MODELING HANFORD-RPP TREATED LAW FEED EVAPORATION

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ABSTRACT/SUMMARY

Previous Hanford-RPP evaporator modeling has focused on the treated LAW feed and eluate evaporation systems without the inclusion of secondary waste recycles.[1-4] This work investigates the potential impact that secondary-waste recycle streams may have on the operation of the treated LAW evaporator. The treated LAW evaporator will concentrate the treated waste effluent streams from the Cs ion exchange blended with the LAW melter offgas scrubbing recycle stream. The Tc ion exchange system (originally part of the test specification) has since been eliminated from the flowsheet. The LAW melter offgas scrubbing recycle stream is the major contributor to the overall recycle volume that is to be mixed with the treated waste feed prior to evaporation. Based on experience at Savannah River Site, the introduction of silica from melter offgas recycle into high sodium/aluminum feeds can produce sodium aluminum-silicate precipitates upon concentration. These sodium-aluminum-silicates can cause operational shutdowns due to plugging of lines and fouling of heat transfer surfaces.

This work examines the potential of the treated waste feed blends to form sodium-aluminum silicate precipitates when evaporated using the zeolite database. To investigate the behavior of the blended pretreated waste feed, an OLI ESP model of the treated LAW evaporator was built. A range of waste feed compositions representative of Envelope A, B, and C were then fed into the OLI model to predict various physical and chemical properties of the evaporator concentrates. Additional runs with treated LAW evaporator were performed to compare chemical and physical property model predictions and experimental results for small scale radioactive tests (S-69) of the treated feed (AW 101) evaporation process.

The objectives of this work were to develop physical property correlations of the concentrated treated feed evaporator bottoms. The model was to simulate the treated LAW evaporator operating at 50°C at the bubble point vacuum with Envelope A, B, or C wastes blended with LAW melter offgas scrubbing recycle (SBS) as feed and the evaporator concentrate or bottoms stream being varied between 15°C and 66°C. The physical property correlations were to be expressed in terms of the waste feed compositions, LAW SBS to waste feed volumetric flow ratio, and the evaporator bottoms temperature and sodium concentration. Simulation results were then regressed to generate predictive equations for density, heat capacity, thermal conductivity, viscosity, and solubility of the Treated LAW evaporator bottoms concentrate. Simulation results were validated with experimental results which had already been completed. Development of these equations was successful based on the goal of developing physical property correlations for each waste envelope with an error no greater

than ±15% between calculated and modeled physical properties. The equation to predict solubility or the amount of total solids in the Treated LAW evaporator bottoms concentrate could not be developed to satisfy this goal. There was not enough information captured by the chosen model inputs to adequately describe the complicated nature of solids precipitation in the bottoms concentrate. However, general trends in solids formation were identified with respect to the bottoms Na molarity and temperature. Another objective of this task was to verify the derived physical property equations with experimental tests with simulated blended LAW feed solutions. The predicted physical properties were compared with experimental results documented in the report Treated LAW Feed Evaporation: Physical Properties and Solubility Determination and with radioactive experiments for AW-101 documented in the report Evaporation of Pretreated Hanford Tank AW-101 Sample Mixed with Recycle. The predicted densities and heat capacities were within +/-15% of the measured values for Envelopes A, B, and C. The Na molarity predictions for Envelope A and B were also within +/-15%. The other predicted physical properties were outside +/-15% of the measured values. This mismatch with measured values was due in part to being outside the range of the predictions, comparing a measured slurry property with a predicted supernate property, and the exclusion of solids in the predictions.

LIST OF ACRONYMS

HLW	High Level Waste
IX	Ion Exchange
LAW	Low Activity Waste
NASGEL	Sodium Aluminosilicate gelatin
OLH	Orthogonal Latin Hypercube
OLI/ESP	OLI Environmental Simulation Package Software
RPP	River Protection Project
SBS	Submerged Bed Scrubber
Sr/TRU	Strontium/Transuranic
TFE	Hanford RPP-WTP Treated Feed Evaporator
TF-COUP	Tank Farm - Contractor Operation and Utilization Plan
UF	Ultra-Filtration

DESCRIPTION OF THE PROCESS

The Waste Treatment Plant process is described in detail in the document “WTP Material Balance and Process Flowsheet Bases, Requirements, and Results”.[5] To summarize, evaporation is used throughout the Waste Treatment Plant pretreatment process to minimize the volume of waste that must be vitrified on the back side of the process. Evaporation is used throughout the process to help reduce the volume of waste, as in the first unit process in pretreatment (Waste Feed Evaporators) which has been modeled in earlier work.[6] Evaporation is also employed before the LAW vitrification (Treated Feed Evaporator) step. The treated LAW evaporator will concentrate the treated waste effluent stream from the Cs ion exchange blended with the LAW melter offgas scrubbing recycle stream. The goal of the Treated Feed Evaporation process is removal of the as much water as possible while maintaining a reasonably low insoluble solid content.

A major goal of this modeling task was to validate the experimental work on the treated feed evaporator.[7] To that end, the waste feeds for envelopes A, B, and C were taken from this prior report.[7] To simulate the pretreatment of these waste feeds, they were first diluted to a density of 1.22 g/ml for the aqueous phase. Additionally, as in the experimental work, the waste feeds were filtered to simulate the pretreatment process. This filtering action was duplicated in the modeling. The OLI modeling is described next.

OLI/ESP MODEL FLOWSHEET AND CHEMISTRY MODEL

The treated feed evaporation process was simulated using the OLI Environmental Simulation Program (OLI/ESP) version 6.6 using the CARBONAT, HNO3DB, SILICA, URANIUM, and ZEOLITE private databases, along with the public database. OLI ESP only performs steady state calculations.

A schematic of the OLI treated feed evaporator model is shown in Figure 1. The model fits were done using JMP® version 5.0.1[8] using linear and nonlinear least squares fit routines.

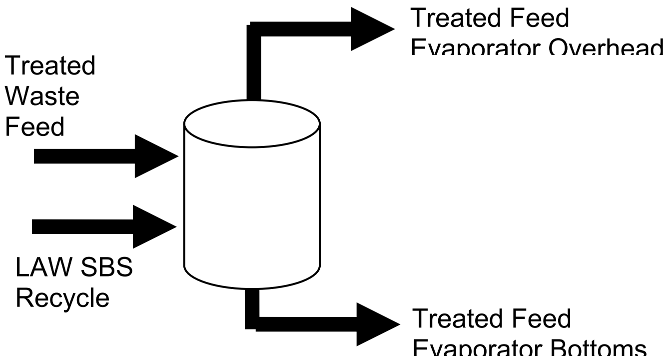

Figure 1. OLI Treated Feed Evaporator Model

The treated feed evaporator was modeled as a flash calculation.[6] To simulate the pretreatment of LAW waste feeds, all waste feeds were first diluted to reach the UF permeate target density of 1.22 g/ml, which corresponds to a sodium molarity of about 5. The waste feeds were then filtered to approximate the Cs effluent resulting from the pre-treatment steps. The SBS feed rate was controlled to match a specified volume ratio between 0 and 2. A range of SBS/Feed ratios were chosen to accommodate the expected variations in flow ratio during actual plant operations.

The supernate from the pretreatment waste feeds along with the ratioed SBS stream were then evaporated at 50^{o}C at the bubble point pressure. The evaporator bottoms stream was then cooled at 1 atm to a temperature in the desired range of 15 to 66 °C. The Na M of this cooled evaporator bottoms (product) stream was then checked against desired values of 6, 8, or 10. If the desired Na M was not reached, the evaporator molar vapor fraction was adjusted until the desired set point was achieved.

The waste feed flow rates used in the OLI simulations were based on a LAW glass production rate of 30 metric tons per day (two melters) at a Na_2O loading of 19.5, 5.0, and 11.2 wt% for Envelope A, B, and C respectively (from Table A-15 of the TF COUP document[9] and Min Prod Rate from Flow sheet Bases Assumptions and Requirements 24590-WTP-RPT-PT-02-005), where only the sodium content of the waste stream was used to calculate the Na_2O loading. This production rate was chosen as a matter of convenience and any mass flow rate could have been used.

The LAW SBS flow rate is not tied directly to the treated feed evaporator process but to the downstream LAW vitrification off gas treatment. Based on run data from Duratek SBS Run Data from VSL-02R8800-2 Rev 0 and input from the customer, the SBS flow rate was treated as an independent variable for the physical property models developed here. It is expressed in terms of its volumetric flow relative to that of the treated waste feed stream, having a range of 0 – 2 (i.e., up to twice the volumetric flow rate of the treated waste feed stream). The composition was based on the analytical results from the VSL melter pilot testing, Mark Crowder's AW-101 testing[10] and from prior experimental work.[7]

OLI/ESP does not have the ability to calculate the heat capacity of a stream directly, so this was accomplished for the evaporator bottoms concentrate stream using the OLI Scratch Pad tool in OLI/Express. The scratch pad tool was used to generate an enthalpy vs. temperature plot at each calculated steady-state composition for the temperature range 15 – 66^{o}C in one-degree increments.

DETERMINATION OF THE FACTOR SPACE FOR THE DESIGNS OF EXPERIMENT

The simulation design matrices were derived from a model factor space defined by certain model variables and their ranges. The design matrices consist of two types of design points – fit points and validation points. The fit points are used for the model fits and consist of the extreme (minimum and maximum) values of each of the variable ranges. This minimum/maximum choice assumes a linear response. The validation points are generated using the Orthogonal Latin Hypercube (OLH) technique[11], which produces points uniformly distributed over the linear factor space. The validation points are used to validate the property model predictions against the simulation results or they are used to improve the model fit when the response appears to be non-linear. The model variables, their constraints, and the corresponding factor spaces used to derive the design matrices are described next.

The physical property models are expressed the in terms of two variable types, 1) mixture variables, which define the composition of the waste feed stream, and 2) process variables which define the "state" of the process, the evaporator bottoms temperature and Na molarity and the SBS to Feed volume ratio.

For all envelopes, the temperature range used for the bottoms concentrate was 15-66^{o}C and the LAW SBS to treated waste feed volume flow ratio was 0 to 2. The bottoms concentrate Na molarity was varied between 6 and 10 molarity based on the prior experimental work.[7]

Given the broad range of compositions between Envelopes A, B, and C, physical property models were developed for each envelope. The significant species and concentration ranges for each of the envelopes were based on the characterization done in the parallel experimental work.[7]

Envelope A was based on prior work done for the Waste Feed Evaporator;[6] Envelope B was represented by the tanks AZ-101 and AZ-102; and Envelope C was represented by the tanks AN-102 and AN-107, as described in the prior experimental work.[7]

The treated waste feed will be concentrated to various endpoint Na molarities depending on operational and processing constraints. From prior modeling work[6] it was shown that the waste feed should be expressed in terms of the mass of its non-water species since the amount of water evaporated will change depending on the dilution of the waste feed via pre-treatment and/or the addition of LAW SBS recycle. However, the non-water species will always be present and thus have the greatest impact on the properties of the bottoms concentrate.

