May resin batch by comparing the results to test 5 within the two tables. Initial Re concentration was varied at each potassium concentration for better definition of the isotherm.

Table 3-5. Batch Contact Initial Conditions at 35 °C

Test	Solution Volume, mL	Resin Mass, g	Phase Ratio, mL/g	Initial Re, mg/L
1 – 35C	20.38	0.2002	101.8	9.31
2 – 35C	20.01	0.1994	100.4	18.6
3 – 35C	20.01	0.1998	100.1	27.9
4 – 35C	20.02	0.2010	99.6	9.31
5 – 35C	20.04	0.2006	99.9	18.6
6 – 35C	20.02	0.1996	100.3	27.9
7 – 35C	20.09	0.1993	100.8	9.31
8 – 35C	20.15	0.1999	100.8	18.6
9 – 35C	20.09	0.2002	100.3	27.9
10 – 35C	20.04	0.2003	100.0	18.6

Table 3-6. Batch Contact Results at 35 °C:

Test	Potassium, M	NO_3^-, M	Final Re, mg/L	Loading, mmol/g	Batch Kd, mL/g
1 – 35C	0.02	2.53	3.81	3.01E-03	146.8
2 – 35C	0.02	2.53	7.34	6.08E-03	154.2
3 – 35C	0.02	2.53	11.2	9.01E-03	150.0
4 – 35C	0.15	2.66	3.86	2.92E-03	140.7
5 – 35C	0.15	2.66	7.16	6.15E-03	160.0
6 – 35C	0.15	2.66	10.6	9.31E-03	163.0
7 – 35C	0.25	2.76	3.77	3.00E-03	148.5
8 – 35C	0.25	2.76	7.10	6.24E-03	163.7
9 – 35C	0.25	2.76	10.7	9.29E-03	161.8
10 – 35C	0.15	2.66	5.69	6.94E-03	227.1

Tables 3-7 and 3-8 provide conditions and results at 45 °C. Performance is in the lowest for this set, though the IBC July 2013 lot of resin again shows a better ability to remove perrhenate (i.e, compare test 10 to 12 and test 11 to 9). Some samples were mixed for up to 72 hours to confirm that sorption was at equilibrium.

Table 3-7. Batch Contact Initial Conditions at 45 °C

Test	Solution Volume, mL	Resin Mass, g	Phase Ratio, mL/g	Initial Re, mg/L
1 – 45C	20.03	0.1999	100.2	9.15
2 – 45C	19.97	0.2008	99.5	18.3
3 – 45C	20.01	0.2008	99.7	27.5
4 – 45C	20.03	0.2007	99.8	9.15
5 – 45C	19.99	0.2009	99.5	18.3
6 – 45C	19.98	0.1996	100.1	27.5
7 – 45C	20.02	0.1997	100.3	9.15
8 – 45C	20.31	0.2003	101.4	18.3
9 – 45C	19.98	0.2002	99.9	27.5
10 – 45C	19.90	0.2007	99.5	18.3
11 – 45C	19.94	0.1997	99.7	27.5
12 – 45C*	19.98	0.2005	99.4	18.3
13 – 45C*	20.01	0.1995	100.2	9.15

*These were agitated for 72 hours for equilibrium verification

Table 3-8. Batch Contact Results at 45 °C:

Test	Potassium, M	NO_3^-, M	Final Re, mg/L	Loading, mmol/g	Batch Kd, mL/g
1 – 45C	0.019	2.53	6.53	1.41E-03	40.3
2 – 45C	0.02	2.53	12.3	3.21E-03	48.5
3 – 45C	0.02	2.53	18.0	5.08E-03	52.7
4 – 45C	0.143	2.66	6.54	1.40E-03	39.9
5 – 45C	0.143	2.66	12.5	3.13E-03	46.7
6 – 45C	0.138	2.66	17.9	5.14E-03	53.4
7 – 45C	0.232	2.76	6.52	1.42E-03	40.5
8 – 45C	0.232	2.76	11.9	3.48E-03	54.5
9 – 45C	0.262	2.76	18.8	4.64E-03	46.0
10 – 45C	0.139	2.66	9.84	4.53E-03	85.7
11 – 45C	0.258	2.76	14.4	6.98E-03	90.3
12 – 45C*	0.141	2.66	12.6	3.04E-03	45.0
13 – 45C*	0.232	2.76	6.31	1.53E-03	45.1

*These were agitated for 72 hours for equilibrium verification

The viscosity of the simulant was measured on another batch of simulant, and results are shown in Table 3-9, below.

Table 3-9 Density and Viscosity Measurement Results of Filtered 7.8 M Average Salt Solution Simulant

Parameter (units)	Temperature (°C)	Result	Std. Deviation
Density (g/cm^3)	25	1.348	0*
Viscosity (cP)	25	6.1	0
Viscosity (cP)	45	3.5	0

*standard deviation of zero indicates that the duplicate analysis results were identical

4.0 Conclusions

Although the resin floats in the solution, the agitation of the bottles ensured that the resin and liquid were in good contact. The replicate tests were generally very similar to each other, indicating good reproducibility.

The new batches of SuperLig® 639 exhibited good performance. The May 2013 batch was in line with prior batches, and the July 2013 batch exhibited improved performance. Both batches meet the performance criteria, and are consistent with prior observations [Nash, 2013; Bruening, 2013].

Distribution coefficient results with the high ionic strength LAW simulant were in the range of prior testing using 5.0 M [Na^+] simulants. Direct comparison to the 5.0 M [Na^+] simulant requires consideration of the initial and final Re concentration, i.e., the isotherms must be compared. This is explained in the Appendix. The loading of Re on the resin is slightly lower at 7.8 M [Na^+] compared to 5.0 M [Na^+].

The results in Appendix C indicate that the breakthrough profile is nearly linear, unlike prior test results that showed a more “S” shaped profile. This is due to the high viscosity of the liquid, which results in low diffusivity of the ions, slowing their transport for absorption onto the active sites in the resin pores. To achieve a good decontamination factor while minimizing eluate generation and maximizing cycle times, using three columns in series is recommended. Furthermore, operation at 25 °C is recommended to avoid early breakthrough of Tc. If these conditions are not feasible, other options could be pursued, such as using smaller particle size resin (although this would increase the pressure drop in the columns). Conversely, building larger columns and then slowing the flow rate may also be an option, although neither of these options has been tested or modeled.

5.0 Path Forward

Although this testing comprehensively examined the resin equilibrium performance, it is not possible to examine kinetics or resin bed packing issues. These parameters can best be studied using ion exchange columns. Planned testing will examine the performance of 7.8 M [Na^+] simulant in columns and allow comparison to the modeling results.

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Appendix A. Simulant Formulation

Attachment A – 7.8 M Sodium Simulant Analyses

Analyses of the simulant used for all work in this memo report are reported here. The target molarities are for the base simulant before further adjustments (potassium and perrhenate additions). The target potassium concentration, 0.02 M, is the minimum value. Higher potassium concentrations were reached using solid potassium nitrate. Perrhenate was added using a 0.04 M solution of sodium perrhenate with microliter pipettes.

Analyte	**Target, M**	**Average, M***	**Comments**
Sodium	7.8	7.63 +/- 2%	Average of 26 ICPES measurements
Potassium	0.02	0.02 +/- 3%	Average of 5 ICPES measurements
Aluminum	0.48	0.495 +/- 3%	Average of 22 ICPES measurements
NO_3^-	2.53	2.60 +/- 2%	Average of 3 IC Anions measurements
SO_4^{-2}	0.13	0.102 +/- 2%	Average of 3 IC Anions measurements
NO_2^-	0.88	0.903 +/- 1%	Average of 3 IC Anions measurements
F^-	0.049	0.029 +/- 2%	Average of 3 IC Anions measurements
PO_4^{-3}	0.076	0.014 +/- 7%	Average of 3 IC Anions measurements
Cl^-	0.066	0.068 +/- 1%	Average of 3 IC Anions measurements

*Uncertainties are relative standard deviations from the data (precision). Stated analytical accuracies are 10%.

