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WASTE FEED EVAPORATION PHYSICAL PROPERITIES MODELING (U)

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF ACRONYMS

FEP	Hanford RPP-WTP Waste Feed Evaporator Process
GCWB	The Geochemist's Workbench
IX	Ion Exchange
HLW	High Level Waste
LAW	Low Activity Waste
NAS gel	Sodium Aluminosilicate gelatin
OLH	Orthogonal Latin Hypercube
OLI/ESP	OLI Environmental Simulation Package Software
TF-COUP	Tank Farm - Contractor Operation and Utilization Plan
SBS	Submerged Bed Scrubber
Sr/TRU	Strontium/Transuranic
UF	Ultra-Filtration
VRF	Volume Reduction Factor
XRD	X-Ray Diffraction

1.0 SUMMARY OF TESTING

1.1 OBJECTIVES

This document describes the waste feed evaporator (FEP) modeling work done as requested in the Waste Feed Evaporation and Physical Properties Modeling[1] test specification and specified in the Task Technical and Quality Assurance Plan for Waste Feed Evaporation and Physical Property Modeling[2] (items C, E, F, G, and H) for the R&T Test Scoping Statement S-89 in support of the Hanford River Protection Project (RPP) Waste Treatment Plant (WTP) project. A private OLI database (ZEOLITE) was developed and used in this work in order to include the behavior of aluminosilicates such a NAS-gel in the OLI/ESP simulations, in addition to the development of the mathematical models.

Mathematical models were developed that describe certain physical properties in the Hanford RPP-WTP waste feed evaporator process (FEP) for envelopes A, B/D, and C. In particular, models were developed for the feed stream to the first ultra-filtration step characterizing it's heat capacity, thermal conductivity, and viscosity (items E, F,and G respectively of the task plan), as well as the density of the evaporator contents (item C of the task plan). The scope of the task was expanded to include the volume reduction factor across the waste feed evaporator (total evaporator feed volume / evaporator bottoms volume). All the physical properties were modeled as functions of the waste feed composition, temperature, and the HLW SBS recycle volumetric flow rate relative to that of the waste feed. The goal for the mathematical models was to predict the physical property to within ±15% of the predicted simulation value with a confidence of 80%.

The simulation model approximating the FEP process used to develop the correlations was relatively complex, and not possible to duplicate within the scope of the bench scale evaporation experiments. Therefore, simulants were made of 13 design points (a subset of the points used in the model fits) using the compositions of the ultra-filtration feed streams as predicted by the simulation model. The chemistry and physical properties of the supernate (the modeled stream) as predicted by the simulation were compared with the analytical results of experimental simulant work as a method of validating the simulation software (item H of the task plan).

Although the task plan calls for the derivation of additional physical property models (items A, B and D of the task plan), the nature of the pre-treatment process made it either unnecessary or irrelevant, and is discussed in section 2.1. Composition data for AY-102 did not exist following the transfer of C106 to AY-102, which was being characterized at the time of this report. Because this tank composition will be used in the upcoming integrated pilot test, a decision was made to include the AY-102 modeling work as part of the pilot test.

1.2 CONDUCT OF TESTING

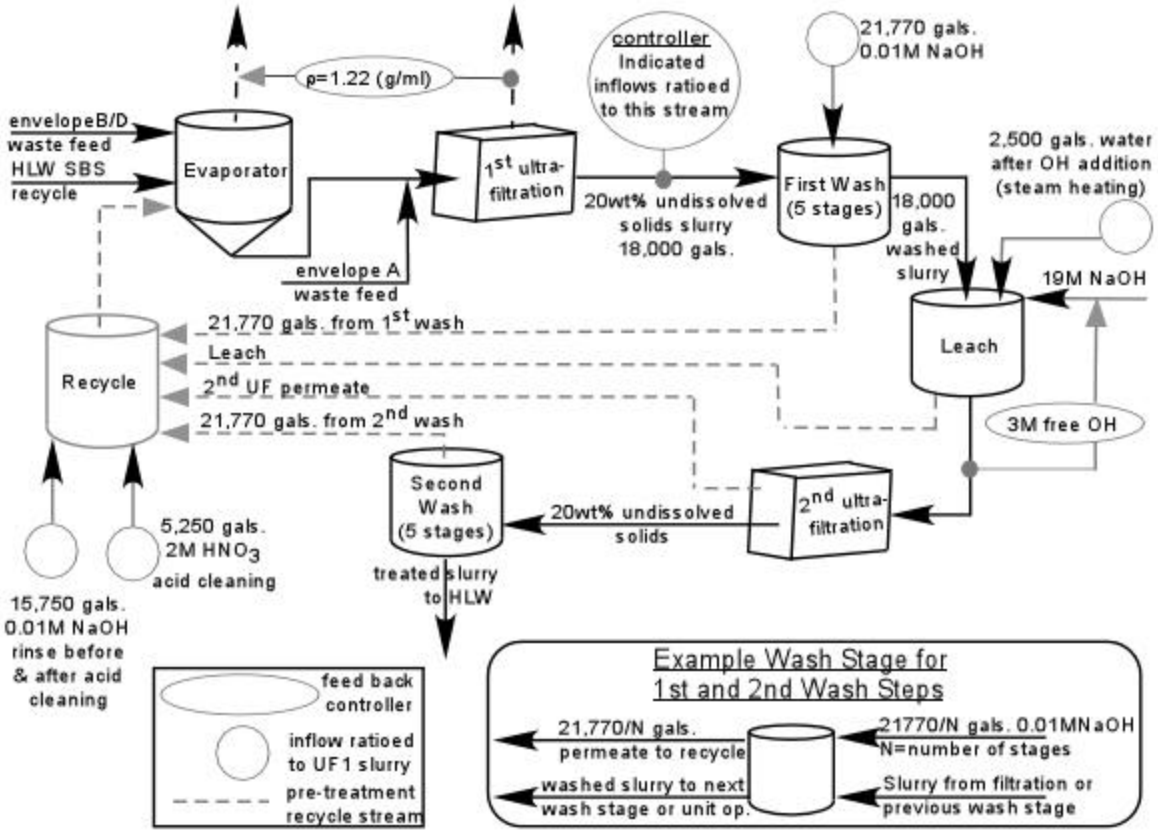
A different set of physical property models were developed for each of the three envelopes. The model variables are the waste feed composition, ultra-filtration feed stream temperature

(20 – 70°C), and the volumetric flow ratio of HLW SBS recycle relative to the waste feed (0 – 2). The matrices were generated assuming that the physical properties could be modeled using polynomials that are linear in composition, and up to second order with respect to the process variables (i.e. temperature, etc.). However, nonlinear (exponential) fits proved better for the viscosity.

Envelope A was divided into what we designate here as sub-envelope A-a (represented by tanks AP-101, AN-104, AN-105, SY-101, AN-103, AW-101, and AW-104) and sub-envelope A-b (represented by tank AY-102, the modeling for this envelope was originally part of this work, but was moved to the integrated pilot testing). Models were also developed for envelope B/D (represented by tanks AZ-101 and AZ-102) and envelope C (represented by tanks AN-102 and AN-107).

The model flow-sheet for the waste feed evaporator varies slightly depending on the envelope being simulated. The simulation flow-sheet for envelopes A and B/D is shown in Figure 1. The flow-sheet for envelope C excludes leach and second wash steps and includes the Sr/TRU precipitation steps.

Figure 1. Simplified Model Flow Diagram for Envelopes A and B/D



The waste feed evaporator process was simulated using the OLI Environmental Simulation Program (OLI/ESP) version 6.6 using the CARBONAT, HNO3DB, SILICA, and ZEOLITE private databases, along with the public database.

The model fits were done using JMP® version 5.0.1[3] using the linear platform (least squares linear regression) for the polynomials and the non-linear platform for the exponential forms of viscosity.

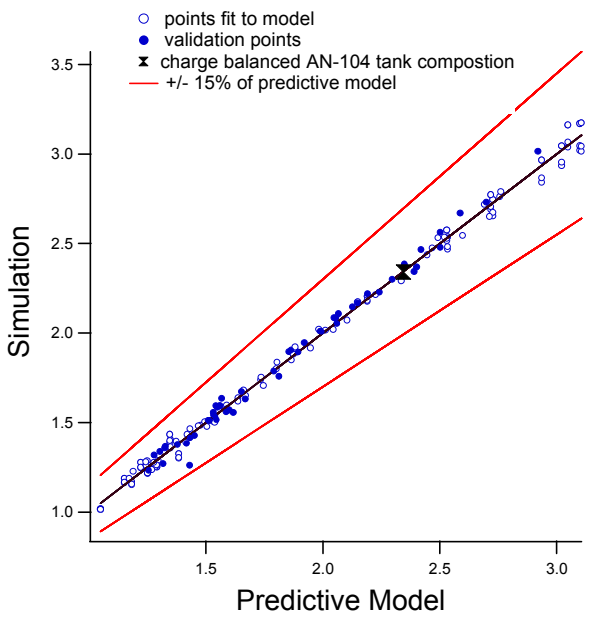
Validation of the models was done in two parts; the physical property model predictions were compared to those of the simulation software for design points not included in the model fit, and the chemistry and physical properties predicted by the simulation software was compared to experimental results for selected simulation design points.

1.3 RESULTS AND PERFORMANCE AGAINST OBJECTIVES

The following figure is an example of the type of plot used to validate the physical property models against the simulation results, showing the viscosity as predicted by the model vs. the simulation viscosity. The plot shows three types of data: the open circles represent data points included in the model fit, the filled circles represent the validation data points (which were not included in the model fit), and the bow-tie represents a simulation based on a actual tank composition using an expanded OLI/ESP chemistry model to include all the minor/trace species (to verify these minor species have, at best, a minor effect on the physical properties being determined). The two red curves are at ±15% of the model prediction as a measure of the model's success at predicting the simulation results. The complete set of results can be found in section 2.6.

As shown in the figure below all the validation points (filled circles) fall between the red curves, showing that the model meets the ±15% with 80% confidence acceptance criteria. In addition, the simulation using the expanded model falls within the curves indicating the variables selected for the correlations are adequate. The model equation is shown immediately following the figure.

Sub-envelope A-a Supernate Viscosity (cP)



134 points fit to model, 54 validation points.

$$\text{viscosity(cP)} = 0.0544[NO_2] + 0.0608[NO_3] - 0.149[OH] + \exp\left(\frac{219}{77.4 + [Temp]} - 0.947 - 0.0678[[NO_2] - 0.134[NO_3] + 0.0611[OH] - 0.0826[NO_3][NO_2]\right)$$

All the physical property models meet the acceptance criteria of ±15% with a confidence of 80%, therefore the physical property models meet the objectives as stated in the task plan, with the exception of the envelope A volume reduction factor, where 68% of the validation points are within ±15%.

The physical properties of the ultra-filtration feed stream supernate showed, in general, good agreement between simulation predictions and analytical results. Three simulants overshot the target sodium molarity (defined as the composition predicted by OLI/ESP) somewhat (by more than 7%) and comparisons with simulation results were consistent with the "higher than target" sodium content of the simulant. The remaining points were generally within 5% of the target sodium molarity. For these points, the difference between the simulation and experimental physical property results were less than 2% for density, 9% for viscosity, and 16% for heat capacity (although the simulation heat capacities were based on the slurry with the experimental was based on the supernate). Both simulation and experimental data predicted a thermal conductivity equal to that of water within the error of experimental measurements and the error of the trial model fits of the simulation data.

The compositions of the ultra-filtration supernate were also in relatively good agreement. The values given below include the three high sodium points mentioned above. The Ca and Fe concentrations were on the order of $1xE^{-5}$ M and $1xE^{-4}$ M respectively for both the simulation and experimental results. S, P and Si were on the order of 0.05, 0.02, and 0.07M respectively for both the experimental and simulation results, with average differences of 8, 34 and 34% respectively. From a chemical point of view, these differences are minor at these small concentrations. Al was on the order of 0.4M for both simulation and experimental results, with an average difference of 16%. This concentration is high enough to suggest that OLI/ESP is under predicting the solubility of Al (by 16%), resulting in a conservative estimate for the formation of NASGel.

1.4 QUALITY REQUIREMENTS

This work was conducted under the applicable requirements of NQA-1, 1989 and NQA-2a 1990, Part 2.7 as described in the technical task plan.

The quality requirements pertaining to OLI/ESP simulation software have been addressed in the document "Software Quality Assurance Plan for Hanford RPP-WTP Evaporator Modeling"[5]. OLI/ESP version 6.6 was used with the private databases CARBONAT, HNO3DB, SILICA, and ZEOLITE. JMP version 5.0.1 was used to fit the simulation physical property data to the mathematical forms.

1.5 ISSUES

None.

2.0 DISCUSSION

2.1 INTRODUCTION AND BACKGROUND

This document describes the waste feed evaporator (FEP) modeling work done as requested in the Waste Feed Evaporation and Physical Properties Modeling[1] test specification and specified in the Task Technical and Quality Assurance Plan for Waste Feed Evaporation and Physical Property Modeling[2] (items C, E, F, G, and H) for the R&T Test Scoping Statement S-89 in support of the Hanford River Protection Project (RPP) Waste Treatment Plant (WTP) project.

Waste currently stored in underground tanks at Hanford is to be pre-treated in preparation for vitrification and permanent storage. Pre-treatment, the first step in separating the HLW from the LAW waste, includes evaporation to reduce the volume sent to the HLW and LAW melters, ultra-filtration to concentrate the slurry sent to HLW, caustic wash steps to reduce the sodium content of the slurry solids, and can include a caustic leach step to reduce the aluminum content of the HLW slurry solids. The wash, leach, and second ultra-filtration steps generate recycle streams which will be returned to the Waste Feed Evaporator along

with recycle streams from other WTP processes, the most significant of these being the HLW SBS recycle stream. The permeate from the first ultra-filtration step will be sent to the LAW process for treatment by the cesium ion-exchange column and eventual vitrification. The treated/concentrated slurry will be sent to HLW for the addition of glass formers in preparation for vitrification.

Savannah River Technology Center personnel have been asked to develop mathematical models for the viscosity, Cp, and thermal conductivity of the feed stream to the first ultra-filtration step as a function of waste feed composition, HLW SBS recycle flow rate, and the ultra-filtration feed stream temperature. The scope of the project was expanded to include modeling of the volume reduction factor across the waste feed evaporator (total evaporator feed volume / evaporator bottoms volume) as a function of the same variables.

Although the task plan calls for the derivation of additional physical property models (items A, B and D of the task plan), the nature of the pre-treatment process made it either unnecessary or irrelevant. These properties include sodium molarity (as a function of density) and bulk solubility of the ultra-filtration feed stream. Because the evaporation was controlled to achieve a filtrate density of 1.22 (g/ml), the density was constant. Also, modeling of the solubility point was unnecessary because the flow-sheet calls for the filtration step to concentrate the stream to 20wt% insoluble/precipitated solids, which presumes solids are already present. Thermal conductivity values were calculated for all the design points and none deviated significantly from that of water (within the error of the trial model fit), therefore, thermal conductivity was not modeled.

Also, models were not developed for a sub-set of envelope A consisting of tank AY-102. This tank was being characterized at the time of this report, and no other data was available since C106 was combined with AY-102. Because this tank composition will be used in the upcoming integrated pilot test, a decision was made to include the AY-102 modeling work as part of the pilot test.

In addition to the flowsheet models just described, this task required a new solubility database for aluminosilicates. Recent operation of the Savannah River Site waste evaporators demonstrated that aluminosilicate minerals can precipitate from caustic waste solutions if aluminum and silicon concentrations are sufficiently high. To model deposition of aluminosilicates in the RPP evaporators, SRTC/ITP contracted OLI Systems, Inc., to create a database to calculate the solubilities of zeolites and related aluminosilicate species in caustic solutions. A version of this database, called ZEOLITE, was used in conjunction with other OLI public and private databases to perform the modeling calculations for this study.

2.2 DEVELOPMENT OF THE OLI DATABASE "ZEOLITE"

The ZEOLITE database contains solubility models for four aluminosilicate species, three of which are crystalline solids and one which is an amorphous gel. The amorphous gel, called sodium aluminosilicate gel or NAS gel, forms as a precursor to the crystallization and

precipitation of zeolite A. The aluminosilicate solid transforms into the three crystalline phases, zeolite A, hydroxysodalite, and cancrinite, in the stated order as it ages.

In the ZEOLITE database, the solubility models for NAS gel and zeolite A are based on data from Ejaz, Jones, and Graham[6]. Ejaz et al. measured solubilities for the dissolution of NAS gel and zeolite A in 3.0 to 4.4 molar NaOH solutions. Temperatures for these measurements ranged from 30°C to 80°C. Solubility models for hydroxysodalite and cancrinite are based on data from Barnes, Addai-Mensah, and Gerson[7]. Barnes et al. precipitated hydroxysodalite and cancrinite by seeding crystals in supersaturated solutions containing approximately 4.3 molal NaOH, 0.4 molal Na_2CO_3, and 1.8 molal $Al(OH)_3$. Temperatures for the Barnes et al. measurements varied from 90°C to 220°C. OLI assigned the stoichiometries given by these date sources to all four modeled species.

OLI developed its solubility models using activity coefficient parameters and standard state Gibbs free energies and entropies to fit these two sets of solubility data. The model for cancrinite solubility is based on simultaneous regression of activity coefficient parameters and standard state properties. Subsequent regression of standard state free energies and entropies with the activity coefficient parameters derived for cancrinite then gave the solubility models for hydroxysodalite, zeolite A, and NAS gel. OLI selected cancrinite as the basis for its correlation of activity coefficients because cancrinite solubility data covered a wider temperature range than the data for the other phases. A regression package embedded in the OLI calculation engine performed the model calculations. OLI included models for the solubilities of both hydrated and anhydrous forms, but recommends that only the hydrated forms be used in solubility calculations.

To improve the solubility models, OLI added an ionic species and several ion-ion interactions to the default set contained in the PUBLIC database and modified properties for other species. The added species is $AlSiO_3(OH)_4^{3-}$. Properties for this species were derived by fitting the solubility data. Spectroscopic evidence presented by Kinrade and Swaddle[8], Swaddle et al.[9], and Gout et al.[10] attest to the existence of this ion and hence support its addition to the database.

Helgeson-Kirkham-Flowers (HKF) parameters[11] were altered for several species, namely, $Al(OH)_3$, $Al(OH)_4^-$, $NaAl(OH)_4$, and H_4SiO_4. Diakanov et al.[12] provided HKF parameters for the first three of these species, and Stefansson[13] gave values for these parameters for H_4SiO_4.

OLI added three pairs of ion-ion interactions to the ZEOLITE database: $Al(OH)_4^-$ /$AlSiO_3(OH)_4^{3-}$, $AlSiO_3(OH)_4^{3-}$/Na^+, and $NaCO_3^-$/OH^-. These interactions are modeled using Bromley activity coefficient parameters[14].

Before the OLI database was used, it was verified by comparing measured and calculated solubilities[15]. Solubilites were compared for the data used to generate the OLI model and for two independent sets of data. Not surprisingly, calculated solubilities agreed closely with most of the Ejaz et al. and Barnes et al. data. The only exceptions were the Ejaz et al. data for NAS gel at 80°C and zeolite A at 30°C, and the Barnes et al. data at 220°C. Calculated

NAS gel solubilities exceeded measured values at 80°C; Ejaz et al. attribute this apparent discrepancy to rapid crystallization of the NAS gel to the much less soluble zeolite A at this temperature. At 30°C, the calculated solubilities for zeolite A were greater than measured values; apparently, at this temperature, crystallization was too slow to achieve equilibrium saturation during the measurement interval. Calculated solubilities also exceeded measured values for the Barnes et al. data at 220°C.

In addition to these comparisons, the OLI model was benchmarked against independent data from Breuer et al. and Park and Englezos[16]. Breuer et al. measured solubilities of zeolite A and hydroxysodalite for simulants of solutions used to process aluminum from ore. For zeolite A, calculated solubilities were an order of magnitude lower than measured solubilities. For hydroxysodalite, agreement between calculated and measured solubilities was close within the range of concentrations for which OLI fit its model, but calculated solubilities were significantly higher as the caustic concentrations dropped. Park and Englezos[17] measured hydroxysodalite solubilities for surrogates of paper pulp liquors. Calculated solubilities significantly exceeded measured values for the Park and Englezos data. This last comparison probably should be given less consideration than the other comparisons, because Park and Englezos did not seed their solutions and in several cases failed to obtain a precipitate with the correct stoichiometric aluminum-to-silicon ratio.

The results of an OLI/ESP simulation using the ZEOLITE database were compared with those from Geochemist's Workbench (GCWB). The GCWB database did not have some of the species used in the OLI simulation (NO_2 was treated as NO_3, and oxalate as CO_2 and CO_3), otherwise the systems were identical. OLI predicted the precipitation of 98 moles of gibbsite and 0.12 moles of NAS gel, where GCWB predicted 184 moles gibbsite and 0.54 moles of NAS gel. While not exact, the values are of the same order of magnitude. Only gibbsite and NAS gel were allowed to precipitate in both simulations (zeolite A, cancrinite, etc. were not allowed to precipitate).

2.3 DESCRIPTION OF PRE-TREATMENT PROCESS

Much of the description below is based on information from the document "WTP Material Balance and Process Flowsheet Bases, Requirements, and Results"[18]. Table 1 outlines the differences the in pre-treatment process for each envelope.

Table 1. Distinctions in the Pre-Treatment Process for each Envelope

Envelope	A-a	B/D	C
Insoluble/precipitated solids concentration in the 1st ultra-filtration feed stream	20wt%	20wt%	15wt%
Point of introduction of waste feed stream to process	Fed to 1st ultra-filtration step (after evaporator)	Fed directly to evaporator with recycle streams	Fed to SR/TRU precipitation, which in turn feeds the 1st ultra-filtration step
1st wash	Yes	Yes	Yes
Leach	Yes	Yes	No
2nd wash	Yes	Yes	No
Sr/TRU precipitation	No	No	Yes

The tank wastes are categorized into three envelopes, A, B, C and D, based on their general composition and the various processes from which the wastes were generated. A, B, and C represent supernates, and D represents the solids of envelope B. Envelope B/D wastes contain higher levels of halides and sulfur, reducing the amount of waste loading possible in the glass, and envelope C wastes contain relatively larger amounts of complexants and Sr/TRU. Because of these variations in composition, the pre-treatment process differs somewhat for each envelope. The process for envelopes A and B/D are described first, then the process for envelope C.

The pre-treatment of envelopes A and B/D are identical except for the point of introduction of the waste feed stream to the pre-treatment process. Envelope A waste will be fed to the pre-treatment process at a sodium concentration greater than 5M. Because the permeate from the first ultra-filtration step has a target density of 1.22 (g/ml) to prevent floatation of the cesium IX resin, and since experience has shown that waste at a concentration of 5M Na has a density in this neighborhood, there is no need to concentrate envelope A waste. In fact, it must be diluted with the evaporator bottoms (HLW SBS and pre-treatment recycles concentrated to less than 5M Na) to achieve the target permeate density. Therefore envelope A tank waste will not be feed to the evaporator, but blended with the evaporator bottoms in the ultra-filtration holding tank following the evaporator. Envelope B/D tank wastes will be sent to the process at less than 5M Na, and therefore combined with the recycle streams prior to evaporation and then concentrated to a supernate density of 1.22 (g/ml).

The contents of the ultra-filtration holding tank will be cycled through the filter until the slurry is concentrated to 20wt% undissolved solids, with the resulting permeate being fed to the LAW for processing by the cesium IX column. The slurry will then be washed with 0.01M NaOH to reduce the sodium content. This is to be done in 22 batches, where one batch consists of adding a volume of 0.01M NaOH, mixing the tank, then filtering an equal volume of supernate to be forwarded to a pre-treatment recycle holding tank and eventually fed to the waste feed evaporator. 21,770 gallons of 0.01M NaOH will be used for every 18,000 gallons of slurry to be washed (~1000 gallons of caustic for each wash batch), generating 21,770 gallons of decanted supernate.

Following the first caustic wash, the envelope A and B/D slurry solids are leached of aluminum by adding sufficient 19M NaOH to achieve a concentration of 3M free OH, followed by heating of the slurry to 50^{o}C with a steam lance. The leached slurry will then be cycled through the second ultra-filtration step to a concentration of 20wt% undissolved solids and the permeate sent to a recycle holding tank and eventually fed to the waste feed evaporator. Finally, the slurry will be washed a second time in a manner identical to the first wash step, with a volume (equal to the wash addition) of filtered supernate being sent to the waste feed evaporator recycle holding tank (as feed to the waste feed evaporator), and the treated slurry sent to HLW in preparation for vitrification.

By definition, envelope C contains higher levels of Sr/TRU than the other envelopes. The tank waste for this envelope will be fed to the Sr/TRU precipitation step where 0.1M $SrNO_3$ and 0.1M $NaMnO_4$ solutions are added to achieve a slurry concentration of 0.01M Sr and 0.075M MnO_4. In addition, 19M NaOH will be added to achieve a concentration of 1M free OH to enhance the precipitation. The resulting slurry will then be fed to the ultra-filtration holding tank where it will be combined with the evaporator bottoms and then concentrated to 15wt% undissolved solids by ultra-filtration and the permeate sent to LAW for processing by the cesium IX columns. Unlike envelopes A and B/D, the concentrated slurry is processed through the first wash step only, and will not go through the leach, 2nd filtration, nor the 2nd caustic wash steps. The first wash step is identical to that for envelopes A and B/D. The slurry from the single wash step will be sent to HLW for eventual vitrification.

For every 18,000 gallons of concentrated slurry produced by the first ultra-filtration step, the filters will be cleaned with 5,250 gallons of 2M HNO_3 (acid cleaning) and 15,750 gallons of 0.01M NaOH (caustic rinse). This is based on two acid cleaning cycles and pre/post acid cleaning caustic washes (verbal communication from Ivan Papp, Aug. 2002 quarterly meeting). These resulting streams are then sent to a waste feed evaporator recycle holding tank and eventually fed to the waste feed evaporator.

19M NaOH is added to the recycle generated from the pre-treatment process (by the wash, leach, and acid cleaning steps) to adjust the pH to 13 prior to being fed to the waste feed evaporator.

Additional recycle streams are sent to pre-treatment from other processes. The most significant of these is the HLW SBS recycle which has been included in the simulation model. Other recycle streams are either extremely dilute or relatively small, and were not included in the simulation flow-sheet described in the following.

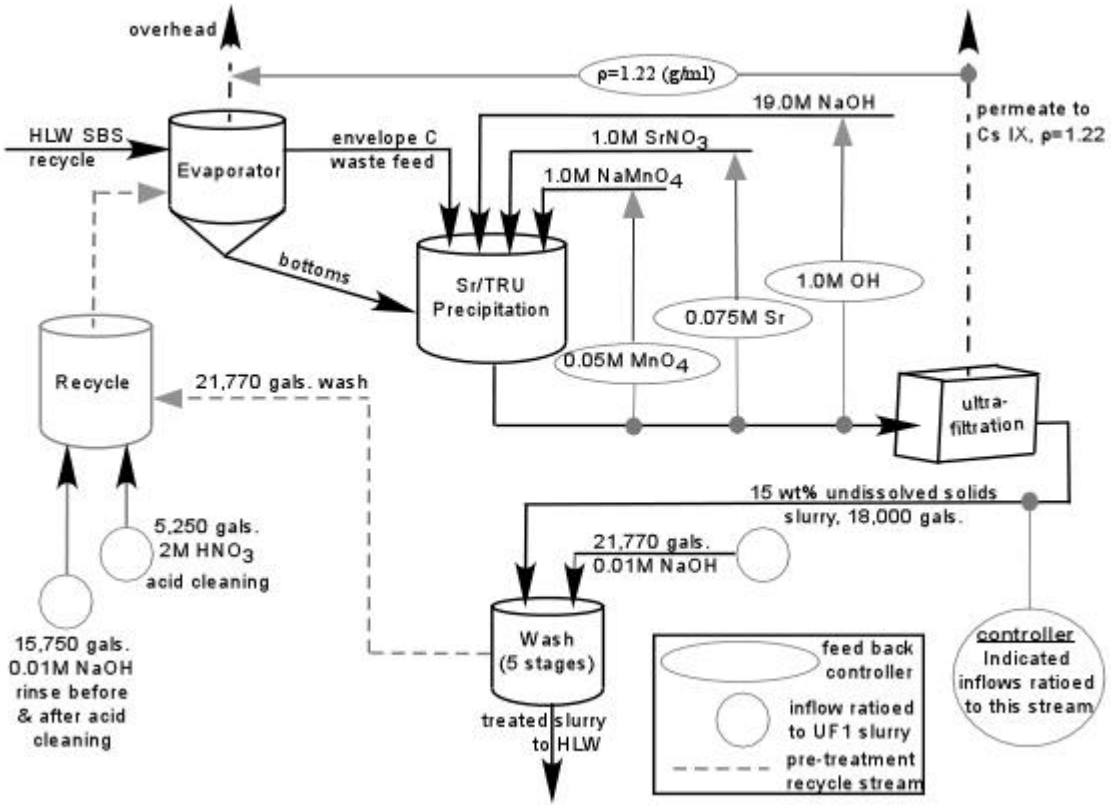
2.4 OLI/ESP MODEL FLOWSHEET AND CHEMISTRY MODEL

The RPP pre-treatment process was simulated using the OLI Environmental Simulation Program (OLI/ESP) version 6.6 using the CARBONAT, HNO3DB, SILICA, and ZEOLITE private databases, along with the public database. The simulation was set up as a steady-state process, and included iterations on the recycle streams generated by the pre-treatment process from the wash, leach, and acid cleaning steps until the entire flow-sheet converged.