Using the recipes and tank characterizations from the prior experimental work,[7] the waste feed compositions for each envelope were analyzed and the significant species which varied the most were chosen to define the waste feed composition factor space. The waste feed composition factor space for Envelope A was defined in earlier modeling work[6] and is shown in Table 1. The constraints were defined such that $[AlO_2]/[OH] \le 0.7$, $[PO_4] + 0.07[F] \le 0.05$, and the sum of the molar charge of the mixture variables must be equal to 4.73648. The concentrations are in terms of a 5M Na solution (i.e., a concentration of 0.1M OH in a 7M Na solution is adjusted to $0.1x\,5/7 = 0.0714$ M OH).

Table 1. Definition for Envelope A Factor Space

	Mixture Variable Molar Ranges **Normalized to equivalent molarity at 5M Na**							**Process Variables**		
Variable	**$[AlO_2]$ (molar at 5M Na)**	**$[CO_3]$ (molar at 5M Na)**	**[F] (molar at 5M Na)**	**$[NO_2]$ (molar at 5M Na)**	**$[NO_3]$ (molar at 5M Na)**	**[OH] (molar at 5M Na)**	**$[PO_4]$ (molar at 5M Na)**	**[Na] (molar)**	**SBS / Feed (volumetric)**	**Temp (°C)**
minimum	0.207	0.326	0.00927	0.731	0.991	0.983	0.00632	6	0.0	15
maximum	1.12	0.686	0.236	1.59	2.08	2.89	0.0436	10	2.0	66
constraints	$[AlO_2]/[OH] \le 0.7$		$[PO_4] + 0.07[F] \le 0.05$		charge equivalent: $[AlO_2] + 2[CO_3] + [F] + [NO_3] + [NO_2] + [OH] + 3[PO_4] = 4.73648$					

Fixed Molar Concentrations

$[SO_4]$ (molar at 5M Na)	$[C_2O_4]$ (molar at 5M Na)	[Cl] (molar at 5M Na)	$[SiO_3]$ (molar at 5M Na)
0.0544	0.02	0.102	0.00636

The composition factor space for Envelope B is shown in Table 2, along with the concentration of the species that were held fixed relative to that of sodium. Note that the Envelope B waste feed input to OLI was targeted at a Na molarity of 6.5 to avoid convergence issues with the dilution to 1.22 g/ml step. To calculate the molarity of the fixed species at another initial Na Molarity, simply multiply the ratio term shown in Table 2 by the new desired initial Na molarity.

Table 2.   Definition for Envelope B Factor Space

	Mixture Variable Mass Fraction Ranges **Mass fraction relative to total mass of mixture variables**						**Process Variables**		
Variable	AlO_2^{-1} **mass fraction**	CO_3^{-2} **mass fraction**	NO_3^{-1} **mass fraction**	OH^{-1} **mass fraction**	SO_4^{-2} **mass fraction**	$C_2O_4^{-2}$ **mass fraction**	**[Na] (molar)**	**SBS / Feed (volumetric)**	**Temp (°C)**
Min	0.0380	0.2529	0.3603	0.0928	0.1438	0.0000	6	0.0	15
Max	0.1107	0.2785	0.3755	0.1074	0.2152	0.0248	10	2.0	66
charge constraint	$-0.0270 \le -0.016955 \cdot AlO_2^{-1} - 0.033328 \cdot CO_3^{-2} \text{-} 0.016128 \cdot NO_3^{-1} - 0.058798 \cdot OH^{-1} - 0.02082 \cdot SO_4^{-2} - 0.02272 \cdot C_2O_4^{-2} \le -0.0251$								

Molar Ratios Fixed Relative to Sodium Molarity

$[NO_2]$	[K]	[F]	[COOH]	$[CrO_4]$	$[C_6H_7O_7]$ (citrate)	$[HOCH_2COO]$ (glycolate)	$[PO_4]$
0.267	0.0271	0.0197	0.0190	0.00419	0.00423	0.0212	0.00262

The composition factor space for Envelope C is shown in Table 3, along with the concentration of the species that were held fixed relative to that of sodium. Note that the Envelope C waste feed input to OLI was targeted at a Na molarity of 6.5 to avoid convergence issues with the dilution to 1.22 g/ml step. To calculate the molarity of the fixed species at another initial Na Molarity simply multiply the ratio term shown in Table 3 by the new desired initial Na molarity.

Table 3.   Definition for Envelope C Factor Space

	Mixture Variable Mass Fraction Ranges **Mass fraction relative to total mass of mixture variables**					**Process Variables**		
Variable	AlO_2^{-1} **mass fraction**	CO_3^{-2} **mass fraction**	NO_2^{-1} **mass fraction**	OH^{-1} **mass fraction**	SO_3^{-2} **mass fraction**	**[Na] (molar)**	**SBS / Feed (volumetric)**	**Temp (°C)**
minimum	0.0052	0.2984	0.3926	0.0828	0.0644	6	0.0	15
maximum	0.1319	0.3282	0.5131	0.1099	0.0733	10	2.0	66
charge constraint	$-0.0310 \le -0.016955 \cdot AlO_2^{-1} - 0.0333 \cdot CO_3^{-2} \text{ - } 0.02174 \cdot NO_2^{-1} - 0.058798 \cdot OH^{-1} \text{ - } 0.02082 \cdot SO_4^{-2} \le -0.0260$							

Molar Ratios Fixed Relative to Sodium Molarity

[Cl]	[F]	$[PO_4]$	$[C_2O_4]$	[K]	$[NO_3]$	[COOH]
0.0114	0.0168	0.00336	0.00241	0.00732	0.394	0.0238

In the treated feed evaporator experimental work, the waste feeds for all envelopes were created from recipes and then filtered. Since the state of the treated evaporator waste feed could be characterized in a number of ways, the choice was made to dilute the characterized waste feeds to 1.22 g/ml density to provide a common basis for the modeling. It is expected that the treated waste feed will be at or near this density after the pre-treatment. This density corresponds to a feed roughly at 5 Na M. The filtration step just simulates the pre-treatment filtration and precipitation removal with the outlet streams ultimately representing the treated waste feeds.

Predictive Physical Property Models and Validation Phase 1

This section shows the predictive models derived from the OLI simulations along with graphs of the simulation results versus the physical model predictions for each waste envelope. In each graph the design points used to fit the model are identified with blue open circles, the validation (OLH) points are identified by red asterisks, a solid red line identifies the predicted value +15%, and a solid green line identifies the predicted value -15%.

The physical property models for all the waste envelopes were able to meet the ±15% of predicted values criterion except for the Na molarity prediction for Envelope C. Even in this case, 96% of OLH points still fell within the ±15% border. So the model still does a fair job at predicting the sodium molarity for most cases.

Envelope A Predictive Models

All concentrations are in terms of molarity as shown in Table 4. The concentrations of the mixture variables (all species except Na) are expressed relative to a stream at a 5M Na concentration. (e.g., an [AlO_2] concentration of 2M in an 8M Na stream is first adjusted to an equivalent concentration in a 5M stream: 2M AlO_2*(5M Na / 8M Na) = 1.25M AlO_2) and then applied to the equation. The three process variables are [Na] (the bottoms concentrate Na molarity, as opposed to the treated evaporator feed stream Na concentration just mentioned), SBS/Feed (volumetric ratio of LAW SBS to treated waste feed flow, and Temp (the bottoms concentrate temperature).

Table 4. Valid Variable Ranges for Envelope A Models

	Mixture Variable Molar Ranges **Normalized to equivalent molarity at 5M Na**							**Process Variables**		
Variable	**[AlO_2] (molar at 5M Na)**	**[CO_3] (molar at 5M Na)**	**[F] (molar at 5M Na)**	**[NO_2] (molar at 5M Na)**	**[NO_3] (molar at 5M Na)**	**[OH] (molar at 5M Na)**	**[PO_4] (molar at 5M Na)**	**[Na] (molar)**	**SBS / Feed (volumetric)**	**Temp (^oC)**
minimum	0.207	0.326	0.00927	0.731	0.991	0.983	0.00632	6	0.0	15
maximum	1.12	0.686	0.236	1.59	2.08	2.89	0.0436	10	2.0	66

Envelope A bottoms concentrate slurry density at its steady state endpoint condition is represented by Equation 1 and shown in Figure 2.

Equation 1

$$\begin{aligned}\text{density}_{\text{EnvA}}\left[\frac{\text{g}}{\text{ml}}\right] = {} & 1.117\cdot x_{AlO2} + 1.110\cdot x_{CO3} + 1.075\cdot x_{F} + 1.072\cdot x_{NO2} + 1.096\cdot x_{NO3} + \\ & 0.9813\cdot x_{OH} + 1.141\cdot \text{x}_{\text{PO4}} \text{ -1.119E-3}\cdot Temp + \text{7.046E-3}\cdot SBS/Feed + \\ & 0.03258\cdot[Na] \text{ - 4.438E-5}\cdot(SBS/Feed\text{-1})\cdot(Temp\text{-40.5}) \text{ -} \\ & \text{1.150E-4}\cdot([Na]\text{-8})\cdot(Temp\text{-40.5})\end{aligned}$$

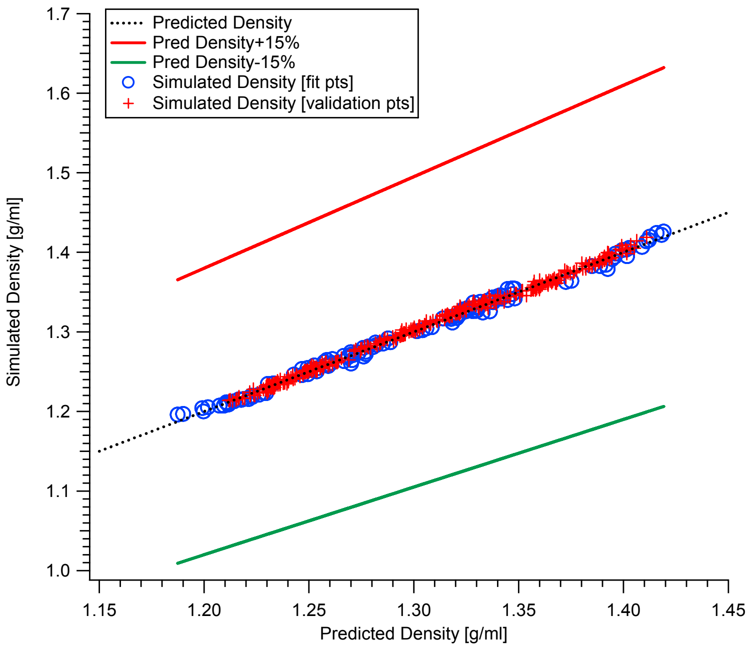

Figure 2. Simulated Density versus Predicted Density for Envelope A

Envelope A bottoms concentrate slurry conductivity at its steady state endpoint condition is represented by Equation 2 and shown in Figure 3.