Appendix B – Resin Batch Assessment

The experimental batch contact testing provided in this report focused on the behavior of a more recent batch of resin provided by IBC (i.e., a May 2013 batch with lot #130611552-56). Earlier isotherm model development (Hamm et al., 2013 and Nash et al., 2013) included all prior resin batch data within its assessment. In this appendix, the isotherm model (i.e., limited to only the algebraic model) is reexamined and updated to reflect this more recent 2014 database. In the most recent version of CERMOD (Hamm et al., 2013) the temperature dependence for TcO_4^- absorption was not addressed and was limited to approximately 20˚C to 25˚C operation. Both CERMOD and the algebraic isotherm models now include temperature dependence over the range of most interest (i.e., 25˚C to 45˚C).

Analytic Isotherm Model

From the previous modeling report (Hamm et al., 2013), the analytic isotherm is

$$Q_x = \frac{Q_T c_x}{c_x + \beta} , \qquad \text{(B-1)}$$

where

Q_T - Total available solid-phase loading sites on resin (mmole of sites per gram resin)

Q_x - Solid-phase loading of species x onto resin

c_x - Liquid-phase concentration of species x in solution

β - Beta factor representing the composite impact associated with enhancers and competitors

x - Shorthand notation for species of interest (i.e., ReO_4^- or TcO_4^-)

The estimated beta parameter is expressed as

$$\beta = \frac{1 + (K_{no}c_n + K_{ko}c_k)c_o + (K_{np}c_n + K_{kp}c_k)c_p}{\eta\left[K_{nx}c_n + K_{kx}c_k\right]} . \qquad \text{(B-2)}$$

Note that η represents the Re versus Tc “surrogate” factor:

$$\eta = \begin{bmatrix} 1.980 = 1/0.505 & \text{for} & \text{Tc} \\ 1.000 & \text{for} & \text{Re} \end{bmatrix} .$$

where

η - A “surrogate” factor representing the chemical differences between Re versus Tc

n, k, o, p - Shorthand notation for Na^+, K^+, NO_3^-, and NO_2^-

K_{ij} - Thermodynamic equilibrium coefficient in mass action equation for species i and j

For convenience within this report the surrogate factor has been redefined as the reciprocal of the factor listed in Hamm et al., 2013.

Within Nash et al. (2013) a total capacity value for the newer resin batch provided by IBC within the range of waste compositions of interest was established. The total capacity of this resin was set to

$$Q_T = 0.6518 \ \ (\text{mmole/g}_{\text{resin}}) \quad . \tag{B-3}$$

For column performance assessments using the VERSE-LC code the total capacity is placed on a per bed volume, rather than on a per resin mass, basis where the VERSE-LC inputted isotherm becomes

$$Q_{XO4} = \frac{\rho_{bed} Q_T c_{XO4}}{c_{XO4} + \beta} = \frac{a \cdot c_{XO4}}{c_{XO4} + \beta} \quad , \tag{B-4}$$

where

$$a = \rho_{bed} Q_T \quad . \tag{B-5}$$

In Eq. (B-3)

ρ_{bed} - Bed density defined as the total resin mass in bed per total volume of bed

a - VERSE parameter representing the total available sites in bed per total volume of bed

For this particular resin batch (IBC Lot #130611552-56) the expected bed density is set to

$$\rho_{bed} = 0.4498 \ \ (\text{g}_{\text{resin}}/\text{ml}_{\text{bed}}) \quad . \tag{B-6}$$

This results in the “a” coefficient employed in VERSE-LC of

$$a = \rho_{bed} Q_T = 0.29318 \, (\text{mmole}_{\text{resin}}/\text{ml}_{\text{bed}}) \quad . \tag{B-7}$$

To accommodate temperature effects the van’t Hoff expression is employed as

$$K_i(T) = K_i^o \exp\left\{ \frac{\Delta H_i^o}{R} \left[\frac{1}{T} - \frac{1}{T_o} \right] \right\} \quad , \tag{B-8}$$

where

K_i - Thermodynamic equilibrium coefficient for a specific species at temperature T

K_i^o - Thermodynamic equilibrium coefficient for a specific species at the reference temperature

T_o - Absolute temperature at the reference state (here set to 25 ˚C)

ΔH_i^o - Heat of absorption for the ith mass action equation at a specific reference state

R - Universal gas constant

In Nash et al. (2013) three batch contact tests were performed at 25 ˚C using the chosen resin (i.e., lot #130611552-56). These batch contact tests were performed using a 5 M sodium HTWOS Avg simulant. Within this report the more concentrated 7.8 M sodium HTWOS Avg simulant was tested along with the same resin batch. Here three separate temperatures (i.e., 25 ˚C, 35 ˚C, and 45 ˚C) were studied where all testing was based on the anion ReO_4^-. A brief summary of these batch contact test results are provided in Tables B-1, B-2, and B-3.

Table B-1. ReO_4^- batch contact results for resin lot #130611552-56 at 25 ˚C.

[Na] [M]	[K] [M]	[NO$_3$] [M]	[NO$_2$] [M]	[OH] [M]	[Re] [M]	Q (mmol/g)	NO$_3$/Re (-)
7.8	0.021	2.53	0.88	2.43	1.506E-05	3.45E-03	1.680E+05
	0.02	2.53	0.88	2.43	1.473E-05	3.31E-03	1.717E+05
	0.174	2.66	0.88	2.43	1.414E-05	3.49E-03	1.882E+05
	0.173	2.66	0.88	2.43	1.423E-05	3.51E-03	1.869E+05
	0.266	2.76	0.88	2.43	1.425E-05	3.53E-03	1.937E+05
	0.267	2.76	0.88	2.43	1.421E-05	3.54E-03	1.942E+05
	0.049	2.56	0.88	2.43	1.536E-05	3.48E-03	1.667E+05
5.0	0.0328	1.60	0.565	1.611	8.002E-06	2.371E-03	2.000E+05
					8.217E-06	2.346E-03	1.947E+05
					8.109E-06	2.358E-03	1.973E+05

Table B-2. ReO_4^- batch contact results for resin lot #130611552-56 at 35 ˚C.

[Na] [M]	[K] [M]	[NO$_3$] [M]	[NO$_2$] [M]	[OH] [M]	[Re] [M]	Q (mmol/g)	NO$_3$/Re (-)
7.8	0.02	2.53	0.88	2.43	2.048E-05	3.01E-03	1.236E+05
					3.942E-05	6.08E-03	6.417E+04
					6.004E-05	9.01E-03	4.214E+04
	0.15	2.66	0.88	2.43	2.073E-05	2.92E-03	1.283E+05
					3.844E-05	6.15E-03	6.920E+04
					5.714E-05	9.31E-03	4.655E+04
	0.25	2.76	0.88	2.43	2.022E-05	3.00E-03	1.365E+05
					3.812E-05	6.24E-03	7.241E+04
					5.741E-05	9.29E-03	4.808E+04

Table B-3. ReO_4^- batch contact results for resin lot #130611552-56 at 45 ˚C.

[Na] [M]	[K] [M]	[NO$_3$] [M]	[NO$_2$] [M]	[OH] [M]	[Re] [M]	Q (mmol/g)	NO$_3$/Re (-)
7.8	0.019	2.53	0.88	2.43	3.504E-05	1.41E-03	7.220E+04
	0.02				6.606E-05	3.21E-03	3.830E+04
	0.02				9.640E-05	5.08E-03	2.625E+04
	0.143	2.66	0.88	2.43	3.510E-05	1.40E-03	7.579E+04
	0.143				6.686E-05	3.13E-03	3.978E+04
	0.138				9.613E-05	5.13E-03	2.767E+04
	0.232	2.76	0.88	2.43	3.499E-05	1.42E-03	7.888E+04
	0.232				6.391E-05	3.48E-03	4.319E+04
	0.262				1.010E-04	4.64E-03	2.734E+04

The algebraic isotherm model [Eq. (B-1)], along with the expression for the beta parameter [Eq. (B-2)], and the equilibrium coefficient temperature dependences [Eq. (B-8)], were fitted to the data provided in Tables B-1, B-2 and B-3 above. To ensure that the new algebraic isotherm model yields very similar results as those employed in Nash et al. (2013), the fitting process was weighted heavily (i.e., a factor of ten) towards the 5 M data listed in Table B-1. Other weighting schemes were tested and indicated that the final fitted parameters were very similar in value.

A comparison of the algebraic isotherm model versus the above database is shown in Figure B-1. As expected, the isotherm model falls through the 25 ˚C data taken by Nash et al. (2013) using a 5 M sodium HTWOS Avg simulant (i.e., forced by weighting scheme chosen and labeled "B5 (25 C) data"). Isotherm curves for each set of batch contact tests are provided (i.e., five sets at 25 ˚C, three sets at 35 ˚C, and three sets at 45 ˚C). Details on each set of batch contact tests can be found in either this report or in Nash et al. (2013).