The evaporator was modeled as a flash calculation [19] (as opposed to a dynamic simulation) since the overhead is essentially water and its composition does not vary with bottoms composition. The evaporation rate was controlled such that the density of the 1st ultra-filtration permeate (sent to LAW) was 1.22(g/ml) at the design point temperature. The evaporator was operated at 50°C at the bubble point pressure, and the 1st filter was operated at 1 atm. and the design point temperature. All other unit operations and streams were set to 1 atm. and 25°C.

The actual pre-treatment process described in Section 2.3 is approximated in the OLI/ESP simulation flowsheet by using a series of unit operations to represent each of the steps as shown in Figure 1 and Figure 2.

Figure 2. Simplified Model Flow Diagram for Envelope C



To reduce the simulation execution time, the number of stages simulated for each of the two wash steps was reduced from 22 to 5. The actual process will use about 22,000 gallons of 0.01M NaOH for every 18,000 gallons of concentrated slurry (or about 1000 gallons per wash stage). For the purpose of the simulation, the 22,000 gallons of wash was divided by the number of stages simulated in order keep the volume of wash used per 18000 gallons of concentrated slurry constant, e.g. for five stages, 4,400 gallons of 0.01M NaOH were used in each wash stage. Trial simulations in which the number of stages was varied showed 5 stages to give the best combination of reduced execution time with a minimum of error due

to approximating the 22 wash stages of the actual process with fewer stages in the simulation, with less than a 5% difference in a number of measurements (such as Na molarity, flow rates, etc.) as compared to the full 22 stage model (see Appendix E).

The waste feed flow rates used in the simulations were based on a LAW glass production rate of 30 metric tons per day at a Na_2O loading of 19.5, 7.5, and 17.0wt% for envelope A, B/D, and C respectively (from Table A-15 of the TF COUP document[20]), where only the sodium content of the waste stream was used to calculate the Na_2O loading. This was not necessary for the model (any flow rate could have been used), but was a choice of convenience.

The HLW SBS flow rate is not tied directly to the pre-treatment process, and therefore 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 waste feed stream, having a range of 0 – 2 (i.e. up to twice the volumetric flow rate of the waste feed stream). The composition was fixed for all simulations, and based on the analytical results from the VSL melter pilot testing.

The remaining inflows are set to the rates/flow ratios as described in Section 2.3, that is, 19M NaOH is added at the leach step to achieve 3M OH, and for every 18,000 gallons of concentrated slurry from the first filter, 1) 2,500 gallons of water is added to represent the steam heating during the leach step, 2) 21,770 gallons of caustic wash for each of the 1st and 2nd wash steps, and 3), 15,750 gallons of caustic wash and 5,250 gallons of acid for cleaning of the filters.

For all the design points simulated, the recycle stream generated from the pre-treatment process had a pH of 13 or greater, so no pH adjustment was done.

Because OLI/ESP does not yet have the capability to calculate the heat capacity of a stream directly, this was done for the ultra-filtration feed stream using the OLI Scratch Pad tool in OLI/Express to generate an enthalpy vs. temperature plot at the calculated steady-state composition. This was done from 15 – 75^{o}C in one degree increments.

The chemistry models used for all simulations include the species given in Table 2, Table 3, and Table 4 of the next section. Additional simulations (beyond those of the design points) were done based on actual tank compositions which used an expanded chemistry model to include the very minor species. (In both cases a patch was required from OLI to increase the number of allowed anion-cation interactions due to the large chemistry models).

Because NAS gel is a necessary precursor to crystalline aluminosilicates (zeolite A, hydroxysodalite, and cancrinite), only the precipitation of NAS gel was modeled. The residence time of the evaporator bottoms is short relative to the kinetics of crystalline aluminosilicate formation; it is not anticipated that these will form to a significant degree in the evaporator. However, when NAS gel is predicted, the crystalline forms will eventually form, possibly in holding tanks and downstream processes if conditions are not significantly different.

2.5 DETERMINATION OF THE FACTOR SPACE FOR THE DESIGNS OF EXPERIMENT

The simulation design matrix was derived from the model factor space, which in turn is defined by model variables and their ranges. The design matrices are given in Appendix C and described briefly below. Their derivation is more fully described in other documents[21-23].

The design matrices consist of two types of design points. One type is used exclusively in the model fits, and consist only of the extreme (minimum and maximum) values of the variable ranges (this assumes a linear response). The second type is generated using the Orthogonal Latin Hypercube (OLH) technique[24], which produces points uniformly distributed over the linear factor space. These points are used to either improve the model fit if the response is found to be non-linear, or (when not included in the model fit) to validate the property model prediction against the simulation results. The model variables and corresponding factor spaces and constraints from which these matrices were derived are described in the following.

The physical property models are given in terms of two types of variables, 1) mixture variables which define the composition of the waste feed stream, and 2) process variables which define the "state" of the stream, these being the temperature, SBS/Feed ratio, and a waste feed dilution factor (expressed in terms of Na molarity as described below). The dilution of the waste feed stream was included as a variable since the volume reduction factor (VRF) is a strong function of this, and the tank waste may be diluted prior to being sent to the pre-treatment process.

For all envelopes, the temperature range was given to be 20-70^{o}C and the range for the HLW SBS volumetric flow rate was chosen to be 0-2 times that of the waste feed stream. The ranges for the waste feed stream sodium molarity (the "dilution factor") were based on the tank waste analysis and the sodium molarities of the diluted waste feed sent to pre-treatment as specified in the "WTP Mass Balance and Process flow-sheet"[18].

Given the broad range in composition, attempting to capture the behavior of all three envelopes in a single model would likely result in models with unacceptably large error. Therefore, a separate set of physical property models was developed for each of the three envelopes. The significant species and corresponding concentration ranges for each of the envelopes were determined using various sources of tank characterization data.

Envelope A was divided into what we designate here as sub-envelope A-a (represented by tanks AP-101, AP-104, AN-104, AN-105, SY-101, AN-103, AW-101, and AW-104) and sub-envelope A-b (represented by tank AY-102), the composition of AY-102 being distinct (much older waste) from the other A tanks. The factor space of envelope B/D is represented by the compositions of tanks AZ-101 and AZ-102, and envelope C by tanks AN-102 and AN-107.

In order to derive the composition (mixture variable) ranges for each envelope, it was necessary to "normalize" the concentrations by some common value. This is because the models predict properties of the filtration feed stream based, in large part, on the composition of the waste feed stream, and the feed is either directly or indirectly (via pre-treatment recycle) concentrated through the evaporator. The models should predict very similar physical property value for waste feeds of identical compositions but different dilutions, since in each case enough water will be evaporated to achieve a permeate density of 1.22 (g/ml), resulting in identical permeates. (The prediction would be identical except for the difference in the SBS flow rate relative to the amount of waste feed solids at different waste feed dilutions). Therefore, the models should not be a function of the amount of water present in the feed. Normalizing the concentrations removes this water dependence from the models. This was born out in the model fits in that only the VRF models included the "dilution factor" variable (described below) since it is of course a strong function of the dilution of the waste feed stream. For all other models, this "dilution factor" was determined to be a statistically insignificant by the JMP software, and not included as a variable.

Normalization of the mixture variable concentrations was done using two different approaches (either approach would have been satisfactory for all envelopes, but this was not apparent to the author at the time the factor spaces were being developed). The analytical tank compositions (expressed in molarities) for envelopes A and C were adjusted to an otherwise identical stream at 5M Na. That is, all molar concentrations were multiplied by the ratio of 5 divided by the analytical sodium molarity value. The choice of normalizing to a value of 5M Na stream was somewhat arbitrary; it is roughly the mid-point of the streams fed to the pre-treatment process and corresponds to the target permeate density. These "normalized" mixture values defined the factor space used to generate the design matrix. For envelope B/D models, a mixture variable is expressed in terms of its mass fraction relative the total mass of the model's mixture variables (e.g. $[\mathrm{AlO2}] = \frac{\mathrm{mass}_{\mathrm{ALO2}}}{\mathrm{mass}_{\mathrm{ALO2}}+\mathrm{mass}_{\mathrm{CO3}}+\mathrm{mass}_{\mathrm{Fe}}+\mathrm{mass}_{\mathrm{NO3}}+\mathrm{mass}_{\mathrm{OH}}+\mathrm{mass}_{\mathrm{SO4}}}$), and these values defined the factor space used to generate the design matrix. Given these forms of expression, the species to be included as mixture variables were determined.

The significant species of sub-envelope A-a, their corresponding concentration ranges, and constraints had already been determined based on the tank waste compositions as given in the TF-COUP[20] document as part of the experimental simulant work[25, 26]. With minor modifications (fixing SO_4 and oxalate concentration to the maximum value of the range, 0.0554M and 0.02M respectively), the same factor space was used for this modeling work and is given in Table 2. 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 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 $0.1x5/7 = 0.0714$ M OH).

Table 2. Definition for Sub-envelope A-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	5.6	0.0	20
maximum	1.12	0.686	0.236	1.59	2.08	2.89	0.0436	7.0	2.0	70
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/D was based on tank characterization reports for AZ-101[27] and AZ-102[28]. Analytical data of both dissolved and undissolved solids were combined to represent the total solids in the slurry. Because the undissolved solids are in equilibrium with the supernate and calculated by the simulation, the factor space must be in terms of the total slurry solids. Therefore, the mixture variables for the envelope B/D physical property models are in terms of the total slurry solids. However, the "dilution factor, expressed as the process variable "sodium molarity", is the molarity of the supernate. A constraint was imposed on the net charge of the mixture variables based on the ranges observed in the data. These ranges are in Table 3, along with the concentration of several species that were fixed relative to that of sodium, either because they were relatively small or showed little variation in the analytical data.

Table 3. Definition for Envelope B/D Factor Space

	Mixture Variable Mass Fraction Ranges Mass fraction relative to total mass of mixture variables						Process Variables		
Variable	$[AlO_2]$ (mass fraction)	$[CO_3]$ (mass fraction)	[Fe] (mass fraction)	$[NO_3]$ (mass fraction)	[OH] (mass fraction)	$[SO_4]$ (mass fraction)	[Na] (molar)	SBS / Feed (volumetric)	Temp (°C)
minimum	0.129	0.284	0.0411	0.115	0.0508	0.0952	2.33	0.0	20
maximum	0.161	0.500	0.080	0.306	0.113	0.183	4.48	2.0	70
charge constraint	$-0.02355 \le -0.016955[AlO2] + 0.053718[Fe] - 0.016128[NO3] - 0.020820[SO4] - 0.058798[OH] - 0.033328[CO3] \le -0.02094$								
Molar Ratios Fixed Relative to Sodium									
$[NO_2]$	[K]		[F]	[Zr]		$[CrO_4]$	$[SiO_3]$		$[C_2O_4]$
0.27	0.027		0.018	0.005		0.0044	0.0041		0.008

The composition factor space for envelope C was based on tank waste characterization reports for tanks AN-102[29, 30] and AN-107[31-33]. Only one ionic form of EDTA (ethlylenediaminetetraacetic acid) – dihydrogen EDTA – was available for the purpose of the simulations, hence all reported forms of EDTA in the analytical data were input as this single

anion. Table 4 shows the mixture and process variable ranges, the mixture variable charge constraint, and the species whose concentration was fixed relative to Na due to their small or relatively consistent concentration in the analytical data.

Table 4. Definition for Envelope C 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)	$[NO_2]$ (molar at 5M Na)	$[NO_3]$ (molar at 5M Na)	[OH] (molar at 5M Na)	$[SO_4]$ (molar at 5M Na)	[Na] (molar)	SBS / Feed (volumetric)	Temp (^oC)
minimum	0.015	0.560	0.780	1.50	0.138	0.051	7.0	0.0	20
maximum	0.290	0.940	1.19	2.30	0.295	0.112	8.5	2.0	70
charge constraint	$4.27 \le [AlO2]+[NO2]+[NO3]+[OH]+2[CO3]+2[SO4] \le 5.33$								

Fixed Molar Concentrations										
[Cl] (molar at 5M Na)	[F] (molar at 5M Na)	$[PO_4]$ (molar at 5M Na)]	$[C_2O_4]$ (molar at 5M Na)	$[CrO_4]$ (molar at 5M Na)	$[SiO_3]$ (molar at 5M Na)	[formate] (molar at 5M Na)	[glycolate] (molar at 5M Na)	[acetate] (molar at 5M Na)	[citrate] (molar at 5M Na)	$[H_2EDTA]$ (molar at 5M Na)
0.052	0.0016	0.022	0.0033	0.0011	0.002	0.091	0.01	0.024	0.015	0.025

2.6 RESULTS

The results are given below in three sections, 1) the model fits with plots comparing model predictions with simulation results, 2) comparison of simulation with experimental simulant results of 13 selected design points, and 3) a snapshot of the progression of aluminum and sodium concentrations through the pre-treatment process for each of the envelopes, in addition to the Sr concentrations for envelope C. Included with the model/simulation plots are the results of simulations based on actual tank compositions for each of the three envelopes (AN-104, AZ-102, and AN-107 for A, B/D, and C respectively) which used an expanded chemistry model to include a majority of the constituents given in the analytical reports. This was a measure of the combined effect of the "minor" constituents on the property models.

Because computer experiments have no random error associated with the results, statistics that are normally used to measure the success of a model from a typical lab experiment could not be used here. Also, it is not feasible to run lab experiments duplicating the complicated pre-treatment process being simulated. Therefore, the physical property models were validated in two stages, one to test whether the derived property models give a reasonable representation of the simulation software predictions, and the other comparing the chemistry predicted by the software with results from experimental simulant work.

Validation of the physical property models against the simulation predictions was done using design points generated by the Orthogonal Latin Hypercube technique[24], which produces points uniformly distributed over the linear factor space. If the physical property models

adequately predict a majority of the OLH points which were not included in the model fit, the model is considered to be a fair representation of the simulation software.

Validation of the simulation software was done by making simulants of 13 selected simulation design points based on the composition of the ultra-filtration feed stream predicted by OLI/ESP. The solids and supernate compositions and physical properties of these simulants were compared with the simulation prediction.

It was not possible to predict how certain simulation design points would behave prior to running the simulations. In very few cases, the concentration of the feed stream was such that it was not possible to dilute it to the target 1.22 (g/ml) supernate density with the generated pre-treatment recycle (none of these cases has HLW SBS). In these situations the simulation was modified so that the pre-treatment recycle by-passed the evaporator and the feed stream diluted with water. There were also very few cases where the feed stream was dilute and the evaporator bottoms flow rate too small for the combined streams to achieve the target 1.22 (g/ml) density. In these situations the evaporator bottoms where concentrated to 30wt% total solids, and the initial dilution of the waste feed reduced. These are considered reasonable adjustments as these cases represent extremes in the operating conditions, and waste streams would not be sent to the pre-treatment process in a state of dilution that would make it impossible reach the target density.

For envelope C, 10 points (2, 6, 10, 14, 18, 22, 26, 30, 34, 38) were removed from the design matrix for which the sodium molarity of the waste feed was given at the high value of the factor space. The sodium molarity of these points had to be adjusted to the minimum factor space value to achieve the target permeate density. The matrix already contained these points at the low sodium value. Because this is a process variable, it does not effect the design as these points represent a combination of conditions (no SBS flow and high sodium waste feed) which would not occur under normal operating conditions.

2.6.1 Predictive Models with Model vs. Simulation Plots

Plots of the simulation results vs. the model prediction are shown for each of the models, with curves indicating ±15% (or ±5%) of the model prediction as a measure of the model's success relative to the simulation results.

The heat capacity models were very successful relative to the simulation predictions, and the viscosity models are well within 15% of the simulation predictions. The volume reduction factor (VRF) models for envelopes B/D and C are, with few exceptions, within ±15% of the simulation predictions. The VRF model for sub envelope A-a shows a definite correlation between the model prediction and simulation results, but there is some scatter beyond ±15% of the simulation prediction (note that the VRF range for this envelope is by far the greatest).

2.6.1.1 Sub-Envelope A-a Predictive Models

All concentrations are in terms of molarity. 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. [Na] is used as a process variable to adjust the water content of the feed stream while keeping the amount of solids relative to each other constant. An example calculation is given in Appendix A. Temperature is in ^oC, and the SBS/Feed ratio is a volumetric flow ratio of the HLW SBS relative to the waste feed.

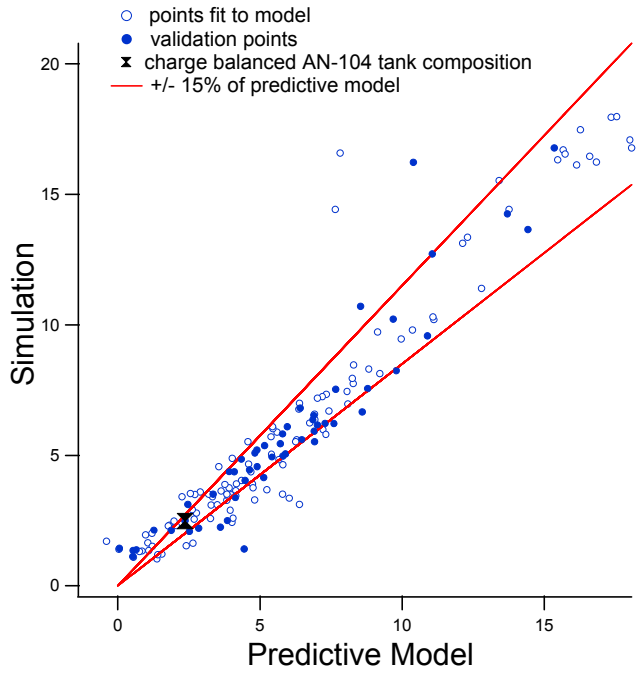
Table 5 Valid Variable Ranges for Sub-Envelope A-a Models

	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	5.6	0.0	20
maximum	1.12	0.686	0.236	1.59	2.08	2.89	0.0436	7.0	2.0	70

The sub-envelope A-a volume reduction factor (VRF: volume of total evaporator feed / volume of evaporator bottoms) at endpoint – steady state conditions is given as:

$$\begin{aligned} VRF = & -35.7 + 7.32[AlO_2] + 37.3[CO_3] + 6.21[F] - 10.1[Na] + 19.1[NO_2] \\ & + 16.5[NO_3] + 28.8[OH] + 2.06[PO_4] + 12.6[SBS] + 0.781[Temp] \\ & - 3.84[CO_3][Na] - 1.92[NO_2][Na] - 1.68[NO_3][Na] - 3.52[OH][Na] \\ & + 1.80[Na]^2 - 2.01[AlO_2][SBS] - 1.17[Na][SBS] - 1.78[SBS]^2 \\ & - 0.165[Na][Temp] + 0.0465[OH][Temp] + 0.0740[SBS][Temp] + 0.00266[Temp]^2 \end{aligned} \quad (1)$$

Figure 3. Sub-envelope A-a Volume Reduction Factor

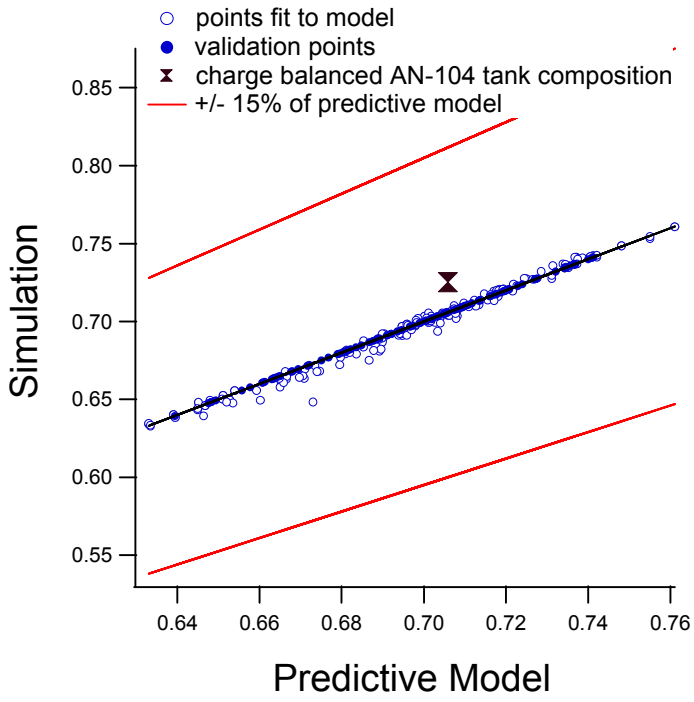


108 points fit to model, 53 validation points.

The sub-envelope A-a slurry heat capacity at endpoint – steady state conditions is given as:

$$\begin{aligned}\mathrm{Cp}\left(\frac{\mathrm{cal}}{\mathrm{gram}\ ^{\mathrm{o}}\mathrm{C}}\right) &= 0.0460 + 0.191[AlO_2] + 0.311[CO_3] + 0.135[F] + 0.140[NO_2] \\ &+0.144[NO_3] + 0.141[OH] + 0.426[PO_4] - 0.00300[SBS] \\ &-0.00206[Temp] + 0.000857[AlO_2][Temp] + 0.000406[F][Temp] \\ &+0.000185[NO_3][Temp] + 0.000231[OH][Temp]\end{aligned} \quad (2)$$

Figure 4. Sub-envelope A-a Slurry Heat Capacity $\left(\mathrm{cal}/\left(\mathrm{gram}\ ^{\mathrm{o}}\mathrm{C}\right)\right)$

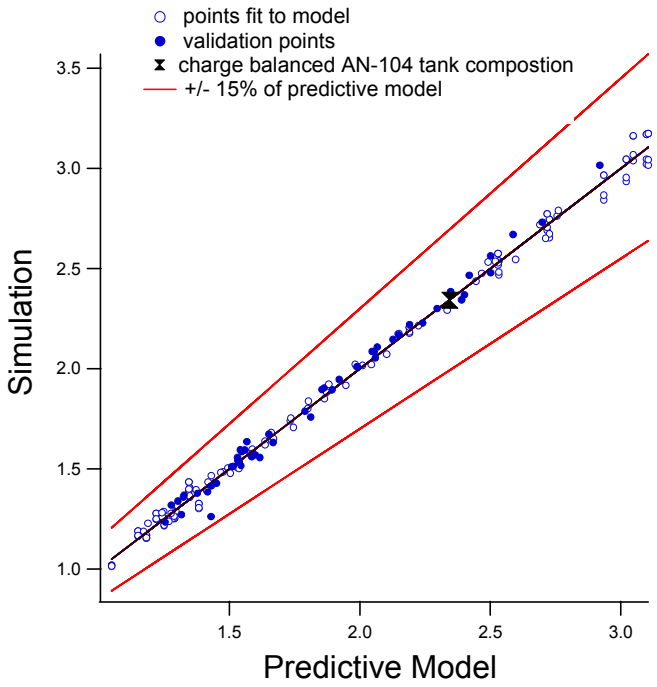


80 points fit to model, 108 validation points.

The sub-envelope A-a supernate viscosity at endpoint – steady state conditions is given as:

$$\begin{aligned}\mathrm{viscosity(cP)} &= 0.0544[NO_2] + 0.0608[NO_3] - 0.149[OH] \\ &+\exp\left(\frac{219}{77.4 + [Temp]} - 0.947 - 0.0678[[NO_2] - 0.134[NO_3]\right. \\ &\left.+0.0611[OH] - 0.0826[NO_3][NO_2]\right)\end{aligned} \quad (3)$$

Figure 5. Sub-envelope A-a Supernate Viscosity (cP)

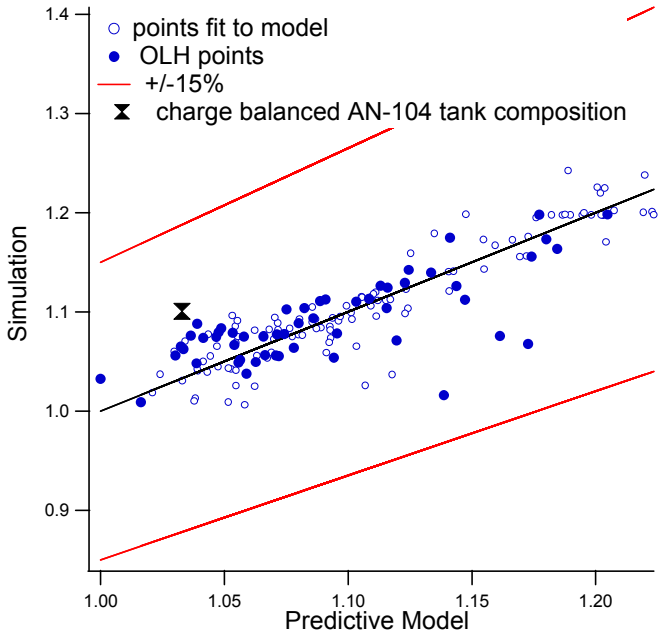


134 points fit to model, 54 validation points.

The envelope A evaporator slurry density at 50°C, endpoint – steady state conditions is given as:

$$\begin{aligned}\text{density}\left(\frac{\text{g}}{ml}\right) = {} & 2.14+0.363[ALO_3]+0.372[CO_3]+0.132[F]+0.187[NO_2] \\ & +0.201[NO_3]+0.377[OH]+0.810[PO_4]-0.686[Na] \\ & +0.0639[SBS]-0.00424[Temp]-0.0251[OH][Na] \\ & +0.00669[CO_3][Temp]+0.00323[F][Temp] \\ & +0.00340[NO_2][Temp]+0.00258[NO_3][Temp] \\ & +0.00310[OH][Temp]-0.00243[Na][Temp] \\ & +0.0579[Na]^2-0.0241[SBS]^2+0.0000945[Temp]^2\end{aligned} \qquad (4)$$

Figure 6. Envelope A Evaporator Bottoms Slurry Density



108 points fit to model, 53 validation points.

2.6.1.2 Envelope B/D Predictive Models

All concentrations for the envelope B/D model mixture variables listed in Table 6 are in terms of weight fraction relative to the total mass of all the mixture variables. [Na] is used as a process variable to, in effect, adjust the water content of the feed stream while keeping the amount of solids relative to each other constant. An example calculation is given in Appendix A. Temperature is in ^{o}C, and the SBS/Feed ratio is a volumetric flow ratio of the HLW SBS relative to the waste feed.

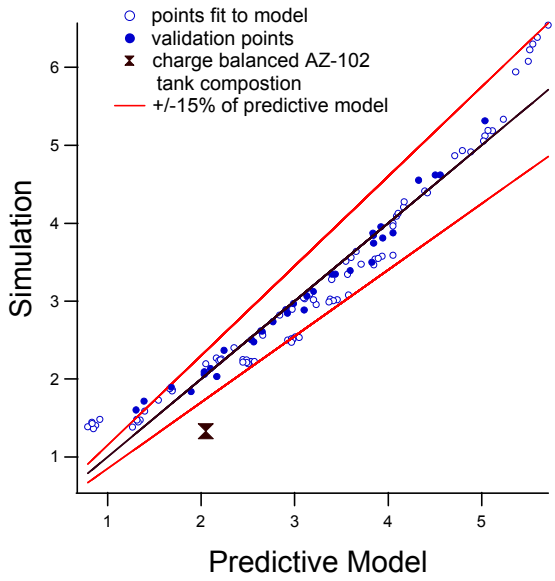
Table 6 Valid Variable Ranges for Envelope B/D Models

	Mixture Variable Mass Fraction Ranges Mass fraction relative to total mass of mixture variables						Process Variables		
Variable	[AlO_2] (mass fraction)	[CO_3] (mass fraction)	[Fe] (mass fraction)	[NO_3] (mass fraction)	[OH] (mass fraction)	[SO_4] (mass fraction)	[Na] (molar)	SBS / Feed (volumetric)	Temp (^{o}C)
minimum	0.129	0.284	0.0411	0.115	0.0508	0.0952	2.33	0.0	20
maximum	0.161	0.500	0.080	0.306	0.113	0.183	4.48	2.0	70

The envelope B/D volume reduction factor (VRF: volume of total evaporator feed / volume of evaporator bottoms) at endpoint – steady state conditions is given as:

$$\begin{aligned} VRF = {} & 1.98 + 3.76[AlO_2] + 4.03[CO_3] + 4.74[Fe] + 3.72[NO_3] + 3.56[OH] \\ & + 3.96[SO_4] - 2.06[Na] + 1.33[SBS] + 0.00958[Temp] + 0.195[Na]^2 \\ & - 3.23[Fe][SBS] + 1.78[OH][SBS] \end{aligned} \quad (5)$$

Figure 7. Envelope B/D Volume Reduction Factor

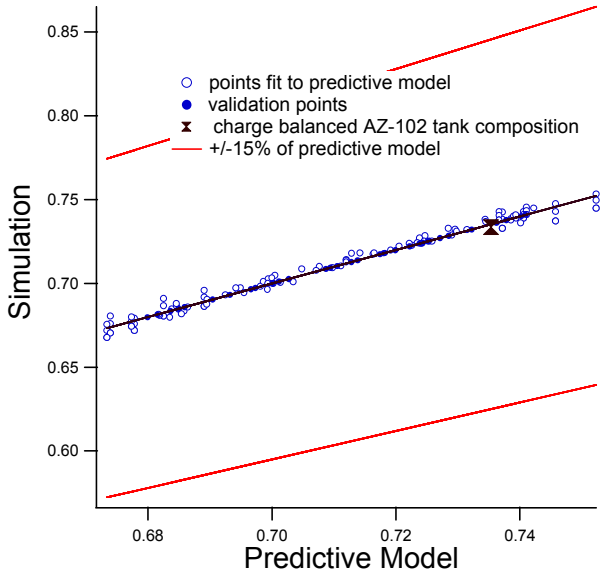


82 points fit to model, 34 validation points.

