

Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

Disclaimer:

This work was prepared under an agreement with and funded by the U.S. Government. Neither the U. S. Government or its employees, nor any of its contractors, subcontractors or their employees, makes any express or implied:

- 1) warranty or assumes any legal liability for the accuracy, completeness, or for the use or results of such use of any information, product, or process disclosed; or
- 2) representation that such use or results of such use would not infringe privately owned rights; or
- 3) endorsement or recommendation of any specifically identified commercial product, process, or service.

Any views and opinions of authors expressed in this work do not necessarily state or reflect those of the United States Government, or its contractors, or subcontractors.

We put science to work.™



Savannah River
National Laboratory™

OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

A U.S. DEPARTMENT OF ENERGY NATIONAL LABORATORY • SAVANNAH RIVER SITE • AIKEN, SC

Evaluation of the Risk of Precipitating Aluminum in Hanford DFLAW Feed Compositions

J. A. Pike
A. Hayrabidian
M. E. Stone

September 25, 2018

SRNL-STI-2018-00446, Revision 0

SRNL.DOE.GOV

DISCLAIMER

This work was prepared under an agreement with and funded by the U.S. Government. Neither the U.S. Government or its employees, nor any of its contractors, subcontractors or their employees, makes any express or implied:

1. warranty or assumes any legal liability for the accuracy, completeness, or for the use or results of such use of any information, product, or process disclosed; or
2. representation that such use or results of such use would not infringe privately owned rights; or
3. endorsement or recommendation of any specifically identified commercial product, process, or service.

Any views and opinions of authors expressed in this work do not necessarily state or reflect those of the United States Government, or its contractors, or subcontractors.

Printed in the United States of America

**Prepared for
U.S. Department of Energy**

Keywords:

Retention: *Permanent*

Evaluation of the Risk of Precipitating Aluminum in Hanford DFLAW Feed Compositions

J. A. Pike
A. Hayrabedian
M. E. Stone

September 25, 2018



Prepared for the U.S. Department of Energy under contract number DE-AC09-08SR22470.

OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

REVIEWS AND APPROVALS

AUTHORS:

J. A. Pike, Environmental Modeling Date

A. Hayrabidian, Environmental Modeling Date

M. E. Stone, Waste Processing Technology Date

TECHNICAL REVIEWER:

D. J. McCabe, Waste Form Processing Technologies Date

APPROVALS:

D. A. Crowley, Date
Manager, Environmental Modeling

C. C. Herman, Date
Director, Waste Form Processing Technologies

EXECUTIVE SUMMARY

The Hanford Tank Operations Contractor (TOC), Washington River Protection Solutions (WRPS), developed the Tank Waste Disposition Integrated Flowsheet that defines process flowsheets during each phase of the Waste Treatment and Immobilization Plant transition to full operation.

The TOC requested Savannah River National Laboratory (SRNL) personnel to perform a review of gibbsite precipitation risks for the Low-Activity Waste Pretreatment System (LAWPS) and Tank Side Cesium Removal (TSCR) processes at Hanford during the Direct Feed Low-Activity Waste (DFLAW) operational phase of the Hanford Low-Activity Waste (LAW) Vitrification Facility.

The planned feed streams to the LAWPS and TSCR processes will consist of soluble tank waste at approximately 5.6 M total sodium concentration that will be filtered and then cesium will be removed via ion exchange using engineered crystalline silicotitanate (CST) media. This evaluation includes a comparison to previous evaluations and experience of functionally equivalent operating facilities at the Savannah River Site (SRS) which include the Actinide Removal Process (ARP) and Modular Caustic-Side Solvent Extraction (CSSX) Unit (MCU).

All 65 unique batch compositions are not likely to precipitate any gibbsite solids above 30°C and at atmospheric pressures. Below 30°C, the risk of precipitation increases significantly with the decrease in temperature for 57 of the 65 compositions such that the solutions may be supersaturated relative to gibbsite solubility by as much as 30% of the aluminum at 25°C. Supersaturation increases to as much as 47% of the aluminum at 20°C.

The risk of other solid precipitation is as significant as or more significant than the risk of gibbsite precipitation. Most notably sodium aluminosilicates and sodium oxalates are significant risks for all batches. For some batches, the risk of precipitating aluminum as sodium aluminosilicates is much greater than precipitating gibbsite. This risk cannot be readily mitigated with a higher free hydroxide concentration. These risks may be mitigated by either reformulating the batch or designing the process to tolerate the solids loading.

Simulation indicates that all 65 unique batch compositions are unlikely to precipitate any gibbsite solids above 30°C and at atmospheric pressures. Below 30°C, the risk of precipitation increases significantly with the decrease in temperature for 57 of the 65 compositions such that the solutions may be supersaturated relative to gibbsite solubility by as much as 30% of the aluminum at 25°C. Supersaturation increases to as much as 47% of the aluminum at 20°C.

Although the task request focused only on the risk of precipitating gibbsite, the risk of other solid precipitation is as significant as or more significant than the risk of gibbsite precipitation. Most notably sodium aluminosilicates and sodium oxalates are significant risks for all batches. For some batches, the risk of precipitating aluminum as sodium aluminosilicates is much greater than precipitating gibbsite. This risk cannot be readily mitigated with a higher free hydroxide concentration. These risks may be mitigated by either reformulating the batch or designing the process to tolerate the solids loading.

The simulation results show many other solids inconsistently identified to precipitate at very low concentrations. Most of these are at trace levels that may or may not be present in the real waste. However, a few batches show a significant amount of a precipitating fluoride-phosphate double salt, $\text{Na}_7\text{F}(\text{PO}_4)_2 \cdot 19\text{H}_2\text{O}$.

The Hanford simulated results are compared to operational history process and equivalent simulation work of ARP-MCU process at the SRS. The following items are conclusions related to specific questions from the TOC's task request:

1. Differences in Hanford and Savannah River Waste compositions that will result in different specific interactions between dissolved ions.