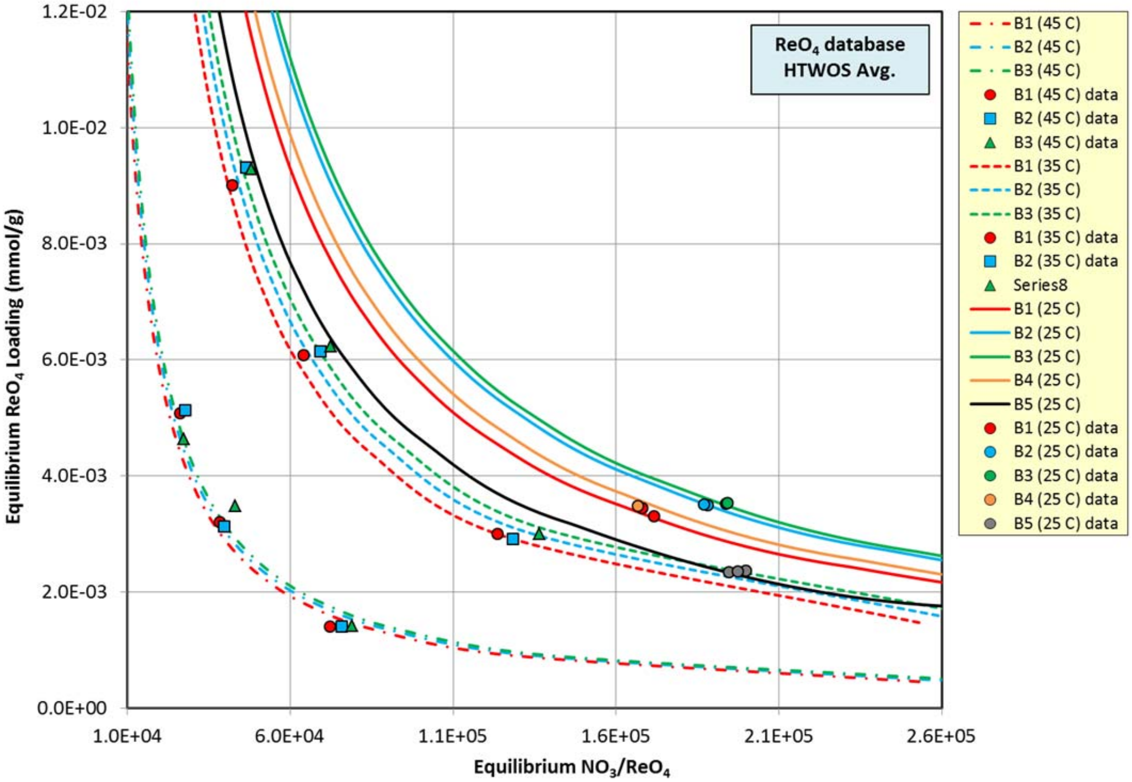

Figure B-1. Comparison of analytic isotherm model to the Re batch contact data at 25˚C, 35˚C, and 45˚C.

The fitting process employed yielded the reference state thermodynamic equilibrium constants and heats of absorption for the six mass actions of interest as listed in Table B-4.

Table B-4. Reference state thermodynamic equilibrium constants and heats of absorption.

Mass Action Eq.	K^o (-)	ΔH^o (kcal/K-gmol)
Na-ReO$_4$	130	-25
K-ReO$_4$	16,190	-100
Na-NO$_3$	0.11	-50
K-NO$_3$	14.5	-180
Na-NO$_2$	0	0
K-NO$_2$	0	0

From the original fitting process, it was observed that NO_2^- played a very minor role as a potential competitor and was omitted from the subsequent fitting process. All of the heats of absorption are negative, indicating that each mass action is an exothermic process, as expected.

Algebraic Isotherm Predictions

For the SRNL 7.8 M sodium HTWOS Avg simulant and the IBC May batch of SuperLig® 639 resin, predicted isotherms for ReO_4^- at 25˚C and for TcO_4^- at temperatures of 25˚C and 45˚C, were computed and are shown in Figure B-2. For comparison, the ReO_4^- isotherm at 25˚C for the 5 M sodium HTWOS Avg simulant is also provided. Also shown in Figure B-2 are the Re data at 25 ˚C for both the 5 M and 7.8 M simulants.

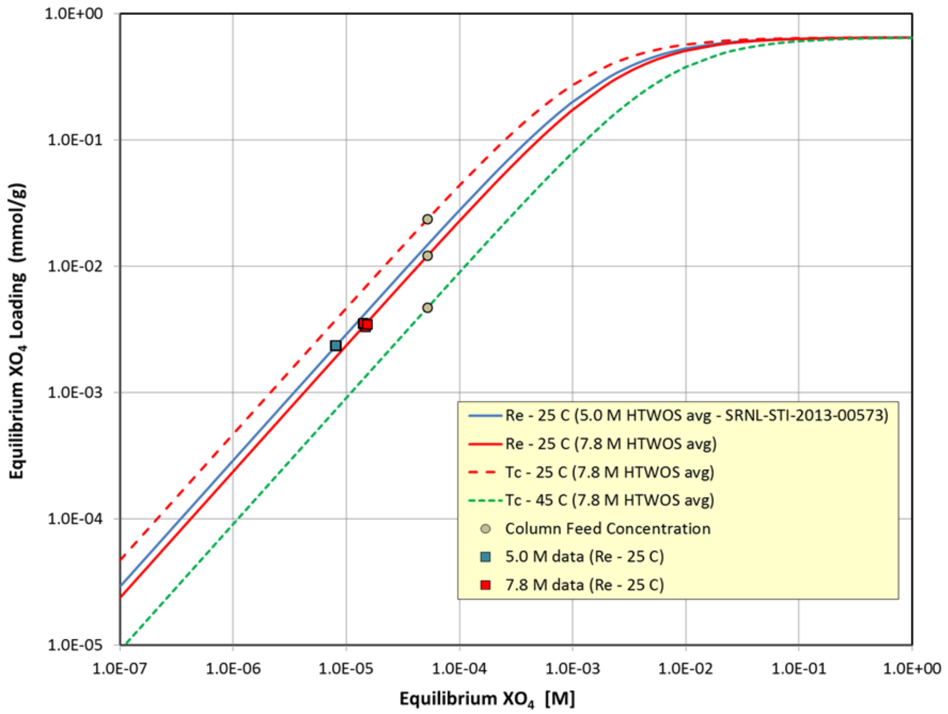

Figure B-2. **Comparison of algebraic model ReO_4 and TcO_4 isotherms at 25˚ and 45˚C for the IBC May batch of SuperLig® 639 resin with a 5 M and 7.8 M HTWOS Avg simulant.**

These isotherms are employed in subsequent VERSE-LC column performance simulations. Table B-5 below provides a listing of these isotherms, and others, along with their specific parameter values. ("SRNL Lab-Scale" refers to an upcoming test)

Table B-5. "Effective" binary isotherms employed in current study.

XO_4	T (˚C)	Simulant Na+ [M]	Qtot (mmol/g)	$a = \rho_{bed} Q_{tot}$ (fit)	Beta (fit)	Application
ReO_4	25	5.0	0.6518	0.29318	2.23277E-03	SRNL Lab-Scale
	25	7.8			2.74050E-03	
	35				4.36780E-03	
	45				1.41654E-02	
TcO_4	25	7.8	0.6518	0.29318	1.38395E-03	Full-Scale
	45				7.15354E-03	

Particle Pore Diffusivity

Prior analyses performed by SRNL (Hamm et al., 2013, and Nash et al., 2013) employed a diluted 5 M sodium simulant referred to as the HTWOS Average simulant. The subsequent analyses presented in this report are looking at an undiluted 7.8 M sodium simulant that still refers to the HTWOS Average simulant. The ionic molar concentrations of the key constituents for both of these simulants are provided for comparison in Table B-6 below.

Table B-6. HTWOS average 5 M and 7.8 M simulant target molar compositions at approximately 25 ˚C.