The envelope B/D slurry heat capacity at endpoint – steady state conditions is given as:

$$\mathrm{Cp}\left(\frac{\mathrm{cal}}{\mathrm{gram}\ ^{\circ}\mathrm{C}}\right) = 0.855[AlO_2] + 0.758[CO_3] + 0.602[Fe] + 0.701[NO_3] + 0.913[OH] + 0.798[SO_4] - 0.00127[Temp] \quad (6)$$

Figure 8. Envelope B/D Slurry Heat Capacity $\left(\mathrm{cal}/\left(\mathrm{gram}\ ^{\circ}\mathrm{C}\right)\right)$

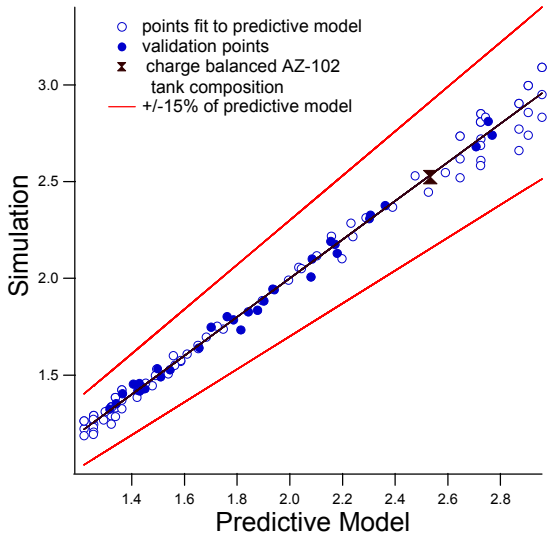


82 points fit to model, 34 validation points.

The envelope B/D supernate viscosity at endpoint – steady state conditions is given as:

$$\text{viscosity(cP)} = \exp\left(\frac{333}{104+[Temp]} - 1.86 + 0.435[CO_3] + 1.63[CO_3][OH]\right) \quad (7)$$

Figure 9. Envelope B/D Supernate Viscosity (cP)

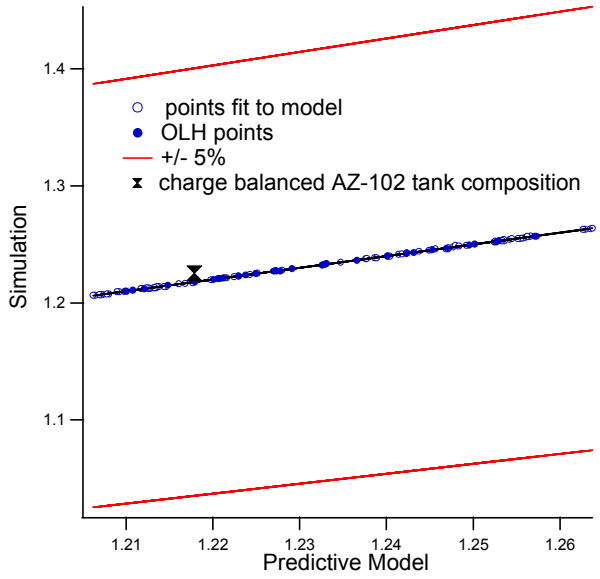


82 points fit to model, 34 validation points.

The envelope B/D evaporator slurry density at 50°C, endpoint – steady state conditions is given as:

$$\begin{aligned}\text{density}\left(\frac{g}{ml}\right) = {} & 0.00243 + 1.24[AlO_2] + 1.16[CO_3] + 1.34[Fe] + 1.19[NO_3] \\ & + 1.144[OH] + 1.19[SO_4] - 0.000117[Na] + 0.000418[SBS] \\ & + 0.000839[Temp] - 0.000442[AlO_2][Temp] \\ & + 0.000310[CO_3][Temp] + 0.00140[Fe][Temp] - 0.00102[OH][Temp]\end{aligned} \quad (8)$$

Figure 10. Envelope B/D Evaporator Bottoms Slurry Density



82 points fit to model, 34 validation points

2.6.1.3 Envelope C Predictive Models

All concentrations are in terms of molarity. The concentrations of the mixture variables (all species except Na) are expressed relative to a stream at a 5M Na concentration. (e.g. an [AlO2] 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. [Na] in then used as a process variable to, in effect, adjust the water content of the feed stream while keeping the amount of solids relative to each other constant. An example calculation is given in Appendix A. Temperature is in ^oC, and the SBS/Feed ratio is a volumetric flow ratio of the HLW SBS relative to the waste feed.

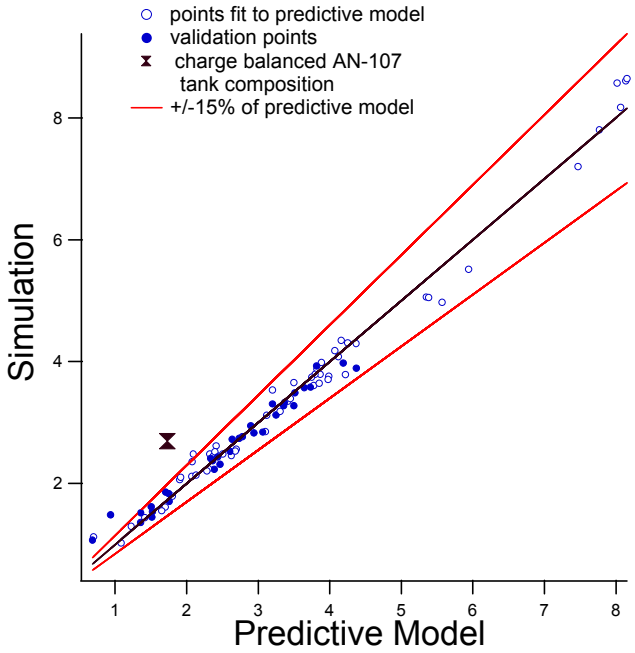
Table 7 Valid Variable Ranges for Envelope C Models

	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)	[NO_2] (molar at 5M Na)	[NO_3] (molar at 5M Na)	[OH] (molar at 5M Na)	[SO_4] (molar at 5M Na)	[Na] (molar)	SBS / Feed (volumetric)	Temp (^oC)
minimum	0.015	0.560	0.780	1.50	0.138	0.051	7.0	0.0	20
maximum	0.290	0.940	1.19	2.30	0.295	0.112	8.5	2.0	70

The envelope C volume reduction factor (VRF: volume of total evaporator feed / volume of evaporator bottoms) at endpoint – steady state conditions is given as:

$$\begin{aligned}\text{VRF} = &-22.2+1.24[AlO_2]+3.79[CO_3]+2.07[NO_2]+1.50[NO_3]\\ &+14.4[OH]+1.98[SO_4]+1.81[Na]-7.44[SBS]+0.264[Temp]\\ &-1.41[Na][OH]-0.852[Na][SBS]-0.0336[Na][Temp]+0.0285[SBS][Temp]\end{aligned} \quad (9)$$

Figure 11. Envelope C Volume Reduction Factor

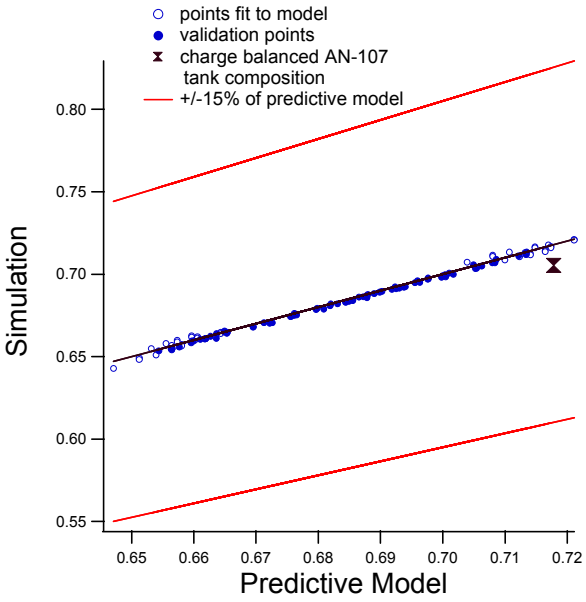


83 points fit to model, 33 validation points.

The envelope C slurry heat capacity at endpoint – steady state conditions is given as:

$$\begin{aligned}\text{Cp}\left(\frac{\text{cal}}{\text{gram}\ ^{\circ}\text{C}}\right) = &\ 0.187[AlO_2]+0.319[CO_3]+0.146[NO_2]+0.160[NO_3]\\ &+0.164[OH]+0.335[SO_4]+0.00207[SBS]-0.00114[Temp]\end{aligned} \quad (10)$$

Figure 12. Envelope C Slurry Heat Capacity $\left(\text{cal}/\left(\text{gram }^{\text{o}}\text{C}\right)\right)$

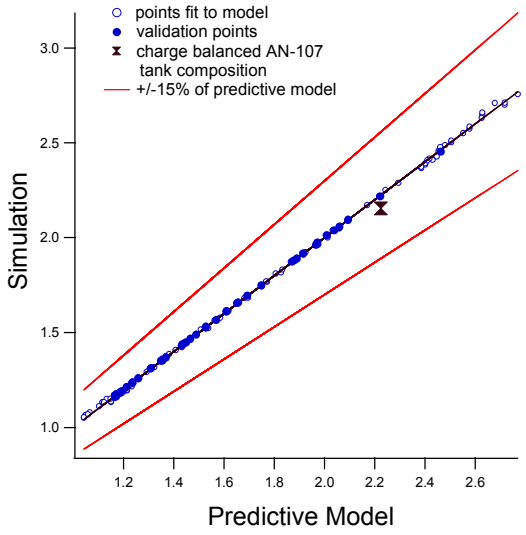


36 points fit to model, 70 validation points.

The envelope C supernate viscosity at endpoint – steady state conditions is given as:

$$\text{viscosity(cP)} = -0.0454[NO_3] + 0.00451[SBS] + \exp\left(\begin{array}{l}\dfrac{312}{98.7+[Temp]} - 1.83 + 0.134[AlO_2] \\ +0.220[CO_3] - 0.0109[SBS]\end{array}\right) \quad (11)$$

Figure 13. Envelope C Supernate Viscosity (cP)

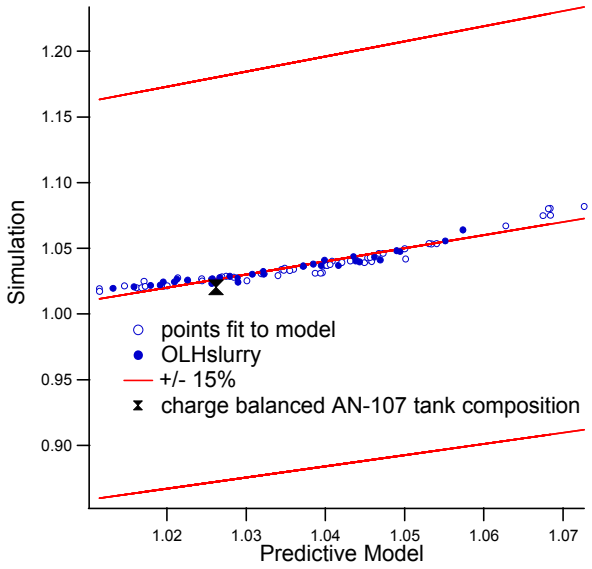


75 points fit to model, 40 validation points.

The envelope C evaporator slurry density at 50°C, endpoint – steady state conditions is given as:

$$\text{density}\left(\frac{g}{ml}\right) = 0.000243[ALO_3] + 0.000481[CO_3] + 0.000243[NO_2] + 0.000234[NO_3] + 0.000262[OH] + 0.000462[SO_4] - 0.0147[Na] + 0.00931[SBS] + 0.000576[Temp] \quad (12)$$

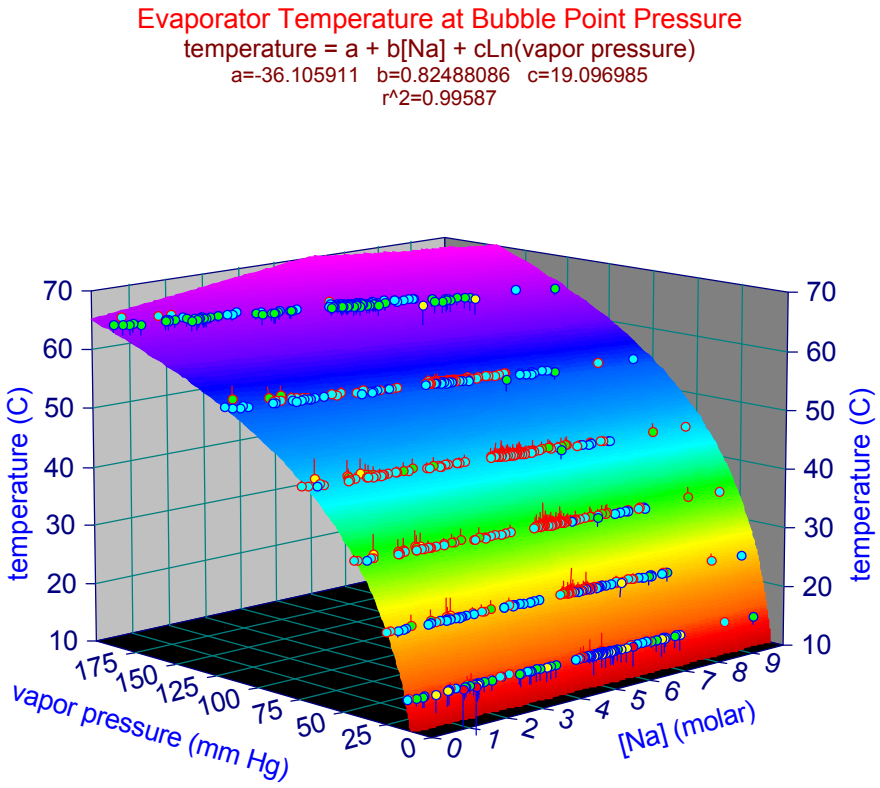
Figure 14. Envelope C Evaporator Bottoms Slurry Density



83 points fit to model, 33 validation points.

The data used to fit the evaporator temperature shown in Figure 15 was not derived from this work. The fit was done using results from the experimental simulant[26] over a broad range of compositions over all three envelopes. The plot gives the evaporator temperature as a function of the evaporator vapor pressure and bottoms sodium molarity. Not shown is a similar plot expressing the vapor pressure as a function of evaporator temperature and bottoms sodium molarity[26].

Figure 15. Evaporator Temperature at Bubble Point Pressure



2.6.2 Comparison of Simulation with Experimental Results

Simulants were made of 13 envelope A-a design points based on the slurry composition of the first ultra-filtration feed stream as predicted by OLI/ESP. The compositions and physical properties of these simulants were compared with those predicted by the simulation as a method of validating the OLI/ESP chemistry.

The experimental and simulation supernate compositions listed in Table 8 show good agreement, though OLI/ESP slightly under predicts the solubility of aluminum. (GCWB predicted an even lower aluminum solubility than OLI/ESP, where OLI/ESP predicted the precipitation of 98 moles of gibbsite and 0.12 moles of NAS gel, and GCWB predicted the precipitation of 184 moles of gibbsite and 0.54 moles of NAS gel for the same system).

Table 8. Comparison of Experimental with Simulation Supernate Compositions

run	Al (molar)			Ca (molar)			Fe (molar)		
	analytical	simulation	% difference	analytical	simulation	% difference	analytical	simulation	% difference
5	0.253	0.216	17.011	1.10E-05	-	N/A	4.98E-05	2.74E-05	N/A
10	1.197	0.989	20.994	3.29E-05	-	N/A	1.59E-04	5.10E-04	N/A
11	0.261	0.224	16.399	4.47E-06	-	N/A	1.38E-04	1.90E-04	N/A
13	0.238	0.205	16.082	8.30E-06	-	N/A	4.14E-05	1.96E-05	N/A
20	1.225	0.989	23.757	3.61E-05	-	N/A	1.63E-04	5.10E-04	N/A
21	0.246	0.211	16.784	9.98E-06	9.82E-05	N/A	1.24E-04	8.64E-04	N/A
25	0.232	0.204	13.331	1.09E-05	1.57E-06	N/A	8.93E-05	7.57E-04	N/A
26	0.222	0.199	11.923	2.41E-05	1.35E-06	N/A	4.07E-05	7.22E-04	N/A
30	1.132	0.926	22.317	3.37E-05	6.08E-07	N/A	1.18E-04	1.11E-03	N/A
33	0.227	0.200	13.216	7.86E-06	6.64E-05	N/A	3.93E-05	5.93E-04	N/A
35	0.244	0.207	18.111	1.13E-05	1.52E-06	N/A	8.49E-05	6.09E-04	N/A
53	0.283	0.237	19.479	3.44E-06	-	N/A	4.28E-05	2.57E-06	N/A
61	0.285	0.243	17.223	7.76E-06	4.85E-05	N/A	1.91E-04	7.58E-04	N/A

run	P (molar)			Si (molar)			S (molar)		
	analytical	simulation	% difference	analytical	simulation	% difference	analytical	simulation	% difference
5	0.0106	0.0350	-69.69	0.00533	0.00665	-19.85	0.0526	0.0568	-7.383
10	0.0049	0.0060	-18.37	0.00431	0.00600	-28.078	0.0414	0.0513	-19.41
11	0.0233	0.0279	-16.68	0.00611	0.00686	-10.85	0.0559	0.0583	-4.083
13	0.0055	0.0062	-10.07	0.00310	0.00288	7.764	0.0485	0.0531	-8.624
20	0.0045	0.0060	-24.01	0.00342	0.00600	-43.016	0.0438	0.0513	-14.75
21	0.0267	0.0290	-8.014	0.01399	0.01532	-8.699	0.0525	0.0566	-7.194
25	0.0124	0.0324	-61.72	0.00714	0.00624	14.40	0.0520	0.0554	-6.067
26	0.0200	0.0303	-33.96	0.00615	0.00256	140.73	0.0482	0.0520	-7.245
30	0.0046	0.0055	-16.15	0.00763	0.00552	38.10	0.0476	0.0507	-6.124
33	0.0053	0.0032	64.60	0.00420	0.00273	54.00	0.0484	0.0523	-7.381
35	0.0123	0.0330	-62.81	0.00493	0.00632	-21.92	0.0517	0.0557	-7.172
53	0.0068	0.0072	-5.606	0.00292	0.00576	-49.24	0.0611	0.0623	-1.888
61	0.0210	0.0434	-51.64	0.01910	0.01918	-0.3799	0.0625	0.0655	-4.616

N/A indicates that the values are so small that relative difference between the experimental and simulation values have little meaning.

The sodium molarity, density, and viscosity experimental and simulation results are given in Table 9. The simulants made to represent the simulation points 10, 20 and 30 overshot the target sodium concentration (defined as the composition predicted by OLI/ESP) by more than 7%, and it is expected that this will be reflected in comparisons between experimental and simulation results. This is apparent in the density and viscosity values, where the simulant values were greater than the corresponding simulation values. The remaining points generally had a difference of less than 5% in sodium molarity, 2% in density, and 9% in viscosity between the experimental and simulation results.

Table 9. Comparison of Experimental with Simulation Na Molarity, Density and Viscosity

envelope A simulation design point	design point temp (°C)	Supernate Na Molarity			Density (g/ml) (target = 1.22)		Viscosity (cP)			
		analytical	target (simulation)	% difference	analytical	% difference	analytical	model (correlation)	simulation (OLI/ESP)	% difference (analytical vs. simulation)
5	20	5.34	5.210	2.493	1.229	0.713	2.86	2.727	2.745	4.079
10	20	5.62	5.246	7.125	1.272	4.252	4.82	3.048	3.162	52.318
11	20	5.72	5.419	5.560	1.241	1.707	3.46	3.099	3.170	9.288
13	20	4.95	4.905	0.915	1.233	1.102	2.41	2.190	2.205	9.271
20	20	5.72	5.246	9.026	1.272	4.257	4.82	3.043	3.162	52.309
21	20	5.48	5.273	3.934	1.238	1.503	3.38	3.099	3.021	11.910
25	20	5.23	5.111	2.319	1.228	0.617	2.77	2.727	2.654	4.447
26	20	4.85	4.835	0.316	1.228	0.695	3.05	2.940	2.842	7.195
30	20	5.56	5.146	8.041	1.267	3.867	4.52	3.048	3.039	48.656
33	20	4.99	4.860	2.682	1.235	1.189	2.45	2.190	2.183	12.308
35	20	5.17	5.132	0.738	1.227	0.572	2.74	2.727	2.674	2.496
53	70	6.21	5.727	8.435	1.244	1.932	1.12	1.049	1.018	9.530
61	70	6.32	6.045	4.558	1.240	1.680	1.47	1.291	1.251	17.680

OLI/ESP generally predicted a somewhat lower heat capacity (13.8% on average) than measured experimentally (Table 10). The experimental heat capacities given are for the supernate, while those calculated by the simulation are for the slurry. Although a supernate would in general be expected to have a higher heat capacity than a slurry, the small amount of undissolved solids is likely to make the difference in heat capacity trivial. Points 10, 20, and 30 show less of a difference between the simulation and experimental values, but this is due to the higher sodium concentration in the simulant, which reduces the heat capacity. Simulations of simple $NaNO_3$-H_2O and NaOH-H_2O systems also showed OLI/ESP to under predict the heat capacity by 2-4% for solutions in the neighborhood of 5M Na as compared to published values (see Appendix D).

The experimental values for thermal conductivity (Table 10) showed a standard deviation about the value of water of 6.5%. No trend was found in the experimental values as a function of sodium concentration, and it is believed the variation is due largely to variability in the measurement. The mean in the percent difference between the experiment results and water is 1.7% with an error of 1.9%, so it is not possible to distinguish the experimental results from the value of water, as was true for the simulation results.

Table 10. Comparison of Experimental with Simulation Heat Capacity and Thermal Conductivity

envelope A design point	temp (°C)	Heat Capacity (cal/(g °C))				Thermal Conductivity (cal/(cm s K))		
		analytical	simulation (OLI/ESP)	model (correlation)	% difference (analytical vs. simulation)	analytical	simulation	% difference from that of water (0.63)
5	20	0.796	0.699	.6993	13.80	0.687	0.630	9.002
10	20	0.804	0.761	.7607	5.73	0.678	0.630	7.660
11	20	0.850	0.703	.7041	20.93	0.728	0.630	15.498
13	20	0.786	0.702	.7020	11.90	0.594	0.630	-5.658
20	20	0.807	0.761	.7608	6.07	0.621	0.630	-1.405
21	20	0.807	0.701	.7007	15.17	0.640	0.630	1.526
25	20	0.798	0.696	.6964	14.65	0.603	0.630	-4.273
26	20	0.812	0.713	.7127	13.95	0.662	0.630	5.066
30	20	0.793	0.753	.7532	5.27	0.658	0.630	4.430
33	20	0.790	0.698	.6976	13.21	0.625	0.630	-0.775
35	20	0.808	0.697	.6970	15.86	0.603	0.630	-4.343
53	70	0.767	0.640	.6401	19.79	0.590	0.630	-6.329
61	70	0.797	0.648	.6477	23.01	0.644	0.630	2.235

Table 11 shows good agreement in the total weight percent solids between the experimental and simulation results (as there should be given the simulant recipes were defined by the simulation composition), with the high sodium simulants (points 10, 20, and 30) having a somewhat higher experimental value. The weight percent insoluble solids show more variation between the experimental and simulation values, but are of the same order of magnitude; measuring such small amounts of insoluble solids experimentally can be very difficult.

Table 11. Comparison of Experimental with Simulation Dissolved and Undissolved Solids

envelope A simulation design point	design point temp (°C)	wt% Total Solids			wt% Insoluble Solids	
		analytical	simulation	% difference	analytical	simulation
5	20	27.51	27.07	1.62	0.694	0.239
10	20	30.82	29.34	5.05	1.147	3.737
11	20	26.59	26.95	-1.34	0.086	1.494
13	20	28.93	28.47	1.64	0.092	0.168
20	20	30.66	29.34	4.52	0.823	3.737
21	20	26.88	26.84	0.15	0.378	1.007
25	20	27.64	27.32	1.17	0.850	0.313
26	20	26.11	25.80	1.21	0.340	0.338
30	20	30.19	29.22	3.33	0.477	3.319
33	20	29.14	28.69	1.58	0.000	0.308
35	20	27.44	27.26	0.67	0.614	0.275
53	70	33.86	33.30	1.67	0.106	0.021
61	70	30.44	29.92	1.75	0.444	0.068

Table 12 compares the forms of precipitated solids. OLI/ESP predicted calcium precipitates, where none was measured by XRD. However, the experimental slurry composition given in

Table 13 shows calcium to be present, whereas the experimental supernate composition (Table 8) shows essentially no calcium, therefore it is believed that calcium did precipitate in the experimental simulants but was not picked up by XRD. There is fairly close agreement on the predictions of sodium oxalate and sodium fluoride. The simulation predicts a greater frequency in the precipitation of gibbsite and NAS gel which is consistent with its lower aluminum solubility prediction (Table 8). The precise form in which the fluorides and phosphates precipitate is often different, but both occur in the simulation and experiment, where the simulation often predicts a calcium form and the experimental XRD results show a sodium form. XRD showed sodium carbonate precipitation occurring in 4 of the 13 points, but this was never predicted by the simulation.

Table 12. Comparison of Experimental with Simulation Precipitated Solid Species

envelope A simulation design point	design point temp	Predicted/Measured Precipitated Solids									
		Na2CO3 .xH20	AlOH3	Na3FSO4	NaF	Na2C2O4	NASGel	Na7FPO42 .19H2O	NaPHOH .12H2O	Ca3PO42	CaF2
5	20	-	-	-	E - S	E - S	-	E - S	-	-	-
10	20	-	S	E	E - S	E - S	S	E	-	-	-
11	20	-	-	-	-	E -S	-	-	S	-	-
13	20	E	E - S	-	-	E	S	-	-	-	-
20	20	-	S	E	E - S	E - S	S	E	-	-	-
21	20	-	-	-	-	E - S	S	E	S	S	-
25	20	-	-	-	-	E - S	E - S	E	-	-	S
26	20	E	S	-	-	S	S	E	-	-	S
30	20	-	S	-	E - S	E - S	E - S	E	-	-	S
33	20	E	S	-	-	E	S	-	-	S	S
35	20	-	-	-	E	E - S	S	E	-	-	S
53	70	E	-	-	-	E	S	-	-	-	-
61	70	-	-	-	-	E	E	E	-	S	-

An "E" indicates the solid was observed experimentally by XRD, "S" indicates the solid was predicted by the simulation.