The composition of the calculated precipitates from simulating the DFLAW feed batches are compared to simulation and operating experience of the SRP-MCU process at SRS. Fundamentally, the feed solutions for both Hanford and SRS are formed from blends of waste that have been stored for decades as concentrated and precipitated electrolyte salts. The SRS batch preparation, at least in part, mitigates the risk of precipitating solids by evaluating blends and adjusting free hydroxide concentrations when viable to reduce risk of precipitating gibbsite, but other solids are not as readily mitigated. Allowing the process to reach low temperatures below 20°C resulted in precipitating sodium oxalate and sodium aluminosilicates and completely plugging the process. At other times, precipitated solids caused reduction in operational efficiency. The solids in ARP-MCU are predominately sodium oxalate and sodium aluminosilicates because most of the risk of gibbsite precipitation is mitigated by batch formulation and addition of sodium hydroxide to adjust the free hydroxide concentration. The DFLAW batches show risk of gibbsite as well as sodium oxalate and sodium aluminosilicates. Hanford wastes have a unique risk of precipitating a significant amount of a fluoride-phosphate double salt that is probably a result of the generally higher phosphate content of the Hanford waste and some batches with high fluoride content.

2. Difference in the impact of gibbsite precipitation on the two facilities.

Gibbsite precipitation is largely mitigated in the SRS process by batch planning preparation because the centrifugal contactors in the MCU can be plugged with high solids loading. Low loadings can pass through the contactors as demonstrated by the fact that the coalescer media has plugged occasionally. Ion exchange columns are sensitive to solids load as the media bed physically acts like a filter bed. In addition, precipitation on CST ion exchange media can cause formation of particle to particle bridging such that the media does not flow out of the column while liquid flow through the column is still viable. Some laboratory test work exists on compatibility of CST media with SRS waste; however, the work identified does not addresses the impact of solids loading on CST columns. It is noted that CST is a non-elutable resin which is replaced completely upon loading; therefore, processing issues caused by solids buildup must occur faster than loading of the column with cesium.

3. Differences in the relative cost impact of adding NaOH to stabilize gibbsite.

The typical batch requires about 70% increase in free hydroxide to mitigate the risk of gibbsite precipitation at 20°C. Each batch would need to be assessed as prepared and adjusted based on the actual composition. Such a large addition of sodium would result in a total increase of

about 15% of the sodium that would be vitrified as low-level waste based on the feed vector provided. At SRS, the primary impact of the sodium additions on cost is due to the increased volume from the sodium hydroxide additions. Since the volume increase in the batch is smaller than the increase in sodium concentrations, the increase in mission length is less. In addition, the cost of grouting the treated supernatant at SRS is much less than the cost of LAW vitrification at Hanford further reducing the cost impact of the hydroxide addition.

It should be noted that the Integrated Solubility Model may underpredict the amount of aluminum in the salt feed vector provided. Thus, the sodium addition could be higher than the 15% determined by this study.

4. Determine if ARP-MCU added acid at any location in their process that could have initiated gibbsite precipitation.

Oxalic acid is added during the ARP-MCU during acid cleaning of the crossflow filter where the spent acid is subsequently neutralized with concentrated sodium hydroxide before removal from ARP-MCU process tanks. Simulation of the process identified that significant amount of sodium oxalate will precipitate and transfer with the spent solution as well remain in the tank heel at the start of normal an operating cycle. Operating experience has realized the risk of precipitating sodium oxalate during a normal ARP-MCU process cycle as well as from increased risk during atypical low temperature excursions that occur during cold weather. No risk of gibbsite precipitation was identified as a result of adding oxalic acid during filter cleaning.

5. Determine if any of the ARP feeds that caused gibbsite precipitation issues originated from high temperature aluminum leaching processes.

High temperature (~90°C) aluminum dissolution was performed as a demonstration for sludge batch preparation in 1982. The leachate was processed through the evaporator system such that the aluminum was mixed with other salt waste that was indistinguishable from typical precipitated salt. Part of that salt waste has been processed through ARP-MCU as feed origin material from Tank 41 dissolved salt solution. The batch blend evaluation and chemical adjustments mitigated risk of precipitating aluminum during processing.

Low temperature (55-80°C) aluminum dissolution was performed during three sludge batch preparations. The leached aluminum has been stored with the intent of maintaining free hydroxide concentration to avoid reprecipitation. None of the leach solution has been processed. The general plan is to blend the waste into salt solution batches with low aluminum content to avoid reprecipitation such that as much of the aluminum as possible ultimately is processed into grout at the salt stone facility.

TABLE OF CONTENTS

EXECUTIVE SUMMARY	v
TABLE OF CONTENTS.....	viii
LIST OF TABLES.....	viii
LIST OF FIGURES	viii
LIST OF ABBREVIATIONS.....	ix
1.0 Introduction.....	1
2.0 Objective	1
3.0 Background	2
3.1 Origination of DFLAW Feed Stream	2
3.2 SRS Salt Batching Strategy	2
4.0 Approach.....	3
4.1 Component List.....	4
4.2 Reconciliation	7
4.3 Survey of Isothermal, Thermodynamic Equilibrium Determinations	7
4.4 Additional Considerations	8
5.0 Results.....	8
5.1 Calculated Precipitated Solids	8
5.2 Comparison of Results to SRS ARP-MCU Experience	12
5.3 Accuracy of the Simulated Results with Analytical Results	16
6.0 Conclusions.....	20
7.0 References.....	22
Appendix A : Initial Composition Vector.....	24
Appendix B : Calculated Gibbsite Precipitation for Each Composition.....	55
Appendix C : Calculated Quantities of Precipitates for Each Composition	67

LIST OF TABLES

Table 4-1: Stream Components and Equivalent Simulated Apparent OLI Components	5
Table 5-1: Simulation of LWHT at the End of ARP Batch 16, Compared with Analytical Results	17
Table 5-2: Simulation of LWPT at the End of Filter Cleaning and Adjustment, Compared with Analytical Results	18

LIST OF FIGURES

Figure 5-1: Gibbsite Equilibrium Isotherms for December 2021 Batch Composition.....	9
Figure 5-2: Projected Total Solids Formed for Each Batch by Mass and Volume.....	9
Figure 5-3: Bivariate Fit of $\text{Na}_7\text{F}(\text{PO}_4)_2 \cdot 19\text{H}_2\text{O}$ By Mass%	11
Figure 5-4: Simplified diagram of the 512-S portion of ARP	12
Figure 5-5: Predicted Solids Concentration in LWHT during One Complete ARP Cycle with Guard Filter Cleaning (Martino, Herman, Pike, & Peters, 2014)	15
Figure 5-6: Oxalate Solubility in Simple $\text{NaNO}_3\text{-NaOH}$ Simulated Waste.....	19
Figure 5-7: Oxalate Solubility in Simple NaNO_3 Simulated Waste	19