Ion	Molarity (M)	Molarity (M)
NO_3^-	1.60	2.53
OH^-	1.611	2.43
SO_4^{-2}	0.086	0.13
$Al(OH)_4^-$	0.307	0.48
NO_2^-	0.565	0.88
CO_3^{-2}	0.274	0.43
K^+	0.0328	0.051
Acetate	0.0385	0.06
F^-	0.0316	0.049
HPO_4^{-2}	0.049	0.076
Cl^-	0.042	0.066
ReO_4^-	4.5E-05	5.23E-05
Total [Na+]	5.0	7.8

In order to compute breakthrough curves one key parameter is the binary pore diffusivity parameter. The basic SuperLig® 639 methodology for computing pore diffusivity was explained by Hamm et al. (2000). To compute a diffusion coefficient for a specific ionic pair mean conductance and mean valance must be computed from individual ionic conductance and valance. A basic listing of available ionic conductance and valance is listed in Table B-7 below.

Table B-7. Ionic conductance and valance of the typical ions of interest.

Ion	Ionic Conductance	Valance
cation		
Cs+	77.30	1.0
K+	73.50	1.0
Na+	50.10	1.0
H+	349.80	1.0
anion		
OH-	198.60	1.0
Cl-	76.35	1.0
NO3-	71.46	1.0
NO2-	72.00	1.0
I-	76.80	1.0
F-	55.40	1.0
CO3-2	69.30	2.0
SO4-2	80.02	2.0
PO4-3	75.00	3.0
Al(OH)4-	70.00	1.0
ReO4-	55.00	1.0

The mean ionic conductance and mean ionic valance are computed based on, respectively:

$$I_{ij} = \frac{I_i \cdot I_j}{I_i + I_j} \quad \text{and} \quad V_{ij} = \frac{V_i \cdot V_j}{V_i + V_j} \,, \qquad \text{(B-9a) and (B-9b)}$$

where

I_i - Ionic conductance of ith species

I_{ij} - Mean ionic conductance for ith and jth species

V_i - Ionic valance of ith species

V_{ij} - Mean ionic valance for ith and jth species

The mean ionic conductance and valance for the two primary binary pairs of interest are listed in Table B-8 below.

Table B-8. Mean ionic conductance and valance for the binary pairs of interest.

Ionic Pair	Mean Ionic Conductance	Mean Ionic Valance
ReO4- / Na+	26.22	0.5
ReO4- / K+	31.46	0.5

The mean diffusion coefficient (in units of cm^2/min) for a specific ionic pair can be expressed as:

$$D_{ij}(T) = N_{const}\left[\frac{I_{ij}}{V_{ij}}\right]T \,, \qquad \text{(B-10)}$$

where

N_{const} - Nernst Constant (= 8.931×10^{-10} times 60 $= 5.3586 \times 10^{-8}$)

T - Thermodynamic temperature (K)

D_{ij} - mean diffusion coefficient of ith and jth ionic binary pair (cm^2/min)

On a mole fraction weighted basis, an uncorrected free stream (i.e., Brownian motion) diffusion coefficient for a mixture of binary pairs can be expressed as:

$$D_{mix}(T) = \sum_{ij} x_{ij} D_{ij}(T) \,, \qquad \text{(B-11)}$$

where

x_{ij} - Mole fraction of specific ionic pair

D_{mix} - Mixture average uncorrected free stream diffusion coefficient (cm^2/min)

A viscosity corrected free stream diffusion coefficient (i.e., a concentration correction factor) can be expressed as:

$$\hat{D}_{mix}(T,\bar{c}) = \frac{D_{mix}(T)}{\left[\dfrac{\mu_{mix}(T,\bar{c})}{\mu_w(T)}\right]} \,, \qquad \text{(B-12)}$$

where

μ_w - Viscosity of water at temperature T

μ_{mix} - Viscosity of aqueous phase mixture at composition $\bar{c}$ and temperature T

$\hat{D}_{mix}$ - Mixture "viscosity corrected" free stream diffusion coefficient (cm^2/min)

The pore diffusion coefficient can then be related to its free stream value through use of the tortuosity factor by the expression:

$$\hat{D}_{pore}(T,\bar{c}) = \tau(T) \cdot \hat{D}_{mix}(T,\bar{c}) \quad , \tag{B-13}$$

where

μ_w - Viscosity of water at temperature T

τ - Tortuosity factor at temperature T

$\hat{D}_{pore}$ - Mixture "viscosity corrected" pore diffusion coefficient (cm^2/min)

The actual S-shape of a VERSE breakthrough curve depends upon the particle kinetics through this particle pore diffusivity value. Historical values for both ReO_4^- and TcO_4^- have been set to 35% of their free stream (i.e., molecular) values (Hamm et al., 2000). This 35% value has been shown repeatedly to be acceptable in prior studies where operating temperatures varied from ~18˚C to 27˚C. However, in the more recent 25˚C and 45˚C testing provided in Nash et al. (2013) the experimental S-shape observed indicated that lower values were more appropriate for the current resin batches (i.e., IBC resin identified as Lot #130611552-56) at the higher temperature. As discussed in Nash et al. (2013) tortuosity values of 35% and 15.4% at 25˚C and 45˚C, respectively, were found to be more appropriate values. At higher temperatures net ionic and neutral species migration appears to be hindered by the ionic pore diffusion processes.

To compute pore diffusivity values, in addition to tortuosity values, free stream diffusivities, compositions, and mixture viscosity must be estimated as indicated in the various equations provided above. As Eq. (B-12) indicates the viscosity of pure water is also required. Prior estimations have assumed this viscosity to be approximately one and corrections are required to update the prior tortuosity factors to yield the pore diffusivity values that were employed within the prior column predictions. Estimated water and aqueous phase simulant viscosity values were computed using the OLI algorithm where the MSE solvent option was chosen. Figure B-3 below shows the OLI generated viscosity values over the range of temperature of potential use.

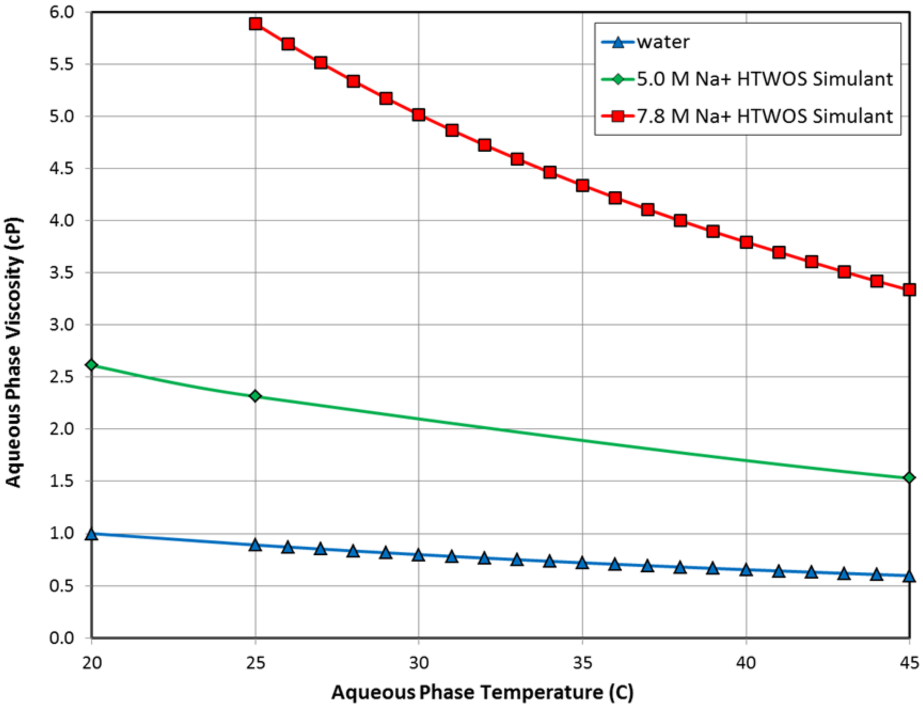

Figure B-3. OLI viscosity estimates for pure water and the 5 M and 7.8 M sodium simulants.

As Figure B-3 indicates, the viscosity of pure water is less than 1.0 cP for temperatures greater than 20 ˚C. In Table B-9 below the series of calculations required to estimate both the free stream and pore diffusion coefficient values are provided (i.e., values shaded in orange are directly employed in VERSE column predictions). For the prior analyses (Hamm et al., 2000 and 2013), the tortuosity factors have been adjusted to retain the pore diffusion coefficient values employed in their column breakthrough calculations. As such, the previous 35% value at 25˚C is now set to 39.3%, while the 15.4% value at 45˚C is now set to 25.77%.