Equation 2

$$\text{conductivity}_{\text{EnvA}}\left[\frac{\text{cal}}{\text{s}\cdot\text{cm}\cdot\text{K}}\right]=1.271\text{E-}3\cdot x_{AlO2}+1.326\text{E-}3\cdot x_{CO3}+1.392\text{E-}3\cdot x_{F}+1.304\text{E-}3\cdot x_{NO2}+$$

$$1.272\text{E-}3\cdot \text{x}_{\text{NO3}}+1.863\text{E-}3\cdot x_{OH}+1.402\text{E-}3\cdot x_{PO4}+3.087\text{E-}6\cdot Temp\ -$$

$$5.159\text{E-}6\cdot SBS/Feed\ -3.590\text{E-}6\cdot[Na]+$$

$$1.639\text{E-}6\cdot(Temp\text{-}40.5)\cdot(x_{OH}\text{-}0.1422)+$$

$$4.555\text{E-}4\cdot(x_{NO3}\text{-}0.4156)\cdot(x_{NO3}\text{-}0.4156)$$

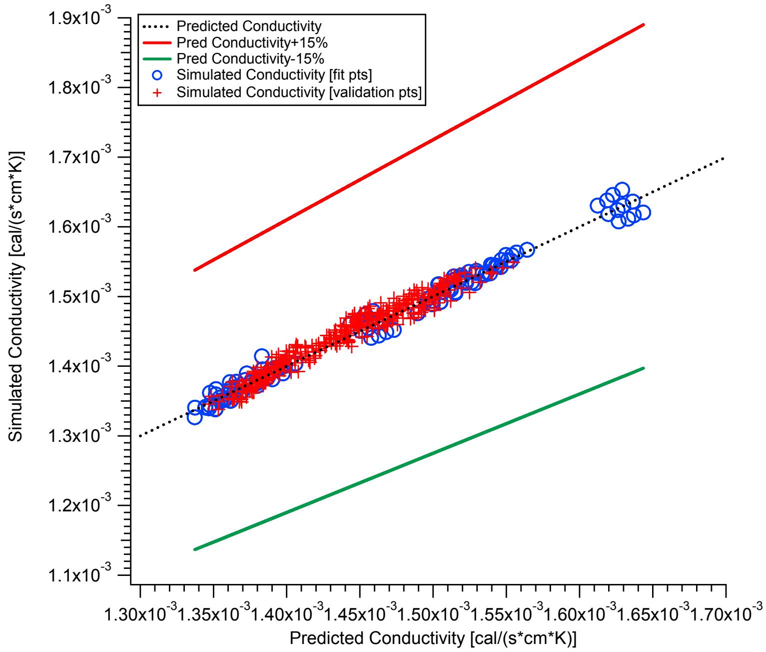

Figure 3. Simulated Conductivity versus Predicted Conductivity for Envelope A

Envelope A bottoms concentrate slurry heat capacity at its steady state endpoint condition is represented by Equation 3 and shown in Figure 4.

Equation 3

$$\mathrm{Cp}_{\mathrm{EnvA}}\left[\frac{\mathrm{cal}}{\mathrm{g}\ {}^{\mathrm{o}}\mathrm{C}}\right] = 0.8824{*}x_{AlO2} + 0.7165{*}x_{CO3} + 0.9227{*}x_{F} + 0.7351{*}x_{NO2} + 0.8640{*}x_{NO3} + 0.9586{*}x_{OH} + 0.8870{*}x_{PO4} - 3.443\mathrm{E}\text{-}3{*}SBS/Feed - 2.020\mathrm{e}\text{-}2{*}[Na] - 0.05588{*}(\mathrm{x}_{\mathrm{CO3}}-0.0510){*}([Na]-8) + -0.03794{*}(x_{NO2}-0.2331){*}([Na]-8) + 0.02999{*}(x_{NO3}-0.4156){*}([Na]-8) + 0.002053{*}(x_{NO3}-0.4156){*}(Temp-40.5) + 9.093\mathrm{e}\text{-}5{*}([Na]-8){*}(Temp-40.5)$$

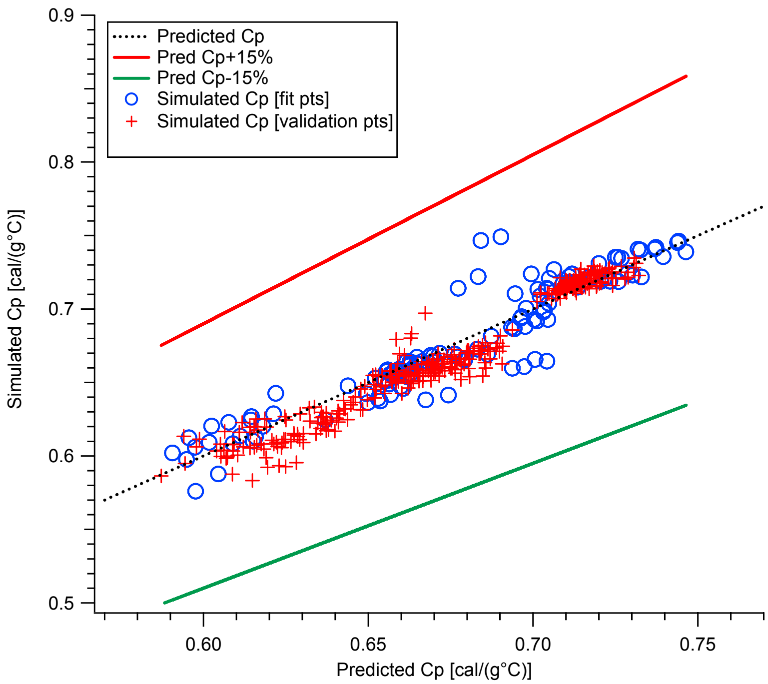

Figure 4. Simulated Cp versus Predicted Cp for Envelope A

Envelope A bottoms concentrate slurry Na molarity at its steady state endpoint condition is represented by Equation 4 and shown in Figure 5.

Equation 4

$$[\mathrm{Na}]_{\mathrm{EnvA}}\left[\frac{\mathrm{gmol}}{\mathrm{L}}\right] = -34.36\cdot x_{AlO2} - 34.10\cdot x_{CO3} - 33.09\cdot x_{F} - 32.95\cdot x_{NO2} - 33.72\cdot x_{NO3} - 30.24\cdot x_{OH} - 35.14\cdot x_{PO4} + 0.03444\cdot Temp - 0.2139\cdot SBS/Feed + 30.82\cdot Density + 0.1106\cdot(Density - 1.300)\cdot(Temp - 40.5) - 0.9262\cdot(Density - 1.300)\cdot(SBS/Feed - 1)$$

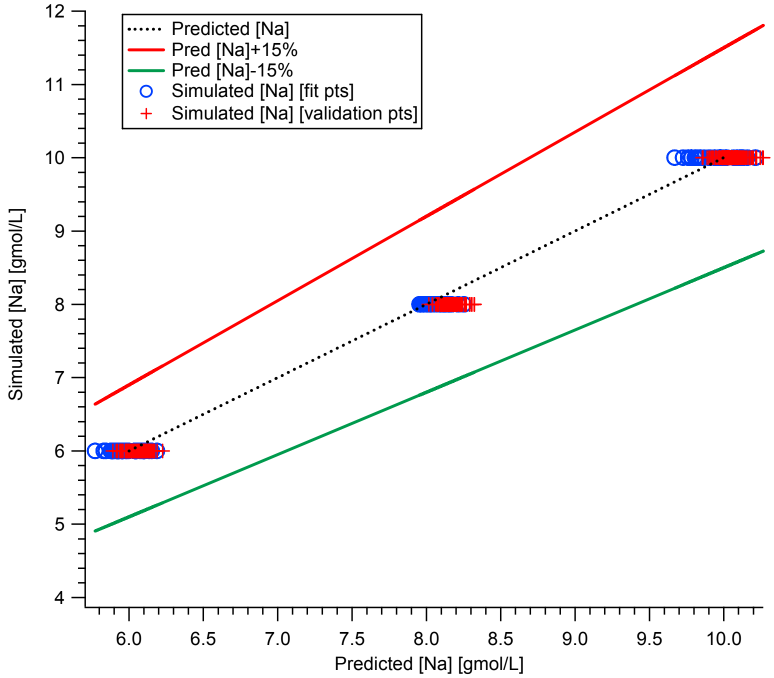

Figure 5. Simulated [Na] versus Predicted [Na] for Envelope A

Although no valid solids prediction model could be developed for the bottoms concentrate stream for Envelope A, the general behavior of the simulated points can be seen in Figure 6. As is evident from the graph, insoluble solids in the bottoms concentrate should not be a concern unless a high Na molarity like 10 M and a low temperature like 20 °C are targeted simultaneously.

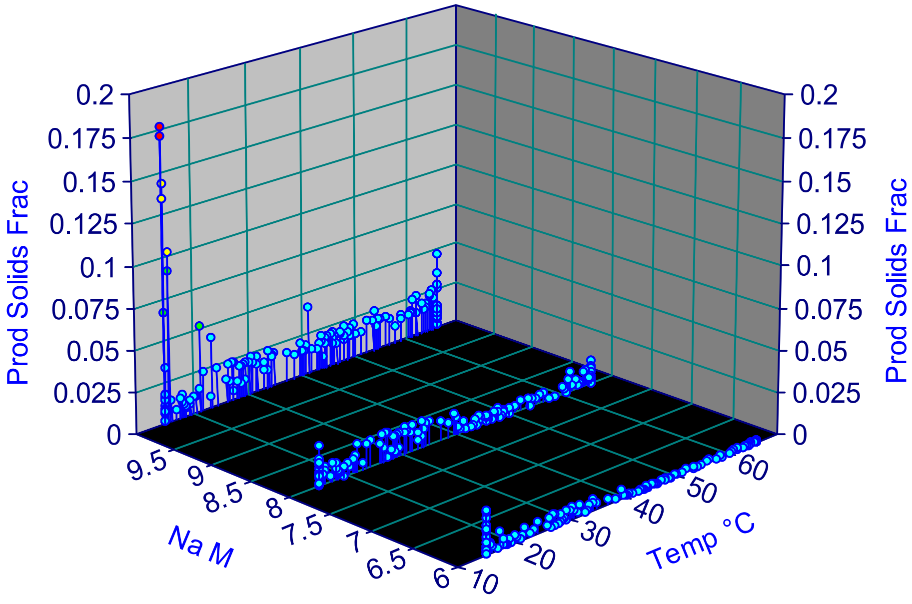

Figure 6. Envelope A Bottoms Solids Fraction versus Na Molarity and Temperature

Envelope B Predictive Models

All concentrations for the Envelope B model mixture variables listed in Table 5 are in terms of weight fraction relative to the total mass of all the mixture variables. The three process variables are [Na] (the bottoms concentrate Na molarity), SBS/Feed (volumetric ratio of LAW SBS to treated waste feed flow, and Temp (the bottoms concentrate temperature).