LIST OF ABBREVIATIONS

ARP	Actinide Removal Process
CSSX	Caustic-Side Solvent Extraction
CST	crystalline silicotitanate
DFLAW	Direct Feed Low-Activity Waste
HLW	High Level Waste
ISM	Integrated Solubility Model
LAW	Low-Activity Waste
LAWPS	Low-Activity Waste Pretreatment System
LWHT	the Late Wash Hold Tank
LWPT	Late Wash Pump Tank
MCU	Modular CSSX Unit
MST	Monosodium Titanate
PUREX	Plutonium Uranium Redox Extraction
RPP	River Protection Project
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
SWPF	Salt Waste Processing Facility
TCCR	Tank Closure Cesium Removal
TOC	Hanford Tank Operations Contractor
TSCR	Tank Side Cesium Removal
WRPS	Washington River Protection Solutions

1.0 Introduction

The Department of Energy (DOE) and predecessor produced and stored approximately 56 million gallons of radioactive and hazardous waste from the production of plutonium during the Second World War and Cold War at the DOE's Hanford site. The waste consists of slurries, precipitated salts and concentrated salt solutions that will be treated and immobilized into a form suitable for disposal as planned by the River Protection Project (RPP). The RPP plans include retrieval of the waste, separate it into high and low radioactive portions and vitrify both for disposal. The low radioactive portion will be dispositioned at Hanford in a near-surface, engineered repository. The high activity portion will be dispositioned in a federal geologic repository.

The Hanford Tank Operations Contractor (TOC), Washington River Protection Solutions (WRPS), developed the Tank Waste Disposition Integrated Flowsheet that defines process flowsheets during each phase of the Waste Treatment and Immobilization Plant transition to full operation.

The TOC requested Savannah River National Laboratory (SRNL) personnel to perform a review of gibbsite precipitation risks for the Low-Activity Waste Pretreatment System (LAWPS) and Tank Side Cesium Removal (TSCR) processes at Hanford during the Direct Feed Low-Activity Waste (DFLAW) operational phase of the Hanford Low-Activity Waste (LAW) Vitrification Facility.

The planned feed streams to the LAWPS and TSCR processes will consist of soluble tank waste at approximately 5.6 M total sodium concentration that will be filtered and then cesium will be removed via ion exchange using engineered crystalline silicotitanate (CST) media. This evaluation includes a comparison to previous evaluations and experience of functionally equivalent operating facilities at the Savannah River Site (SRS) which include the Actinide Removal Process (ARP) and Modular Caustic-Side Solvent Extraction (CSSX) Unit (MCU).

2.0 Objective

Evaluate the potential risk of gibbsite precipitation for the feed stream compositions provided by the TOC and compare the results to an equivalent evaluation of precipitation risks at Savannah River Sites ARP/MCU facility. The evaluation considered the following:

- Differences in Hanford and Savannah River Waste compositions that will result in different specific interactions between dissolved ions.
- Difference in the impact of gibbsite precipitation on the two facilities.
- Differences in the relative cost impact of adding NaOH to stabilize gibbsite.
- Determine if ARP-MCU added acid at any location in their process that could have initiated gibbsite precipitation.
- Determine if any of the ARP feeds that caused gibbsite precipitation issues originated from high temperature aluminum leaching processes.

3.0 Background

3.1 Origination of DFLAW Feed Stream

The material streams considered in this evaluation are provided by the TOC and are shown as received in Appendix A. These stream compositions represent the calculated compositions of the currently planned DFLAW feed stream from the material balance of the One System River Protection Project Integrated Flowsheet (Anderson, et al., 2017). The composition table contains monthly average composition of the filtered feed stream to the ion exchange process.

The DFLAW Feed Stream composition represents the feed to the ion exchange column after solids removal from the TOPSim model used for Hanford's River Protection Project System Plan (Bernards, et al., 2017). The system plan describes TOPSim as a software application developed using a Gensym G2™ platform that simulates the Hanford tank farms and processing plant operations. The simulation includes a chemistry model, the Integrated Solubility Model (ISM), that calculates the solubility of waste constituents at multiple points in the flowsheet and over a wider range of conditions. As such, the calculated composition in Appendix A represents the results of the ISM calculation for chemical equilibrium and removal of the solid phase from the stream.

3.2 SRS Salt Batching Strategy

The batching strategy focuses first on creating a batch that meets all downstream waste acceptance criteria constraints and then makes small adjustments for improving processability by minimizing the risk of unplanned solids precipitation.

SRS batching strategy has evolved with each successive salt solution batch and continues to evolve to make the batch qualification process more efficient while continuing to mitigate process risks. This description represents the process currently practiced before start of the Salt Waste Processing Facility (SWPF). After startup, the rate of generating salt batches will increase from roughly one per year to at least six per year. As such, the process will likely continue evolving to reduce the qualification cycle time.

The following outline describes the general qualification process along with a few important points for each step.

1. Develop a proposed salt batch blend.

Consists of dissolved salt solutions and concentrated supernatant from multiple tanks.

Recipe volumes based on operational transfer logistics as well as waste acceptance constraints.

Tank waste compositions based on both sample data and process knowledge.

TM Gensym, G2, and Gensym G2 are trademarks of Ignite Technologies, Austin, TX.

2. Evaluate proposed blend relative to all downstream waste acceptance criteria.
3. If acceptable, evaluate proposed blend for solids precipitation risk, otherwise start over.

OLI Systems software is used.

4. If significant solids are predicted to form, adjust chemistry to avoid solids

Adjust blend by changing recipe, including adding or removing tanks from the recipe.

Propose chemical addition, usually concentrated sodium hydroxide, to recipe.

Blends are proposed to minimize chemical additions but may not be optimal because of operational constraints.

5. Transfer blend recipe to the blend tank, currently Tank 21.

6. Add any adjustment chemicals identified in the recipe.

7. Sample blend tank composition for waste acceptance qualification.

8. Perform waste acceptance qualification evaluation.

Evaluation includes mixing with current feed tank heel and downstream process related effects such as dilution.

9. If not acceptable, develop mitigation plan/recipe to bring the salt batch into compliance.

This step has not been exercised yet because the initial evaluation steps have identified and mitigated any potential noncompliance before creating the salt batch.

10. If acceptable, evaluate proposed blend for solids precipitation risk.

OLI Systems software is used.

11. If significant solids are predicted to form, adjust chemistry to avoid solids.

Chemical addition is usually concentrated sodium hydroxide.