Table 13. Experimental Slurry Composition

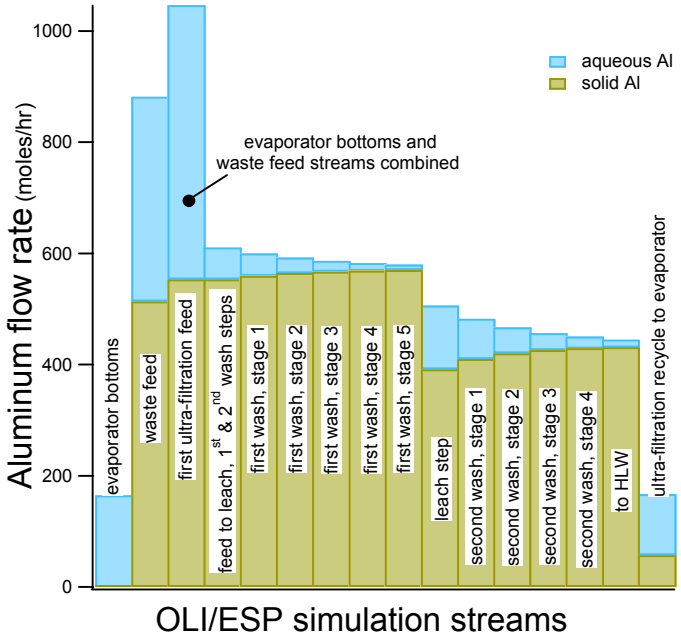
run	Al (molar)	B (molar)	Ca (molar)	Mg (molar)	Na (molar)	P (molar)	Si (molar)	V (molar)	Zn (molar)	Zr (molar)	K (molar)	S (molar)
5	1.69E-01	1.04E+01	-	-	3.79E+00	2.02E-02	3.88E-02	-	-	9.09E-05	4.80E-03	4.01E-02
10	7.47E-01	1.00E+01	-	-	3.90E+00	2.74E-03	2.19E-02	-	-	1.42E-04	1.66E-03	3.31E-02
11	1.74E-01	9.84E+00	-	-	3.66E+00	1.56E-02	3.97E-02	-	-	7.93E-05	3.43E-03	4.08E-02
13	1.60E-01	1.05E+01	-	-	3.56E+00	3.71E-03	3.20E-02	-	-	-	2.98E-03	3.62E-02
20	1.63E-01	1.01E+01	4.52E-03	1.41E-03	3.80E+00	1.83E-02	2.33E-02	2.56E-04	2.47E-03	1.06E-04	8.72E-02	3.81E-02
21	1.60E-01	1.04E+01	4.39E-03	1.36E-03	3.83E+00	1.96E-02	3.39E-02	-	2.51E-03	9.32E-05	9.03E-02	3.93E-02
25	1.57E-01	9.85E+00	4.18E-03	1.34E-03	3.52E+00	1.57E-02	3.00E-02	-	2.46E-03	1.08E-04	8.94E-02	3.93E-02
26	6.91E-01	9.23E+00	-	-	3.63E+00	2.74E-03	1.96E-02	2.58E-04	-	1.96E-04	-	3.06E-02
30	7.10E-01	1.02E+01	3.40E-03	1.06E-03	3.79E+00	2.73E-03	8.87E-02	-	2.18E-03	1.77E-04	7.72E-02	3.31E-02
33	1.53E-01	1.02E+01	3.21E-03	1.06E-03	3.34E+00	3.33E-03	2.34E-02	3.20E-04	1.91E-03	5.85E-05	6.71E-02	3.55E-02
35	1.59E-01	1.03E+01	3.28E-03	1.06E-03	3.50E+00	1.05E-02	2.71E-02	-	1.95E-03	1.11E-04	7.23E-02	3.84E-02
53	1.78E-01	1.03E+01	-	-	3.94E+00	3.69E-03	2.11E-02	-	-	1.16E-04	3.29E-03	3.98E-02
61	1.84E-01	1.08E+01	4.55E-03	1.38E-03	4.25E+00	2.22E-02	3.02E-02	-	2.47E-03	-	8.50E-02	4.42E-02

2.6.3 Fate of Aluminum, Strontium, Sodium and NAS gel Through the Pre-Treatment Process for Three Waste Feed Compositions

Figure 16, Figure 17, and Figure 18 track aluminum through each stage of the pre-treatment process for waste feed from envelopes A (tank AN-104), B/D (tank AZ-102), and C (tank AN-107) respectively.

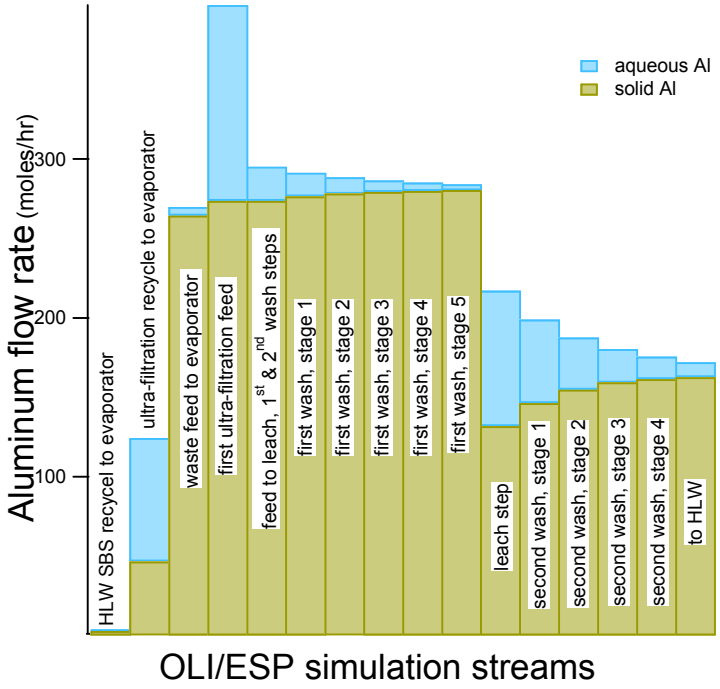
Figure 16 shows that the reduction of aluminum to HLW due to leaching for envelope A is minimal, with approximately 73% of the total aluminum fed to the wash and leach steps being sent to HLW. Most of this reduction occurs immediately following the leach step where a volume of supernate equal to that added as NaOH and steam is decanted from the slurry.

Figure 16. Fate of Aluminum Through Pre-Treatment Process for AN-104



The reduction of aluminum to HLW due to leaching is somewhat greater for envelope B/D (than for A) due to its higher aluminum solids content. Approximately 58% of the total aluminum fed to the wash and leach steps is sent to HLW, as shown in Figure 17.

Figure 17. Fate of Aluminum Through Pre-Treatment Process for AZ-102



Aluminum is not an issue for envelope C tanks and the leach step is not part of the pre-treatment process. Figure 18 is included only for comparison to the other envelopes.

Figure 18. Fate of Aluminum Through Pre-Treatment Process for AN-107

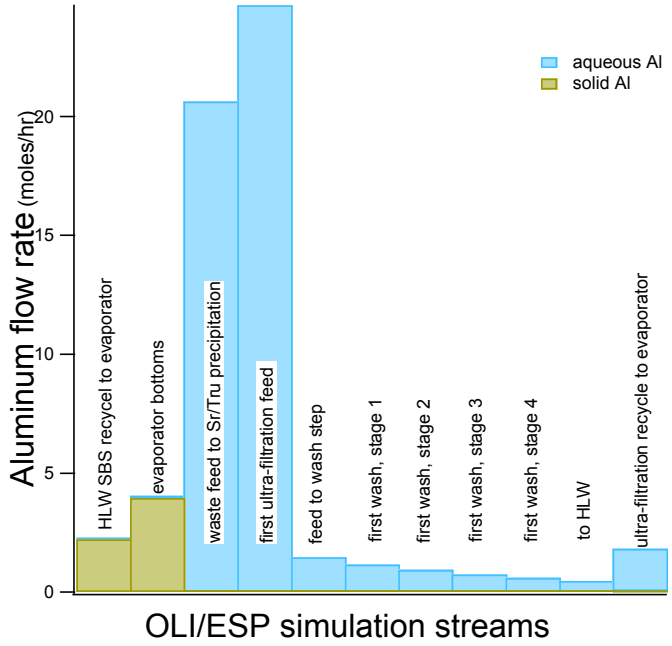
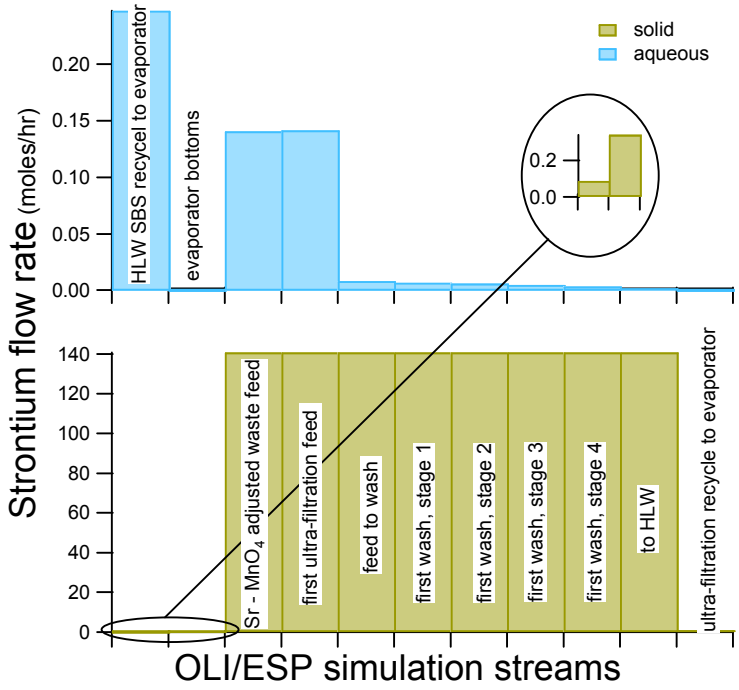


Figure 19 shows strontium in the pre-treatment process for envelope C; not surprisingly, essentially all the strontium remains as a precipitated solid and is sent to HLW.

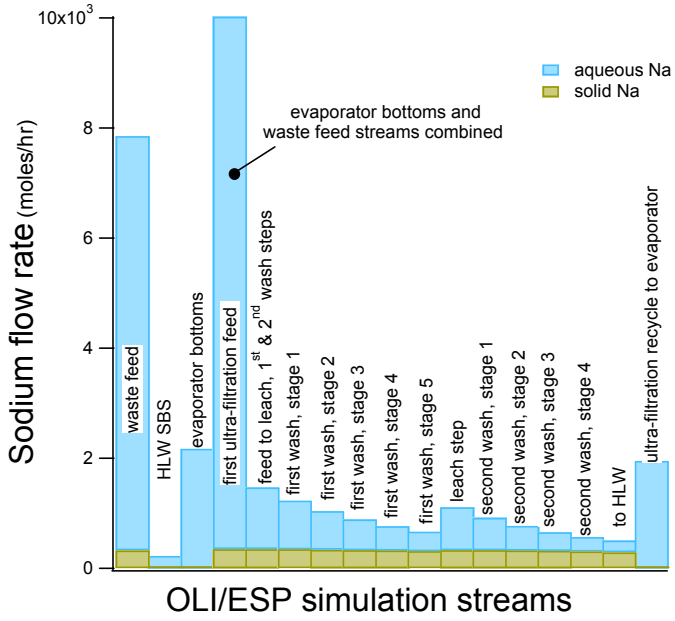
Figure 19. Fate of Strontium Through Pre-Treatment Process for AN-107



Note the difference in scale between the aqueous and solid phases.

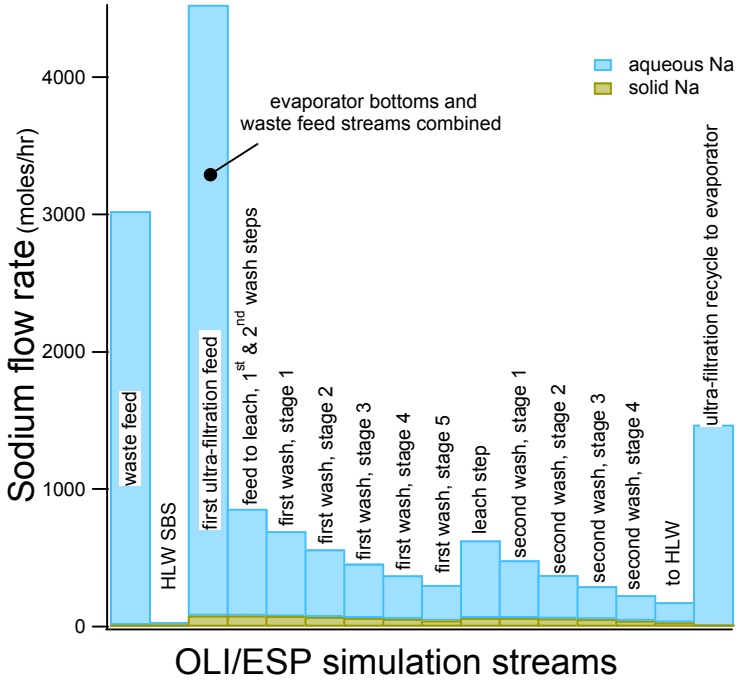
Figure 20, Figure 21, and Figure 22 track sodium through each stage of the pre-treatment process for waste feed from envelopes A (tank AN-104), B/D (tank AZ-102), and C (tank AN-107) respectively. The plots show the sodium is reduced by diluting the supernate, while the amount of sodium in the solids remains relatively constant. 34% of the sodium fed to the leach and wash step for envelope A (tank AN-104) is sent to HLW, as shown in Figure 20.

Figure 20. Fate of Sodium Through Pre-Treatment Process for AN-104



21% of Sodium fed to the leach and wash steps for envelope B/D are sent to HLW, as shown in Figure 21.

Figure 21. Fate of Sodium Through Pre-Treatment Process for AZ-102



32% of Na fed to the leach and wash steps for envelope C is sent to HLW, as shown in Figure 22.

Figure 22. Fate of Sodium Through Pre-Treatment Process for AN-107

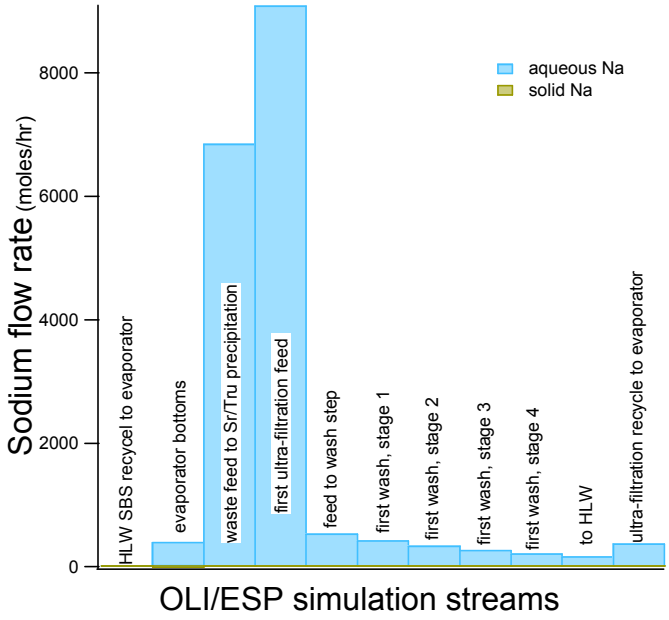


Figure 23 and Figure 24 show the progression of NAS gel through the pre-treatment process for wastes from envelope A and B/D respectively. Envelope C showed a small amount of NAS gel in the evaporator bottoms (0.34 moles/hr), and an insignificant amount in the ultra-filtration recycle (0.008moles/hr), but no NAS gel was present in the streams following the Sr/TRU precipitation step.

Figure 23. Fate of NAS gel Through Pre-Treatment Process for AN-104

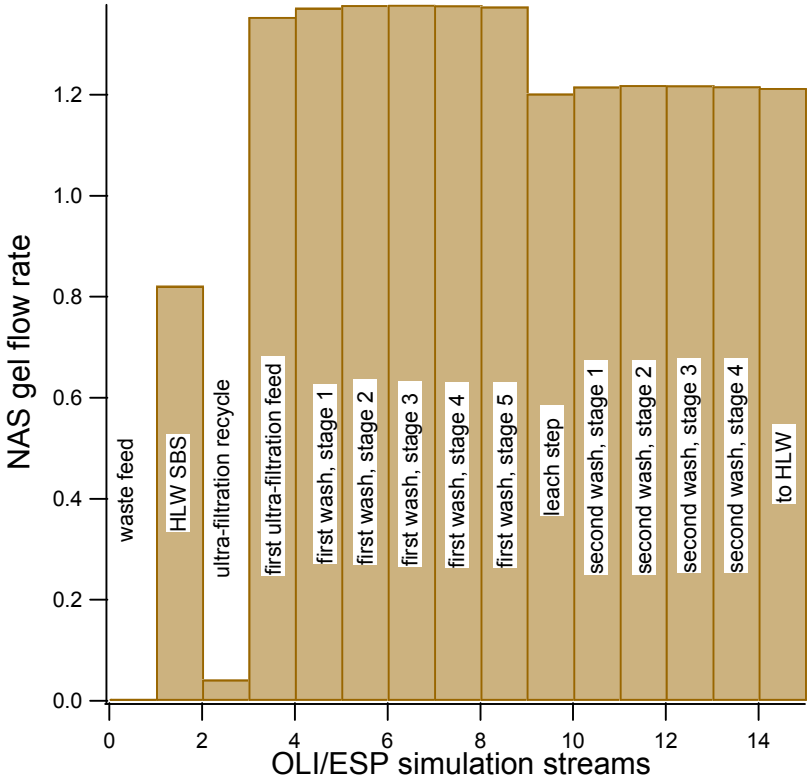
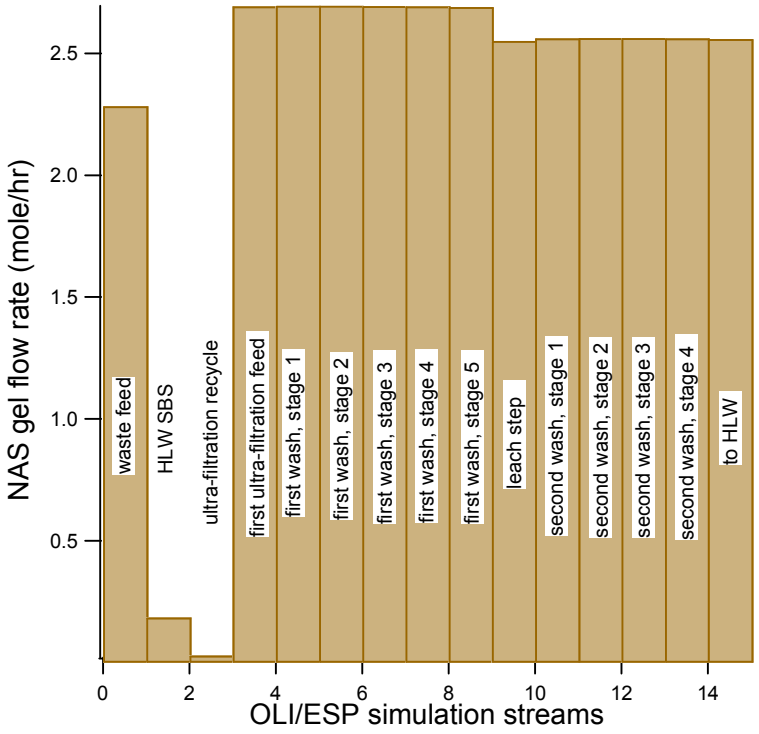


Figure 24. Fate of NAS gel Through Pre-Treatment Process for AZ-102



3.0 FUTURE WORK

Development of physical property models for AY-102 (C106) will be done in conjunction with the integrated pilot testing.

$SrNaPO_4.H_2O$ solids which formed in experimental simulation work for envelope C are not included the OLI databases. This should be included in order to model its behavior in the pre-treatment process.

Blending of envelope A with envelope B/D wastes prior to the pre-treatment process are being considered as a method of generating continuous feed to both the HLW and LAW melters and minimize the HLW melter idle time. Modeling and experimental work could be preformed to predict the compositions and solids precipitation of theses blended feed streams, and the behavior of the blended streams through the pre-treatment process.

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APPENDIX A. EXAMPLE MODEL CALCULATION

Example calculations are shown for envelopes A and B/D. Calculations for envelope C models are done the same as for envelope A.

Envelope A Sample Calculation
The mixture variables used for envelope A and C models are expressed in molar concentrations relative to a 5M Na stream, as shown below.

Below are example analytical molar concentrations for mixture variables of the waste feed stream:
AlO_2 = 0.9408M, CO_3 = 0.2506M, F=0.0322M, NO_2 = 1.246M, NO_3 = 2.2078M,
OH = 1.5904M, PO_4 = 0.03696M

Below are example values for the process variables:
sodium of waste feed stream = 7M Na,
Temp. of feed stream to 1st ultra-filtration = 28°C
waste feed volumetric flow rate = 1,171 L/hr., HLW SBS volumetric flow rate = 1885 L/hr.

1) Normalize mixture variables to a 5M Na stream by multiplying the molar concentration by 5 and dividing by the analytical sodium molar concentration, in this case 7.

$[AlO_2]$ = 0.9408M x 5 / 7 = 0.672M,
$[CO_3]$ = 0.2506M x 5 / 7 = 0.179M,
[F] =0.0322M x 5 / 7 = 0.23M,
$[NO_2]$ = 1.246M x 5 / 7 = 0.89M,
$[NO_3]$ = 2.2078M x 5 / 7 = 1.577M,
[OH] = 1.5904M x 5 / 7 = 1.136M,
$[PO_4]$ = 0.03696M x 5 / 7 = 0.0264,

2) Calculate the waste feed to HLW SBS volumetric ratio:

[SBS] = (HLW SBS flow) / (waste feed flow) = 1885(L/hr.) / 1,171(L/hr) = 1.61

3) Input values into model equation:

$$\text{viscosity(cP)} = 0.0544[NO_2] + 0.0608[NO_3] - 0.149[OH] + \exp\left(\begin{array}{l}\dfrac{219}{77.4+[Temp]} - 0.947 - 0.0678[NO_2] - 0.134[NO_3] \\ +0.0611[OH] - 0.0826[NO_3][NO_2]\end{array}\right)$$

$$= 0.0544(0.89) + 0.0608(1.577) - 0.149(1.136) + \exp\left(\begin{array}{l}\dfrac{219}{77.4+(28)} - 0.947 - 0.0678(0.89) - 0.134(1.577) \\ +0.0611(1.136) - 0.0826(0.89)(1.577)\end{array}\right)$$

$$= 2.229(cP)$$

Although the process variables [SBS] and [Na] were not used in this example, the values applied to the model equations would be 1.16 and 7 respectively.

Envelope B/D Sample Calculation

The mixture variables used for envelope B/D models are expressed in term of their mass fraction relative to the total mass of the mixture variables, as shown below.

Below are example analytical masses given for mixture variables of the waste feed stream based on the *total solids* of the waste stream:
AlO_2 = 0.42825g, CO_3 = 0.9555g, Fe = 0.17526g, NO_3 = 0.87771g, OH = 0.2529g, SO_4 = 0.31038g
(all aluminum and sulfur are treated as AlO_2 and SO_4 and should be assigned be molecular weight of these anions, i.e. grams of AlO_2 = moles of Al x 59)

Below are example values for the process variables:
sodium of waste feed stream = 2.5M Na,
Temp. of feed stream to 1st ultra-filtration = 68°C
waste feed volumetric flow rate = 1,171 L/hr., HLW SBS volumetric flow rate = 1464 L/hr.

1) Normalize mixture variables to a mass fraction by dividing by the total mass of the mixture variables:

Total mixture variable mass = 0.42825g + 0.9555g + 0.17526g + 0.87771g + 0.2529g + 0.31038g
= 3g

$[AlO_2]$ = 0.42825g / 3g = 0.14275,
$[CO_3]$ = 0.9555g / 3g = .3185,
[Fe] = 0.17526g / 3g = 0.05842,

$[NO_3]$ = 0.87771g / 3g = 0.29257,
[OH] = 0.2529g / 3g = 0.0843,
$[SO_4]$ = 0.31038g / 3g = 0.10346,

2) Calculate the waste feed to HLW SBS volumetric ratio:

[SBS] = (HLW SBS flow) / (waste feed flow) = 1464(L/hr.) / 1,171(L/hr) = 1.25

3) Input values into model equation:

$$\text{viscosity(cP)} = -0.0454[NO_3] + 0.0045[SBS] + \exp\left(\begin{array}{l}\dfrac{312}{98.7+[Temp]} - 1.83 + 0.134[AlO_2] \\ +0.22[CO_3] - 0.0109[SBS]\end{array}\right)$$

$$= -0.0454(0.29257) + 0.0045(1.25) + \exp\left(\begin{array}{l}\dfrac{312}{98.7+(68)} - 1.83 + 0.134(0.14275) \\ +0.22(0.3185) - 0.0109(1.25)\end{array}\right)$$

$$= 1.117(cP)$$

Although the process variable [Na] was not used in this example, the value applied to the model equation would be 2.5.

APPENDIX B. DESIGN MATRICIES FOR ENVELOPES A, B/D, AND C

The following tables list the compositions of the waste feed stream, SBS/Feed volumetric flow ratio, and filtration feed stream temperature used in the OLI/ESP computer simulations. The mixture variables for envelopes A-a and C are given in terms of 5M Na stream, and in terms of the mass fraction to the total mass of the mixture variables for envelope B/D. The sodium concentration represents a "dilution factor" of the waste feed stream, water is added or removed to a waste feed stream of a given mixture variable concentration to achieve the target sodium molarity. The Test ID describes the type of design point. MPV indicates a model design point used in the property model fit and are derived using only the minimum and maximum values of the factor space. OLH indicates a design point used to validate the model (though some were occasionally used in the model fits as described in the results section), and were generated to be uniformly distributed over the factor space (as opposed to only the extreme vertices of the MPV points).

Table 14. Sub-envelope A-a Computer Simulation Design Matrix

Test ID	Type	[AlO2] (molar at 5M Na)	[CO3] (molar at 5M Na)	[F] (molar at 5M Na)	[NO2] (molar at 5M Na)	[NO3] (molar at 5M Na)	[OH] (molar at 5M Na)	[PO4] (molar at 5M Na)	SBS/Feed	[Na] (molar)	Temp (°C)
1	MPV	0.206984	0.032611	0.009284	0.73098	0.991014	2.606201	0.042265	0	5.6	20
2	MPV	0.206984	0.032611	0.009284	0.730981	0.991014	2.71405	0.006315	0	5.6	20
3	MPV	0.206984	0.032611	0.009284	1.541582	1.911454	0.983009	0.006315	0	5.6	20
4	MPV	0.206984	0.032611	0.228819	0.730982	2.016651	1.468877	0.006315	0	5.6	20
5	MPV	0.206984	0.032611	0.228819	1.541581	0.991014	1.600911	0.033983	0	5.6	20
6	MPV	0.206984	0.665097	0.228819	0.73098	1.154545	0.983009	0.033983	0	5.6	20
7	MPV	0.673054	0.665097	0.009284	0.73098	0.991014	0.983009	0.006315	0	5.6	20
8	MPV	0.736049	0.032611	0.009284	0.73098	2.016651	1.051499	0.042265	0	5.6	20
9	MPV	0.824593	0.032611	0.009284	1.541582	0.991014	1.17799	0.042265	0	5.6	20
10	MPV	1.085885	0.032611	0.228819	0.730982	0.991014	1.615613	0.006315	0	5.6	20
11	MPV	0.206984	0.032611	0.009284	0.73098	0.991014	2.606201	0.042265	0	7	20
12	MPV	0.206984	0.032611	0.009284	0.730981	0.991014	2.71405	0.006315	0	7	20
13	MPV	0.206984	0.032611	0.009284	1.541582	1.911454	0.983009	0.006315	0	7	20
14	MPV	0.206984	0.032611	0.228819	0.730982	2.016651	1.468877	0.006315	0	7	20
15	MPV	0.206984	0.032611	0.228819	1.541581	0.991014	1.600911	0.033983	0	7	20
16	MPV	0.206984	0.665097	0.228819	0.73098	1.154545	0.983009	0.033983	0	7	20
17	MPV	0.673054	0.665097	0.009284	0.73098	0.991014	0.983009	0.006315	0	7	20
18	MPV	0.736049	0.032611	0.009284	0.73098	2.016651	1.051499	0.042265	0	7	20
19	MPV	0.824593	0.032611	0.009284	1.541582	0.991014	1.17799	0.042265	0	7	20
20	MPV	1.085885	0.032611	0.228819	0.730982	0.991014	1.615613	0.006315	0	7	20
21	MPV	0.206984	0.032611	0.009284	0.73098	0.991014	2.606201	0.042265	2	5.6	20
22	MPV	0.206984	0.032611	0.009284	0.730981	0.991014	2.71405	0.006315	2	5.6	20
23	MPV	0.206984	0.032611	0.009284	1.541582	1.911454	0.983009	0.006315	2	5.6	20
24	MPV	0.206984	0.032611	0.228819	0.730982	2.016651	1.468877	0.006315	2	5.6	20
25	MPV	0.206984	0.032611	0.228819	1.541581	0.991014	1.600911	0.033983	2	5.6	20
26	MPV	0.206984	0.665097	0.228819	0.73098	1.154545	0.983009	0.033983	2	5.6	20
27	MPV	0.673054	0.665097	0.009284	0.73098	0.991014	0.983009	0.006315	2	5.6	20
28	MPV	0.736049	0.032611	0.009284	0.73098	2.016651	1.051499	0.042265	2	5.6	20
29	MPV	0.824593	0.032611	0.009284	1.541582	0.991014	1.17799	0.042265	2	5.6	20
30	MPV	1.085885	0.032611	0.228819	0.730982	0.991014	1.615613	0.006315	2	5.6	20