Table 5. Valid Variable Ranges for Envelope B Models

	Mixture Variable Mass Fraction Ranges **Mass fraction relative to total mass of mixture variables**						**Process Variables**		
Variable	AlO_2^{-1} **mass fraction**	CO_3^{-2} **mass fraction**	NO_3^{-1} **mass fraction**	OH^{-1} **mass fraction**	SO_4^{-2} **mass fraction**	$C_2O_4^{-2}$ **mass fraction**	**[Na] (molar)**	**SBS / Feed (volumetric)**	**Temp (°C)**
Min	0.0380	0.2529	0.3603	0.0928	0.1438	0.0000	6	0.0	15
Max	0.1107	0.2785	0.3755	0.1074	0.2152	0.0248	10	2.0	66

The Envelope B evaporator bottoms concentrate slurry density at its steady state endpoint condition is represented by Equation 5 and shown in Figure 7.

Equation 5

$$\text{density}_{\text{EnvB}}\left[\frac{\text{g}}{\text{ml}}\right] = 3.463\text{E-}3\cdot(\,SBS/Feed\ \text{- }1)\ \text{-}0.02774\cdot(Temp\ \text{- }45)/25) + 1.034\ \cdot x_{AlO2} + 1.009\cdot x_{CO3} + 0.9938\cdot x_{NO3} + 0.9362\cdot x_{OH} + 1.068\cdot x_{SO4} + 1.020\cdot x_{C2O4} + 0.04177\cdot[Na]$$

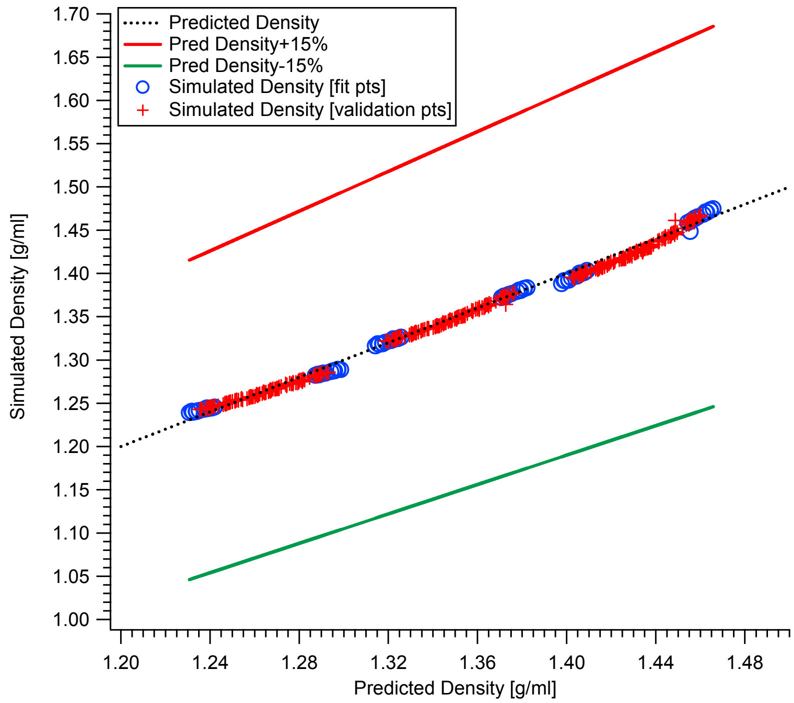

Figure 7. Simulated Density versus Predicted Density for Envelope B

The Envelope B evaporator bottoms supernate viscosity at its steady state endpoint condition is represented by Equation 6 and shown in Figure 8.

Equation 6

$$\text{visc}_{\text{EnvB}}[\text{cP}] = \text{Exp}\left(\frac{2122}{137.5 + \mathit{Temp}} + 0.2318 \cdot [Na] + 5.162 \cdot x_{OH} - 15.24\right) +$$
$$0.5203 \cdot [Na] - 4.817 \cdot x_{OH} + 0.08783 \cdot x_{OH} \cdot \mathit{Temp} - 4.700\text{E-}3 \cdot [Na] \cdot \mathit{Temp}$$

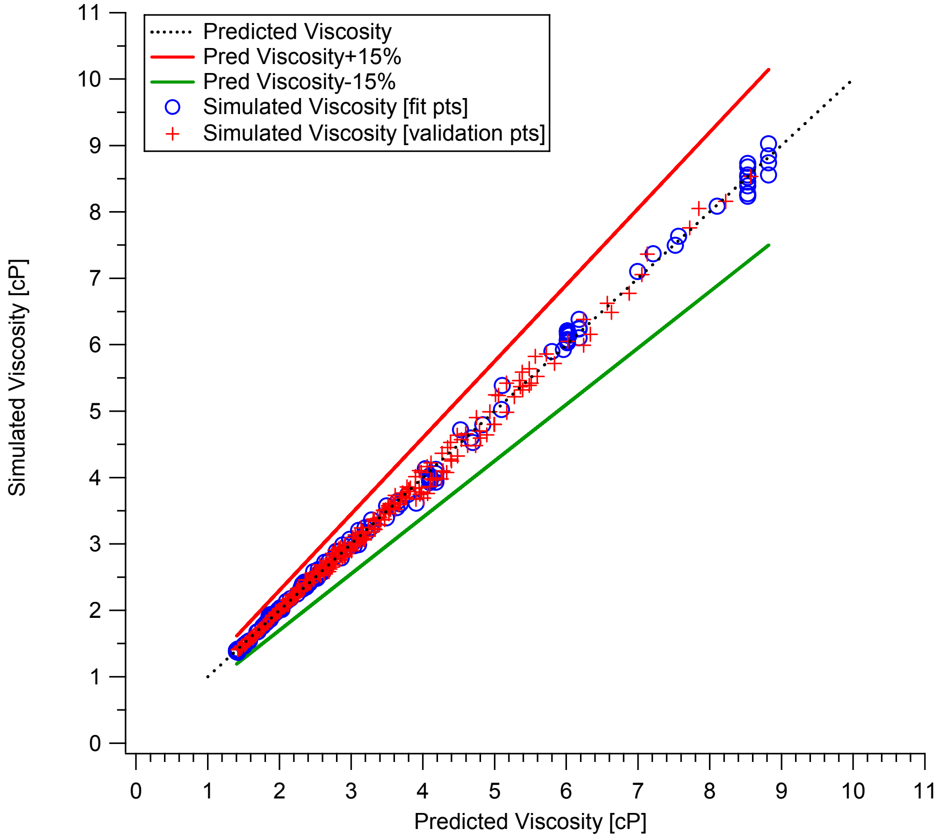

Figure 8. Simulated Viscosity versus Predicted Viscosity for Envelope B

The Envelope B evaporator bottoms concentrate slurry conductivity at its steady state endpoint condition is represented by Equation 7 and shown in Figure 9.

Equation 7

$$\text{conductivity}_{\text{EnvB}}\left[\frac{\text{cal}}{\text{s} \cdot \text{cm} \cdot \text{K}}\right] = 1.274\text{E-}3 \cdot x_{AlO2} + 1.355\text{E-}3 \cdot x_{CO3} + 1.432\text{E-}3 \cdot x_{NO3} + 1.674\text{E-}3 \cdot x_{OH} +$$
$$1.373\text{E-}3 \cdot x_{SO4} + 1.418\text{E-}3 \cdot x_{C2O4} - 1.041\text{E-}6 \cdot (\mathit{SBS} / \mathit{Feed} - 1) -$$
$$6.550\text{E-}6 \cdot [Na] - 1.785\text{E-}5 \cdot ([Na] - 8) \cdot (x_{AlO2} - 0.06883) +$$
$$3.853\text{E-}5 \cdot ([Na] - 8) \cdot (x_{OH} - 0.09767)$$

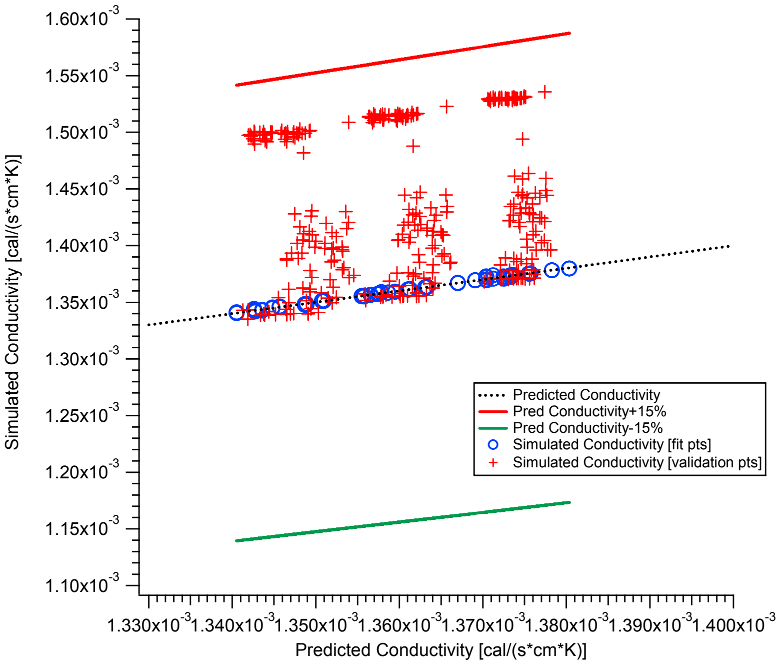

Figure 9. Simulated Conductivity versus Predicted Conductivity for Envelope B

Envelope B bottoms concentrate slurry heat capacity at its steady state endpoint condition is represented by Equation 8 and shown in Figure 10.