Table B-9. Computed free stream and pore diffusivity values.

Reference report	Hamm et al. (2000)	Hamm et al. (2013)	Hamm et al. (2013)	This report	This report
Simulant	**5M Envelope A**	**5M HTWOS Avg**	**5M HTWOS Avg**	**7.8M HTWOS Avg**	**7.8M HTWOS Avg**
Temperature (C)	25	25	45	25	45
density (g/ml)	na	1.223	1.205	1.335	1.329
viscosity (cP)	2.940	2.314	1.530	5.887	3.334
viscosity H_2O (cP)	0.891	0.891	0.597	0.891	0.597
viscosity ratio (cP/cP H_2O)	3.300	2.597	2.563	6.609	5.588
pore/free tortuosity factor	0.393	0.393	0.2577	0.393	0.2577
Na+ conc [M]	5.000	5.0023	5.0023	7.800	7.800
K+ conc [M]	0.115	0.0328	0.0328	0.051	0.051
Na+ mole fraction	0.9775	0.9935	0.9935	0.9935	0.9935
K+ mole fraction	0.0225	0.0065	0.0065	0.0065	0.0065
ReO4- / Na+ diffusion coef (cm^2/min)	8.377E-04	8.377E-04	8.939E-04	8.377E-04	8.939E-04
ReO4- / K+ diffusion coef (cm^2/min)	1.005E-03	1.005E-03	1.073E-03	1.005E-03	1.073E-03
Diffusion coef (cm^2/min)	8.415E-04	8.388E-04	8.951E-04	8.388E-04	8.951E-04
diffusion coef (cm^2/min) (viscosity corrected)	2.550E-04	3.230E-04	3.493E-04	1.269E-04	1.602E-04
particle/pore diffusivity (cm^2/min)	1.002E-04	1.269E-04	9.001E-05	4.988E-05	4.128E-05

The impact on the diffusion coefficient value due to a concentration increase from 5 M to 7.8 M sodium can be seen to be:

- 2.86X reduction at 25˚C
- 3.65X reduction at 45˚C

Reductions in pore diffusion coefficient of this magnitude are expected to distort the S-shaped breakthrough curves significantly towards earlier breakthrough performance.

Aqueous phase density and viscosity measurements have been made for the 7.8 M sodium simulant. A quick comparison of these measurements to OLI estimates is provided in Table B-10 below. The differences in the measured versus computed viscosities are minimal, within <5% of the diffusivity.

Table B-10. Measured versus computed aqueous phase density and viscosity values for the 7.8 M sodium HTWOS Avg simulant.

	Temperature (C)	Measured Value	OLI (MSE database)
Simulant		**7.8 M HTWOS Avg**	**7.8 M HTWOS Avg**
density (g/ml)	25	1.348	1.335
	45	Not measured	1.329
viscosity (cP)	25	6.1	5.887
	45	3.5	3.334

VERSE SRNL Column Pretest Predictions

For the SRNL 7.8 M sodium HTWOS Avg simulant and the IBC May batch of SuperLig® 639 resin, VERSE column pretest predictions were made for the column experiments to be operated at SRNL later in 2015. The same two-column carousel configurations were simulated at 25˚C and at 45˚C. Input details for the three columns are provided in Table B-11, both for the lab-scale and the full-scale facilities. The results of the two column predictions are shown in Figure B-4. The solid lines represent the 25˚C breakthrough curves. The dashed lines represent the 45˚C breakthrough curves.

Table B-11. Key VERSE-LC input parameters for each three column carousel.

	Lab-Scale Columns	Full-Scale Columns
Parameter	**Parameter settings**	**Parameter settings**
Number of finite elements within bed	50 for each bed	50 for each bed
Number of internal collocation points per finite element within bed	4 for each bed	4 for each bed
Number of internal collocation points within pores	6 for each bed	6 for each bed
Components explicitly modeled:	perrhenate	pertechnetate
Axial dispersion, E_b (cm^2/min)	Chung and Wen (1968) correlation	Chung and Wen (1968) correlation
Film coefficient, k_f (cm/min)	Wilson and Geankoplis (1966) correlation	Wilson and Geankoplis (1966) correlation
Flowrate (ml/min)	49.132	75,710.133
Active column lengths, L	21.824 cm for each bed	250.414 cm for each bed
Column diameters, D	7.2746 cm for each bed	83.471 cm for each bed
Headspace volumes	907.05 ml for each bed	1370.3 L for each bed
Particle radius (μm)	387	387
Bed porosities, ε_b (-)	0.363 for each bed	0.363 for each bed
Particle porosities, ε_p (-)	0.437 for each bed	0.437 for each bed
Fluid dynamic viscosity, μ_w	5.887 cP (25˚C) 3.334 cP (45˚C)	5.887 cP (25˚C) 3.334 cP (45˚C)
Fluid density, ρ_w	1.335 g/ml (25˚C) 1.329 g/ml (45˚C)	1.335 g/ml (25˚C) 1.329 g/ml (45˚C)
Lag column switching exit technetium concentration criterion (none for lead)	n.a.	1.0% of feed concentration as cumulative average
Native (initial) concentration	0.0 M	0.0 M
Feed (loading) concentration	5.23x10^{-5} M	5.23x10^{-5} M
Molecular diffusion coefficient	1.269 x10^{-4} cm^2/min (25˚C) 1.602 x10^{-4} cm^2/min (45˚C)	1.269 x10^{-4} cm^2/min (25˚C) 1.602 x10^{-4} cm^2/min (45˚C)
Particle pore diffusion coefficient	4.988 x10^{-5} cm^2/min (25˚C) 4.128 x10^{-5} cm^2/min (45˚C)	4.988 x10^{-5} cm^2/min (25˚C) 4.128 x10^{-5} cm^2/min (45˚C)
Freundlich-Langmuir Hybrid **a** coefficient (batch specific)	2.9318 x10^{-1} gmoles/L$_{BV}$	2.9318 x10^{-1} gmoles/L$_{BV}$
Freundlich-Langmuir Hybrid **b** coefficient	1.0 M^{-1}	1.0 M^{-1}
Freundlich-Langmuir Hybrid $\mathbf{M_a}$ coefficient	1.0 (-)	1.0 (-)

	Lab-Scale Columns	**Full-Scale Columns**
Parameter	**Parameter settings**	**Parameter settings**
Freundlich-Langmuir Hybrid $\mathbf{M_b}$ coefficient	1.0 (-)	1.0 (-)
Freundlich-Langmuir Hybrid β "effective" coefficient for pertechnetate	2.74050 x10^{-3} (-) (25˚C) 1.41654 x10^{-2} (-) (45˚C)	1.38395 x10^{-3} (-) (25˚C) 7.15354 x10^{-3} (-) (45˚C)

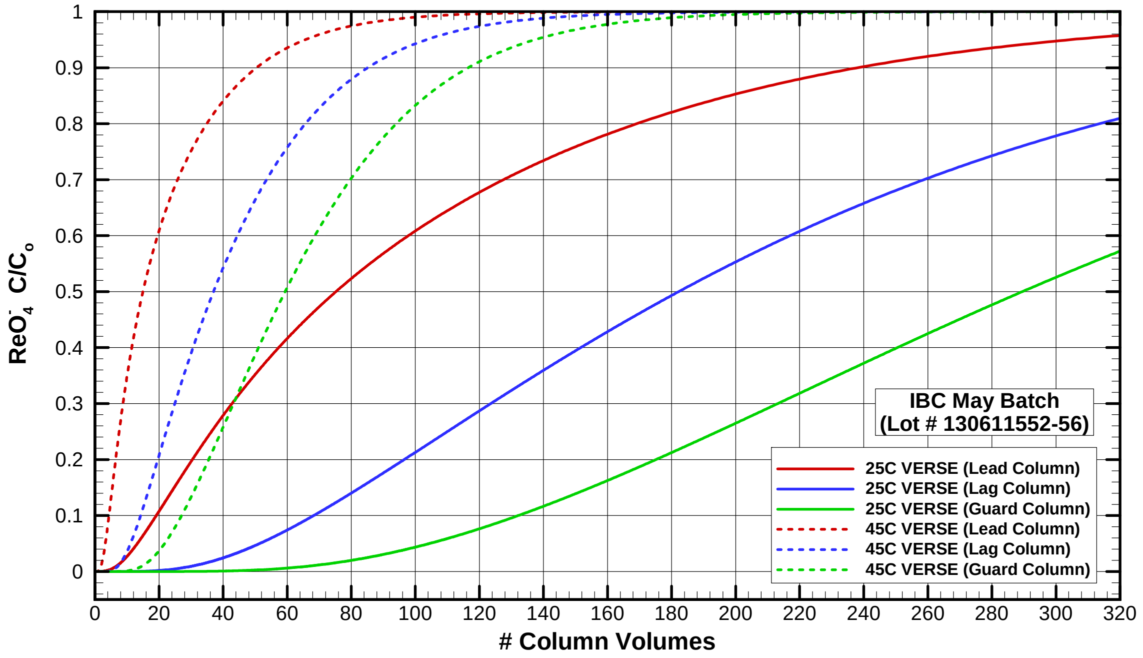

Figure B-4. Comparison of VERSE predicted Lab-scale ReO$_4$ column performance at 25˚C and 45˚C for the IBC May batch of SuperLig$^{®}$ 639 resin using the 7.8 M HTWOS Avg simulant.