Test ID	Type	[AlO2] (molar at 5M Na)	[CO3] (molar at 5M Na)	[F] (molar at 5M Na)	[NO2] (molar at 5M Na)	[NO3] (molar at 5M Na)	[OH] (molar at 5M Na)	[PO4] (molar at 5M Na)	SBS/Feed	[Na] (molar)	Temp (°C)
31	MPV	0.206984	0.032611	0.009284	0.73098	0.991014	2.606201	0.042265	2	7	20
32	MPV	0.206984	0.032611	0.009284	0.730981	0.991014	2.71405	0.006315	2	7	20
33	MPV	0.206984	0.032611	0.009284	1.541582	1.911454	0.983009	0.006315	2	7	20
34	MPV	0.206984	0.032611	0.228819	0.730982	2.016651	1.468877	0.006315	2	7	20
35	MPV	0.206984	0.032611	0.228819	1.541581	0.991014	1.600911	0.033983	2	7	20
36	MPV	0.206984	0.665097	0.228819	0.73098	1.154545	0.983009	0.033983	2	7	20
37	MPV	0.673054	0.665097	0.009284	0.73098	0.991014	0.983009	0.006315	2	7	20
38	MPV	0.736049	0.032611	0.009284	0.73098	2.016651	1.051499	0.042265	2	7	20
39	MPV	0.824593	0.032611	0.009284	1.541582	0.991014	1.17799	0.042265	2	7	20
40	MPV	1.085885	0.032611	0.228819	0.730982	0.991014	1.615613	0.006315	2	7	20
41	MPV	0.206984	0.032611	0.009284	0.73098	0.991014	2.606201	0.042265	0	5.6	70
42	MPV	0.206984	0.032611	0.009284	0.730981	0.991014	2.71405	0.006315	0	5.6	70
43	MPV	0.206984	0.032611	0.009284	1.541582	1.911454	0.983009	0.006315	0	5.6	70
44	MPV	0.206984	0.032611	0.228819	0.730982	2.016651	1.468877	0.006315	0	5.6	70
45	MPV	0.206984	0.032611	0.228819	1.541581	0.991014	1.600911	0.033983	0	5.6	70
46	MPV	0.206984	0.665097	0.228819	0.73098	1.154545	0.983009	0.033983	0	5.6	70
47	MPV	0.673054	0.665097	0.009284	0.73098	0.991014	0.983009	0.006315	0	5.6	70
48	MPV	0.736049	0.032611	0.009284	0.73098	2.016651	1.051499	0.042265	0	5.6	70
49	MPV	0.824593	0.032611	0.009284	1.541582	0.991014	1.17799	0.042265	0	5.6	70
50	MPV	1.085885	0.032611	0.228819	0.730982	0.991014	1.615613	0.006315	0	5.6	70
51	MPV	0.206984	0.032611	0.009284	0.73098	0.991014	2.606201	0.042265	0	7	70
52	MPV	0.206984	0.032611	0.009284	0.730981	0.991014	2.71405	0.006315	0	7	70
53	MPV	0.206984	0.032611	0.009284	1.541582	1.911454	0.983009	0.006315	0	7	70
54	MPV	0.206984	0.032611	0.228819	0.730982	2.016651	1.468877	0.006315	0	7	70
55	MPV	0.206984	0.032611	0.228819	1.541581	0.991014	1.600911	0.033983	0	7	70
56	MPV	0.206984	0.665097	0.228819	0.73098	1.154545	0.983009	0.033983	0	7	70
57	MPV	0.673054	0.665097	0.009284	0.73098	0.991014	0.983009	0.006315	0	7	70
58	MPV	0.736049	0.032611	0.009284	0.73098	2.016651	1.051499	0.042265	0	7	70
59	MPV	0.824593	0.032611	0.009284	1.541582	0.991014	1.17799	0.042265	0	7	70
60	MPV	1.085885	0.032611	0.228819	0.730982	0.991014	1.615613	0.006315	0	7	70
61	MPV	0.206984	0.032611	0.009284	0.73098	0.991014	2.606201	0.042265	2	5.6	70
62	MPV	0.206984	0.032611	0.009284	0.730981	0.991014	2.71405	0.006315	2	5.6	70
63	MPV	0.206984	0.032611	0.009284	1.541582	1.911454	0.983009	0.006315	2	5.6	70
64	MPV	0.206984	0.032611	0.228819	0.730982	2.016651	1.468877	0.006315	2	5.6	70
65	MPV	0.206984	0.032611	0.228819	1.541581	0.991014	1.600911	0.033983	2	5.6	70
66	MPV	0.206984	0.665097	0.228819	0.73098	1.154545	0.983009	0.033983	2	5.6	70
67	MPV	0.673054	0.665097	0.009284	0.73098	0.991014	0.983009	0.006315	2	5.6	70
68	MPV	0.736049	0.032611	0.009284	0.73098	2.016651	1.051499	0.042265	2	5.6	70
69	MPV	0.824593	0.032611	0.009284	1.541582	0.991014	1.17799	0.042265	2	5.6	70
70	MPV	1.085885	0.032611	0.228819	0.730982	0.991014	1.615613	0.006315	2	5.6	70
71	MPV	0.206984	0.032611	0.009284	0.73098	0.991014	2.606201	0.042265	2	7	70
72	MPV	0.206984	0.032611	0.009284	0.730981	0.991014	2.71405	0.006315	2	7	70
73	MPV	0.206984	0.032611	0.009284	1.541582	1.911454	0.983009	0.006315	2	7	70
74	MPV	0.206984	0.032611	0.228819	0.730982	2.016651	1.468877	0.006315	2	7	70
75	MPV	0.206984	0.032611	0.228819	1.541581	0.991014	1.600911	0.033983	2	7	70
76	MPV	0.206984	0.665097	0.228819	0.73098	1.154545	0.983009	0.033983	2	7	70
77	MPV	0.673054	0.665097	0.009284	0.73098	0.991014	0.983009	0.006315	2	7	70
78	MPV	0.736049	0.032611	0.009284	0.73098	2.016651	1.051499	0.042265	2	7	70
79	MPV	0.824593	0.032611	0.009284	1.541582	0.991014	1.17799	0.042265	2	7	70
80	MPV	1.085885	0.032611	0.228819	0.730982	0.991014	1.615613	0.006315	2	7	70
81	OLH	0.62249	0.36313	0.23423	0.99104	0.992554	1.071098	0.032936	0.0391	6.6227	20
82	OLH	0.61535	0.13597	0.23069	1.234319	1.105193	1.211971	0.022339	1.957	6.3656	20.1
83	OLH	0.56899	0.10789	0.17755	0.818246	1.907495	1.011636	0.012261	0.7578	6.6691	20.7
84	OLH	0.71343	0.10534	0.22316	0.769589	1.721739	1.057052	0.01361	0.3008	5.9637	20.9
85	OLH	0.30686	0.31591	0.21297	1.368541	1.021903	1.092212	0.034058	0.0039	6.4531	21.1
86	OLH	0.32291	0.2738	0.11776	1.469197	1.031099	1.228102	0.006604	1.2305	6.3383	22
87	OLH	0.40315	0.44098	0.04735	0.918902	1.135875	1.238342	0.036967	1.5898	6.8742	22.5

Test ID	Type	[AlO2] (molar at 5M Na)	[CO3] (molar at 5M Na)	[F] (molar at 5M Na)	[NO2] (molar at 5M Na)	[NO3] (molar at 5M Na)	[OH] (molar at 5M Na)	[PO4] (molar at 5M Na)	SBS/Feed	[Na] (molar)	Temp (°C)
88	OLH	0.59039	0.50096	0.20057	0.73938	1.109087	1.020913	0.02474	0.7734	5.7832	23
89	OLH	0.78654	0.06833	0.18773	0.841739	1.162892	1.558783	0.020712	1.1641	6.3547	23.1
90	OLH	0.24088	0.13852	0.13592	1.182316	1.331878	1.526356	0.01403	0.6094	6.8934	23.2
91	OLH	0.37997	0.09896	0.10758	1.491016	1.133808	1.38283	0.014452	0.8594	6.866	23.5
92	OLH	0.52263	0.06706	0.07525	1.576571	1.241781	1.132218	0.01797	0.1914	6.2016	23.6
93	OLH	0.38532	0.29677	0.08588	0.999433	1.297449	1.255557	0.039767	1.0195	5.8816	24.2
94	OLH	0.39245	0.30953	0.04647	0.761198	1.717348	1.180829	0.006375	0.5352	6.2043	24.4
95	OLH	0.6528	0.10917	0.22936	1.222574	1.218357	1.102979	0.03069	1.3203	6.1141	24.9
96	OLH	0.57256	0.2521	0.03274	1.467525	1.070218	1.063692	0.008515	1.8398	6.3465	25.4
97	OLH	0.67955	0.3861	0.06285	1.066547	1.007584	1.101807	0.015314	0.1563	6.6391	26.1
98	OLH	0.34609	0.04026	0.0416	0.81991	1.584683	1.754483	0.036398	1.5977	6.3137	26.3
99	OLH	0.65815	0.32995	0.20279	1.041374	1.007769	1.089346	0.025717	0.1719	6.691	26.6
100	OLH	0.67242	0.17936	0.023	0.890377	1.576768	1.135896	0.026433	1.6094	6.7867	27.8
101	OLH	0.49588	0.12321	0.09607	0.984328	1.716215	1.084068	0.037833	0.8633	6.6254	28.3
102	OLH	0.3871	0.38482	0.18463	0.821609	1.361916	1.186076	0.008503	1.0703	6.9234	29.1
103	OLH	0.68846	0.03643	0.06241	1.204122	1.446256	1.163543	0.032943	1.0273	6.8223	30.8
104	OLH	0.50836	0.26359	0.13902	0.756161	1.388419	1.363931	0.017803	1.1758	5.7859	31
105	OLH	0.82042	0.11045	0.05045	1.076613	1.279716	1.236871	0.01717	0.5	5.7148	31.3
106	OLH	0.58861	0.17043	0.20854	1.004464	1.550631	0.989318	0.018019	1.2695	5.6191	31.8
107	OLH	0.87213	0.07089	0.01857	1.257803	1.090504	1.305578	0.016705	0.0195	6.4176	31.9
108	OLH	0.51193	0.12576	0.23334	1.019573	1.45827	1.165067	0.03226	1.4414	6.3055	32
109	OLH	0.65102	0.05174	0.03584	1.286334	1.534695	1.10046	0.008217	1.0547	6.1387	32.8
110	OLH	0.85787	0.14363	0.13238	0.982652	1.181645	1.273241	0.007144	1.2461	6.9754	33
111	OLH	0.26763	0.09386	0.03008	1.314845	1.821059	1.04935	0.021932	1.0977	5.9719	33.2
112	OLH	0.62962	0.15256	0.07614	1.26116	1.351476	1.036881	0.025361	0.6211	6.6309	33.3
113	OLH	0.42455	0.26103	0.08012	1.299764	1.021742	1.263102	0.041714	1.0664	5.7121	33.6
114	OLH	0.43525	0.20105	0.0354	1.103465	1.646617	1.092615	0.007011	0.6563	6.3574	34.1
115	OLH	0.66707	0.07216	0.18507	0.944075	1.527232	1.239094	0.009873	1.3867	6.5324	34.2
116	OLH	0.48696	0.25338	0.14433	1.031317	1.360324	1.184898	0.007297	1.0078	5.991	34.9
117	OLH	0.45665	0.10024	0.15983	1.579929	1.258588	1.012549	0.022818	1.8711	6.4559	35.2
118	OLH	0.84717	0.28528	0.17356	0.781338	1.003718	1.330542	0.009864	0.5664	6.8414	35.3
119	OLH	0.21413	0.12831	0.11245	1.106819	1.118654	1.873912	0.017965	0.6953	6.9563	36.1
120	OLH	0.38175	0.09258	0.21474	1.262849	1.412871	1.231764	0.015782	1.4219	5.8461	36.3
121	OLH	0.54938	0.17298	0.04115	1.142041	1.585056	1.036257	0.012212	1.3555	6.8113	37.4
122	OLH	0.44238	0.52265	0.09916	0.82496	1.095207	1.1899	0.013191	0.2383	6.3246	37.6
123	OLH	0.72591	0.06961	0.03451	0.892064	1.476075	1.380318	0.029461	0.6328	5.8844	38
124	OLH	0.31399	0.36696	0.12573	1.269554	1.033048	1.140457	0.039927	1.5313	6.1496	38.2
125	OLH	0.26406	0.04281	0.21829	0.776296	1.591467	1.764918	0.011943	0.4727	6.1305	38.3
126	OLH	0.68133	0.08109	0.13548	0.986024	1.335708	1.357935	0.025941	0.5195	6.7895	38.8
127	OLH	0.62784	0.16149	0.14212	0.751135	1.042666	1.790615	0.019708	1.9727	6.4887	38.9
128	OLH	0.38889	0.18319	0.13636	1.371889	1.229871	1.169479	0.024537	0.1523	6.0266	39.4
129	OLH	0.53511	0.06323	0.08057	0.772936	1.266101	1.919087	0.012072	1.668	6.877	41.6
130	OLH	0.36571	0.11172	0.0571	0.754483	1.547349	1.758338	0.01002	1.9336	5.9938	42.9
131	OLH	0.55116	0.24189	0.14965	0.811531	1.5033	1.172814	0.021415	1.4258	5.8488	44
132	OLH	0.34966	0.1985	0.10448	0.928971	1.301246	1.541855	0.037756	0.168	5.775	44.5
133	OLH	0.99874	0.0326	0.1895	0.734361	1.006731	1.71952	0.007476	1.6641	6.0621	44.7
134	OLH	0.42098	0.25465	0.11644	0.846772	1.618549	1.197325	0.009038	0.2344	6.2699	45.1
135	OLH	0.29616	0.44863	0.07215	0.767916	1.102341	1.53708	0.021191	1.6914	6.1961	45.6
136	OLH	0.57077	0.23424	0.01813	1.029628	1.337195	1.239566	0.024237	1.125	6.3027	46.1
137	OLH	0.207	0.11938	0.08234	1.259482	1.713387	1.154112	0.027133	0.2813	6.5051	47.2
138	OLH	0.20878	0.42311	0.0664	0.833337	1.584118	1.14865	0.016325	1.7813	6.6582	47.6
139	OLH	0.43347	0.33761	0.14788	1.157126	1.174428	1.095925	0.017477	0.6992	6.0703	48
140	OLH	0.56542	0.27252	0.09651	1.00783	1.510207	0.989144	0.007443	0.957	6.8359	48.1
141	OLH	0.56721	0.04664	0.02521	0.972589	1.842704	1.130946	0.034847	0.3164	6.9617	48.3
142	OLH	0.24623	0.05302	0.18596	1.506112	1.587626	1.076525	0.009329	1.7539	5.8051	48.6
143	OLH	0.54224	0.42949	0.01016	0.907157	1.253655	1.107669	0.018873	0.4375	6.3164	48.7
144	OLH	0.62427	0.09003	0.1709	1.341693	1.341909	1.039446	0.012734	0.7617	5.6656	48.8

Test ID	Type	[AlO2] (molar at 5M Na)	[CO3] (molar at 5M Na)	[F] (molar at 5M Na)	[NO2] (molar at 5M Na)	[NO3] (molar at 5M Na)	[OH] (molar at 5M Na)	[PO4] (molar at 5M Na)	SBS/Feed	[Na] (molar)	Temp (°C)
145	OLH	0.26228	0.35675	0.12042	1.189017	1.096772	1.325559	0.009644	0.6758	5.7996	49
146	OLH	0.45843	0.08748	0.16825	1.524558	1.176813	1.132225	0.033748	1.4922	6.2645	49.8
147	OLH	0.30508	0.41035	0.12972	0.8434	1.498217	1.06436	0.025001	1.168	6.9863	50
148	OLH	0.68312	0.17553	0.03805	1.053127	1.495258	0.993723	0.040714	0.7852	5.9281	50.1
149	OLH	0.21948	0.38227	0.08898	1.412166	1.023316	1.110599	0.039133	0.9219	6.4148	50.2
150	OLH	0.72056	0.31081	0.07791	0.737703	1.363814	1.161719	0.017718	1.2031	6.1086	50.4
151	OLH	0.52084	0.14873	0.04691	1.361835	1.427181	1.059517	0.007579	0.6289	6.5516	50.9
152	OLH	0.78297	0.11555	0.1864	0.875294	1.408075	1.192179	0.020154	0.0078	5.6082	51.4
153	OLH	0.54581	0.05812	0.16603	0.804829	1.428592	1.573822	0.033719	1.2773	6.7594	51.5
154	OLH	0.36749	0.36951	0.05975	1.07997	1.110003	1.323304	0.018981	0.9531	6.732	52.1
155	OLH	0.24801	0.23551	0.2205	1.113529	1.144487	1.444008	0.031642	1.6328	6.9645	52.2
156	OLH	0.45308	0.17681	0.01636	1.37021	1.415263	1.044424	0.027841	1.1289	6.2371	52.3
157	OLH	0.77049	0.13087	0.08101	1.192368	1.270483	1.122409	0.01266	1.7773	5.7039	52.8
158	OLH	0.56007	0.22785	0.02831	1.356811	1.019968	1.221595	0.031342	1.1602	5.7914	53.1
159	OLH	0.59217	0.10279	0.16692	0.93736	1.235711	1.487652	0.037029	1.1172	6.3848	53.2
160	OLH	0.50301	0.09513	0.14743	0.934017	1.188525	1.704913	0.022775	1.8945	5.7422	54.1
161	OLH	0.24445	0.08237	0.07082	0.803146	1.753188	1.580697	0.039813	1.5391	5.827	54.4
162	OLH	0.43168	0.32867	0.02565	0.759533	1.402306	1.402887	0.019028	0.0547	5.8215	55.4
163	OLH	0.48518	0.37972	0.10492	1.024601	1.064157	1.191376	0.035602	1.9258	6.7211	56.3
164	OLH	0.8543	0.19212	0.08765	0.801471	1.155341	1.344821	0.036219	1.4766	6.4367	57.7
165	OLH	0.6207	0.5252	0.0385	0.913877	1.05046	0.998535	0.021336	0.457	6.2262	57.8
166	OLH	0.66528	0.13342	0.05842	0.930654	1.616645	1.092894	0.035249	1.2734	6.4422	58.3
167	OLH	0.3764	0.28656	0.11511	1.152109	1.161995	1.330884	0.008954	0.625	5.7449	58.5
168	OLH	0.48875	0.42566	0.09341	0.774616	1.411179	1.029989	0.029072	1.1484	6.784	59.1
169	OLH	0.37284	0.28018	0.08367	1.220886	1.082858	1.294234	0.040544	1.7695	6.9781	60.1
170	OLH	0.90958	0.16277	0.01148	0.865225	1.214781	1.370421	0.013151	1.918	6.3438	60.7
171	OLH	0.29794	0.07471	0.02743	0.903813	1.836202	1.447266	0.024803	0.207	6.5625	61.9
172	OLH	0.32647	0.18957	0.03761	1.49773	1.330579	1.067334	0.032539	1.7266	6.4121	62.9
173	OLH	0.22483	0.08875	0.08809	1.556455	1.073476	1.580309	0.01194	1.0898	6.3902	63
174	OLH	0.22662	0.42821	0.05621	1.032993	1.373037	1.091264	0.033312	0.8945	6.6801	64.5
175	OLH	0.63497	0.23168	0.03363	0.838374	1.695376	1.000486	0.023428	1.6758	6.6773	64.8
176	OLH	0.97199	0.05685	0.10359	0.868576	1.151791	1.407376	0.039819	1.0625	5.6574	65
177	OLH	0.47805	0.20488	0.16205	1.143724	1.265418	1.252239	0.008413	1.9492	5.857	65.3
178	OLH	0.74018	0.39759	0.19924	0.848435	0.99162	1.060125	0.0339	1.7852	5.9801	66
179	OLH	0.40137	0.05429	0.15319	1.200774	1.718693	1.052632	0.033747	0.2422	6.1797	66.1
180	OLH	0.80081	0.18829	0.12928	0.994405	1.193109	1.157507	0.028263	0.4961	6.7922	67.1
181	OLH	0.32469	0.07982	0.13326	1.044738	1.829275	1.171242	0.024545	0.6367	5.6328	67.4
182	OLH	0.37819	0.07727	0.07968	1.101768	1.108598	1.814296	0.033136	1.4102	6.9508	67.6
183	OLH	0.79546	0.12704	0.12795	0.746088	1.41424	1.288166	0.036832	0.4453	6.0102	67.8
184	OLH	0.51014	0.22147	0.11156	0.806515	1.653769	1.185381	0.008725	0.1836	5.6684	68.2
185	OLH	0.46021	0.19978	0.21386	0.920584	1.483154	1.22751	0.010534	1.6563	6.1059	68.5
186	OLH	0.47448	0.3274	0.17046	0.977619	1.052056	1.332875	0.02473	0.1875	6.0977	68.7
187	OLH	0.43703	0.31336	0.23556	1.056477	1.280749	1.037244	0.0209	1.7969	6.9262	68.8
188	OLH	0.51906	0.11428	0.18153	1.328266	1.146931	1.257442	0.024897	1.0508	6.6445	69.4

Table 15. Envelope B/D Computer Simulation Design Matrix

Test ID	Type	[AlO2] (mass fract)	[CO3] (mass fract)	[Fe] (mass fract)	[NO3] (mass fract)	[OH] (mass fract)	[SO4] (mass fract)	SBS/Feed	[Na] (molar)	Temp (°C)
1	MPV	0.129000	0.387890	0.072110	0.115000	0.113000	0.183000	2	2.33	20
2	MPV	0.161000	0.284370	0.041100	0.305330	0.113000	0.095200	2	2.33	20
3	MPV	0.129000	0.284000	0.078000	0.300800	0.113000	0.095200	2	2.33	20
4	MPV	0.161000	0.498000	0.080000	0.115000	0.050800	0.095200	2	2.33	20
5	MPV	0.129000	0.440210	0.041100	0.243690	0.050800	0.095200	2	2.33	20
6	MPV	0.161000	0.284000	0.046280	0.274920	0.050800	0.183000	2	2.33	20

Test ID	Type	[AlO2] (mass fract)	[CO3] (mass fract)	[Fe] (mass fract)	[NO3] (mass fract)	[OH] (mass fract)	[SO4] (mass fract)	SBS/Feed	[Na] (molar)	Temp (°C)
7	MPV	0.129000	0.387890	0.072110	0.115000	0.113000	0.183000	2	4.48	70
8	MPV	0.161000	0.284370	0.041100	0.305330	0.113000	0.095200	2	4.48	70
9	MPV	0.129000	0.284000	0.078000	0.300800	0.113000	0.095200	2	4.48	70
10	MPV	0.161000	0.498000	0.080000	0.115000	0.050800	0.095200	2	4.48	70
11	MPV	0.129000	0.440210	0.041100	0.243690	0.050800	0.095200	2	4.48	70
12	MPV	0.161000	0.284000	0.046280	0.274920	0.050800	0.183000	2	4.48	70
13	MPV	0.129000	0.387890	0.072110	0.115000	0.113000	0.183000	2	4.48	20
14	MPV	0.161000	0.284370	0.041100	0.305330	0.113000	0.095200	2	4.48	20
15	MPV	0.129000	0.284000	0.078000	0.300800	0.113000	0.095200	2	4.48	20
16	MPV	0.161000	0.498000	0.080000	0.115000	0.050800	0.095200	2	4.48	20
17	MPV	0.129000	0.440210	0.041100	0.243690	0.050800	0.095200	2	4.48	20
18	MPV	0.161000	0.284000	0.046280	0.274920	0.050800	0.183000	2	4.48	20
19	MPV	0.129000	0.387890	0.072110	0.115000	0.113000	0.183000	0	2.33	20
20	MPV	0.161000	0.284370	0.041100	0.305330	0.113000	0.095200	0	2.33	20
21	MPV	0.129000	0.284000	0.078000	0.300800	0.113000	0.095200	0	2.33	20
22	MPV	0.161000	0.498000	0.080000	0.115000	0.050800	0.095200	0	2.33	20
23	MPV	0.129000	0.440210	0.041100	0.243690	0.050800	0.095200	0	2.33	20
24	MPV	0.161000	0.284000	0.046280	0.274920	0.050800	0.183000	0	2.33	20
25	MPV	0.129000	0.387890	0.072110	0.115000	0.113000	0.183000	0	2.33	70
26	MPV	0.161000	0.284370	0.041100	0.305330	0.113000	0.095200	0	2.33	70
27	MPV	0.129000	0.284000	0.078000	0.300800	0.113000	0.095200	0	2.33	70
28	MPV	0.161000	0.498000	0.080000	0.115000	0.050800	0.095200	0	2.33	70
29	MPV	0.129000	0.440210	0.041100	0.243690	0.050800	0.095200	0	2.33	70
30	MPV	0.161000	0.284000	0.046280	0.274920	0.050800	0.183000	0	2.33	70
31	MPV	0.129000	0.387890	0.072110	0.115000	0.113000	0.183000	0	4.48	70
32	MPV	0.161000	0.284370	0.041100	0.305330	0.113000	0.095200	0	4.48	70
33	MPV	0.129000	0.284000	0.078000	0.300800	0.113000	0.095200	0	4.48	70
34	MPV	0.161000	0.498000	0.080000	0.115000	0.050800	0.095200	0	4.48	70
35	MPV	0.129000	0.440210	0.041100	0.243690	0.050800	0.095200	0	4.48	70
36	MPV	0.161000	0.284000	0.046280	0.274920	0.050800	0.183000	0	4.48	70
37	MPV	0.129000	0.387890	0.072110	0.115000	0.113000	0.183000	0	4.48	20
38	MPV	0.161000	0.284370	0.041100	0.305330	0.113000	0.095200	0	4.48	20
39	MPV	0.129000	0.284000	0.078000	0.300800	0.113000	0.095200	0	4.48	20
40	MPV	0.161000	0.498000	0.080000	0.115000	0.050800	0.095200	0	4.48	20
41	MPV	0.129000	0.440210	0.041100	0.243690	0.050800	0.095200	0	4.48	20
42	MPV	0.161000	0.284000	0.046280	0.274920	0.050800	0.183000	0	4.48	20
43	MPV	0.129000	0.387890	0.072110	0.115000	0.113000	0.183000	2	2.33	70
44	MPV	0.161000	0.284370	0.041100	0.305330	0.113000	0.095200	2	2.33	70
45	MPV	0.129000	0.284000	0.078000	0.300800	0.113000	0.095200	2	2.33	70
46	MPV	0.161000	0.498000	0.080000	0.115000	0.050800	0.095200	2	2.33	70
47	MPV	0.129000	0.440210	0.041100	0.243690	0.050800	0.095200	2	2.33	70
48	MPV	0.161000	0.284000	0.046280	0.274920	0.050800	0.183000	2	2.33	70
49	OLH	0.150000	0.419580	0.073620	0.158270	0.061500	0.137030	0.125	3.3882	21.953125
50	OLH	0.153750	0.376330	0.049310	0.240340	0.065900	0.114370	0.7969	3.11945	39.53125
51	OLH	0.160500	0.449170	0.049610	0.125450	0.050800	0.164470	0.625	3.67375	27.421875
52	OLH	0.145750	0.332010	0.043230	0.264220	0.062000	0.152790	0.5781	3.37141	33.28125
53	OLH	0.155250	0.404650	0.070280	0.176180	0.083400	0.110240	0.0469	2.58195	34.84375
54	OLH	0.153250	0.379120	0.066020	0.147830	0.098900	0.154880	0.8125	2.66594	41.09375
55	OLH	0.148000	0.384100	0.046570	0.247800	0.075600	0.097930	1.5156	2.76672	25.46875
56	OLH	0.160000	0.444160	0.069970	0.119480	0.059100	0.147290	1.3594	2.54836	43.046875
57	OLH	0.156750	0.297970	0.053260	0.250790	0.111100	0.130130	1.5625	3.28742	41.484375
58	OLH	0.151000	0.361420	0.074830	0.216470	0.097000	0.099280	1.9688	3.55617	42.265625
59	OLH	0.159500	0.325520	0.056600	0.198560	0.104300	0.155520	1.5781	4.27844	29.375
60	OLH	0.148250	0.387570	0.078180	0.126940	0.087700	0.171360	1.5469	2.73313	24.6875
61	OLH	0.159000	0.301310	0.058120	0.229900	0.094000	0.157670	1.3125	2.51477	29.765625
62	OLH	0.154750	0.466510	0.076660	0.132910	0.067800	0.101370	0.0781	3.27063	66.875
63	OLH	0.158000	0.334380	0.048390	0.268700	0.057600	0.132930	0.7813	2.43078	50.078125