Equation 8

$$
\begin{aligned}
\mathrm{Cp}_{\mathrm{EnvB}}\left[\frac{\mathrm{cal}}{\mathrm{g}\ {}^{\mathrm{o}}\mathrm{C}}\right] = {} & -0.01526 \cdot x_{AlO2} + 1.168 \cdot x_{CO3} + 1.149 \cdot x_F + 0.9522 \cdot x_{NO2} + \\
& 1.398 \cdot x_{NO3} + 1.188 \cdot x_{OH} + 1.228 \cdot x_{PO4} - 7.754\mathrm{E}\text{-}2 \cdot SBS / Feed\ - \\
& 2.020\mathrm{e}\text{-}2 \cdot [Na] - 0.05588 \cdot (\mathrm{x}_{\mathrm{CO3}} - 0.0510) \cdot ([Na]-8) + \\
& -0.03794 \cdot (x_{NO2} - 0.2331) \cdot ([Na]-8) + 0.02999 \cdot (x_{NO3} - 0.4156) \cdot ([Na]-8) + \\
& 0.002053 \cdot (x_{NO3} - 0.4156) \cdot (Temp - 40.5) + 9.093\mathrm{e}\text{-}5 \cdot ([Na]-8) \cdot (Temp - 40.5)
\end{aligned}
$$

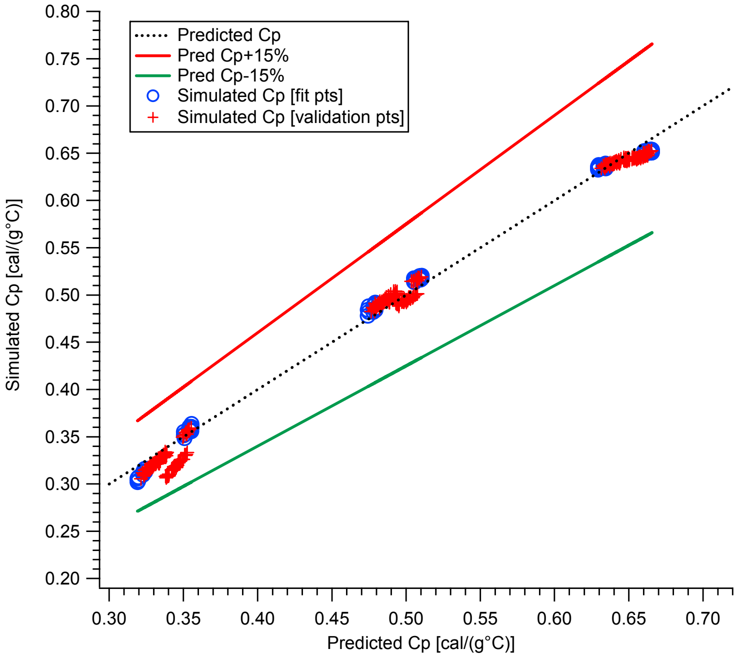

Figure 10. Simulated Cp versus Predicted Cp for Envelope B

The Envelope B evaporator bottoms concentrate slurry Na molarity at its steady state endpoint condition is represented by Equation 9 and shown in Figure 11.

Equation 9

$$[\mathrm{Na}]_{\mathrm{EnvB}}\left[\frac{\mathrm{gmol}}{\mathrm{L}}\right] = -0.08268\cdot(SBS/Feed\ -1) + 0.6680\cdot\frac{(Temp\ -45)}{25} - 25.34\cdot x_{AlO2} - 24.70\cdot x_{CO3} - 24.41\cdot x_{NO3} - 22.97\cdot x_{OH} - 26.14\cdot x_{SO4} - 25.03\cdot x_{C2O4} + 24.41\cdot Density - 0.3649\cdot(SBS/Feed\ -1)\cdot(Density - 1.348) + 1.854\cdot\frac{(Temp\ -45)}{25}\cdot(Density - 1.348)$$

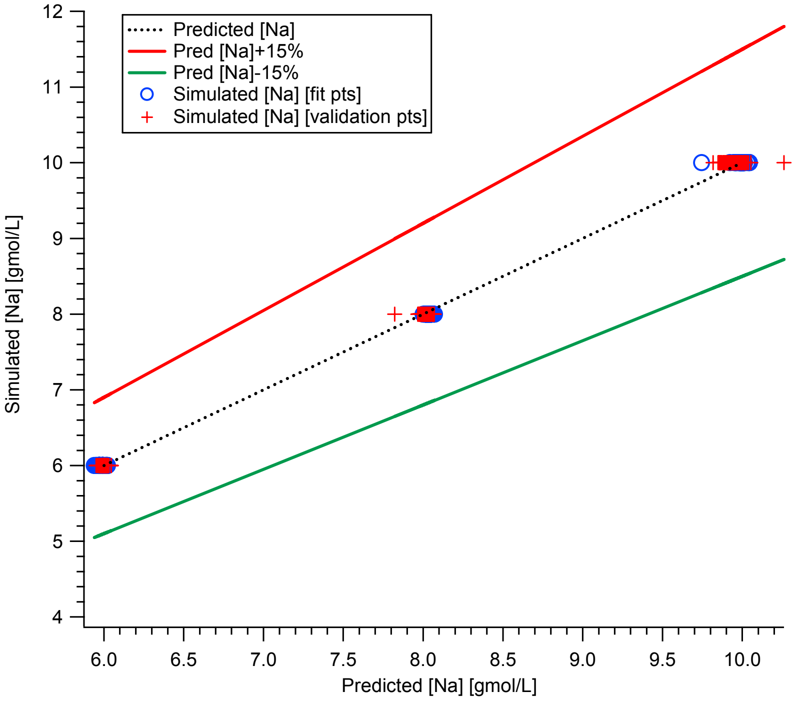

Figure 11. Simulated [Na] versus Predicted [Na] for Envelope B

Although no valid solids prediction model could be developed for the bottoms concentrate stream for Envelope B, the general behavior of the simulated points can be seen in Figure 12. The graph shows that for a temperature range of 15 to 66°C and a Na molarity range of 6 to 10 Na M, the fraction of insoluble solids in the bottoms stream is always below 3 wt-%. The graph also shows that the bottoms Na molarity concentration has the biggest impact on the amount solids that forms compared to temperature. The graph also shows that the majority of solids precipitate out between 20 and 40°C.

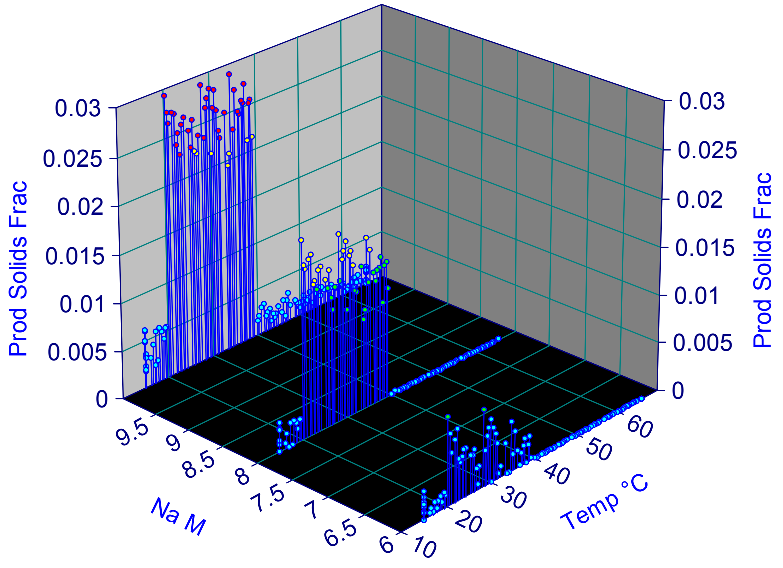

Figure 12. Envelope B Bottoms Solids Fraction versus Na Molarity and Temperature

Envelope C Predictive Models

Concentrations for the Envelope C model mixture variables listed in Table 6 are in terms of weight fraction relative to the total mass of all the mixture variables. The three process variables are [Na] (the bottoms concentrate Na molarity), SBS/Feed (volumetric ratio of LAW SBS to treated waste feed flow, and Temp (the bottoms concentrate temperature).

Table 6. Valid Variable Ranges for Envelope C Models

	Mixture Variable Mass Fraction Ranges **Mass fraction relative to total mass of mixture variables**					**Process Variables**		
Variable	AlO_2^{-1} **mass fraction**	CO_3^{-2} **mass fraction**	NO_2^{-1} **mass fraction**	OH^{-1} **mass fraction**	SO_3^{-2} **mass fraction**	**[Na] (molar)**	**SBS / Feed (volumetric)**	**Temp (°C)**
minimum	0.0052	0.2984	0.3926	0.0828	0.0644	6	0.0	15
maximum	0.1319	0.3282	0.5131	0.1099	0.0733	10	2.0	66

The Envelope C evaporator bottoms concentrate slurry density at its steady state endpoint condition is represented by Equation 10 and shown in Figure 13.

Equation 10

$$\begin{aligned}\text{density}_{\text{EnvC}}\left[\frac{\text{g}}{\text{ml}}\right] ={}& 0.01257\cdot(\mathit{SBS}/\mathit{Feed}\ -1) - 0.03233\cdot\frac{\mathit{Temp}\ -45}{25}\ - \\ & 1.765\text{E-}3\cdot(\mathit{SBS}/\mathit{Feed}\ -1)\cdot\frac{\mathit{Temp}\ -45}{25} + \\ & 1.074\cdot\ x_{\text{AlO2}} + 1.051\cdot x_{\text{CO3}} + 1.042\cdot x_{\text{NO2}} + 1.018\cdot x_{\text{OH}} + 1.132\cdot x_{\text{SO4}} + \\ & 0.03275\cdot[\mathit{Na}] - 2.685\text{E-}3\cdot([\mathit{Na}]-8)\cdot\frac{\mathit{Temp}\ -45}{25}\end{aligned}$$

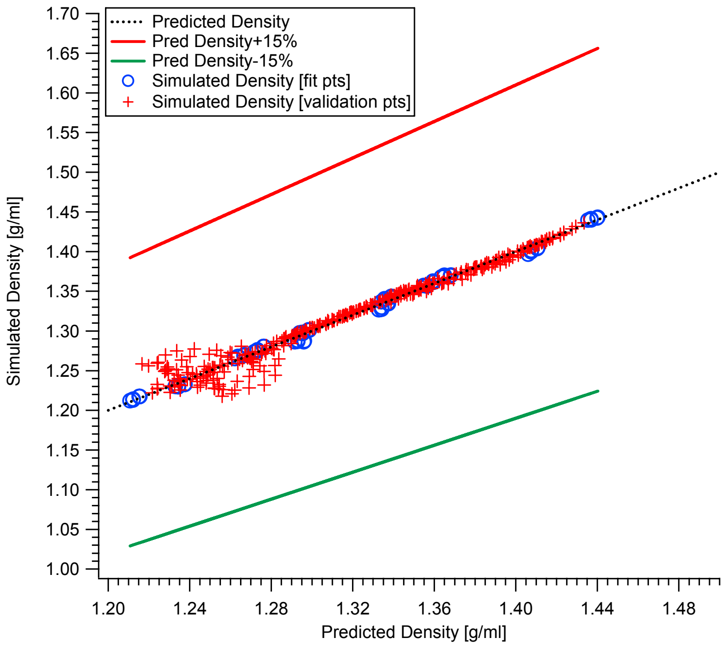

Figure 13. Simulated Density versus Predicted Density for Envelope C

The Envelope C evaporator bottoms supernate viscosity at its steady state endpoint condition is represented by Equation 11 and shown in Figure 14.