The actual S-shape of the VERSE breakthrough curves depends upon the particle kinetics through the particle pore diffusivity value. The reduced pore diffusivity values due to increased viscosity of the 7.8 M sodium solution tends to greatly eliminate the S-shape yielding early breakthrough behavior as seen in Figure B-4.

Full-Scale Column Performance Assessment

Full-scale 3-column run calculations were performed where 1% cumulative breakthrough of TcO_4^- concentration was used as the exit criterion. The "cumulative" average concentration (i.e., cumulative breakthrough sum, "bucket" average) was computed and once this 1% value was reached in the liquid exiting the last column, the first column in the configuration was removed and replaced with a clean column at the end. This model step mathematically represents removing the lead column out of the system for elution. Conceptually, the process operates as a carousel, with the lead column valved out of series when it is saturated, and replaced by a new column in the last position (i.e., guard position).

Parameter values chosen were taken from the previously issued engineering study performed by WRPS [Russell, 2013; see Section 2.3]:

- A 3-Column configuration (i.e., lead, lag, and polish columns);
- 25˚C and 45˚C operating temperature;
- 362 gallon active bed volume for each column; and
- 20 gpm feed stream flowrate (i.e., corresponds to a 3.315 BV/hr).

The other key assumptions being made are:

- Average HTWOS feed composition at 7.8 M [Na^+];
- L/D ratio assumed to be fixed at 3.0; and
- Resin batch assumed to be consistent behavior with SuperLig® 639 Lot #130611552-56.

A similar set of results were provided in Nash et al. (2013) for the 5 M sodium HTWOS Avg simulant at T = 25˚C and 45˚C, as well. Table B-12 provides the geometrical and flow conditions of the full-scale columns considered.

Table B-12. Full-Scale three column configuration considered.

Flowrate (BV/hr)	Volume (gal)	Diameter (cm)	3-Column Length (cm)	Flowrate (ml/min)	CSTR-Volume (ml)
3.315	362.0	83.471	250.414	75,710.133	1,370,319.144

The results of these simulations are provided in Table B-13 for the 7.8 M sodium composition results generated in this report and for comparison the 5.0 M sodium composition results taken from Nash et al. (2013). These results represent the third cycle values where near stabilized repeatable performance is achieved.

Table B-13. Comparison of volumes of simulant processed based the 5.0 M versus the 7.8 M sodium HTWOS Avg composition at both 25˚C and 45˚C.

Temperature (C)	Simulant HTWOS Avg Na+ [M]	# Bed Volumes Processed (-)	Processed Volume (kgal)	Waste Na^+ processed (moles)
25	**5.0**	207.6	75.2	1.42E6
	7.8	120.1	43.5	1.28E6
45	**5.0**	103.4	37.4	7.07E5
	7.8	20.9	7.6	2.2E5

To demonstrate that near repeatable performance is achieved in three cycles, the bucket average algorithm was run for five cycles and the results of these runs are provided in Table B-14.

Table B-14. Volumes of solution processed for five cycles based on the 7.8 M sodium HTWOS Avg composition at both 25˚C and 45˚C.

	Waste Volume Processed at 25 C (1000 gal)	Waste Volume Processed at 45 C (1000 gal)
Cycle 1	79.6	15.1
Cycle 2	33.2	5.1
Cycle 3	43.5	7.6
Cycle 4	43.4	7.6
Cycle 5	43.5	7.6
Total	243.2	43.0
5-cycle avg	48.64	8.60

Breakthrough behavior for the 5-cycle bucket average runs are plotted in Figure B-5 and B-6 for the 25˚C and 45˚C cases, respectively.

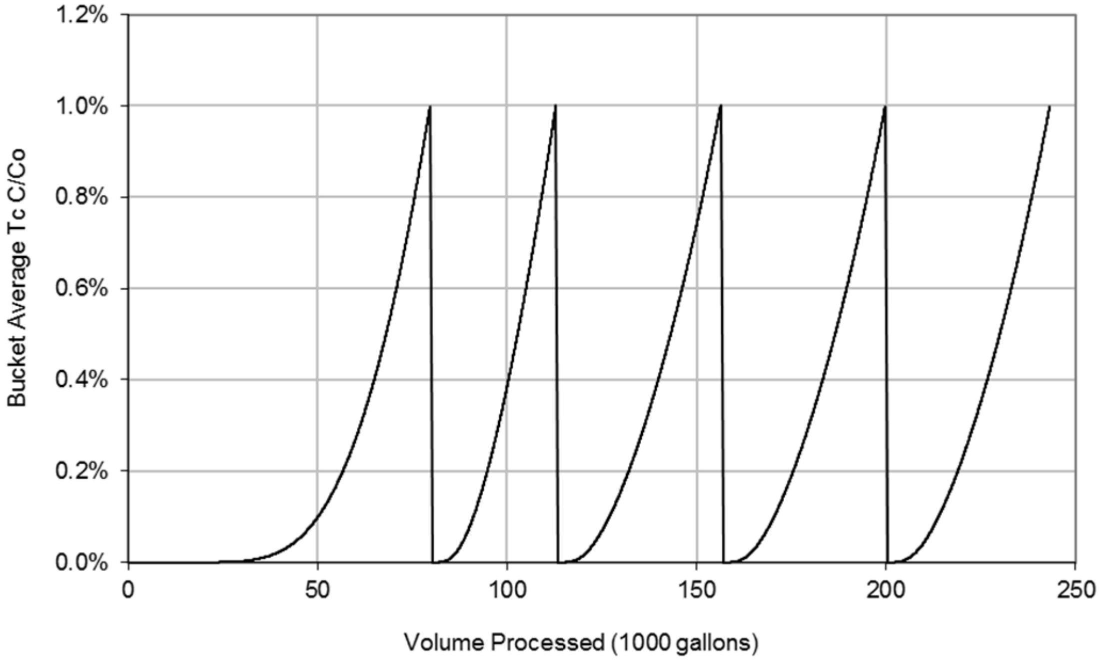

Figure B-5. Five-cycle VERSE predicted TcO_4 breakthrough performance at 25˚C for the IBC May batch of SuperLig® 639 resin and using the 7.8 M HTWOS Avg composition.