Test ID	Type	[AlO2] (mass fract)	[CO3] (mass fract)	[Fe] (mass fract)	[NO3] (mass fract)	[OH] (mass fract)	[SO4] (mass fract)	SBS/Feed	[Na] (molar)	Temp (°C)
64	OLH	0.146750	0.383660	0.057810	0.188120	0.057100	0.166560	0.2969	4.19445	54.375
65	OLH	0.147250	0.407400	0.062680	0.128430	0.079500	0.174740	0.75	3.00188	63.359375
66	OLH	0.158750	0.318920	0.055990	0.223930	0.076600	0.165810	0.5313	3.33781	55.546875
67	OLH	0.147750	0.355050	0.066320	0.203040	0.108600	0.119240	0.5938	2.93469	68.828125
68	OLH	0.157750	0.342990	0.062070	0.238850	0.085300	0.113040	0.25	4.41281	57.109375
69	OLH	0.157500	0.353480	0.072100	0.167230	0.107200	0.142490	0.8438	2.63234	49.6875
70	OLH	0.150500	0.408540	0.070880	0.195580	0.053200	0.121300	1.4531	3.05227	61.40625
71	OLH	0.147500	0.351910	0.047180	0.243330	0.075100	0.134980	1.7813	3.10266	57.890625
72	OLH	0.156000	0.339360	0.063590	0.261230	0.073600	0.106220	1.5938	3.9593	52.03125
73	OLH	0.157000	0.417580	0.058730	0.137380	0.060000	0.169310	1.7969	3.79133	70
74	OLH	0.146500	0.386580	0.075140	0.171700	0.074100	0.145980	1.0781	2.33	53.984375
75	OLH	0.151500	0.361880	0.045660	0.219450	0.067300	0.154210	1.1719	2.8675	61.015625
76	OLH	0.152500	0.406550	0.061160	0.186630	0.094500	0.098660	1.8594	2.44758	46.171875
77	OLH	0.149000	0.334550	0.046870	0.255270	0.084800	0.129510	1.1406	2.36359	59.0625
78	OLH	0.156250	0.332190	0.065410	0.213480	0.105200	0.127470	1.1094	4.00969	69.21875
79	OLH	0.149250	0.312200	0.056300	0.209010	0.103300	0.169940	1.625	3.99289	59.453125
80	OLH	0.148500	0.426490	0.065720	0.122460	0.086800	0.150030	1.8125	2.78352	58.671875
81	OLH	0.159750	0.296340	0.060250	0.231390	0.092600	0.159670	1.6094	2.68273	52.8125
82	OLH	0.145000	0.362950	0.060550	0.210500	0.081900	0.139100	1	3.405	45
83	OLH	0.140000	0.306320	0.047480	0.262730	0.102300	0.141170	1.875	3.4218	68.046875
84	OLH	0.136250	0.349570	0.071790	0.180660	0.097900	0.163830	1.2031	3.69055	50.46875
85	OLH	0.144250	0.393890	0.077870	0.156780	0.101800	0.125410	1.4219	3.43859	56.71875
86	OLH	0.134750	0.321250	0.050830	0.244820	0.080400	0.167950	1.9531	4.22805	55.15625
87	OLH	0.139250	0.405290	0.080000	0.149320	0.064400	0.161740	1.9375	4.21125	47.34375
88	OLH	0.129000	0.451470	0.053560	0.162750	0.051800	0.151420	1.4844	3.30422	63.75
89	OLH	0.140500	0.387960	0.070580	0.241840	0.063900	0.095220	1.7188	3.23703	62.1875
90	OLH	0.136750	0.346780	0.055080	0.273170	0.064900	0.123320	1.1875	4.14406	48.90625
91	OLH	0.134500	0.454150	0.066930	0.161260	0.072200	0.110960	1.3906	3.97609	53.59375
92	OLH	0.142000	0.341800	0.074530	0.173200	0.088200	0.180270	0.4844	4.04328	64.53125
93	OLH	0.133250	0.427930	0.067840	0.170210	0.052700	0.148070	0.4375	3.52258	48.515625
94	OLH	0.139000	0.364480	0.046270	0.204530	0.066800	0.178920	0.0313	3.25383	47.734375
95	OLH	0.130500	0.400380	0.064500	0.222440	0.059500	0.122680	0.4219	2.53156	60.625
96	OLH	0.141750	0.338330	0.042920	0.294060	0.076100	0.106840	0.4531	4.07688	65.3125
97	OLH	0.131000	0.424590	0.062980	0.191100	0.069800	0.120530	0.6875	4.29523	60.234375
98	OLH	0.132000	0.391520	0.072710	0.152300	0.106200	0.145270	1.2188	4.37922	39.921875
99	OLH	0.143250	0.342240	0.063290	0.232880	0.106700	0.111640	1.7031	2.61555	35.625
100	OLH	0.142750	0.318500	0.058420	0.292570	0.084300	0.103460	1.25	3.80813	26.640625
101	OLH	0.131250	0.406980	0.065110	0.197070	0.087200	0.112390	1.4688	3.47219	34.453125
102	OLH	0.142250	0.370850	0.054780	0.217960	0.055200	0.158960	1.4063	3.87531	21.171875
103	OLH	0.132250	0.382910	0.059030	0.182150	0.078500	0.165160	1.75	2.39719	32.890625
104	OLH	0.132500	0.372420	0.049000	0.253770	0.056600	0.135710	1.1563	4.17766	40.3125
105	OLH	0.137750	0.454900	0.076960	0.135890	0.062900	0.131600	1.3438	4.4632	35.234375
106	OLH	0.142500	0.373990	0.073920	0.177670	0.088700	0.143220	0.2188	3.70734	32.109375
107	OLH	0.134000	0.386540	0.057510	0.159770	0.090200	0.171980	0.4063	2.8507	37.96875
108	OLH	0.133000	0.308320	0.062370	0.283620	0.103800	0.108890	0.2031	3.01867	20
109	OLH	0.143500	0.339330	0.045960	0.249300	0.089700	0.132210	0.9219	4.48	36.015625
110	OLH	0.138500	0.364020	0.075440	0.201550	0.096500	0.123990	0.8281	3.9425	28.984375
111	OLH	0.137500	0.319350	0.059940	0.234380	0.069300	0.179530	0.1406	4.36242	43.828125
112	OLH	0.141000	0.391350	0.074230	0.165730	0.079000	0.148690	0.8594	4.44641	30.9375
113	OLH	0.133750	0.393710	0.055690	0.207520	0.058600	0.150730	0.8906	2.80031	20.78125
114	OLH	0.140750	0.413700	0.064800	0.211990	0.060500	0.108260	0.375	2.81711	30.546875
115	OLH	0.141500	0.299410	0.055380	0.298540	0.077000	0.128170	0.1875	4.02648	31.328125
116	OLH	0.130250	0.429560	0.060850	0.189610	0.071200	0.118530	0.3906	4.12727	37.1875

Table 16. Envelope C Computer Simulation Design Matrix

Test ID	Type	[AlO2] (molar at 5M Na)	[CO3] (molar at 5M Na)	[NO2] (molar at 5M Na	[NO3] (molar at 5M Na	[OH] (molar at 5M Na	[SO4] (molar at 5M Na	SBS/Feed	[Na] (molar)	Temp (oC)
1	MPV	0.015	0.94	0.78	1.5	0.2438	0.112	0	7	20
2	MPV	0.015	0.94	0.78	1.5	0.2438	0.112	0	8.5	20
3	MPV	0.015	0.94	0.78	1.5	0.2438	0.112	2	7	20
4	MPV	0.015	0.94	0.78	1.5	0.2438	0.112	2	8.5	20
5	MPV	0.015	0.94	0.78	1.5	0.2438	0.112	0	7	70
6	MPV	0.015	0.94	0.78	1.5	0.2438	0.112	0	8.5	70
7	MPV	0.015	0.94	0.78	1.5	0.2438	0.112	2	7	70
8	MPV	0.015	0.94	0.78	1.5	0.2438	0.112	2	8.5	70
9	MPV	0.0888	0.56	0.78	2.3	0.13	0.112	0	7	20
10	MPV	0.0888	0.56	0.78	2.3	0.13	0.112	0	8.5	20
11	MPV	0.0888	0.56	0.78	2.3	0.13	0.112	2	7	20
12	MPV	0.0888	0.56	0.78	2.3	0.13	0.112	2	8.5	20
13	MPV	0.0888	0.56	0.78	2.3	0.13	0.112	0	7	70
14	MPV	0.0888	0.56	0.78	2.3	0.13	0.112	0	8.5	70
15	MPV	0.0888	0.56	0.78	2.3	0.13	0.112	2	7	70
16	MPV	0.0888	0.56	0.78	2.3	0.13	0.112	2	8.5	70
17	MPV	0.015	0.5754	0.78	2.3	0.295	0.051	0	7	20
18	MPV	0.015	0.5754	0.78	2.3	0.295	0.051	0	8.5	20
19	MPV	0.015	0.5754	0.78	2.3	0.295	0.051	2	7	20
20	MPV	0.015	0.5754	0.78	2.3	0.295	0.051	2	8.5	20
21	MPV	0.015	0.5754	0.78	2.3	0.295	0.051	0	7	70
22	MPV	0.015	0.5754	0.78	2.3	0.295	0.051	0	8.5	70
23	MPV	0.015	0.5754	0.78	2.3	0.295	0.051	2	7	70
24	MPV	0.015	0.5754	0.78	2.3	0.295	0.051	2	8.5	70
25	MPV	0.015	0.8529	1.19	1.5	0.13	0.051	0	7	20
26	MPV	0.015	0.8529	1.19	1.5	0.13	0.051	0	8.5	20
27	MPV	0.015	0.8529	1.19	1.5	0.13	0.051	2	7	20
28	MPV	0.015	0.8529	1.19	1.5	0.13	0.051	2	8.5	20
29	MPV	0.015	0.8529	1.19	1.5	0.13	0.051	0	7	70
30	MPV	0.015	0.8529	1.19	1.5	0.13	0.051	0	8.5	70
31	MPV	0.015	0.8529	1.19	1.5	0.13	0.051	2	7	70
32	MPV	0.015	0.8529	1.19	1.5	0.13	0.051	2	8.5	70
33	MPV	0.29	0.9204	0.78	1.5	0.13	0.051	0	7	20
34	MPV	0.29	0.9204	0.78	1.5	0.13	0.051	0	8.5	20
35	MPV	0.29	0.9204	0.78	1.5	0.13	0.051	2	7	20
36	MPV	0.29	0.9204	0.78	1.5	0.13	0.051	2	8.5	20
37	MPV	0.29	0.9204	0.78	1.5	0.13	0.051	0	7	70
38	MPV	0.29	0.9204	0.78	1.5	0.13	0.051	0	8.5	70
39	MPV	0.29	0.9204	0.78	1.5	0.13	0.051	2	7	70
40	MPV	0.29	0.9204	0.78	1.5	0.13	0.051	2	8.5	70
41	MPV	0.29	0.56	1.19	1.5238	0.295	0.112	0	7	20
42	MPV	0.29	0.56	1.19	1.5238	0.295	0.112	0	8.5	20
43	MPV	0.29	0.56	1.19	1.5238	0.295	0.112	2	7	20
44	MPV	0.29	0.56	1.19	1.5238	0.295	0.112	2	8.5	20
45	MPV	0.29	0.56	1.19	1.5238	0.295	0.112	0	7	70
46	MPV	0.29	0.56	1.19	1.5238	0.295	0.112	0	8.5	70
47	MPV	0.29	0.56	1.19	1.5238	0.295	0.112	2	7	70
48	MPV	0.29	0.56	1.19	1.5238	0.295	0.112	2	8.5	70
49	OLH	0.015	0.68172	0.8825	2.05674	0.13258	0.09627	1.75	8.32	42.66
50	OLH	0.02145	0.83313	0.79281	1.79107	0.2473	0.061955	1.17	7.81	52.42
51	OLH	0.02359	0.65797	1.18039	1.70871	0.27309	0.07054	1.08	7.62	64.92

Test ID	Type	[AlO2] (molar at 5M Na)	[CO3] (molar at 5M Na)	[NO2] (molar at 5M Na	[NO3] (molar at 5M Na	[OH] (molar at 5M Na	[SO4] (molar at 5M Na	SBS/Feed	[Na] (molar)	Temp (oC)
52	OLH	0.02574	0.75297	0.94016	1.861	0.18414	0.06291	0.69	8.16	61.8
53	OLH	0.02789	0.78859	1.01063	1.74616	0.1532	0.06387	1.63	8.37	24.69
54	OLH	0.03004	0.74109	0.78641	1.9236	0.25375	0.08341	1.03	7.22	33.28
55	OLH	0.03219	0.77375	0.94336	1.79554	0.18027	0.07197	1.61	8.36	65.7
56	OLH	0.03434	0.79453	0.95617	1.64496	0.22668	0.095795	0.58	8.3	46.56
57	OLH	0.03648	0.66391	0.86328	2.07564	0.14418	0.0977	0.02	7.21	35.23
58	OLH	0.04078	0.86875	0.86008	1.55114	0.27695	0.088175	0.8	7.09	67.66
59	OLH	0.04293	0.73516	0.92414	1.79319	0.20348	0.10437	0.52	8.08	21.56
60	OLH	0.04508	0.63719	1.07789	1.92746	0.14547	0.08626	0.81	7.46	62.97
61	OLH	0.04723	0.67281	0.83125	2.05873	0.21508	0.072445	0.5	7	28.98
62	OLH	0.04938	0.76781	1.14195	1.53095	0.27051	0.057195	0	8.13	36.02
63	OLH	0.05152	0.82125	0.89852	1.78642	0.13516	0.06434	1.14	7.11	47.73
64	OLH	0.05367	0.71438	0.7832	1.94407	0.28727	0.072915	1.59	8.38	25.47
65	OLH	0.05582	0.7025	0.97859	1.89643	0.15063	0.078165	0.03	8.42	30.94
66	OLH	0.05797	0.72031	0.87609	1.90692	0.23441	0.063395	0.72	8	32.11
67	OLH	0.06227	0.81234	0.8793	1.703	0.18672	0.093415	1.34	7.87	58.28
68	OLH	0.06441	0.655	1.05867	1.77994	0.20863	0.110575	1.41	7.82	64.14
69	OLH	0.06656	0.59563	0.81523	2.12907	0.26148	0.0896	0.09	7.84	39.92
70	OLH	0.06871	0.59266	1.15156	1.7681	0.24988	0.109615	0.13	7.9	48.13
71	OLH	0.07301	0.64609	0.84727	1.97635	0.2357	0.109145	1.27	7.76	39.53
72	OLH	0.07516	0.56594	0.99461	1.99121	0.24215	0.103895	1.25	7.4	62.58
73	OLH	0.0816	0.69656	1.11953	1.70672	0.16738	0.087225	1.16	7.49	62.19
74	OLH	0.08805	0.74406	1.03625	1.74082	0.17898	0.05529	0.95	8.17	67.27
75	OLH	0.0902	0.91031	0.82484	1.56094	0.16223	0.091985	0.61	7.89	69.61
76	OLH	0.09234	0.56891	0.8857	2.17678	0.21766	0.06625	1.3	7.15	40.7
77	OLH	0.09449	0.73813	1.13555	1.6425	0.13387	0.080065	1.86	7.86	50.86
78	OLH	0.09879	0.56297	1.02344	1.98698	0.28469	0.06148	1.45	8.34	66.09
79	OLH	0.10094	0.61047	0.97219	2.07229	0.17254	0.05195	1.11	7.93	41.48
80	OLH	0.10523	0.64906	1.01703	1.7985	0.28855	0.067685	0.34	8.14	53.2
81	OLH	0.10738	0.62531	0.92734	1.97733	0.15707	0.11153	1.53	7.23	36.41
82	OLH	0.10953	0.62234	1.09711	1.70846	0.26664	0.10819	1.92	7.91	45.39
83	OLH	0.11598	0.79156	0.9882	1.67484	0.15578	0.06244	0.42	8.25	31.33
84	OLH	0.11813	0.88359	0.88891	1.50939	0.20477	0.07721	0.44	7.71	69.22
85	OLH	0.12027	0.58672	0.96258	1.98461	0.23699	0.082455	0.94	7.47	34.45
86	OLH	0.12242	0.69953	1.17398	1.63428	0.19961	0.056725	0.45	7.52	59.45
87	OLH	0.12457	0.57781	1.16438	1.87156	0.19703	0.06482	1.81	7.29	60.63
88	OLH	0.12887	0.69359	1.00102	1.79635	0.1416	0.09389	0.05	8.45	55.94
89	OLH	0.13531	0.58375	0.79922	2.28746	0.13129	0.06101	1.83	7.28	29.77
90	OLH	0.13961	0.6075	1.06828	1.82855	0.23313	0.079115	0.64	7.27	70
91	OLH	0.15035	0.57484	0.93055	2.13106	0.16867	0.056245	0.33	7.32	37.19
92	OLH	0.1525	0.75	0.985	1.6298	0.2125	0.0815	1	7.75	45
93	OLH	0.1568	0.66094	0.84086	1.87031	0.27566	0.088645	1.89	8.48	46.17
94	OLH	0.15895	0.58078	1.10031	1.92507	0.15965	0.06863	0.53	7.56	44.22
95	OLH	0.16109	0.66984	0.90813	1.76797	0.24859	0.10867	0.77	7.83	66.48
96	OLH	0.16324	0.59859	1.02023	1.88075	0.2241	0.07865	1.94	8.46	32.89
97	OLH	0.16754	0.72328	0.93695	1.82488	0.14676	0.060055	1.38	7.7	63.36
98	OLH	0.17184	0.77078	0.80883	1.76677	0.20605	0.073875	1.73	8.07	35.63
99	OLH	0.17398	0.61938	1.05547	1.76949	0.19445	0.105325	1.52	8.24	37.97
100	OLH	0.17828	0.61344	1.06508	1.78237	0.19574	0.097225	0.22	8.09	30.16
101	OLH	0.18258	0.80047	0.79602	1.62532	0.22539	0.106275	1.55	7.98	30.55
102	OLH	0.18688	0.61641	1.08109	1.75021	0.22023	0.085785	1.56	7.79	20.78
103	OLH	0.18902	0.70844	0.9818	1.58476	0.26922	0.10056	1.58	7.25	58.67
104	OLH	0.19117	0.65203	0.91773	1.85048	0.2602	0.05958	0.31	7.35	48.91

Test ID	Type	[AlO2] (molar at 5M Na)	[CO3] (molar at 5M Na)	[NO2] (molar at 5M Na	[NO3] (molar at 5M Na	[OH] (molar at 5M Na	[SO4] (molar at 5M Na	SBS/Feed	[Na] (molar)	Temp (oC)
105	OLH	0.19332	0.71734	0.82164	1.84502	0.23184	0.05815	1.44	8.11	68.83
106	OLH	0.19547	0.87766	0.87289	1.55114	0.15836	0.05481	0.08	7.59	44.61
107	OLH	0.20191	0.56	1.11633	1.83984	0.25891	0.052905	0.91	8.05	26.25
108	OLH	0.20836	0.60453	1.00422	1.87385	0.17383	0.08674	1.64	7.48	32.5
109	OLH	0.21051	0.76188	0.83445	1.6171	0.29113	0.082925	0.14	7.64	39.14
110	OLH	0.2148	0.58969	1.14516	1.69866	0.26277	0.071015	1.39	7.61	20.39
111	OLH	0.21695	0.75594	0.93375	1.51878	0.24602	0.10771	1.05	7.33	22.73
112	OLH	0.2191	0.57188	0.89531	1.97907	0.18156	0.112	0.2	7.53	46.95
113	OLH	0.22125	0.62828	0.78	1.9627	0.28598	0.068155	0.23	8.31	55.16
114	OLH	0.2234	0.80344	0.85047	1.55288	0.25762	0.075775	0.84	8.01	27.81
115	OLH	0.22555	0.68469	0.84406	1.77814	0.21121	0.10723	1.33	7.96	61.41
116	OLH	0.2277	0.64016	1.04906	1.76516	0.16996	0.0753	0.78	8.44	38.36
117	OLH	0.23414	0.60156	0.81203	2.00838	0.26406	0.060535	1.72	7.01	49.69
118	OLH	0.24273	0.68766	1.0907	1.5566	0.23828	0.069585	0.66	7.63	31.72
119	OLH	0.24488	0.69063	0.86648	1.80938	0.18543	0.077685	0.98	7.95	68.05
120	OLH	0.25563	0.73219	0.82805	1.72865	0.15449	0.1058	2	7.38	53.98
121	OLH	0.26422	0.63125	1.10992	1.70846	0.14805	0.074825	1.2	8.41	22.34
122	OLH	0.26637	0.63422	0.85688	1.94618	0.14289	0.08102	1.13	8.43	66.88
123	OLH	0.27066	0.70547	1.01383	1.61464	0.19832	0.067205	1.42	7.2	43.44
124	OLH	0.27711	0.71141	0.95938	1.51344	0.2718	0.099125	0.38	7.13	65.31
125	OLH	0.28141	0.84203	0.78961	1.55089	0.15191	0.09246	0.92	7.88	25.08
126	OLH	0.2857	0.64313	0.80242	1.9983	0.13	0.07006	0.3	7.73	51.25
127	OLH	0.28785	0.67578	0.83766	1.78053	0.20219	0.091505	0.16	8.2	56.33

APPENDIX C. UNDISSOLVED SOLIDS PREDICTED BY OLI/ESP FOR ENVELOPES A-a, B/D, AND C

The following tables list the solids present in the feed to the 1st ultra-filtration step as the mass fraction of the total undissolved (insoluble) solids. NAS gel was the only form of sodium aluminosilicate turned on during the simulations as it is the precursor to all other forms (i.e. cancrinite). The last row of each table lists the number of simulations for which the solids was present.

Table 17. Sub-Envelope A-a Solids

Run#	MGOH2	NASGEL	CAF2	ALOH3	NIOH2	NA2C2O4	CA3PO42	NAF	NAPHOH .12H2O	CAOH2	CACO3	NAFPO4 .19H2O	sum
1	4.11E-05	-	-	-	-	1.67E-01	-	-	8.33E-01	-	-	-	1.00E+00
2	4.11E-05	-	-	-	-	1.00E+00	-	-	-	-	-	-	1.00E+00
3	4.74E-05	2.69E-01	-	7.31E-01	-	-	-	-	-	-	-	-	1.00E+00
4	4.51E-05	4.29E-01	-	-	-	5.71E-01	-	-	-	-	-	-	1.00E+00
5	4.26E-05	-	-	-	-	5.13E-01	-	3.26E-01	-	-	-	1.61E-01	1.00E+00
6	4.69E-05	2.60E-01	-	6.65E-01	-	7.49E-02	-	-	-	-	-	-	1.00E+00
7	4.60E-05	1.13E-02	-	9.32E-01	6.38E-05	5.61E-02	-	-	-	-	-	-	1.00E+00
8	4.61E-05	8.59E-03	-	9.53E-01	7.50E-05	3.79E-02	-	-	-	-	-	-	1.00E+00
9	4.59E-05	6.88E-03	-	9.29E-01	5.96E-05	6.39E-02	-	-	-	-	-	-	1.00E+00
10	4.59E-05	1.23E-03	-	8.16E-01	6.87E-05	5.68E-02	-	1.26E-01	-	-	-	-	1.00E+00
11	4.11E-05	-	-	-	-	1.67E-01	-	-	8.33E-01	-	-	-	1.00E+00
12	4.11E-05	-	-	-	-	1.00E+00	-	-	-	-	-	-	1.00E+00
13	4.74E-05	2.69E-01	-	7.31E-01	-	-	-	-	-	-	-	-	1.00E+00
14	4.51E-05	4.29E-01	-	-	-	5.71E-01	-	-	-	-	-	-	1.00E+00
15	4.26E-05	-	-	-	-	5.25E-01	-	3.33E-01	-	-	-	1.42E-01	1.00E+00
16	4.69E-05	2.60E-01	-	6.65E-01	-	7.49E-02	-	-	-	-	-	-	1.00E+00
17	4.60E-05	1.13E-02	-	9.32E-01	6.38E-05	5.61E-02	-	-	-	-	-	-	1.00E+00
18	4.61E-05	8.59E-03	-	9.53E-01	7.50E-05	3.78E-02	-	-	-	-	-	-	1.00E+00
19	4.59E-05	6.88E-03	-	9.29E-01	5.97E-05	6.39E-02	-	-	-	-	-	-	1.00E+00
20	4.59E-05	1.23E-03	-	8.16E-01	6.86E-05	5.68E-02	-	1.26E-01	-	-	-	-	1.00E+00
21	1.19E-02	5.30E-02	-	-	-	1.98E-01	6.86E-02	-	6.69E-01	-	-	-	1.00E+00
22	4.23E-02	1.25E-01	-	-	-	6.57E-01	-	-	-	1.76E-01	-	-	1.00E+00
23	2.66E-02	5.50E-01	3.80E-02	2.82E-01	-	-	1.04E-01	-	-	-	-	-	1.00E+00
24	3.82E-02	6.89E-01	1.68E-01	-	-	1.05E-01	-	-	-	-	-	-	1.00E+00
25	3.05E-02	4.92E-01	1.35E-01	-	-	3.43E-01	-	-	-	-	-	-	1.00E+00
26	2.66E-02	5.56E-01	1.17E-01	2.55E-01	-	4.55E-02	-	-	-	-	-	-	1.00E+00
27	3.53E-03	6.68E-02	-	8.63E-01	6.99E-05	4.72E-02	-	-	-	-	1.97E-02	-	1.00E+00
28	3.17E-03	5.84E-02	-	8.88E-01	8.00E-05	3.22E-02	1.81E-02	-	-	-	-	-	1.00E+00
29	3.01E-03	5.43E-02	-	8.65E-01	6.59E-05	6.05E-02	1.71E-02	-	-	-	-	-	1.00E+00
30	2.31E-03	3.80E-02	1.00E-02	8.64E-01	6.22E-05	5.90E-02	-	2.65E-02	-	-	-	-	1.00E+00
31	9.53E-03	1.50E-02	-	-	-	1.99E-01	5.46E-02	-	7.22E-01	-	-	-	1.00E+00
32	4.05E-02	-	-	-	-	7.91E-01	-	-	-	1.69E-01	-	-	1.00E+00
33	2.39E-02	5.20E-01	2.54E-02	3.26E-01	-	-	1.04E-01	-	-	-	-	-	1.00E+00
34	3.65E-02	6.77E-01	1.61E-01	-	-	1.25E-01	-	-	-	-	-	-	1.00E+00
35	2.79E-02	4.51E-01	1.23E-01	-	-	3.98E-01	-	-	-	-	-	-	1.00E+00
36	2.36E-02	5.21E-01	1.04E-01	3.01E-01	-	5.04E-02	-	-	-	-	-	-	1.00E+00
37	2.87E-03	5.63E-02	-	8.76E-01	6.86E-05	4.84E-02	-	-	-	-	1.60E-02	-	1.00E+00
38	2.58E-03	4.90E-02	-	9.00E-01	7.91E-05	3.33E-02	1.46E-02	-	-	-	-	-	1.00E+00
39	2.45E-03	4.53E-02	-	8.77E-01	6.47E-05	6.12E-02	1.38E-02	-	-	-	-	-	1.00E+00
40	1.75E-03	2.88E-02	7.54E-03	8.31E-01	6.62E-05	5.84E-02	-	7.22E-02	-	-	-	-	1.00E+00