12. Transfer acceptable salt solution to salt process feed tank.

4.0 Approach

The feed stream composition provided by the TOC includes 264 individual stream compositions to evaluate which would take more time to evaluate than was available. The compositions provided by the TOC in terms of mole quantities with an associated total mass and volume. The monthly compositions are converted to molar concentrations by dividing the mole quantities by the total volume. Examination of the resulting concentrations reveals several compositions repeat consecutively, indicating several batch sizes greater than the expected monthly process rate. The monthly compositions are consolidated to monthly ranges such that 65 unique compositions in

terms of apparent molar concentration remained for analysis. For convenience, many of the identified components with zero content are eliminated from the listing.

The method to evaluate the precipitation risk is an adaptation of a method used to evaluate the risks in the ARP at SRS. The results of the evaluation may then be compared to the results of the ARP evaluation. However, the ARP evaluation evaluated the complete process cycle and relied on developing starting compositions from analytical data from various samples such that the feed stream is derived as the most probable composition, not a presumed composition or the direct analytical result of a specific sample. OLI StudioTM and OLI ESPTM were used to derive the feed stream composition and then simulate an entire process cycle. Analytical samples were available and compared to the simulation only for a couple of points near the end of the process cycle. The simulation proved an accurate composition match and clearly explained why solids were frequently found after the cross-flow filter unit operation (Martino, Herman, Pike, & Peters, 2014). The source of the stream composition for this evaluation is a calculated material balance, however, it is provided as ionic components with some additional stream characterization data. The ionic components suggest chemical compounds, but many of the components are not likely to exist as described in the solutions. For this evaluation, the provided compositions are treated as an apparent composition and a “true” composition is derived using the same techniques applied to analytical data.

The following sections describe the details of the methods used to evaluate the precipitation risk using electrolyte thermodynamic modeling. Each unique composition is examined using OLI StudioTM version 9.5.4 in three parts:

- parsing of component list,
- composition reconciliation, and
- survey of isothermal, thermodynamic equilibrium determinations.

4.1 Component List

The component vector of the stream compositions provided in Appendix A consists of 334 ionic components, which is intractable to run the simulations within time constraints for this evaluation. Many components have zero content and are parsed from the list. In addition, all the radionuclides are parsed from the list as most of the components are already accounted for in the chemical components or have such a low chemical concentration that will have negligible effect on the bulk chemistry and potential precipitation of aluminum compounds. This initial parsing of components results in 63 components as identified in Table 4-1.

Many metals in the component list are identified as cations but are very unlikely to exist in solution. Many form anions in the high pH solution. Using the cation as input to the simulation causes results in a simulated solution chemistry that does not closely resemble the bulk chemistry of the input streams because resulting calculated equilibrium resolves cation reactions to form the equilibrium anions. The objective is to achieve a simulated composition that would resemble the

TM OLI Analyzer is a trademark of OLI Systems, Inc., of Cedar Knolls, New Jersey.

TM OLI ESP is a trademark of OLI Systems, Inc., of Cedar Knolls, New Jersey.

Table 4-1: Stream Components and Equivalent Simulated Apparent OLI Components

Stream Component	Presumed OLI Species	Notes
	Neutral	
CrOOH	CrOOH	Negligible, not simulated
H ₂ O	H ₂ O	
Sb ⁺⁵	Sb(OH) ₅	Negligible, not simulated
Si ⁺⁴	Na ₂ SiO ₃	
Te ⁺⁶	Na ₂ TeO ₄	Negligible, not simulated
	Cations	
Ag ⁺¹	Ag ⁺¹	
Ba ⁺²	Ba ⁺²	
Be ⁺²	Be ⁺²	
Bi ⁺³	Bi ⁺³	
Ca ⁺²	Ca ⁺²	
Cd ⁺²	Cd ⁺²	
Co ⁺³	Co ⁺³	
Cs ⁺¹	Cs ⁺¹	
Cu ⁺²	Cu ⁺²	
Fe ⁺³	Fe ⁺³	
Hg ⁺²	Hg ⁺²	
K ⁺¹	K ⁺¹	
La ⁺³	La ⁺³	
Li ⁺¹	Li ⁺¹	
Mg ⁺²	Mg ⁺²	
Mn ⁺⁴	Mn ⁺²	
Na ⁺¹	Na ⁺¹	
Nd ⁺³	Nd ⁺³	
NH ₃	NH ₄ ⁺¹	Negligible, not simulated
Ni ⁺²	Ni ⁺²	
Pb ⁺²	Pb ⁺²	
Pd ⁺²	Pd ⁺²	
Pr ⁺³	Pr ⁺³	
Rb ⁺¹	Rb ⁺¹	
Rh ⁺³	Rh ⁺³	
Ru ⁺³	Ru ⁺³	
Sr ⁺²	Sr ⁺²	
Th ⁺⁴	Th ⁺⁴	
Ti ⁺⁴	Ti(H ₂ O) ₄ ⁺⁴	
Tl ⁺³	Tl ⁺³	
Y ⁺³	Y ⁺³	
Zr ⁺⁴	Zr ⁺⁴	

**Table 4-1: Stream Components and Equivalent Simulated Apparent OLI Components
(Continued)**

Stream Component	Presumed OLI Species	Notes
Anions		
Al(OH)_4^{-1}	Al(OH)_4^{-1}	
Al^{+3}	Al(OH)_4^{-1}	Negligible, not simulated
As^{+5}	AsO_4^{-3}	Negligible, not simulated
B^{+3}	B(OH)_4^{-1}	
$\text{C}_2\text{O}_4^{-2}$	$\text{C}_2\text{O}_4^{-2}$	
Ce^{+3}	Ce(OH)_4^{-1}	
Cl^{-1}	Cl^{-1}	
CN^{-1}	CN^{-1}	Negligible, not simulated
CO_3^{-2}	CO_3^{-2}	
CrO_4^{-2}	CrO_4^{-2}	
F^{-1}	F^{-1}	
HCOO^{-1}	HCOO^{-1}	
MnO_4^{-1}	MnO_4^{-1}	See note 1.
Mo^{+6}	MoO_4^{-2}	
NO_2^{-}	NO_2^{-1}	
NO_3^{-}	NO_3^{-1}	
OH^{-1}	OH^{-1}	Interpreted as free hydroxide
PO_4^{-3}	PO_4^{-3}	
Se^{+6}	SeO_4^{-2}	Negligible, not simulated
SO_4^{-2}	SO_4^{-2}	
Ta^{+5}	TaO_3^{-1}	Negligible, not simulated
V^{+5}	VO_4^{-3}	
W^{+6}	WO_4^{-2}	Negligible, not simulated
Zn^{+2}	ZnO_2^{-2}	