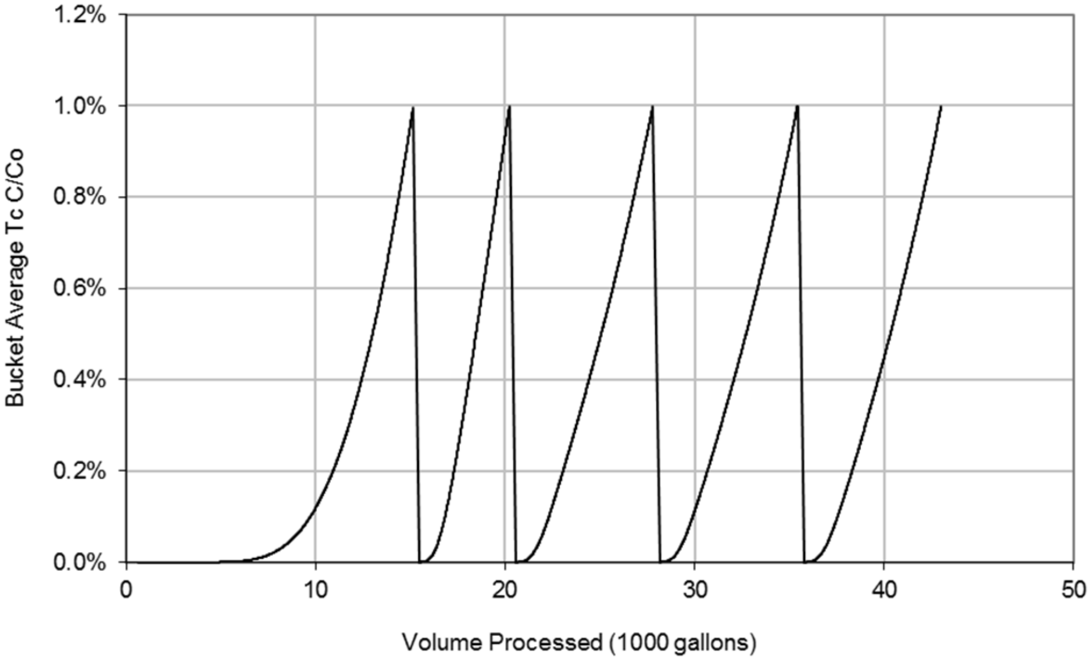

Figure B-6. Five-cycle VERSE predicted TcO_4 breakthrough performance at 45˚C for the IBC May batch of SuperLig® 639 resin and using the 7.8 M HTWOS Avg simulant.

Appendix B References

Bruening, R.L., Final Resin Property and Performance Report on Quality control Tests and Data for Two 4+ Liter Batches of SuperLig® 639; August 15, 2013

Hamm, L.L., Smith, F.G., and McCabe, D.J., 2000, Preliminary Ion Exchange Modeling for Removal of Technetium from Hanford Waste Using SuperLig 639 Resin, WSRC-TR-2000-00305, SRT-RPP-2000-00011, August.

Hamm, L.L., Smith, F.G. III, Aleman, S.E., McCabe, D.J., Upgrade to Ion Exchange Modeling for Removal of Technetium from Hanford Waste Using SuperLig® 639 Resin, SRNL-STI-2013-00160, May, 2013

Nash, C.A., Morse, M.M., McCabe, D.J., Hamm, L.L., Smith, and F.G. III, Aleman, S.E., Upgrade to Ion Exchange Modeling for Technetium Removal Resin Maturation, SRNL-STI-2013-00573, Rev. 1, December, 2013

Russell, R.M., Supplemental LAW Immobilization Technetium Removal Pre Conceptual Engineering Study, RPP-RPT-555855, Rev. 0, November 2013

Appendix C – Laboratory-Scale Column Input and Output Files

For reference the VERSE-LC input and output files for the laboratory-scale (SRNL) column benchmarking (i.e., 25˚C and 45˚C runs) are provided in this appendix. Both column tests were performed using perrhenate. The input and output files for each temperature run are listed below:

VERSE Input File for Lab-Scale 25C Perrhenate Column (SRNL) Test

```
Simulation at 25C of ReO4- removal on experimental SL639 3 column system
1 component (ReO4-) isotherm (7.8M HTWOS Avg simulant)
1, 150, 4, 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
65.4710, 7.2746, 49.132, 907.05  Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
387.0, 0.363, 0.437,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - conc step change
1, 0.0, 5.23d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.05887, 1.3350                  fluid viscosity(posie), density(g/cm^3)
m                                COMMAND - subcolumns
50, 150, 0, 1, 0.1, 0.0, 10000.0 elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
6, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
D
-1, 3000.0, 1, 0.0
-                                end of commands
6000.0, 0.1                      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
4.988d-5                         part-pore diffusivities(cm^2/min) 39.3% of free values
1.269d-4                         Brownian diffusivities(cm^2/min)
0.29318                          Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                              Freundlich/Langmuir Hybrid b    (1/M)
1.0                              Freundlich/Langmuir Hybrid Ma   (-)
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
2.74050E-03                             Freundlich/Langmuir Hybrid beta (-) 25C and 7.8M
simulant
```

VERSE Output File for Lab-Scale 25˚C Perrhenate Column (SRNL) Test

```
===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: case
 Simulation at 25C of ReO4- removal on experimental SL639 3 column system
 1 component (ReO4-) isotherm (HTWOS simulant)
 Begin Run:  14:07:21 on 11-17-2014   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)        =   6000.00000 min         dtheta max     =       .10000 BV
abs. tol.      =       .10000E-06         rel. tol.      =       .10000E-03
Total Length   =     25.77600 cm          D              =      2.86400 cm
Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =    166.05480 mL
F              =      2.99800 mL/min      Uo (linear)    =      1.28200 cm/min
R              =    387.00000 microns     L/R            =    666.04651
Bed Void frac. =       .36300             Pcl. Porosity  =       .43700
Spec. Area     =     49.37984 1/cm        Time/BV        =      6.70201 min
Vol CSTRs      =     55.35000 mL

Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .17885E+00
Dp  [cm2/min]  =  .49880E-04
Doo [cm2/min]  =  .12690E-03
kf  [cm/min]   =  .32354E-01
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .13481E-01
Sc(i)          =  .21055E+05
Peb(i)         =  .61587E+02
Bi(i)          =  .57443E+02
Nf(i)          =  .29497E+02
Np(i)          =  .97542E-01
Pep(i)         =  .22761E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .29318E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .27405E-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 .5230E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .5887E-01 poise and density to 1.322     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+05 min.
     When comp.  1 reaches .1000     M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  6: Monitor conc. history at stream  6.  Filename = case.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  7: Dump full profile file at  3000.     min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in  8983 steps.  Average step size .6679     minutes
End run:  14:08:45 on 11-17-2014
Integrated Areas in History Files:
case.h01                   .214364
case.h02                   .128769
case.h03                   .665588E-01
```

VERSE Input File for Lab-Scale 45˚C Perrhenate Column (SRNL) Test

```
Simulation at 45C of ReO4- removal on experimental SL639 3 column system
1 component (ReO4-) isotherm (7.8M HTWOS Avg simulant)
1, 150, 4, 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
65.4710, 7.2746, 49.132, 907.05  Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
387.0, 0.363, 0.437,  0.0        part-rad(um), bed-void, part-void, sorb-cap()
0.0                              initial concentrations (M)
S                                COMMAND - conc step change
1, 0.0, 5.23d-5, 1, 0.0          spec id, time(min), conc(M), freq, dt(min)
V                                COMMAND - viscosity/density change
0.03334, 1.3290                  fluid viscosity(posie), density(g/cm^3)
m                                COMMAND - subcolumns
50, 150, 0, 1, 0.1, 0.0, 10000.0 elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-e,t-ee
h                                COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
h                                COMMAND - effluent history dump
6, 1.0, 1.0, 0.25, 0.1           unit op#, ptscale(1-4) filtering
D
-1, 3000.0, 1, 0.0
-                                end of commands
6000.0, 0.1                      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
4.128d-5                         part-pore diffusivities(cm^2/min) 25.77% of free values
1.602d-4                         Brownian diffusivities(cm^2/min)
0.29318                          Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                              Freundlich/Langmuir Hybrid b    (1/M)
1.0                              Freundlich/Langmuir Hybrid Ma   (-)
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
1.41654E-02                             Freundlich/Langmuir Hybrid beta (-) 45C and 7.8M
simulant
```