Equation 11

$$\text{visc}_{\text{EnvC}}[\text{cP}] = \text{Exp}\left(\frac{7418}{31.70 + \mathit{Temp}} + 0.2390 \cdot [Na] - 0.7285 \cdot x_{NO2} + \atop - 22.96 + -0.08727 \cdot SBS/Feed \right) + \\ 0.4093 \cdot [Na] - 0.4685 \cdot x_{NO2} - 2.672\text{E-}3 \cdot [Na] \cdot \mathit{Temp} - 0.04042 \cdot SBS/Feed$$

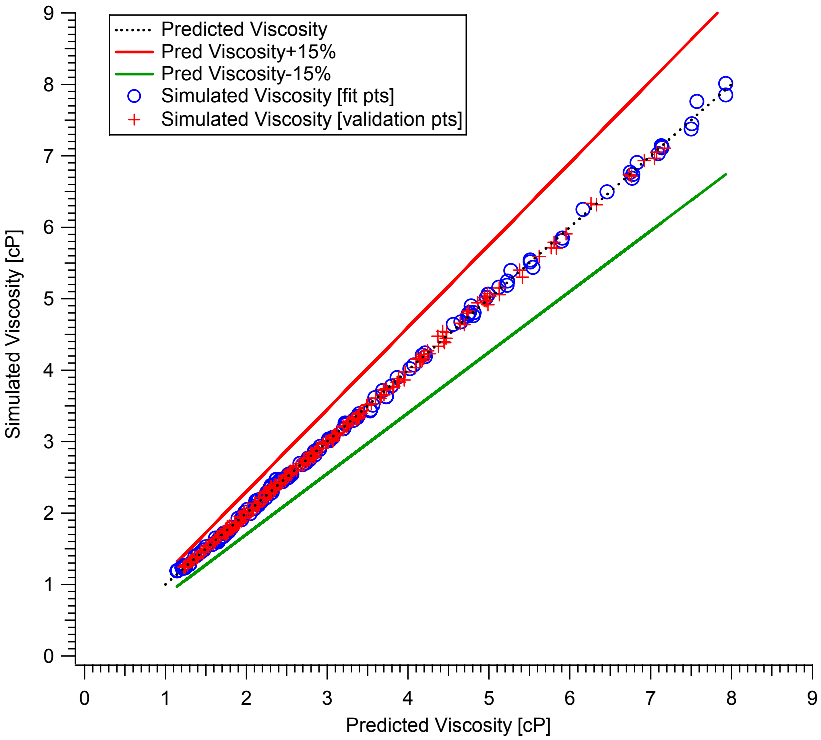

Figure 14. Simulated Viscosity versus Predicted Viscosity for Envelope C

The Envelope C evaporator bottoms concentrate slurry conductivity at its steady state endpoint condition is represented by Equation 12 and shown in Figure 15.

Equation 12

$$\text{conductivity}_{\text{EnvC}}\left[\frac{\text{cal}}{\text{s}\cdot\text{cm}\cdot\text{K}}\right] = \text{-7.282E-6}\cdot(\mathit{SBS/Feed}\text{ - 1}) \text{ - 1.498E-6}\cdot\frac{\text{Temp - 45}}{25} + -9.488\text{E-7}\cdot(\mathit{SBS/Feed}\text{ - 1})\cdot\frac{\mathit{Temp}\text{ - 45}}{25} + 1.318\text{E-3}\cdot x_{AlO2} + 1.468\text{E-3}\cdot x_{CO3} + 1.385\text{E-3}\cdot x_{NO2} + 1.602\text{E-3}\cdot x_{OH} + 1.258\text{E-3}\cdot x_{SO4} \text{ - 1.110E-5}\cdot[\text{Na}]$$

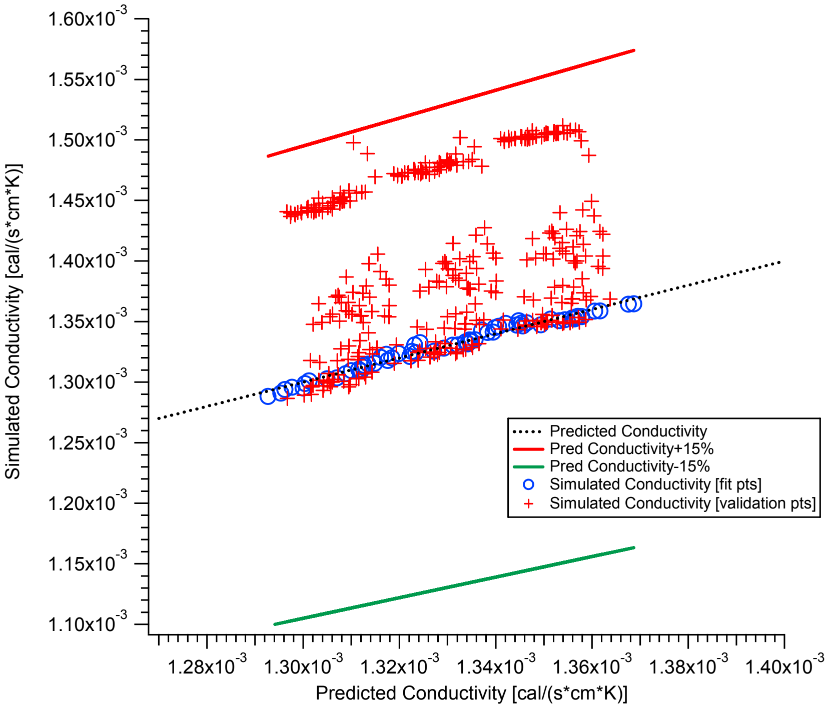

Figure 15. Simulated Conductivity versus Predicted Conductivity for Envelope C

Envelope C bottoms concentrate slurry heat capacity at its steady state endpoint condition is represented by Equation 13 and shown in Figure 16.

Equation 13

$$\text{Cp}_{\text{EnvC}}\left[\frac{\text{cal}}{\text{g }^{\text{o}}\text{C}}\right] = -0.008923\cdot\frac{\mathit{Temp}\text{ - 45}}{25} + 0.9093\cdot x_{AlO2} + 0.8587 * x_{CO3} + 0.8621\cdot x_{NO2} + 1.005\cdot x_{OH} + 0.9629\cdot x_{SO4} \text{ -0.03087}\cdot[\mathit{Na}]$$

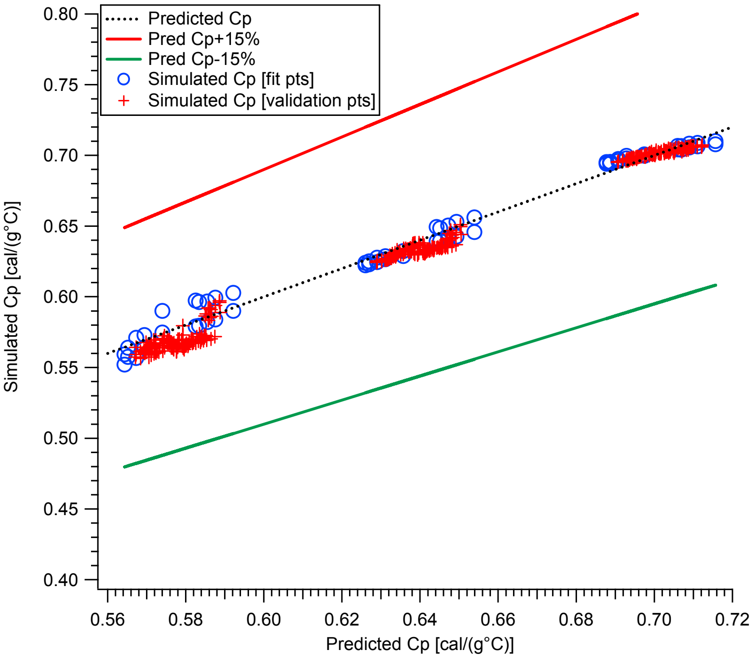

Figure 16. Simulated Cp versus Predicted Cp for Envelope C

The Envelope C evaporator bottoms concentrate slurry Na molarity at its steady state endpoint condition is represented by Equation 14 and shown in Figure 17.

Equation 14

$$[\mathrm{Na}]_{\mathrm{EnvC}}\left[\frac{\mathrm{gmol}}{\mathrm{L}}\right] = -0.3663\cdot(\mathit{SBS}/\mathit{Feed} - 1) + 0.9644\cdot\frac{\mathit{Temp} - 45}{25} - 33.00\cdot x_{AlO2} - 31.33\cdot x_{CO3} - 31.88\cdot \mathrm{x}_{\mathrm{NO2}} - 32.29\cdot \mathrm{x}_{\mathrm{OH}} - 34.16\cdot \mathrm{x}_{\mathrm{SO4}} + 30.49\cdot \mathit{Density} - 1.764\cdot(\mathit{SBS}/\mathit{Feed} - 1)\cdot(\mathit{Density} - 1.322) + 2.327\cdot\frac{\mathit{Temp} - 45}{25}\cdot(\mathit{Density} - 1.322)$$

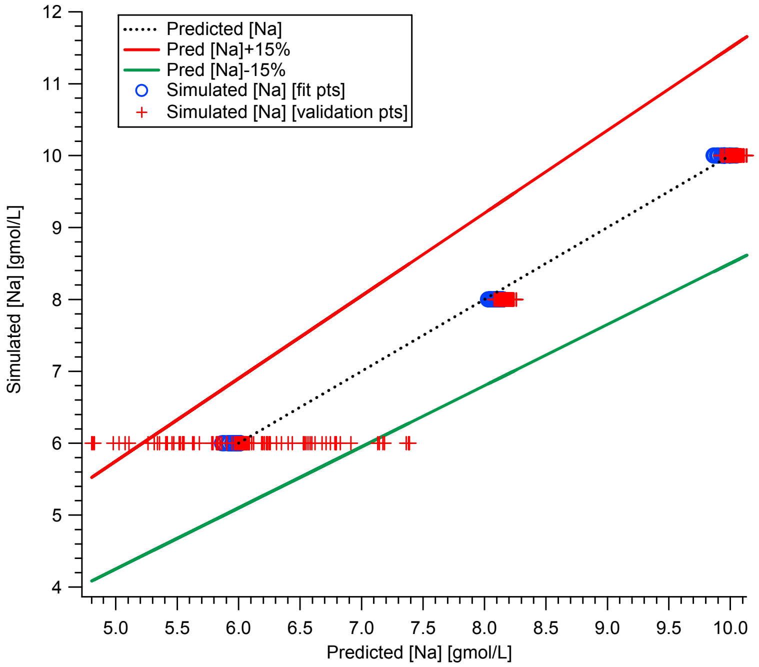

Figure 17. Simulated [Na] versus Predicted [Na] for Envelope C

Although no valid solids prediction model could be developed for the bottoms concentrate stream for Envelope C, the general behavior of the simulated points can be seen in Figure 18 and Figure 19. The graphs show that the bottoms Na molarity concentration and the SBS/Feed ratio have the biggest impact on the amount solids that form compared to temperature. As the Na molarity or the SBS/Feed ratio increase the amount of insoluble solids also increases.