Note 1: MnO_4^- concentration is small, but inclusion affects amount of gibbsite precipitation greater than 1% because practically all the MnO_4^- is reduced to MnO_2 in the simulated results and alters the apparent free hydroxide concentration enough to affect the aluminum equilibrium solubility.

composition as if it was an analytical result from a sample. Some judgment is applied to the stream components to determine the most likely compatible ionic species. As such, the apparent components are converted to the equivalent OLI component for simulation input as identified in Table 4-1. All stream components are intended to be included in the simulation, but the calculation time increased exponentially such that the few thousand calculations needed to complete the evaluation would be intractable. A few components with very small concentrations and no practical effect on gibbsite precipitation are neglected.

4.2 Reconciliation

Reconciliation converts the apparent ionic compositions into input for the solubility calculations. The stream composition is characterized as ion concentrations with some additional stream characterization data that must be converted into a charge balanced composition of chemical compounds. The calculated stream composition is then used as input for calculating solubility isotherms as described in the next section. OLI Analyzer™ version 9.5.4 reconciliation function is used to develop this input composition.

The reconciliation function accepts ionic components, elemental components, and any compounds found in the databases. The user selects criteria to direct how the input is charge balanced. For these calculations, charge balance was achieved by allowing the sodium concentration to be automatically adjusted. This method of charge balance was chosen for three reasons. First, the method is consistent with the evaluation of SRS waste. Second, sodium is the most dominate ion such that the adjustment amounts to a small fraction of the total sodium. Third, adjusting the sodium concentration has the least effect, if any, on the quantity of calculated solids.

The output of the calculation provides the likely composition of the solution in terms of ionic species, e.g. true composition, as well as an equivalent chemical compound composition, e.g. apparent composition. The calculated apparent composition contains chemical forms that are the least hydrated and sometimes will appear arbitrary, but will be mass, charge, and oxidation state balanced. The software readily recreates the true composition from the apparent composition. Because the apparent composition list is substantially shorter than the true composition list, the calculated apparent composition is the input for all further calculations for each unique stream composition.

4.3 Survey of Isothermal, Thermodynamic Equilibrium Determinations

Several types of calculations may be performed using OLI Analyzer™. Each type calculates thermodynamic equilibrium conditions for the given inputs. An isothermal calculation restrains the conditions of the calculation to maintain temperature to a specified value and is used here. A survey of isothermal calculations where one variable is changed will trace an isotherm for that variable. By making a series of calculations over a range of temperatures, multiple isotherms will be traced. The survey calculation provides the information needed to evaluate the propensity or risk to form solid precipitates.

This evaluation is focused on gibbsite or aluminum precipitates, but the simulation estimates all solids species formed. Because the focus is on aluminum precipitates, the evaluation includes the characterization of all the precipitates above a de minimis concentration of 1E-10 mole per liter of total apparent composition and reports concentrations of the all precipitates 1E-5 mole per liter of total apparent composition as these components may influence the amount of calculated gibbsite precipitate by greater than 1%.

In addition to identifying formation of solid precipitates, OLI software calculates relative saturation as a scaling tendency. A scaling tendency value of 1.0 indicates saturation, values less than 1.0 indicate calculated equilibrium concentration relative to the calculated saturation concentration, and values above 1.0 would indicate a supersaturated concentration. However, the

calculated results are at equilibrium which means all calculated compositions are at or below saturation so none of the results include scaling tendencies above 1.0 unless the user identifies solids to exclude from the calculation.

For each unique composition, a survey relative to temperature and hydroxide ion concentration provides information to determine the relative risk to form solids as the temperature changes as well as provides information to evaluate the potential risk of solids formation based on variance of in-situ solution from the baseline values. Hydroxide was selected as the component most likely to affect solubility in this solution. Because sodium is used to reconcile charge balance, the NaOH concentration varies over a range such that the calculated free hydroxide varies 20% above and below the calculated component composition from the reconciliation calculation. The temperature ranged from 15 to 50 °C in 5 °C increments, which represents a nominal operating temperature range where the generated information could be used to determine a minimum operating temperature to minimize the risk of gibbsite solids formation.