VERSE Output File for Lab-Scale 45˚C Perrhenate Column (SRNL) Test

```
===============================================================================
 VERSE v7.80  by R. D. Whitley and N.-H. L. Wang, c1999 PRF
 ===============================================================================
 Input file: case
 Simulation at 45C of ReO4- removal on experimental SL639 3 column system
 1 component (ReO4-) isotherm (HTWOS simulant)
 Begin Run:  14:40:33 on 11-17-2014   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)        =   6000.00000 min        dtheta max     =       .10000 BV
 abs. tol.      =       .10000E-06        rel. tol.      =       .10000E-03
 Total Length   =     25.77600 cm          D              =      2.86400 cm
 Tot. Capacity  =       .00000 eq/L solid  Col. Vol.      =    166.05480 mL
 F              =      2.99800 mL/min      Uo (linear)    =      1.28200 cm/min
 R              =    387.00000 microns     L/R            =    666.04651
 Bed Void frac. =       .36300             Pcl. Porosity  =       .43700
 Spec. Area     =     49.37984 1/cm        Time/BV        =      6.70201 min
 Vol CSTRs      =     55.35000 mL
```

```
Component no.  =      1
Ke  [-]        =  .10000E+01
Eb  [cm2/min]  =  .17846E+00
Dp  [cm2/min]  =  .41280E-04
Doo [cm2/min]  =  .16020E-03
kf  [cm/min]   =  .37792E-01
Ds  [cm2/min]  =  .00000E+00

Dimensionless Groups:
Re             =  .23930E-01
Sc(i)          =  .93957E+04
Peb(i)         =  .61722E+02
Bi(i)          =  .81075E+02
Nf(i)          =  .34455E+02
Np(i)          =  .80724E-01
Pep(i)         =  .27503E+04

Isotherm       =  Freundlich/Langmuir Hybrid
Iso. Const. 1  =  .29318E+00
Iso. Const. 2  =  .10000E+01
Iso. Const. 3  =  .10000E+01
Iso. Const. 4  =  .10000E+01
Iso. Const. 5  =  .14165E-01
Init. Conc.    =  .00000E+00
Conc. at eqb.  =  .00000E+00
Conc. units          M
===============================================================================
COMMAND LIST:
  1: Step conc. of component 1 at .0000     min to .5230E-04 M
     Execute   1 times, every .0000     mins.
  2: User set viscosity to .3334E-01 poise and density to 1.329     g/cm3
  3: Carousel (conc.). Active between t = .0000     and .1000E+05 min.
     When comp.  1 reaches .1000     M     at end of node 150,
     shift  50 axial elements out the feed end
  4: Monitor conc. history at stream  2.  Filename = case.h01
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  5: Monitor conc. history at stream  4.  Filename = case.h02
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  6: Monitor conc. history at stream  6.  Filename = case.h03
     Output density adjustments:
     1.0    *default abs conc delta,      1.0    *default rel conc delta,
     .25    *default force w/ conc delta, .10    *default force w/o conc delta
  7: Dump full profile file at  3000.     min
     Execute   1 times, every .0000     mins.
===============================================================================
VERSE-LC finished in  8957 steps.  Average step size .6699     minutes
End run:  14:41:49 on 11-17-2014
Integrated Areas in History Files:
case.h01                 .292304
case.h02                 .270807
case.h03                 .249311
```

Appendix D – Full-Scale Column Input Files

For reference VERSE-LC input files for full-scale column simulations are provided in this appendix. Output files are not included here since cumulative average calculations were performed. To perform a cumulative average calculation requires multiple VERSE-LC runs where the timing of carousel operations is iteratively determined. Thus, no single VERSE-LC output file exists. The cases presented here correspond to an "effective" single component isotherm modeling approach where the pertechnetate ion is modeled assuming the nitrate concentration remains essentially constant throughout the columns. Note that the maximum number of internal collocation points within the pores allowed by VERSE-LC was used. Early numerical testing to establish the minimum usable number of finite elements and collocation points that maintains acceptable accuracy indicated that radial concentration gradients within the particle pores were large and sharp.

VERSE Input File for Full-Scale 25˚C Pertechnetate 3-Column System

```
Simulation of TcO4- removal on full-scale SL639 3 column system [May IBC Batch Lot
#130611552-56]
1 component (TcO4-) isotherm (7.8M HTWOS simulant) at 25C
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA
NNNYY                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
751.241, 83.471, 75710.133, 1370319.144 Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
387.0, 0.363, 0.437,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentrations (M)
S                                 COMMAND - conc step change
1, 0.0, 5.23d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.05887, 1.335                    fluid viscosity(posie), density(g/cm3)
m                                 COMMAND - subcolumns
50, 150, 0, 1, 5.23d+7, 0.0, 10000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-
e,t-ee
h                                 COMMAND - effluent history dump
1, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
3, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
5, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
h                                 COMMAND - effluent history dump
6, 1.0, 1.0, 0.25, 0.1            unit op#, ptscale(1-4) filtering
D
-1, 2173.8, 1, 0.0
-                                end of commands
2173.8, 0.1                      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
4.988d-5                         part-pore diffusivities(cm2/min) 39.3% of free values
1.269d-4                         Brownian diffusivities(cm2/min)
0.29318                          Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                              Freundlich/Langmuir Hybrid b    (1/M)
1.0                              Freundlich/Langmuir Hybrid Ma   (-)
1.0                              Freundlich/Langmuir Hybrid Mb   (-)
1.38395E-03                      Freundlich/Langmuir Hybrid beta (-)  25C and 7.8M
```

VERSE Input File for Full-Scale 45˚C Pertechnetate 3-Column System

```
Simulation of TcO4- removal on full-scale SL639 3 column system [May IBC Batch Lot
#130611552-56]
1 component (TcO4-) isotherm (7.8M HTWOS simulant) at 45C
1, 150, 4, 6                      ncomp, nelem, ncol-bed, ncol-part
FCWNA                             isotherm,axial-disp,film-coef,surf-diff,BC-col  FCUNA

NNNYY                             input-only,perfusable,feed-equil,datafile.yio
M                                 comp-conc units
751.241, 83.471, 75710.133, 1370319.144 Length(cm),Diam(cm),Q-flow(ml/min),CSTR-vol(ml)
387.0, 0.363, 0.437,  0.0         part-rad(um), bed-void, part-void, sorb-cap()
0.0                               initial concentrations (M)
S                                 COMMAND - conc step change
1, 0.0, 5.23d-5, 1, 0.0           spec id, time(min), conc(M), freq, dt(min)
V                                 COMMAND - viscosity/density change
0.03334, 1.329                    fluid viscosity(posie), density(g/cm3)
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m                                  COMMAND - subcolumns
50, 150, 0, 1, 5.23d+7, 0.0, 10000.0  elem-shift,elem-watch,pp-watch,c-watch,c-thresh,t-
e,t-ee
h                                  COMMAND - effluent history dump
1, 1.0, 1.0, 0.25, 0.1             unit op#, ptscale(1-4) filtering
h                                  COMMAND - effluent history dump
2, 1.0, 1.0, 0.25, 0.1             unit op#, ptscale(1-4) filtering
h                                  COMMAND - effluent history dump
3, 1.0, 1.0, 0.25, 0.1             unit op#, ptscale(1-4) filtering
h                                  COMMAND - effluent history dump
4, 1.0, 1.0, 0.25, 0.1             unit op#, ptscale(1-4) filtering
h                                  COMMAND - effluent history dump
5, 1.0, 1.0, 0.25, 0.1             unit op#, ptscale(1-4) filtering
h                                  COMMAND - effluent history dump
6, 1.0, 1.0, 0.25, 0.1             unit op#, ptscale(1-4) filtering
D
-1, 378.24, 1, 0.0
-                                 end of commands
 378.24, 0.1                       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
4.128d-5                          part-pore diffusivities(cm2/min) 25.77% of free values
1.602d-4                          Brownian diffusivities(cm2/min)
0.29318                           Freundlich/Langmuir Hybrid a    (moles/L B.V.)
1.0                               Freundlich/Langmuir Hybrid b    (1/M)
1.0                               Freundlich/Langmuir Hybrid Ma   (-)
1.0                               Freundlich/Langmuir Hybrid Mb   (-)
7.15354E-03                       Freundlich/Langmuir Hybrid beta (-)  45C and 7.8
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Distribution:

S. L. Marra, 773-A
F. M. Pennebaker, 773-42A
T. B. Brown, 773-A
E. N. Hoffman, 999-W
D. H. McGuire, 999-W
S. D. Fink, 773-A
C. C. Herman, 773-A
K. M. L. Taylor-Pashow, 773-A
C. A. Nash, 773-42A
C. L. Crawford, 773-42A
D. J. McCabe, 773-42A
W. R. Wilmarth, 773-A
D. T. Herman, 735-11A
A. D. Cozzi, 999-W
D. K. Peeler, 999-W
K. M. Fox, 999-W
K. H. Subramanian, WRPS
Records Administration (EDWS)
J. A. Diediker. DOE-ORP
L. Holton, DOE-ORP
W. F. Hamel, DOE-ORP
T. W. Fletcher, DOE-ORP
S. H. Pfaff, DOE-ORP
S. T. Arm, WRPS
P. A. Cavanah, WRPS
T. W. Crawford, WRPS
W. G. Ramsey, WRPS
D. J. Swanberg, WRPS
N. P. Machara, DOE-EM
J. A. Poppiti, DOE-EM
D. J. Koutsandreas, DOE-EM
R. A. Gilbert, DOE-ORP
C. J. Winkler, WRPS
R. H. Spires, WRPS