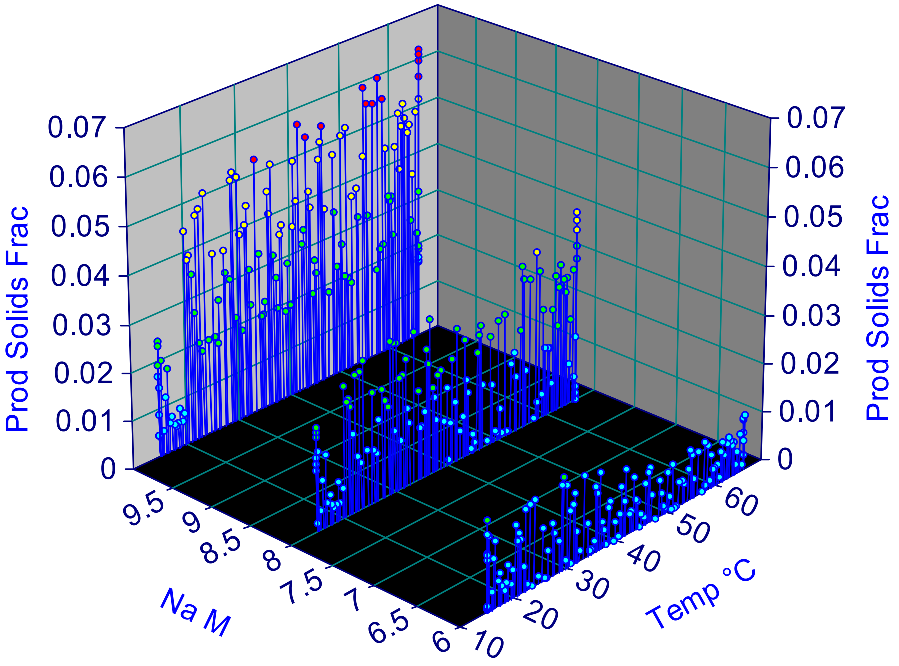

Figure 18. Envelope C Bottoms Solids Fraction versus Na Molarity and Temperature

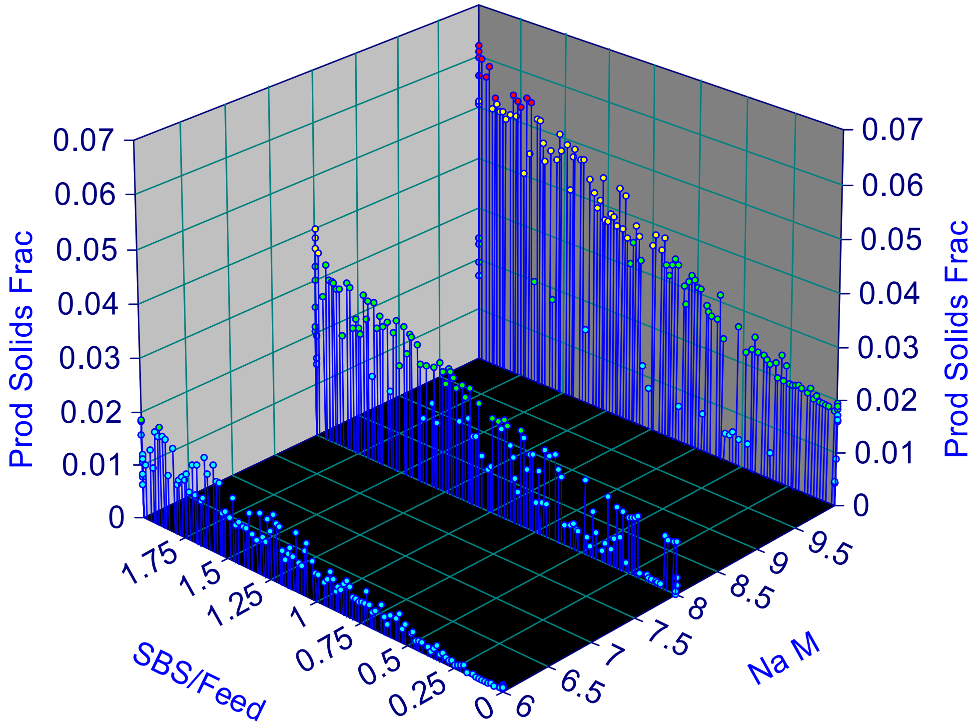

Figure 19. Envelope C Bottoms Solids Fraction versus Na Molarity and SBS/Feed

Comparison of Simulation Results with Experimental Results

Experimental work was completed as part of Task S-94 to generate data concerning the evaporation of the LAW treated wastes for Envelopes A, B, and C.[7] Several physical properties were measured for the various waste feeds against which the prediction models discussed earlier can be compared.

The density predictions for Envelope A were within +/-6% of the measured values for the bottoms concentrate with a Na molarity between 2 and 10.

The comparison of the measured versus predicted viscosities was not as good as for the densities. The best predictions were for 25°C and for Na molarities between 6 and 10. The viscosity predictions for Envelope A were within +/-20% for the 25°C measurements but only +/-50% for 15°C and 60°C tests. It is expected that the lower and higher temperature extremes produced solids that are not accounted for by the viscosity prediction since it is based only on the supernate phase of the bottoms concentrate. For the 15°C and 60°C viscosity measurements versus predictions, less than 40% of the test points had the large +/-50% error while the remaining 60% of the test points fell within +/-20%. Another factor contributing to the difference is that the viscosity prediction model was based on bottoms concentrate ranging from 6 to 10 M Na while the test data covered 2 to 10 M Na.

The thermal conductivity predictions for Envelope A were within +/-25% of all the measured values for the bottoms concentrate with a Na molarity between 2 and 8 except for 3 samples. This large discrepancy is due in part to the fact that the simulated conductivity is for the supernate only, whereas the measured conductivity is for the entire slurry (supernate plus solids). Prior modeling work[6] showed that the experimental conductivity has a standard deviation of 6.5% (about the value of water). The simulated conductivities are based on correction factors for the conductivity of water using various anions/cations as defined in Perry's Chemical Handbook.[12] The simulated conductivities for all envelopes fell within a 3% standard deviation of the value of water. Since the measurement error is higher than this value, the predicted conductivities cannot be distinguished from those of water. Therefore, there is no need to use the complicated prediction equation for conductivity when statistically a prediction for the conductivity of water is just as accurate.

The heat capacity predictions for Envelope A were within +/-15% of all the measured values for the bottoms concentrate with a Na molarity between 2 and 8 except for 4 samples. Part of the reason for the 4 points that exceeded +/-15% is that the experimental heat capacities are for the supernate, while those predicted are for the slurry (supernate plus solids). Analyses of the experimental samples show evidence of solids which in turn helps explain some of the deviation from predicted values.

The sodium molarity predictions for Envelope A were within +/-15% of the measured values for the bottoms concentrate with a Na molarity between 6 and 10. However, for the initial samples at 2 molar, the predicted values are within +/-50%. This discrepancy is due to the prediction being derived from data with Na M between 6 and 10, and thus should not be expected to do well when extrapolated down to 2 M. Another reason for the large discrepancy is that it is difficult to derive a predictive relationship relating waste feed composition (dry basis), SBS/Feed ratio, bottoms temperature, and bottoms density to bottoms Na molarity.

No accurate prediction equations for the solubility of the evaporator bottoms stream in terms of the total insoluble solids present could be derived in either linear or nonlinear forms for Envelopes A, B, or C. Several attempts were made to include nonlinear and linear terms in the prediction fits, but the waste feed compositions, SBS to Waste Feed ratio, the bottoms temperature, and Na molarity did not provide enough data about this phenomena. However, some general observations were made from the simulations.

For Envelope A, about 35% of the simulated values (16 out of 336 total – including fit and validation points) had bottoms insoluble solids greater than 1 wt% but only about 10% of the simulated values (33 points) had insoluble solids greater than 2 wt%. Of this 10% segment, 64% of the values were between 2 wt% and 5 wt%, 9% of the values were between 5 wt% and 10 wt%, and 27% were between 10 wt% and 20wt%. The high weight percent insoluble solids were only observed at bottoms temperatures less than 20°C and sodium molarities greater than 8. The primary salts were sodium oxalate, sodium carbonate, sodium sulfate-carbonate, sodium fluoride, sodium aluminosilicate gelatin (NASGEL), and sodium nitrate. The sodium nitrate only came out at 10 M Na concentrations. For the simulated runs, NASGEL solids appear in the bottoms concentrate stream over a wider % range at 6 Na M than 8 Na M and 10 Na M. In fact at 10 Na M, no NASGEL forms for the simulated runs performed. The NASGEL solids appear at all tested bottoms temperatures. The SBS/Feed ratio has no effect on NASGEL formation at 10 Na M. Increasing the SBS/Feed ratio above 1.75 slightly increases the chance of NASGEL formation. Increasing the SBS/feed ratio above 0.5 greatly increases the chance of NASGEL formation at 6 Na M. Please note that due to the variability in the data, a low Na M like 6 and a high SBS/Feed ratio does not guarantee that NASGEL will form. The experimental solids measurements from prior work[7] were only qualitative and not quantitative. This fact makes comparison of simulated solids predictions with experimental results difficult.

The density predictions for Envelope B were within +/-5% of the measured values for the bottoms concentrate with a Na molarity between 1.2 and 8.