Run#	MGOH2	NASGEL	CAF2	ALOH3	NIOH2	NA2C2O4	CA3PO42	NAF	NAPHOH .12H2O	CAOH2	CACO3	NAFPO4 .19H2O	sum
41	-	-	-	-	-	-	-	-	-	-	-	-	-
42	-	-	-	-	-	-	-	-	-	-	-	-	-
43	5.01E-05	1.00E+00	-	-	-	-	-	-	-	-	-	-	1.00E+00
44	-	-	-	-	-	-	-	-	-	-	-	-	-
45	-	-	-	-	-	-	-	-	-	-	-	-	-
46	4.98E-05	1.00E+00	-	-	-	-	-	-	-	-	-	-	1.00E+00
47	5.05E-05	1.00E+00	-	-	-	-	-	-	-	-	-	-	1.00E+00
48	4.76E-05	3.61E-01	-	6.39E-01	6.88E-05	-	-	-	-	-	-	-	1.00E+00
49	5.01E-05	1.00E+00	-	-	-	-	-	-	-	-	-	-	1.00E+00
50	-	-	-	-	-	-	-	-	-	-	-	-	-
51	-	-	-	-	-	-	-	-	-	-	-	-	-
52	-	-	-	-	-	-	-	-	-	-	-	-	-
53	5.01E-05	1.00E+00	-	-	-	-	-	-	-	-	-	-	1.00E+00
54	-	-	-	-	-	-	-	-	-	-	-	-	-
55	-	-	-	-	-	-	-	-	-	-	-	-	-
56	4.98E-05	1.00E+00	-	-	-	-	-	-	-	-	-	-	1.00E+00
57	5.05E-05	1.00E+00	-	-	-	-	-	-	-	-	-	-	1.00E+00
58	4.76E-05	3.62E-01	-	6.38E-01	6.90E-05	-	-	-	-	-	-	-	1.00E+00
59	5.01E-05	1.00E+00	-	-	-	-	-	-	-	-	-	-	1.00E+00
60	-	-	-	-	-	-	-	-	-	-	-	-	-
61	1.47E-01	-	-	-	-	-	8.53E-01	-	-	-	-	-	1.00E+00
62	1.53E-01	-	-	-	-	-	7.30E-01	-	-	1.17E-01	-	-	1.00E+00
63	4.07E-02	7.22E-01	-	-	1.25E-04	-	2.37E-01	-	-	-	-	-	1.00E+00
64	5.86E-02	6.83E-01	2.59E-01	-	4.16E-05	-	-	-	-	-	-	-	1.00E+00
65	8.16E-02	5.59E-01	3.60E-01	-	-	-	-	-	-	-	-	-	1.00E+00
66	4.20E-02	7.73E-01	1.85E-01	-	1.21E-04	-	-	-	-	-	-	-	1.00E+00
67	3.54E-02	7.64E-01	-	-	1.43E-04	-	-	-	-	-	2.00E-01	-	1.00E+00
68	3.59E-02	7.56E-01	-	-	1.40E-04	-	2.08E-01	-	-	-	-	-	1.00E+00
69	3.71E-02	7.47E-01	-	-	1.18E-04	-	2.16E-01	-	-	-	-	-	1.00E+00
70	4.63E-02	7.49E-01	2.04E-01	-	6.67E-05	-	-	-	-	-	-	-	1.00E+00
71	1.47E-01	-	-	-	-	-	8.53E-01	-	-	-	-	-	1.00E+00
72	1.51E-01	-	-	-	-	-	7.69E-01	-	-	7.96E-02	-	-	1.00E+00
73	4.02E-02	7.25E-01	-	-	1.15E-04	-	2.34E-01	-	-	-	-	-	1.00E+00
74	6.10E-02	6.70E-01	2.69E-01	-	-	-	-	-	-	-	-	-	1.00E+00
75	8.94E-02	5.16E-01	3.94E-01	-	-	-	-	-	-	-	-	-	1.00E+00
76	4.13E-02	7.76E-01	1.82E-01	-	1.10E-04	-	-	-	-	-	-	-	1.00E+00
77	3.43E-02	7.72E-01	-	-	1.35E-04	-	-	-	-	-	1.94E-01	-	1.00E+00
78	3.38E-02	7.46E-01	-	2.45E-02	1.32E-04	-	1.96E-01	-	-	-	-	-	1.00E+00
79	3.63E-02	7.53E-01	-	-	1.07E-04	-	2.11E-01	-	-	-	-	-	1.00E+00
80	4.66E-02	7.48E-01	2.05E-01	-	3.67E-05	-	-	-	-	-	-	-	1.00E+00
81	1.16E-04	1.47E-02	3.25E-04	9.19E-01	4.67E-05	6.60E-02	-	-	-	-	-	-	1.00E+00
82	3.77E-03	7.25E-02	1.65E-02	8.39E-01	3.47E-05	6.83E-02	-	-	-	-	-	-	1.00E+00
83	1.52E-03	3.93E-02	6.53E-03	9.25E-01	5.82E-05	2.77E-02	-	-	-	-	-	-	1.00E+00
84	5.40E-04	1.78E-02	2.20E-03	9.35E-01	7.48E-05	4.41E-02	-	-	-	-	-	-	1.00E+00
85	8.25E-05	7.67E-02	1.68E-04	7.93E-01	-	1.30E-01	-	-	-	-	-	-	1.00E+00
86	1.03E-02	2.37E-01	4.53E-02	5.64E-01	-	1.43E-01	-	-	-	-	-	-	1.00E+00
87	6.58E-03	1.41E-01	2.86E-02	7.52E-01	-	7.18E-02	-	-	-	-	-	-	1.00E+00
88	1.79E-03	4.47E-02	7.74E-03	8.97E-01	6.51E-05	4.86E-02	-	-	-	-	-	-	1.00E+00
89	2.06E-03	3.95E-02	8.90E-03	8.82E-01	4.01E-05	6.71E-02	-	-	-	-	-	-	1.00E+00
90	1.97E-02	4.41E-01	8.67E-02	-	-	4.52E-01	-	-	-	-	-	-	1.00E+00
91	6.41E-03	1.63E-01	2.81E-02	6.55E-01	-	1.47E-01	-	-	-	-	-	-	1.00E+00
92	6.14E-04	3.18E-02	2.52E-03	9.02E-01	2.15E-05	6.36E-02	-	-	-	-	-	-	1.00E+00
93	6.33E-03	1.49E-01	2.77E-02	7.57E-01	-	6.02E-02	-	-	-	-	-	-	1.00E+00
94	2.90E-03	8.99E-02	1.26E-02	8.95E-01	-	-	-	-	-	-	-	-	1.00E+00

Run#	MGOH2	NASGEL	CAF2	ALOH3	NIOH2	NA2C2O4	CA3PO42	NAF	NAPHOH .12H2O	CAOH2	CACO3	NAFPO4 .19H2O	sum
95	2.68E-03	5.70E-02	1.17E-02	8.78E-01	7.47E-05	5.05E-02	-	-	-	-	-	-	1.00E+00
96	4.40E-03	8.94E-02	1.92E-02	8.37E-01	6.18E-05	5.00E-02	-	-	-	-	-	-	1.00E+00
97	3.45E-04	1.96E-02	1.33E-03	9.27E-01	7.58E-05	5.14E-02	-	-	-	-	-	-	1.00E+00
98	3.41E-02	6.38E-01	1.48E-01	-	-	1.80E-01	-	-	-	-	-	-	1.00E+00
99	3.84E-04	2.19E-02	1.51E-03	9.24E-01	7.69E-05	5.22E-02	-	-	-	-	-	-	1.00E+00
100	3.12E-03	6.45E-02	-	9.15E-01	8.72E-05	-	1.77E-02	-	-	-	-	-	1.00E+00
101	2.82E-03	7.45E-02	1.22E-02	9.10E-01	5.33E-05	-	-	-	-	-	-	-	1.00E+00
102	6.99E-03	1.78E-01	3.07E-02	7.84E-01	-	-	-	-	-	-	-	-	1.00E+00
103	2.23E-03	5.27E-02	9.59E-03	9.35E-01	9.13E-05	-	-	-	-	-	-	-	1.00E+00
104	6.29E-03	1.39E-01	2.76E-02	8.27E-01	-	-	-	-	-	-	-	-	1.00E+00
105	1.07E-03	2.87E-02	4.49E-03	9.40E-01	1.02E-04	2.58E-02	-	-	-	-	-	-	1.00E+00
106	3.70E-03	8.29E-02	1.62E-02	8.97E-01	1.02E-04	-	-	-	-	-	-	-	1.00E+00
107	8.13E-05	1.19E-02	-	9.43E-01	9.94E-05	4.44E-02	-	-	-	-	-	-	1.00E+00
108	5.64E-03	1.26E-01	2.47E-02	8.44E-01	5.30E-05	-	-	-	-	-	-	-	1.00E+00
109	2.80E-03	6.57E-02	1.21E-02	9.19E-01	9.82E-05	-	-	-	-	-	-	-	1.00E+00
110	2.09E-03	4.52E-02	9.07E-03	9.15E-01	1.09E-04	2.84E-02	-	-	-	-	-	-	1.00E+00
111	3.17E-02	7.98E-01	3.50E-02	-	-	-	1.35E-01	-	-	-	-	-	1.00E+00
112	1.63E-03	4.98E-02	6.99E-03	9.42E-01	1.00E-04	-	-	-	-	-	-	-	1.00E+00
113	1.33E-02	3.20E-01	5.83E-02	6.08E-01	-	-	-	-	-	-	-	-	1.00E+00
114	4.01E-03	1.24E-01	1.73E-02	8.55E-01	2.08E-05	-	-	-	-	-	-	-	1.00E+00
115	3.71E-03	8.11E-02	1.62E-02	8.99E-01	9.23E-05	-	-	-	-	-	-	-	1.00E+00
116	5.92E-03	1.47E-01	2.60E-02	8.21E-01	2.70E-05	-	-	-	-	-	-	-	1.00E+00
117	9.29E-03	2.02E-01	4.08E-02	7.48E-01	5.91E-05	-	-	-	-	-	-	-	1.00E+00
118	1.14E-03	3.26E-02	4.84E-03	9.29E-01	1.06E-04	3.21E-02	-	-	-	-	-	-	1.00E+00
119	5.60E-02	-	2.47E-01	-	-	6.97E-01	-	-	-	-	-	-	1.00E+00
120	3.01E-02	6.80E-01	1.33E-01	1.58E-01	-	-	-	-	-	-	-	-	1.00E+00
121	4.71E-03	1.12E-01	2.05E-02	8.63E-01	9.94E-05	-	-	-	-	-	-	-	1.00E+00
122	2.77E-03	1.60E-01	1.20E-02	8.25E-01	-	-	-	-	-	-	-	-	1.00E+00
123	2.20E-03	5.87E-02	-	9.27E-01	9.04E-05	-	1.22E-02	-	-	-	-	-	1.00E+00
124	3.63E-02	8.04E-01	1.60E-01	-	-	-	-	-	-	-	-	-	1.00E+00
125	6.84E-02	6.30E-01	3.02E-01	-	-	-	-	-	-	-	-	-	1.00E+00
126	1.93E-03	6.22E-02	8.31E-03	9.27E-01	7.59E-05	-	-	-	-	-	-	-	1.00E+00
127	2.62E-02	5.15E-01	1.16E-01	2.86E-01	-	5.73E-02	-	-	-	-	-	-	1.00E+00
128	1.13E-02	9.33E-01	4.90E-02	6.30E-03	-	-	-	-	-	-	-	-	1.00E+00
129	4.23E-02	7.71E-01	1.86E-01	-	-	-	-	-	-	-	-	-	1.00E+00
130	4.61E-02	7.51E-01	2.03E-01	-	-	-	-	-	-	-	-	-	1.00E+00
131	9.56E-03	2.17E-01	4.20E-02	7.31E-01	8.15E-05	-	-	-	-	-	-	-	1.00E+00
132	2.45E-02	8.70E-01	1.05E-01	-	-	-	-	-	-	-	-	-	1.00E+00
133	5.57E-03	1.08E-01	2.44E-02	8.62E-01	1.04E-04	-	-	-	-	-	-	-	1.00E+00
134	1.50E-02	9.19E-01	6.58E-02	-	-	-	-	-	-	-	-	-	1.00E+00
135	4.58E-02	7.53E-01	2.01E-01	-	-	-	-	-	-	-	-	-	1.00E+00
136	1.02E-02	2.56E-01	-	6.75E-01	4.15E-05	-	5.88E-02	-	-	-	-	-	1.00E+00
137	2.75E-02	8.54E-01	1.18E-01	-	-	-	-	-	-	-	-	-	1.00E+00
138	4.15E-02	7.76E-01	1.82E-01	-	-	-	-	-	-	-	-	-	1.00E+00
139	2.70E-02	8.54E-01	1.19E-01	-	-	-	-	-	-	-	-	-	1.00E+00
140	5.04E-03	1.46E-01	2.21E-02	8.27E-01	1.20E-04	-	-	-	-	-	-	-	1.00E+00
141	2.28E-03	1.19E-01	-	8.66E-01	8.80E-05	-	1.22E-02	-	-	-	-	-	1.00E+00
142	3.99E-02	7.84E-01	1.76E-01	-	-	-	-	-	-	-	-	-	1.00E+00
143	4.81E-03	1.99E-01	-	7.69E-01	5.00E-05	-	2.69E-02	-	-	-	-	-	1.00E+00
144	4.71E-03	1.36E-01	2.06E-02	8.38E-01	1.20E-04	-	-	-	-	-	-	-	1.00E+00
145	4.07E-02	7.80E-01	1.79E-01	-	-	-	-	-	-	-	-	-	1.00E+00
146	3.49E-02	8.11E-01	1.54E-01	-	-	-	-	-	-	-	-	-	1.00E+00
147	3.28E-02	8.23E-01	1.44E-01	-	-	-	-	-	-	-	-	-	1.00E+00
148	3.39E-03	9.82E-02	-	8.79E-01	1.44E-04	-	1.91E-02	-	-	-	-	-	1.00E+00

Run#	MGOH2	NASGEL	CAF2	ALOH3	NIOH2	NA2C2O4	CA3PO42	NAF	NAPHOH .12H2O	CAOH2	CACO3	NAFPO4 .19H2O	sum
149	3.81E-02	7.95E-01	1.67E-01	-	-	-	-	-	-	-	-	-	1.00E+00
150	5.68E-03	1.37E-01	2.48E-02	8.32E-01	1.32E-04	-	-	-	-	-	-	-	1.00E+00
151	9.56E-03	3.36E-01	4.15E-02	6.13E-01	2.18E-05	-	-	-	-	-	-	-	1.00E+00
152	8.50E-05	4.39E-02	1.64E-04	9.56E-01	1.34E-04	-	-	-	-	-	-	-	1.00E+00
153	3.71E-02	8.00E-01	1.63E-01	-	-	-	-	-	-	-	-	-	1.00E+00
154	3.57E-02	8.09E-01	1.55E-01	-	-	-	-	-	-	-	-	-	1.00E+00
155	4.95E-02	7.32E-01	2.18E-01	-	-	-	-	-	-	-	-	-	1.00E+00
156	3.03E-02	7.95E-01	-	-	-	-	1.75E-01	-	-	-	-	-	1.00E+00
157	8.63E-03	1.84E-01	3.78E-02	7.69E-01	1.42E-04	-	-	-	-	-	-	-	1.00E+00
158	3.23E-02	7.81E-01	-	-	-	-	1.86E-01	-	-	-	-	-	1.00E+00
159	3.51E-02	8.11E-01	1.54E-01	-	-	-	-	-	-	-	-	-	1.00E+00
160	4.42E-02	7.61E-01	1.95E-01	-	-	-	-	-	-	-	-	-	1.00E+00
161	5.34E-02	6.91E-01	1.64E-01	-	-	-	9.19E-02	-	-	-	-	-	1.00E+00
162	7.95E-03	9.57E-01	-	-	-	-	3.51E-02	-	-	-	-	-	1.00E+00
163	3.73E-02	7.99E-01	1.64E-01	-	-	-	-	-	-	-	-	-	1.00E+00
164	1.16E-02	2.57E-01	5.03E-02	6.81E-01	1.15E-04	-	-	-	-	-	-	-	1.00E+00
165	6.11E-03	2.58E-01	-	7.02E-01	9.72E-05	-	3.45E-02	-	-	-	-	-	1.00E+00
166	1.16E-02	2.90E-01	-	6.32E-01	1.24E-04	-	6.66E-02	-	-	-	-	-	1.00E+00
167	4.03E-02	7.82E-01	1.77E-01	-	-	-	-	-	-	-	-	-	1.00E+00
168	3.08E-02	8.34E-01	1.35E-01	-	-	-	-	-	-	-	-	-	1.00E+00
169	4.04E-02	7.71E-01	1.37E-01	-	-	-	5.22E-02	-	-	-	-	-	1.00E+00
170	1.71E-02	3.48E-01	-	5.36E-01	1.19E-04	-	9.92E-02	-	-	-	-	-	1.00E+00
171	4.60E-02	7.03E-01	-	-	-	-	2.51E-01	-	-	-	-	-	1.00E+00
172	3.69E-02	7.49E-01	-	-	6.54E-05	-	2.14E-01	-	-	-	-	-	1.00E+00
173	1.06E-01	4.30E-01	4.65E-01	-	-	-	-	-	-	-	-	-	1.00E+00
174	3.68E-02	7.51E-01	-	-	-	-	2.12E-01	-	-	-	-	-	1.00E+00
175	2.85E-02	6.75E-01	-	1.31E-01	1.15E-04	-	1.65E-01	-	-	-	-	-	1.00E+00
176	2.42E-02	5.26E-01	1.05E-01	3.44E-01	5.55E-05	-	-	-	-	-	-	-	1.00E+00
177	4.03E-02	7.82E-01	1.78E-01	-	7.61E-05	-	-	-	-	-	-	-	1.00E+00
178	3.62E-02	8.04E-01	1.59E-01	-	1.05E-04	-	-	-	-	-	-	-	1.00E+00
179	1.70E-02	9.10E-01	7.34E-02	-	-	-	-	-	-	-	-	-	1.00E+00
180	2.34E-02	8.75E-01	1.02E-01	-	-	-	-	-	-	-	-	-	1.00E+00
181	3.40E-02	8.17E-01	1.49E-01	-	-	-	-	-	-	-	-	-	1.00E+00
182	6.45E-02	5.62E-01	-	-	-	-	3.73E-01	-	-	-	-	-	1.00E+00
183	2.62E-02	8.60E-01	1.13E-01	-	-	-	-	-	-	-	-	-	1.00E+00
184	1.59E-02	9.15E-01	6.91E-02	-	-	-	-	-	-	-	-	-	1.00E+00
185	3.93E-02	7.87E-01	1.73E-01	-	8.34E-05	-	-	-	-	-	-	-	1.00E+00
186	2.16E-02	8.84E-01	9.40E-02	-	-	-	-	-	-	-	-	-	1.00E+00
187	3.66E-02	8.02E-01	1.61E-01	-	1.03E-04	-	-	-	-	-	-	-	1.00E+00
188	3.61E-02	8.05E-01	1.59E-01	-	-	-	-	-	-	-	-	-	1.00E+00
number of occurrences	178	166	108	87	83	60	38	6	4	4	4	2	

Mass fraction of total undissolved solids present in 1st ultra filtration slurry. The last row lists the number of simulations for which the particular solid was present. The right-hand most column is a sum of the mass fractions as a check.

Table 18. Envelope B/D Solids

Run#	FEIIIOH3	ZRO2	NASGEL	MGOH2	NIOH2	ALOH3	SRCO3	CAF2	NA2C2O4	MNOH2	CACO3	sum
1	3.97E-01	5.53E-02	9.55E-02	4.55E-05	1.49E-04	3.59E-01	5.00E-03	1.59E-03	8.65E-02	-	-	1.00E+00
2	2.65E-01	6.33E-02	1.07E-01	4.57E-05	1.34E-04	4.67E-01	5.73E-03	1.82E-03	8.94E-02	-	-	1.00E+00

Run#	FEIIIOH3	ZRO2	NASGEL	MGOH2	NIOH2	ALOH3	SRCO3	CAF2	NA2C2O4	MNOH2	CACO3	sum
3	4.21E-01	4.86E-02	8.34E-02	4.55E-05	1.51E-04	3.71E-01	4.39E-03	1.40E-03	7.01E-02	-	-	1.00E+00
4	3.44E-01	4.05E-02	7.14E-02	4.56E-05	1.68E-04	4.73E-01	3.65E-03	1.16E-03	6.57E-02	-	-	1.00E+00
5	2.60E-01	6.20E-02	1.09E-01	4.58E-05	1.61E-04	4.86E-01	5.59E-03	1.77E-03	7.55E-02	-	-	1.00E+00
6	2.56E-01	4.87E-02	8.48E-02	4.57E-05	1.60E-04	5.37E-01	4.40E-03	1.40E-03	6.75E-02	-	-	1.00E+00
7	6.95E-01	1.07E-01	1.55E-01	4.54E-05	1.84E-04	-	4.93E-03	1.56E-03	3.57E-02	-	-	1.00E+00
8	5.75E-01	1.72E-01	2.42E-01	4.59E-05	1.83E-04	-	7.91E-03	2.50E-03	-	-	-	1.00E+00
9	7.43E-01	9.37E-02	1.35E-01	4.55E-05	1.85E-04	2.21E-02	4.32E-03	1.37E-03	-	-	-	1.00E+00
10	4.78E-01	6.02E-02	8.86E-02	4.57E-05	1.92E-04	3.69E-01	2.78E-03	-	-	1.32E-04	1.13E-03	1.00E+00
11	4.05E-01	1.10E-01	1.59E-01	4.60E-05	1.92E-04	3.19E-01	5.06E-03	1.60E-03	-	4.93E-05	-	1.00E+00
12	3.90E-01	8.47E-02	1.23E-01	4.59E-05	1.91E-04	3.97E-01	3.91E-03	1.24E-03	-	1.40E-05	-	1.00E+00
13	4.15E-01	5.89E-02	8.08E-02	4.53E-05	1.42E-04	3.49E-01	2.72E-03	8.72E-04	9.31E-02	-	-	1.00E+00
14	2.76E-01	6.80E-02	9.09E-02	4.56E-05	1.25E-04	4.64E-01	3.15E-03	1.01E-03	9.71E-02	-	-	1.00E+00
15	4.37E-01	5.12E-02	6.97E-02	4.54E-05	1.45E-04	3.64E-01	2.38E-03	7.65E-04	7.47E-02	-	-	1.00E+00
16	3.54E-01	4.23E-02	5.98E-02	4.55E-05	1.64E-04	4.72E-01	1.96E-03	6.32E-04	6.94E-02	-	-	1.00E+00
17	2.70E-01	6.62E-02	9.29E-02	4.56E-05	1.55E-04	4.85E-01	3.06E-03	9.80E-04	8.22E-02	-	-	1.00E+00
18	2.63E-01	5.13E-02	7.13E-02	4.56E-05	1.55E-04	5.39E-01	2.38E-03	7.67E-04	7.21E-02	-	-	1.00E+00
19	4.37E-01	6.32E-02	6.31E-02	4.57E-05	1.35E-04	3.35E-01	-	-	1.02E-01	-	-	1.00E+00
20	2.89E-01	7.37E-02	7.08E-02	4.59E-05	1.15E-04	4.59E-01	-	-	1.07E-01	-	-	1.00E+00
21	4.57E-01	5.43E-02	5.35E-02	4.52E-05	1.38E-04	3.55E-01	-	-	8.01E-02	-	-	1.00E+00
22	3.66E-01	4.44E-02	4.62E-02	4.54E-05	1.59E-04	4.69E-01	-	-	7.37E-02	-	-	1.00E+00
23	2.81E-01	7.15E-02	7.36E-02	4.55E-05	1.46E-04	4.83E-01	-	-	9.03E-02	-	-	1.00E+00
24	2.71E-01	5.44E-02	5.52E-02	4.55E-05	1.49E-04	5.42E-01	-	-	7.74E-02	-	-	1.00E+00
25	7.09E-01	1.14E-01	1.22E-01	4.51E-05	1.83E-04	-	-	-	5.44E-02	-	-	1.00E+00
26	6.03E-01	1.96E-01	2.01E-01	4.57E-05	1.80E-04	-	-	-	-	-	-	1.00E+00
27	7.88E-01	1.02E-01	1.10E-01	4.53E-05	1.84E-04	-	-	-	-	-	-	1.00E+00
28	5.18E-01	6.67E-02	7.38E-02	4.56E-05	1.92E-04	3.42E-01	-	-	-	1.19E-04	-	1.00E+00
29	4.65E-01	1.32E-01	1.44E-01	4.58E-05	1.90E-04	2.58E-01	-	-	-	-	-	1.00E+00
30	4.32E-01	9.75E-02	1.06E-01	4.58E-05	1.90E-04	3.65E-01	-	-	-	-	-	1.00E+00
31	7.09E-01	1.14E-01	1.22E-01	4.51E-05	1.83E-04	-	-	-	5.44E-02	-	-	1.00E+00
32	6.03E-01	1.96E-01	2.01E-01	4.57E-05	1.80E-04	-	-	-	-	-	-	1.00E+00
33	7.88E-01	1.02E-01	1.10E-01	4.53E-05	1.84E-04	-	-	-	-	-	-	1.00E+00
34	5.18E-01	6.67E-02	7.38E-02	4.56E-05	1.92E-04	3.42E-01	-	-	-	7.63E-05	-	1.00E+00
35	4.65E-01	1.32E-01	1.44E-01	4.58E-05	1.91E-04	2.58E-01	-	-	-	-	-	1.00E+00
36	4.32E-01	9.75E-02	1.06E-01	4.58E-05	1.90E-04	3.65E-01	-	-	-	-	-	1.00E+00
37	4.37E-01	6.32E-02	6.31E-02	4.57E-05	1.35E-04	3.35E-01	-	-	1.02E-01	-	-	1.00E+00
38	2.89E-01	7.37E-02	7.08E-02	4.59E-05	1.15E-04	4.59E-01	-	-	1.07E-01	-	-	1.00E+00
39	4.57E-01	5.43E-02	5.35E-02	4.52E-05	1.37E-04	3.55E-01	-	-	8.02E-02	-	-	1.00E+00
40	3.66E-01	4.44E-02	4.62E-02	4.54E-05	1.59E-04	4.69E-01	-	-	7.37E-02	-	-	1.00E+00
41	2.81E-01	7.15E-02	7.36E-02	4.55E-05	1.46E-04	4.83E-01	-	-	9.03E-02	-	-	1.00E+00
42	2.71E-01	5.44E-02	5.52E-02	4.55E-05	1.49E-04	5.42E-01	-	-	7.74E-02	-	-	1.00E+00
43	6.66E-01	9.96E-02	1.78E-01	4.57E-05	1.87E-04	4.25E-02	8.95E-03	2.82E-03	1.39E-03	3.34E-05	-	1.00E+00
44	5.49E-01	1.53E-01	2.71E-01	4.61E-05	1.85E-04	9.21E-03	1.38E-02	4.35E-03	-	-	-	1.00E+00
45	6.68E-01	8.27E-02	1.47E-01	4.56E-05	1.88E-04	9.22E-02	7.43E-03	2.35E-03	-	-	-	1.00E+00
46	4.47E-01	5.52E-02	1.00E-01	4.58E-05	1.93E-04	3.90E-01	4.95E-03	-	-	1.75E-04	2.01E-03	1.00E+00
47	3.64E-01	9.45E-02	1.70E-01	4.61E-05	1.93E-04	3.60E-01	8.48E-03	2.68E-03	-	1.10E-04	-	1.00E+00
48	3.60E-01	7.54E-02	1.35E-01	4.61E-05	1.92E-04	4.20E-01	6.77E-03	2.15E-03	-	6.97E-05	-	1.00E+00
49	3.75E-01	4.88E-02	5.19E-02	4.54E-05	1.59E-04	4.50E-01	1.89E-04	7.25E-05	7.37E-02	-	-	1.00E+00
50	3.49E-01	7.23E-02	9.07E-02	4.57E-05	1.76E-04	4.43E-01	1.92E-03	6.18E-04	4.23E-02	-	-	1.00E+00
51	2.91E-01	6.10E-02	7.20E-02	4.55E-05	1.64E-04	4.95E-01	1.08E-03	3.53E-04	7.96E-02	-	-	1.00E+00
52	3.13E-01	7.25E-02	8.52E-02	4.56E-05	1.68E-04	4.69E-01	1.29E-03	4.21E-04	5.81E-02	-	-	1.00E+00
53	4.25E-01	6.12E-02	6.42E-02	4.54E-05	1.70E-04	3.85E-01	1.17E-04	4.82E-05	6.45E-02	-	-	1.00E+00
54	4.50E-01	7.13E-02	9.20E-02	4.54E-05	1.75E-04	3.18E-01	2.27E-03	7.26E-04	6.52E-02	-	-	1.00E+00
55	2.98E-01	6.43E-02	9.46E-02	4.56E-05	1.58E-04	4.63E-01	3.68E-03	1.17E-03	7.49E-02	-	-	1.00E+00
56	3.89E-01	5.52E-02	8.33E-02	4.56E-05	1.84E-04	4.23E-01	3.07E-03	9.79E-04	4.46E-02	-	-	1.00E+00