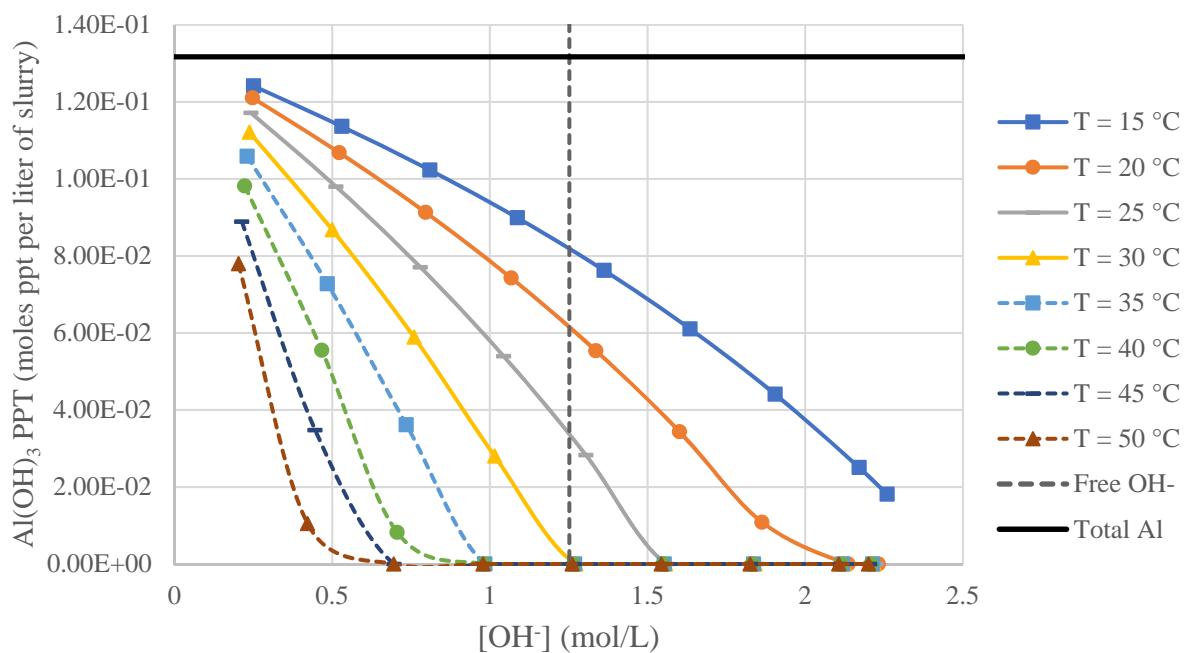
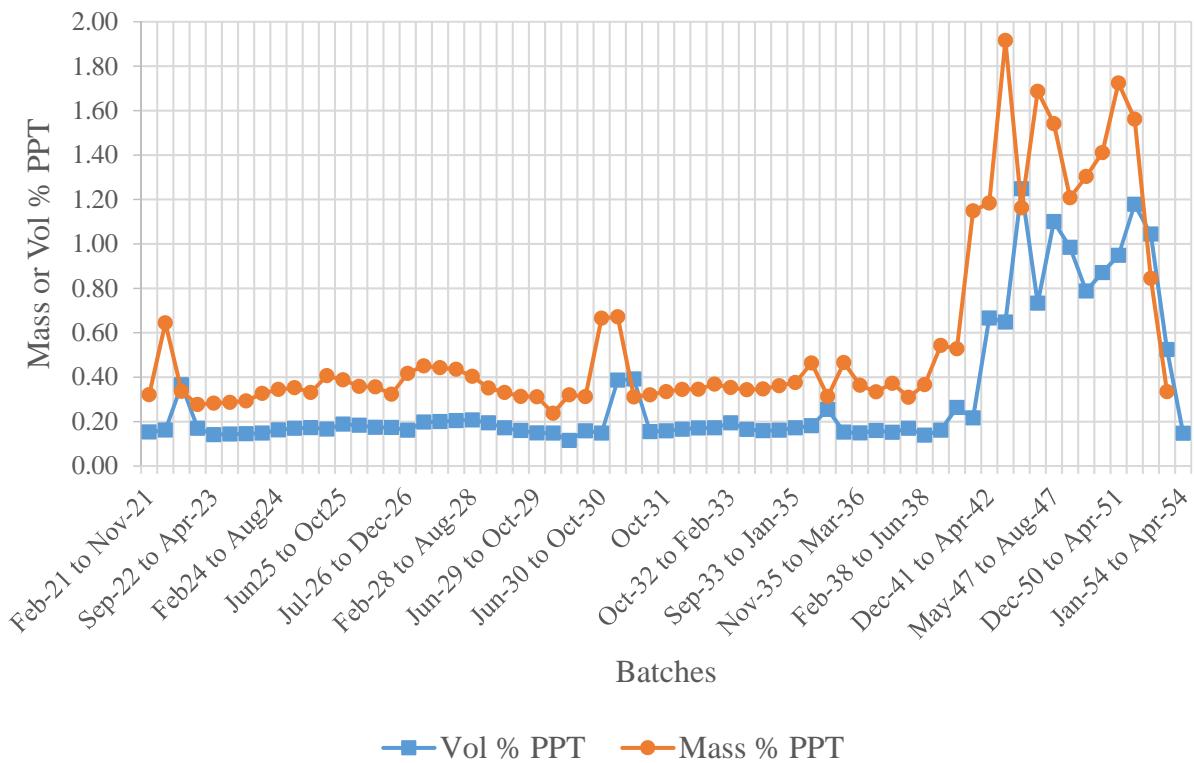
4.4 Additional Considerations

Earlier work indicated that all High Level Waste (HLW) calculations should include the public database for the Mixed Solvent Electrolyte (MSE) model/database with default redox chemistry active (Wilmarth, et al., 2013). The effect of active redox allows inclusion of reactions in the database that change oxidation state. Allowing default selection includes database reactions for the following metals for the inputs used in this analysis: Al, Bi, Cd, Cr, Co, Cu, Fe, Pb, Mn, Hg, Mo, Ni, Ag, Th, Ti, V, Zn, and Zr. However, activation of the redox chemistry slows the calculations substantially and would not allow completion of the survey calculations in a reasonable time. Test calculations showed that the redox chemistry has no practical effect on the gibbsite except for the compositions containing MnO_4^{-1} . Practically all the MnO_4^{-1} ions react to form MnO_2 which precipitates in the solid phase at equilibrium conditions, substantially increasing the total solids for several batches. Gibbsite precipitation is up to 4% lower at equilibrium when accounting for reduction of MnO_4^{-1} , most likely due to a small difference in the ionic strength at equilibrium. Since there is no effect on the results, all the surveys without MnO_4^{-1} were run without redox chemistry activated.

5.0 Results

5.1 Calculated Precipitated Solids

Appendix B contains graphical representations of the risk of gibbsite precipitation for each unique composition. Nearly every feed composition shows significant risk of precipitation below 30°C. Each graph in the appendix shows the amount of gibbsite calculated to form per liter of feed solution for a range of free hydroxide concentration around the feed stream concentration for isotherms every 5°C from 15 to 50°C. Figure 5-1 shows an example graph with an extended free hydroxide concentration range for the December 2021 batch composition. The precipitation trend is typical of nearly all the batches where the composition is approximately saturated in aluminum at 30°C. Colder operating conditions risk precipitating around ½ of the aluminum when dropping to ~20°C that can be mitigated with ~70% increase in the free hydroxide concentration, from 1.25 to 2.1 M in this case for a total of 15% increase in total sodium. These calculations suggest that the risk of gibbsite precipitation may be mitigated by either maintaining the solution temperature

**Figure 5-1: Gibbsite Equilibrium Isotherms for December 2021 Batch Composition****Figure 5-2: Projected Total Solids Formed for Each Batch by Mass and Volume**

through the ion exchange process at or above 30°C or increasing the free hydroxide concentration. The precise increase would depend on the minimum protected operating temperature. Since performance of CST decreases with increasing temperature, operating temperatures could become constrained to a very narrow range but quantifying the effect is beyond the scope of this report.