The viscosity predictions for Envelope B did not match the experimental values as well as those for Envelope A. At a temperature of 15°C the predicted viscosity varied +/-60% of the measured value. At a temperature of 25°C the predicted viscosity varied +/-70% of the measured value. At a temperature of 60°C the predicted viscosity varied +/-50% of the measured value. These bad matches are all at points less than 6 Na M and the viscosity prediction model was based on bottoms concentrate ranging from 6 to 10 M Na. It is also expected that the lower and higher temperature extremes produced solids that are not accounted for by the viscosity prediction since it is based only on the supernate phase of the bottoms concentrate. To obtain a better predictor of viscosity, an accurate count of the solids in each sample plus a solids correction term derived from experimental results would need to be included. Prior modeling work[6] for the waste feed evaporator showed that when the supernate viscosity was measured experimentally and compared with modeling predictions there was relatively good agreement (within +/- 15%).

The thermal conductivity predictions for Envelope B were within +/-25% of the measured values for the bottoms concentrate with a Na molarity between 1.2 and 5 except for four samples. This large discrepancy is due in part that the simulated conductivity is for the supernate only, whereas the measured conductivity is for the entire slurry (supernate plus solids). Prior modeling work[6] showed that the experimental conductivity has a standard deviation of 6.5% (about the value of water). The simulated conductivities are based on correction factors for the conductivity of water using various anions/cations as defined in Perry's Chemical Handbook.[12] The simulated conductivities for all envelopes fell within a 3% standard deviation of the value of water. Since the measurement error is higher than this value, the predicted conductivities cannot be distinguished from those of water. Therefore there is no need to use the complicated prediction equation for conductivity when statistically a prediction for the conductivity of water is just as accurate.

The heat capacity predictions for Envelope B were within +/-15% of the measured values for the bottoms concentrate with a Na molarity between 1.2 and 5.

The sodium molarity predictions for Envelope B were within +/-15% of the measured values for the bottoms concentrate with a Na molarity between 6 and 10. . However, for the initial samples at 2 molar, the predicted values are within +/-55%. This discrepancy is again due to the fact that the model prediction was based on simulated data with Na M between 6 and 10. Another reason for the large discrepancy is that it is difficult to derive a predictive relationship relating waste feed composition (dry basis), SBS/Feed ratio, bottoms temperature, and bottoms density to bottoms Na molarity.

No accurate prediction equations for the solubility of the evaporator bottoms stream in terms of the total insoluble solids present could be derived for Envelopes A, B, or C. Several attempts were made to include nonlinear and linear terms in the prediction fits, but the waste feed compositions, SBS to waste feed ratio, the bottoms temperature and Na molarity did not provide enough data to characterize these phenomena. However, some general observations were made from the simulations. For Envelope B, about 21% of the simulated values (83 out of 399 total – including fit and validation points) had bottoms insoluble solids greater than 1 wt% but only about 11% of the simulated values (42 points) had insoluble solids greater than 2 wt%. None of the predicted values went over 3 wt%. The insoluble solids only went above 2 wt% when the Na molarity went above 8 M. At 6 M Na the solids stayed below 1 wt%, at 8 M the solids stayed below 2 wt%, and at 10 M Na the solids stayed below 3 wt%. More solids appear to come out between 20 °C and 40 °C than the other temperatures. The primary salts were aluminum hydroxide, sodium oxalate, sodium fluorosulfate, and sodium fluoride.

The density predictions for Envelope C were within +/- 11% of the measured values for the bottoms concentrate with a Na molarity between 2 and 10.

The viscosity predictions for Envelope C were not good as Envelope A, with errors between the measured and predicted values ranging from 20% to 70%. It is estimated that part of this error is due to the prediction being based on simulated values between 6 and 10 molar. It is also expected that the lower and higher temperature extremes produced solids that are not accounted for by the viscosity prediction since it is based only on the supernate phase of the bottoms concentrate. A better predictor of viscosity could be obtained by getting an accurate count of the solids in each sample plus a solids correction term derived from experimental results would need to be included. Prior modeling work[6] for the waste feed evaporator showed that when the supernate viscosity was measured experimentally and compared with modeling predictions, relatively good agreement (within +/- 15%) was obtained.

The thermal conductivity predictions for Envelope C were within +/- 20% of the measured values for the bottoms concentrate with a Na molarity between 2 and 8 except for 3 samples. The discrepancy for the 3 samples outside the +/-20% range is due in part to the fact that the simulated conductivity is for the supernate only where as the measured conductivity is for the entire slurry (supernate plus solids). Prior modeling work[6] showed that the experimental conductivity has a standard deviation of 6.5% (about the value of water). The simulated conductivities are based on correction factors for the conductivity of water using various anions/cations as defined in Perry's Chemical Handbook.[12] The simulated conductivities for all envelopes fell within a 3% standard deviation of the value of water. Since the measurement error is higher than this value, the predicted conductivities cannot be distinguished from those of water. Therefore there is no need to use the complicated prediction equation for conductivity when statistically a prediction for the conductivity of water is just as accurate.

The heat capacity predictions for Envelope C were within +/- 10% of the measured values for the bottoms concentrate with a Na molarity between 2 and 8.

The sodium molarity predictions for envelope C were worse than for the other envelopes only coming within +/- 32% of the measured values for the bottoms concentrate with a Na molarity between 2 and 10. This poor comparison was expected since the Na molarity prediction did not satisfy the +/-15% of the predicted values criterion even after adding some of the validation points to the fits to try to capture some nonlinear behavior. One reason for the large discrepancy is because it is difficult to derive a predictive relationship relating waste feed composition (dry basis), SBS/Feed ratio, bottoms temperature, and bottoms density to bottoms Na molarity.

Because of slight differences in experimental runs and simulation runs no points are exact matches. For Envelope C, about 60% of the simulated values (242 our of 405 points – including fit and validation points) had bottoms insoluble solids greater than 1 wt%, but only about 36% of the simulated values (145 points) had insoluble solids greater than 2 wt%. Of this 36% segment, 83% of the values were between 2 wt% and 5 wt%, while the remaining 17% of the values were between 5 wt% and 7 wt%. The higher solids weight percents were observed at NA M greater than 8. Temperatures have a much smaller impact on the solubility than the Na molarity. The primary salts were calcium fluoride, hydrosodalite, sodium oxalate, sodium carbonate, sodium fluorosulfate, sodium sulfate-carbonate, sodium fluoride, sodium aluminosilicate gelatin (NASGEL), and sodium nitrate. For the simulated runs, NASGEL solids appear in the bottoms concentrate stream over a wider % range at 10 Na M than 8 Na M and 6 Na M. For all sodium molarities simulated, the % NASGEL in the bottoms stream stays below 1.2%. The NASGEL solids range between 0 and 1.2% for bottoms temperatures between 15°C and 66 °C. Increasing the SBS/Feed ratio above 0.5 for the 10 Na M bottoms concentrate increases the chance of NASGEL formation. Increasing the SBS/Feed ratio above 0.25 for the 8 Na M bottoms concentrate increases the chance of NASGEL formation. For the 8 Na M bottoms concentrate NASGEL begins to form at lower SBS/Feed ratios but the % NASGEL at the highest SBS/Feed ratio is less than at 10 Na M. The 6 Na M bottoms concentrate shows NASGEL formation starting around SBS/Feed of 0.15 and increasing as SBS/Feed ratio increases. Going from 10 Na M bottoms concentrate down to 8 Na M then 6 Na M, the maximum amount of NASGEL formed at the highest SBS/Feed ratio decreases along with the Na M. Please note that due to the variability in the data, a low Na M like 6 and a high SBS/Feed ratio like 2 can still form more NASGEL than a higher Na M at the same SBS/Feed ratio.

Additional experiments were performed with AW-101 radioactive simulant.[8] The physical property prediction models for Envelope A were used to compare measured versus predicted values from this experimental work. These comparisons are shown in Table 7. The Na M predictions for the experimental samples other than the feed are not very good. Since the experimental samples were taken as the process was still being evaporated and not at steady state, the Na M predictions would not be expected to be very good since they are based on steady state simulated conditions. The density predictions are within +/-15% which is a good indicator of the ability of OLI to predict density, at least within an acceptable range.

The predicted viscosities are off by as much as 50% from the measured values. Since the viscosity prediction has a strong dependence on Na molarity and represents the equilibrium value, it is not surprising the predicting values are off as indicated. In the experiment, samples were pulled at various bottom concentrations which most likely did not represent the process at equilibrium. OLI is a steady state simulator and thus any predictions derived from its results represent steady state points. Also the viscosity can be strongly influenced by solids which can cause the large discrepancies seen here. The predicted heat capacities are within +/-20%.

Table 7. Comparisons of AW-101 Radioactive Experimental Measured Values versus Envelope A Predictions

AW101 Test ID	Meas Temp	Meas Press [mmHg]	SBS/Feed	Measured Na M	Predicted Na M	% Diff b/n Meas/ & Pred Na M	Measured Density [g/ml]	Predicted Density [g/ml]	% Diff b/n Meas/Pred Density	Meas visc [cP]	Pred Visc [cP]	% Diff b/n Meas/Pred Visc	Meas Cp [supernate] [cal/g°C]	Meas Cp [slurry] [cal/g°C]	Pred Cp [supernate] [cal/g°C]	% Diff b/n Meas/Pred Cp
AW101007	44.9	64.0	1.2	7.0	10.3	-48.5%	1.36	1.25	7.8%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
AW101008	47.1	72.9	1.2	7.0	10.4	-49.8%	1.36	1.25	8.0%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
AW101009	50.1	80.5	1.2	7.0	10.6	-51.6%	1.36	1.25	8.2%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
AW101010	52.3	60.2	1.9	7.6	11.1	-46.0%	1.38	1.27	7.9%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
feed	25	760.0	1.9	2.1	1.4	33.2%	1.08	1.11	-3.1%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
AW101011	55.6	71.6	1.9	7.6	11.2	-47.9%	1.38	1.27	8.2%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
AW101012	58.4	80.5	1.9	7.6	11.4	-49.5%	1.38	1.26	8.4%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
AW101013	62.7	75.4	1.2	10.4	18.0	-73.2%	1.57	1.34	14.7%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
feed	25	760.0	1.2	2.2	2.0	8.8%	1.10	1.11	-1.0%	n/a	n/a	n/a	n/a	n/a	n/a	n/a
visc pt	25	760.0	1.2	n/a	n/a	n/a	n/a	n/a	n/a	7.1	3.7	47.9%	n/a	n/a	n/a	n/a
visc pt 2	25	760.0	1.9	n/a	n/a	n/a	n/a	n/a	n/a	8.7	4.2	52.2%	n/a	n/a	n/a	n/a
Cp pt-Blend 1	50	760.0	1.2	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.78	0.81	0.64	20.97%
Cp pt 2-Blend 2	50	760.0	1.9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	0.79	0.76	0.65	14.70%

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