Run#	FEIIIOH3	ZRO2	NASGEL	MGOH2	NIOH2	ALOH3	SRCO3	CAF2	NA2C2O4	MNOH2	CACO3	sum
57	4.23E-01	8.26E-02	1.17E-01	4.56E-05	1.71E-04	3.19E-01	4.08E-03	1.30E-03	5.29E-02	-	-	1.00E+00
58	4.67E-01	6.11E-02	9.15E-02	4.56E-05	1.79E-04	3.41E-01	3.51E-03	1.12E-03	3.38E-02	-	-	1.00E+00
59	3.64E-01	6.57E-02	8.58E-02	4.55E-05	1.56E-04	4.00E-01	2.51E-03	8.03E-04	8.06E-02	-	-	1.00E+00
60	3.96E-01	4.87E-02	7.29E-02	4.55E-05	1.63E-04	4.06E-01	2.89E-03	9.23E-04	7.23E-02	-	-	1.00E+00
61	3.56E-01	5.95E-02	8.60E-02	4.56E-05	1.62E-04	4.26E-01	3.25E-03	1.04E-03	6.81E-02	-	-	1.00E+00
62	5.61E-01	7.72E-02	8.60E-02	4.56E-05	1.90E-04	2.76E-01	1.92E-04	-	-	4.92E-07	8.49E-05	1.00E+00
63	3.67E-01	7.57E-02	1.01E-01	4.59E-05	1.85E-04	4.53E-01	2.55E-03	8.14E-04	-	-	-	1.00E+00
64	4.47E-01	7.95E-02	9.02E-02	4.57E-05	1.87E-04	3.82E-01	5.83E-04	1.93E-04	-	-	-	1.00E+00
65	5.38E-01	9.37E-02	1.20E-01	4.56E-05	1.89E-04	2.16E-01	2.44E-03	7.75E-04	2.86E-02	-	-	1.00E+00
66	4.70E-01	8.67E-02	1.03E-01	4.57E-05	1.85E-04	3.38E-01	1.44E-03	4.62E-04	-	-	-	1.00E+00
67	7.25E-01	1.21E-01	1.50E-01	4.55E-05	1.84E-04	-	2.55E-03	8.08E-04	-	-	-	1.00E+00
68	5.31E-01	8.95E-02	9.92E-02	4.56E-05	1.85E-04	2.79E-01	5.25E-04	1.74E-04	-	-	-	1.00E+00
69	5.27E-01	7.59E-02	9.97E-02	4.55E-05	1.81E-04	2.49E-01	2.54E-03	8.11E-04	4.45E-02	-	-	1.00E+00
70	4.53E-01	6.20E-02	9.20E-02	4.58E-05	1.91E-04	3.88E-01	3.07E-03	9.76E-04	-	5.45E-05	-	1.00E+00
71	4.21E-01	9.43E-02	1.45E-01	4.60E-05	1.88E-04	3.32E-01	5.63E-03	1.78E-03	-	-	-	1.00E+00
72	4.50E-01	6.89E-02	9.61E-02	4.58E-05	1.86E-04	3.81E-01	2.88E-03	9.19E-04	-	-	-	1.00E+00
73	4.61E-01	8.36E-02	1.24E-01	4.58E-05	1.92E-04	3.27E-01	4.11E-03	1.30E-03	-	3.63E-05	-	1.00E+00
74	4.94E-01	6.43E-02	9.38E-02	4.57E-05	1.88E-04	3.43E-01	3.11E-03	9.91E-04	-	-	-	1.00E+00
75	4.18E-01	9.89E-02	1.39E-01	4.59E-05	1.89E-04	3.38E-01	4.21E-03	1.34E-03	-	-	-	1.00E+00
76	4.25E-01	7.26E-02	1.22E-01	4.57E-05	1.82E-04	3.35E-01	5.76E-03	1.83E-03	3.75E-02	-	-	1.00E+00
77	4.61E-01	1.06E-01	1.55E-01	4.59E-05	1.87E-04	2.71E-01	5.36E-03	1.70E-03	-	-	-	1.00E+00
78	6.80E-01	1.13E-01	1.46E-01	4.55E-05	1.85E-04	5.58E-02	3.24E-03	1.02E-03	-	-	-	1.00E+00
79	5.76E-01	1.11E-01	1.54E-01	4.57E-05	1.85E-04	1.54E-01	4.66E-03	1.48E-03	-	-	-	1.00E+00
80	4.91E-01	7.98E-02	1.28E-01	4.57E-05	1.89E-04	2.62E-01	5.42E-03	1.72E-03	3.16E-02	-	-	1.00E+00
81	4.67E-01	7.75E-02	1.20E-01	4.58E-05	1.85E-04	3.29E-01	4.85E-03	1.54E-03	-	-	-	1.00E+00
82	4.44E-01	7.47E-02	9.66E-02	4.56E-05	1.80E-04	3.48E-01	2.28E-03	7.31E-04	3.37E-02	-	-	1.00E+00
83	6.15E-01	1.45E-01	2.20E-01	4.59E-05	1.84E-04	9.15E-03	8.24E-03	2.60E-03	-	-	-	1.00E+00
84	5.50E-01	7.78E-02	1.03E-01	4.55E-05	1.83E-04	2.39E-01	2.63E-03	8.40E-04	2.71E-02	-	-	1.00E+00
85	5.85E-01	7.80E-02	1.10E-01	4.55E-05	1.87E-04	2.05E-01	3.35E-03	1.07E-03	1.74E-02	-	-	1.00E+00
86	4.71E-01	9.59E-02	1.38E-01	4.59E-05	1.86E-04	2.89E-01	4.57E-03	1.45E-03	-	-	-	1.00E+00
87	4.73E-01	5.61E-02	8.16E-02	4.57E-05	1.87E-04	3.79E-01	2.67E-03	8.52E-04	7.02E-03	-	-	1.00E+00
88	4.38E-01	8.71E-02	1.27E-01	4.59E-05	1.91E-04	3.42E-01	4.06E-03	1.29E-03	-	4.49E-05	-	1.00E+00
89	4.85E-01	6.66E-02	1.01E-01	4.58E-05	1.91E-04	3.42E-01	3.67E-03	1.17E-03	-	2.86E-05	-	1.00E+00
90	4.32E-01	7.77E-02	1.01E-01	4.58E-05	1.85E-04	3.86E-01	2.31E-03	7.38E-04	-	-	-	1.00E+00
91	4.92E-01	7.72E-02	1.05E-01	4.57E-05	1.87E-04	3.14E-01	2.79E-03	8.89E-04	7.07E-03	-	-	1.00E+00
92	6.34E-01	8.66E-02	1.02E-01	4.55E-05	1.88E-04	1.76E-01	1.08E-03	3.46E-04	-	-	-	1.00E+00
93	4.60E-01	6.73E-02	7.96E-02	4.57E-05	1.87E-04	3.92E-01	8.68E-04	2.83E-04	-	-	-	1.00E+00
94	4.10E-01	9.54E-02	1.02E-01	4.56E-05	1.80E-04	3.56E-01	9.65E-05	4.02E-05	3.64E-02	-	-	1.00E+00
95	5.03E-01	7.89E-02	9.66E-02	4.57E-05	1.90E-04	3.19E-01	1.37E-03	4.41E-04	-	-	-	1.00E+00
96	5.18E-01	1.37E-01	1.59E-01	4.58E-05	1.87E-04	1.83E-01	1.58E-03	5.03E-04	-	-	-	1.00E+00
97	5.33E-01	8.97E-02	1.09E-01	4.57E-05	1.89E-04	2.66E-01	1.49E-03	4.75E-04	-	-	-	1.00E+00
98	5.09E-01	7.29E-02	9.23E-02	4.53E-05	1.73E-04	2.57E-01	2.09E-03	6.70E-04	6.62E-02	-	-	1.00E+00
99	4.23E-01	6.71E-02	1.05E-01	4.56E-05	1.70E-04	3.41E-01	4.56E-03	1.45E-03	5.79E-02	-	-	1.00E+00
100	3.67E-01	6.01E-02	7.72E-02	4.55E-05	1.58E-04	4.26E-01	2.05E-03	6.62E-04	6.67E-02	-	-	1.00E+00
101	4.25E-01	6.64E-02	9.20E-02	4.55E-05	1.72E-04	3.51E-01	2.92E-03	9.31E-04	6.10E-02	-	-	1.00E+00
102	3.14E-01	5.48E-02	7.30E-02	4.56E-05	1.58E-04	4.81E-01	2.07E-03	6.67E-04	7.43E-02	-	-	1.00E+00
103	3.75E-01	6.29E-02	1.04E-01	4.56E-05	1.74E-04	3.91E-01	4.80E-03	1.53E-03	6.07E-02	-	-	1.00E+00
104	3.72E-01	7.60E-02	9.75E-02	4.58E-05	1.80E-04	4.36E-01	2.18E-03	6.98E-04	1.47E-02	-	-	1.00E+00
105	4.23E-01	5.39E-02	7.06E-02	4.53E-05	1.78E-04	3.94E-01	1.68E-03	5.40E-04	5.54E-02	-	-	1.00E+00
106	4.45E-01	5.95E-02	6.42E-02	4.54E-05	1.67E-04	3.63E-01	3.66E-04	1.27E-04	6.74E-02	-	-	1.00E+00
107	4.37E-01	8.10E-02	9.35E-02	4.54E-05	1.70E-04	3.12E-01	1.20E-03	3.90E-04	7.47E-02	-	-	1.00E+00
108	3.96E-01	6.21E-02	6.48E-02	4.53E-05	1.34E-04	3.88E-01	4.38E-04	1.53E-04	8.83E-02	-	-	1.00E+00
109	3.69E-01	8.47E-02	1.01E-01	4.56E-05	1.65E-04	3.75E-01	1.80E-03	5.79E-04	6.71E-02	-	-	1.00E+00
110	4.43E-01	5.74E-02	6.85E-02	4.54E-05	1.62E-04	3.60E-01	1.25E-03	4.07E-04	6.90E-02	-	-	1.00E+00

Run#	FEIIIOH3	ZRO2	NASGEL	MGOH2	NIOH2	ALOH3	SRCO3	CAF2	NA2C2O4	MNOH2	CACO3	sum
111	4.53E-01	7.40E-02	8.00E-02	4.56E-05	1.80E-04	3.80E-01	2.48E-04	9.00E-05	1.22E-02	-	-	1.00E+00
112	4.24E-01	5.58E-02	6.67E-02	4.54E-05	1.69E-04	3.87E-01	1.12E-03	3.64E-04	6.51E-02	-	-	1.00E+00
113	3.29E-01	5.75E-02	7.46E-02	4.55E-05	1.57E-04	4.59E-01	1.91E-03	6.17E-04	7.79E-02	-	-	1.00E+00
114	3.83E-01	5.78E-02	6.68E-02	4.55E-05	1.71E-04	4.32E-01	8.04E-04	2.65E-04	5.92E-02	-	-	1.00E+00
115	3.82E-01	6.65E-02	7.04E-02	4.55E-05	1.64E-04	4.23E-01	3.23E-04	1.15E-04	5.80E-02	-	-	1.00E+00
116	4.22E-01	7.20E-02	8.12E-02	4.55E-05	1.74E-04	3.65E-01	7.06E-04	2.33E-04	5.87E-02	-	-	1.00E+00
number of occurrences	116	116	116	116	116	107	92	89	70	14	3	

Mass fraction of total undissolved solids present in 1st ultra filtration slurry. The last row lists the number of simulations for which the particular solid was present. The right-hand most column is a sum of the mass fractions as a check.

Table 19. Envelope C Solids

Run#	MNOH2	MGOH2	SRCO3	FEIIIOH3	ZRO2	NASGEL	ALOH3	sum
1	1.28E-02	6.14E-05	9.40E-01	4.73E-02	-	-	-	1.00E+00
3	1.23E-02	6.14E-05	9.28E-01	6.01E-02	-	-	-	1.00E+00
4	1.24E-02	6.14E-05	9.30E-01	5.79E-02	-	-	-	1.00E+00
5	1.23E-02	5.69E-05	9.87E-01	-	3.22E-04	-	-	1.00E+00
7	1.25E-02	5.73E-05	9.87E-01	-	3.22E-04	-	-	1.00E+00
8	1.25E-02	5.72E-05	9.87E-01	-	3.22E-04	-	-	1.00E+00
9	1.24E-02	6.13E-05	9.41E-01	4.61E-02	-	-	-	1.00E+00
11	1.19E-02	6.14E-05	9.30E-01	5.85E-02	-	-	-	1.00E+00
12	1.19E-02	6.14E-05	9.32E-01	5.64E-02	-	-	-	1.00E+00
13	1.02E-02	5.63E-05	9.89E-01	-	3.22E-04	-	-	1.00E+00
15	1.06E-02	5.68E-05	9.89E-01	-	3.23E-04	-	-	1.00E+00
16	1.05E-02	5.67E-05	9.89E-01	-	3.23E-04	-	-	1.00E+00
17	1.29E-02	6.13E-05	9.39E-01	4.82E-02	-	-	-	1.00E+00
19	1.23E-02	6.14E-05	9.27E-01	6.09E-02	-	-	-	1.00E+00
20	1.25E-02	6.14E-05	9.29E-01	5.88E-02	-	-	-	1.00E+00
21	1.04E-02	5.60E-05	9.89E-01	-	3.23E-04	-	-	1.00E+00
23	1.09E-02	5.65E-05	9.89E-01	-	3.23E-04	-	-	1.00E+00
24	1.08E-02	5.64E-05	9.89E-01	-	3.23E-04	-	-	1.00E+00
25	1.26E-02	6.14E-05	9.41E-01	4.65E-02	-	-	-	1.00E+00
27	1.20E-02	6.14E-05	9.29E-01	5.93E-02	-	-	-	1.00E+00
28	1.21E-02	6.14E-05	9.31E-01	5.71E-02	-	-	-	1.00E+00
29	1.20E-02	5.49E-05	9.88E-01	-	3.22E-04	-	-	1.00E+00
31	1.22E-02	5.73E-05	9.87E-01	-	3.23E-04	-	-	1.00E+00
32	1.22E-02	5.72E-05	9.87E-01	-	3.23E-04	-	-	1.00E+00
33	1.02E-02	6.18E-05	7.68E-01	3.73E-02	-	-	1.84E-01	1.00E+00
35	9.75E-03	6.18E-05	7.64E-01	4.77E-02	-	1.93E-02	1.59E-01	1.00E+00
36	9.83E-03	6.18E-05	7.66E-01	4.60E-02	-	1.38E-02	1.64E-01	1.00E+00
37	1.17E-02	5.70E-05	9.88E-01	-	3.28E-04	-	-	1.00E+00
39	1.16E-02	5.76E-05	9.69E-01	-	3.33E-04	1.91E-02	-	1.00E+00
40	1.17E-02	5.75E-05	9.77E-01	-	3.31E-04	1.08E-02	-	1.00E+00
41	1.03E-02	6.19E-05	7.35E-01	3.79E-02	-	-	2.16E-01	1.00E+00
43	9.87E-03	6.19E-05	7.29E-01	4.81E-02	-	2.06E-02	1.92E-01	1.00E+00
44	9.95E-03	6.19E-05	7.32E-01	4.65E-02	-	1.51E-02	1.96E-01	1.00E+00
45	1.17E-02	5.66E-05	9.88E-01	-	3.28E-04	-	-	1.00E+00
47	1.18E-02	5.74E-05	9.67E-01	-	3.34E-04	2.11E-02	-	1.00E+00
48	1.18E-02	5.72E-05	9.75E-01	-	3.31E-04	1.27E-02	-	1.00E+00
49	1.41E-02	6.04E-05	9.77E-01	8.67E-03	-	-	-	1.00E+00
50	1.43E-02	5.96E-05	9.86E-01	-	8.51E-05	-	-	1.00E+00
51	1.28E-02	5.77E-05	9.87E-01	-	2.77E-04	-	-	1.00E+00

Run#	MNOH2	MGOH2	SRCO3	FEIIIOH3	ZRO2	NASGEL	ALOH3	sum
52	1.28E-02	5.83E-05	9.87E-01	-	2.43E-04	-	-	1.00E+00
53	1.30E-02	6.13E-05	9.36E-01	5.07E-02	-	-	-	1.00E+00
54	1.42E-02	6.10E-05	9.51E-01	3.52E-02	-	-	-	1.00E+00
55	1.23E-02	5.77E-05	9.87E-01	-	2.85E-04	-	-	1.00E+00
56	1.48E-02	6.02E-05	9.85E-01	-	-	-	-	1.00E+00
57	1.42E-02	6.08E-05	9.63E-01	2.23E-02	-	-	-	1.00E+00
58	1.27E-02	5.74E-05	9.87E-01	-	3.02E-04	-	-	1.00E+00
59	1.28E-02	6.13E-05	9.39E-01	4.85E-02	-	-	-	1.00E+00
60	1.23E-02	5.80E-05	9.87E-01	-	2.57E-04	-	-	1.00E+00
61	1.38E-02	6.11E-05	9.47E-01	3.96E-02	-	-	-	1.00E+00
62	1.51E-02	6.09E-05	9.64E-01	2.09E-02	-	-	-	1.00E+00
63	1.43E-02	6.01E-05	9.86E-01	-	-	-	-	1.00E+00
64	1.34E-02	6.12E-05	9.35E-01	5.11E-02	-	-	-	1.00E+00
65	1.40E-02	6.11E-05	9.54E-01	3.20E-02	-	-	-	1.00E+00
66	1.41E-02	6.10E-05	9.51E-01	3.48E-02	-	-	-	1.00E+00
67	1.35E-02	5.90E-05	9.86E-01	-	1.97E-04	-	-	1.00E+00
68	1.26E-02	5.80E-05	9.87E-01	-	2.69E-04	-	-	1.00E+00
69	1.46E-02	6.05E-05	9.75E-01	1.01E-02	-	-	-	1.00E+00
70	1.47E-02	5.99E-05	9.85E-01	-	-	-	-	1.00E+00
71	1.43E-02	6.06E-05	9.67E-01	1.89E-02	-	-	-	1.00E+00
72	1.25E-02	5.81E-05	9.87E-01	-	2.53E-04	-	-	1.00E+00
73	1.29E-02	5.83E-05	9.87E-01	-	2.48E-04	-	-	1.00E+00
74	1.20E-02	5.74E-05	9.88E-01	-	2.99E-04	-	-	1.00E+00
75	1.20E-02	5.71E-05	9.88E-01	-	3.19E-04	-	-	1.00E+00
76	1.41E-02	6.05E-05	9.70E-01	1.59E-02	-	-	-	1.00E+00
77	1.41E-02	5.99E-05	9.86E-01	-	4.25E-05	-	-	1.00E+00
78	1.19E-02	5.74E-05	9.88E-01	-	2.89E-04	-	-	1.00E+00
79	1.42E-02	6.05E-05	9.76E-01	9.84E-03	-	-	-	1.00E+00
80	1.42E-02	5.94E-05	9.86E-01	-	1.16E-04	-	-	1.00E+00
81	1.39E-02	6.08E-05	9.56E-01	2.97E-02	-	-	-	1.00E+00
82	1.47E-02	6.03E-05	9.85E-01	-	-	-	-	1.00E+00
83	1.40E-02	6.11E-05	9.53E-01	3.32E-02	-	-	-	1.00E+00
84	1.22E-02	5.71E-05	9.87E-01	-	3.16E-04	-	-	1.00E+00
85	1.41E-02	6.09E-05	9.54E-01	3.15E-02	-	-	-	1.00E+00
86	1.35E-02	5.87E-05	9.86E-01	-	2.14E-04	-	-	1.00E+00
87	1.28E-02	5.85E-05	9.87E-01	-	2.31E-04	-	-	1.00E+00
88	1.35E-02	5.91E-05	9.86E-01	-	1.62E-04	-	-	1.00E+00
89	1.31E-02	6.11E-05	9.41E-01	4.55E-02	-	-	-	1.00E+00
90	1.12E-02	5.66E-05	9.88E-01	-	3.22E-04	-	-	1.00E+00
91	1.41E-02	6.07E-05	9.67E-01	1.91E-02	-	-	-	1.00E+00
92	1.47E-02	6.03E-05	9.85E-01	-	-	-	-	1.00E+00
93	1.44E-02	6.02E-05	9.86E-01	-	-	-	-	1.00E+00
94	1.43E-02	6.03E-05	9.86E-01	-	-	-	-	1.00E+00
95	1.21E-02	5.75E-05	9.88E-01	-	2.92E-04	-	-	1.00E+00
96	1.38E-02	6.10E-05	9.46E-01	3.99E-02	-	-	-	1.00E+00
97	1.23E-02	5.82E-05	9.87E-01	-	2.62E-04	-	-	1.00E+00
98	1.40E-02	6.09E-05	9.54E-01	3.20E-02	-	-	-	1.00E+00
99	1.42E-02	6.08E-05	9.62E-01	2.40E-02	-	-	-	1.00E+00
100	1.40E-02	6.11E-05	9.51E-01	3.52E-02	-	-	-	1.00E+00
101	1.37E-02	6.11E-05	9.44E-01	4.22E-02	-	-	-	1.00E+00
102	1.24E-02	6.14E-05	9.28E-01	5.53E-02	-	4.18E-03	-	1.00E+00
103	1.36E-02	5.90E-05	9.86E-01	-	2.04E-04	-	-	1.00E+00
104	1.43E-02	5.99E-05	9.86E-01	-	-	-	-	1.00E+00
105	1.15E-02	5.71E-05	9.88E-01	-	3.14E-04	-	-	1.00E+00

Run#	MNOH2	MGOH2	SRCO3	FEIIIOH3	ZRO2	NASGEL	ALOH3	sum
106	1.47E-02	6.04E-05	9.85E-01	-	-	-	-	1.00E+00
107	1.35E-02	6.12E-05	9.40E-01	4.61E-02	-	-	-	1.00E+00
108	1.36E-02	6.10E-05	9.41E-01	3.92E-02	-	5.76E-03	-	1.00E+00
109	1.49E-02	6.07E-05	9.73E-01	1.25E-02	-	-	-	1.00E+00
110	1.25E-02	6.14E-05	9.25E-01	5.52E-02	-	7.23E-03	-	1.00E+00
111	1.29E-02	6.13E-05	9.35E-01	5.09E-02	-	8.34E-04	-	1.00E+00
112	1.41E-02	6.00E-05	9.86E-01	-	-	-	-	1.00E+00
113	1.35E-02	5.91E-05	9.86E-01	-	1.54E-04	-	-	1.00E+00
114	1.37E-02	6.12E-05	9.43E-01	4.28E-02	-	-	-	1.00E+00
115	1.27E-02	5.85E-05	9.87E-01	-	2.41E-04	-	-	1.00E+00
116	1.42E-02	6.07E-05	9.68E-01	1.74E-02	-	-	-	1.00E+00
117	1.37E-02	5.99E-05	9.75E-01	-	7.35E-06	1.16E-02	-	1.00E+00
118	1.41E-02	6.10E-05	9.51E-01	3.50E-02	-	-	-	1.00E+00
119	1.15E-02	5.72E-05	9.88E-01	-	3.09E-04	-	-	1.00E+00
120	1.33E-02	5.97E-05	9.70E-01	-	1.41E-04	1.61E-02	-	1.00E+00
121	1.21E-02	6.14E-05	9.03E-01	4.86E-02	-	4.84E-03	3.11E-02	1.00E+00
122	1.13E-02	5.74E-05	9.88E-01	-	3.00E-04	-	-	1.00E+00
123	1.42E-02	6.05E-05	9.72E-01	4.21E-03	-	9.79E-03	-	1.00E+00
124	1.26E-02	5.78E-05	9.87E-01	-	2.86E-04	-	-	1.00E+00
125	1.25E-02	6.14E-05	9.09E-01	4.41E-02	-	2.48E-03	3.14E-02	1.00E+00
126	1.34E-02	5.96E-05	9.86E-01	-	4.94E-05	-	-	1.00E+00
127	1.33E-02	5.91E-05	9.86E-01	-	1.75E-04	-	-	1.00E+00
number of occurrences	115	115	115	54	51	17	8	

Mass fraction of total undissolved solids present in 1st ultra-filtration slurry. The last row lists the number of simulations for which the particular solid was present. The right-hand most column is a sum of the mass fractions as a check.

APPENDIX D. OLI PREDICTION OF HEAT CAPACITY FOR SIMPLE NAOH-H2O AND NANO3-H2O SYSTEMS

OLI/ESP prediction of Cp was consistently below the value measured experimentally of simulants. Simulations of simple binary systems were run and compared with data published in the "International Critical Tables"[34], Vol. 5, pp 115 and 125. These results indicate the OLI/ESP under-predicts the Cp by 2-4% for a 5M Na solution.

Figure 25. OLI/ESP Prediction of Cp Compared to Published Values for $NaNO_3$-H_2O System at 20°C and Various Concentrations

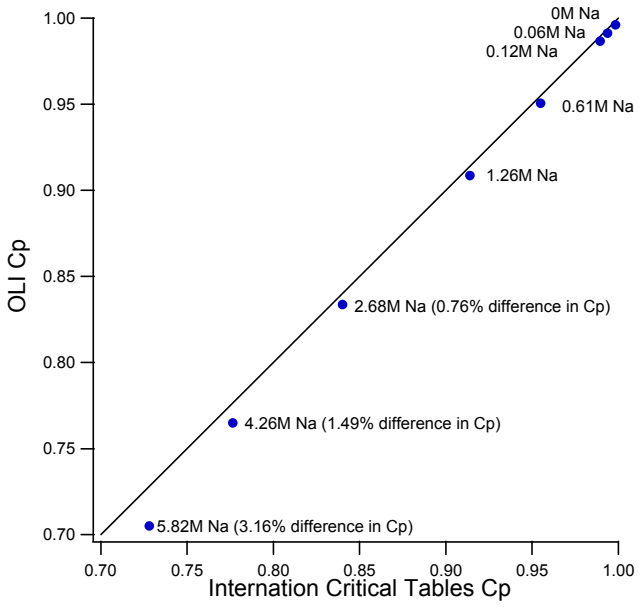
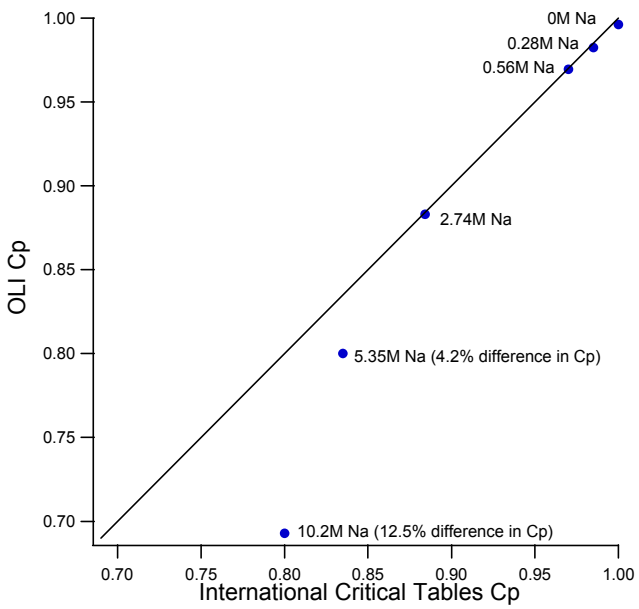


Figure 26. OLI/ESP Prediction of Cp Compared to Published Values for NaOH-H_2O System at 20°C and Various Concentrations



APPENDIX E. RESULTS OF TRIAL SIMULATIONS FOR WHICH THE NUMBER OF WASH STAGES WAS VARIED

The RPP pre-treatment flow-sheet calls for the concentrated slurry to be washed in 22 stages (for each wash step) with 0.01M NaOH. Simulating this many stages would take a tremendous amount of time with little comparative gain in the accuracy of the simulations. A series of trial simulations were run in which the number of wash stages was varied (1, 3, 5, 8, 10, 12, 15, 18, 20, and 22). The plots below show the results of selected streams as a function of the number of wash stages. The left axis of all the plots is the percent difference of the stream property at the given number of stages (x-axis) and the full 22 stages. Based on these trial simulations, 5 wash stages were used in simulation flow-sheet to approximate the 22 stages of the actual process.

Figure 27. UF1 Slurry

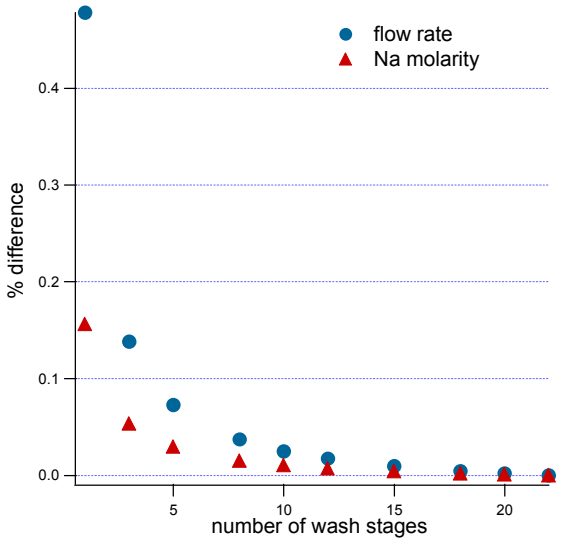


Figure 28. UF Recycle

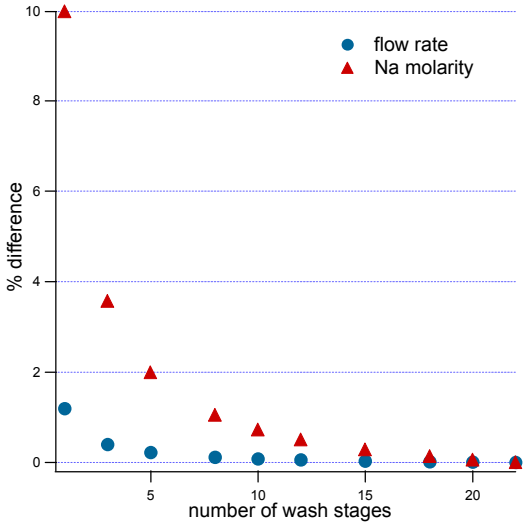


Figure 29. UF2 Slurry

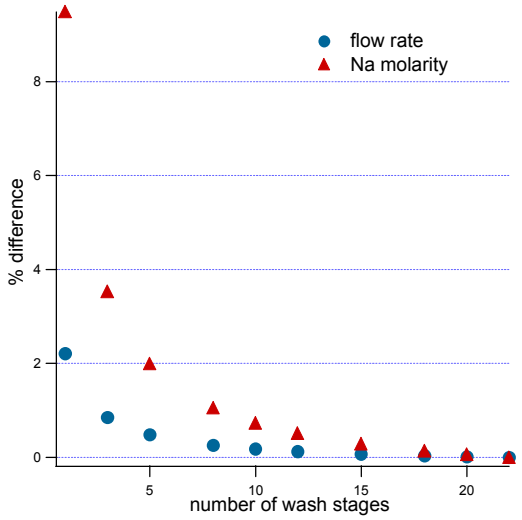


Figure 30. Slurry to HLW

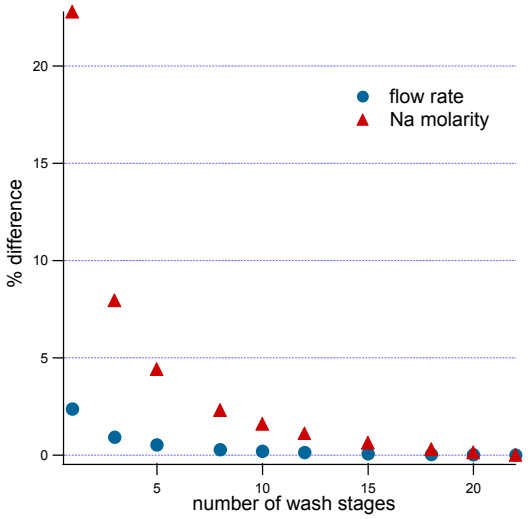


Figure 31. Evaporator Overhead