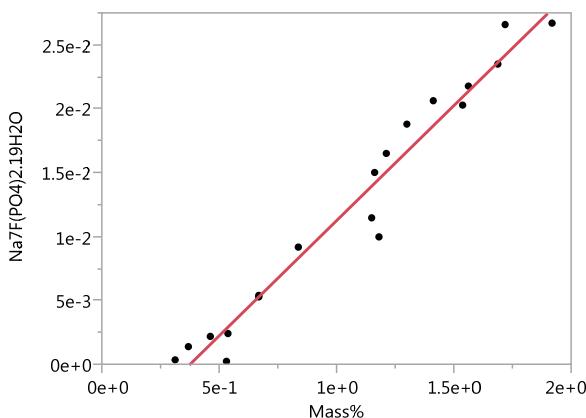
Generally, a 70% increase in free hydroxide minimizes the solids precipitation risk but the batch free hydroxide concentration varies from around 0.5 to 2.3 M such that the increase in total sodium will vary from batch to batch from about 6% to 27%. The average batch free hydroxide concentration is 1.08 M which suggests that the minimum increase in total sodium for the lifecycle could be somewhat less than 15%. A thorough evaluation to determine the minimum increase for every batch is needed to determine the total increase in sodium added to the life-cycle. 15% is a reasonable first-order estimate of the lifecycle increase if this mitigation strategy is pursued.

As noted, this type of calculation identifies all calculated precipitates as shown in Appendix C. Dominant precipitating solids include gibbsite, sodium oxalate, and sodium aluminosilicates. However, many very low and trace level solids are identified too. Little or no data is available to validate the propensity of forming these precipitates in waste solutions. Note that in some cases, practically all the identified metal ion in the input composition, such as copper, is predicted to precipitate. The complete list is provided for information.

Figure 5-2 shows the amount of total solids projected for each batch by mass and equivalent volume. Volume is calculated from the OLI software built-in physical property estimation methods for density. The calculated solids density is an estimate of crystalline density whereas bulk densities of a precipitate will tend to be at least 1/3 less dense when accounting for interstitial spaces between particles. Therefore, the solid slurry volume would be expected to be at least 50% larger than the calculated crystalline volumes.

The mass of precipitated solids has a step increase starting with the December-41 to April-42 batch. The feed compositions in Appendix A indicate a corresponding decrease in free hydroxide concentration from an approximate nominal 1.5 M to 0.5 M with total sodium remaining around 5.6 M but does not correlate with the increase in calculated precipitated mass. In fact, the risk of gibbsite precipitation decreases for many of the later batches and goes to zero for a few batches as indicated in Appendix B. Examination of the precipitated solids provides some indication of what might be causing the increase in precipitated mass. A statistical evaluation of the data shown in Appendix C reveals only one precipitating solid that shows high correlation with total mass and that is a fluoride-phosphate double salt (see Figure 5-3). Since these streams represent the planned feed stream to the ion exchange column, this salt represents a significant risk of plugging the column for the later batches. The risk of this double salt forming appears to correspond with an increase in fluoride concentration of an order of magnitude. Determining the source of the increase is beyond the scope of this report.

Section 3.1 indicates that the DFLAW feed stream composition in Appendix A is estimated by a method intended to produce compositions at or near equilibrium, thus, minimizing risk of precipitating significant solids. The methods used in this analysis reveals a consistent supersaturated condition for aluminum which could reflect a difference in the ISM and the OLI Analyzer MSE model. However, it could also reflect differences in the component parameter

**Linear Fit**

$$\text{Na}_7\text{F}(\text{PO}_4)_2.19\text{H}_2\text{O} = -0.006662 + 0.0180084 * \text{Mass\%}$$

where Na₇F(PO₄)₂.19H₂O is in kmoles.

Summary of Fit

RSquare	0.962493
RSquare Adj	0.960287
Root Mean Square Error	0.001847
Mean of Response	0.012512
Observations (or Sum Wgts)	19

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	0.00148844	0.001488	436.2511
Error	17	0.000005800	3.412e-6	Prob > F
C. Total	18	0.00154644	-	<0.0001*

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob> t
Intercept	-0.006662	0.001011	-6.59	<0.0001*
Mass%	0.0180084	0.000862	20.89	<0.0001*

Figure 5-3: Bivariate Fit of Na₇F(PO₄)₂.19H₂O By Mass%

database, the methods employed to ensure charge balance or lack thereof in the ISM inputs, lumped separation factors for some components considered non-impactive in the ISM model whereas all components are rigorously simulated in the OLI MSE model, or other differences not yet identified. By inspection, several components provided in Appendix A should not exist or exist at vanishingly small concentrations at equilibrium, suggestive that the compositions are not at equilibrium. For example, MnO₄⁻ is identified in significant amounts for some batches but is extremely unlikely. In some batches, Al⁺³ is identified simultaneously with Al(OH)₄⁻ where Al⁺³ is extremely unlikely although the amount of Al⁺³ is too small to make any difference to the results. Boron, molybdenum, vanadium, cerium, and zinc are identified as cationic species, but are much more likely aqueous anionic species. The cumulative effect of all components considered to have a low impact on mission metrics and converted to wash and leach factors in the TOPsim model and ISM may result in the differences observed in this evaluation. The OLI MSE model calculates concentrations for all possible species for a given input chemistry, but identification of possible species depends on the existence of the species in the database or a database extension. A chemical species that forms in the aqueous phase in Hanford waste that does not in SRS and is not in the OLI MSE database, but is accounted in the ISM model, would account for the consistent difference. Detailed examination of the ISM and TOPsim models are needed to discern the reasons for the significant difference in precipitation. The analysis methods used here have been applied successfully to identify supersaturated conditions in SRS salt waste processes and is discussed in Section 5.3.

5.2 Comparison of Results to SRS ARP-MCU Experience

Disposition paths to treat soluble salt waste at SRS include the ARP-MCU (currently operating), the SWPF (currently in startup testing), and Tank Closure Cesium Removal (TCCR – preparing for deployment and start up). The ARP-MCU process has operated for more than 5 years. ARP-MCU and the SWPF are based on the same process technology of reducing soluble actinide and strontium content of the waste by adsorption onto Monosodium Titanate (MST) and removal by filtration followed by cesium removal by solvent extraction. The ARP-MCU is small scale, interim operating facility providing early waste processing, freeing operating space in the tank farms before SWPF start up. TCCR process is also a portable, supplemental process based on cesium removal using Crystalline Silicotitanate media to sorb the cesium and then store the media for future disposition.

The ARP and the MCU have both had problems with unexpected solids forming and interfering with proper operation. In the ARP, the down-stream (dead-end) guard filter after the cross-flow filter (see Figure 5-4) has been plugged with solids. In addition, solids have been found in the Late Wash Hold Tank (LWHT) and Late Wash Pump Tank (LWPT); the LWHT feeds MCU.

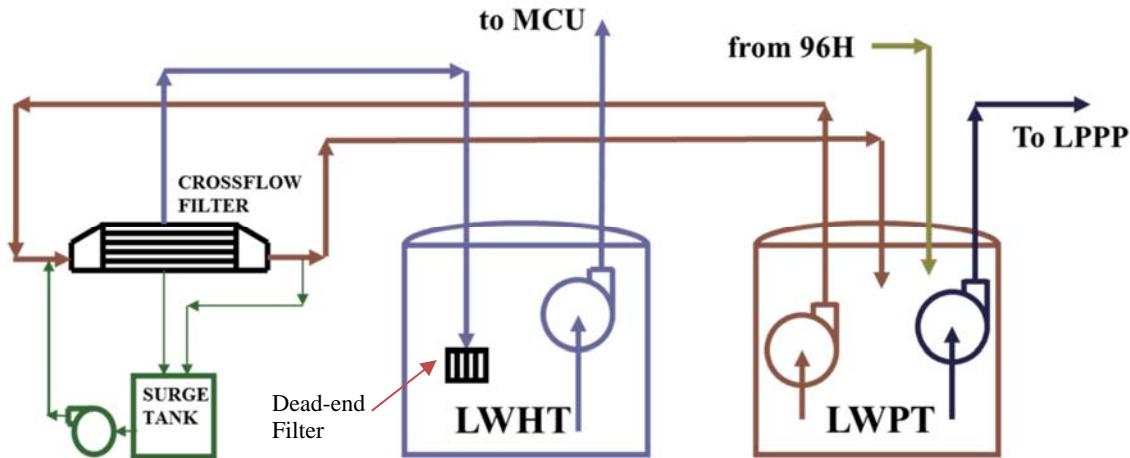


Figure 5-4: Simplified diagram of the 512-S portion of ARP

MCU has experienced unintended solids formation during start up where a poorly formulated chemical simulant caused significant amount of sodium aluminosilicates to form, plating process tank walls. The tanks were flushed to remove as much of the solids as possible before startup, but the plated solids remained, broke off into smaller pieces over time and caused some process issues. Solids have also formed after the ARP filters that then plugged the initial centrifugal contactor, causing complete process shut-down for recovery.

In 2013 and 2014, after plugging the LWHT dead-end filter several times and poor cross-flow filter performance, SRNL personnel along with Savannah River Remediation personnel performed extensive investigation of the performance and plugging problems (Wilmarth, et al., 2013) (Martino, Herman, Pike, & Peters, 2014). Guard filters removed from the LWHT and the coalescer media removed from the MCU contained qualitative evidence of aluminum (primarily as bayerite

or boehmite), sodium, silicon, and titanium, in oxide and/or hydroxide forms as well as aluminosilicate solids. Some solids were described as likely to be carbonate salts and MST (Peters, Fondeur, & Fink, 2010), (Peters, Fondeur, & Fink, 2011), (Peters, Fondeur, & Fink, 2012). The solids that plugged the MCU contactor were found to be predominately sodium oxalate solids which was not significant in the samples from the filter or coalescer media (Fondeur & Fink, 2012). The filter and coalescer media were flushed before removal to reduced radiation rates which would have also washed away any marginally soluble salts such as sodium oxalate. As such, sodium oxalate may have been present in those instances too, but not confirmed.

The SRNL study concluded the following about the process stream compositions:

1. Aluminum concentration was practically at saturation in the ARP feed stream and in ARP during filtering.

Due to a high concentration of soluble aluminum in the samples causing analytical interference, there was no direct evidence of precipitated aluminum compounds from sample analysis. OLI modeling showed that aluminum was practically at saturation in Tank 49 and in ARP during filtration. With minor fluctuations in temperature or hydroxide concentration, there was a risk of precipitating aluminum hydroxide (gibbsite) solids during processing.

2. Sodium oxalate was significantly supersaturated in the ARP feed stream and throughout the ARP.

The oxalates were significantly supersaturated in the ARP feed stream and throughout the ARP which presents a risk of precipitating sodium oxalate within ARP and in the downstream MCU process.

3. Silicon was supersaturated in the ARP feed stream relative to sodium aluminosilicate (cancrinite).

Silicon was present in the solids isolated from all LWPT samples. From these observations, a small quantity of sodium aluminosilicate solids was expected in the ARP strike tanks and the LWPT. OLI modeling showed that silicon was supersaturated in the ARP feed stream relative to sodium aluminosilicate (cancrinite).

The OLI simulation calculates saturation levels for a total of 3 relevant sodium aluminosilicates, two carbonate forms, $\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}\text{CO}_3 \cdot 1\text{H}_2\text{O}$, $\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}\text{CO}_3 \cdot 2\text{H}_2\text{O}$, and one hydroxide form, $\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}(\text{OH})_2 \cdot 2\text{H}_2\text{O}$. $\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}\text{CO}_3 \cdot 1\text{H}_2\text{O}$ was calculated to be above saturation in the ARP feed tank sample but was not determined in the other 512-S samples as there are no liquid phase concentration results for silicon above the detection limits in the other samples. Experience in the laboratory and in the HLW waste tanks demonstrate that the precipitation reaction requires temperatures approaching boiling for the reaction formation of these solids to occur quickly. Supersaturating conditions for sodium aluminosilicates have persisted for months at nominal waste tank temperatures; thus, it is reasonable to assume that the silicon in the feed remained

approximately at this concentration through filtration and feed to MCU as minimal dilution or heating occurs in this part of the process.

4. Measured iron, magnesium, and copper are well above saturation.

Iron is commonly found as a bulk component of sludge whereas magnesium and copper are commonly identified in sludge samples at low concentrations. Iron is a common steel component too. All three have very low solubility in the aqueous phase. A small amount of sludge is entrained with dissolved salt solution such that the aqueous phase is expected to be near or at saturation for any of these components but is difficult to verify if supersaturated analytically because the aqueous phase concentrations tend to be close to detection levels although iron is consistently found in aqueous phase analysis. Examination of the solids found in the MCU coalescer media (Fondeur & Fink, 2012) show presence of iron, magnesium and copper which suggests precipitation after the ARP filter. Because iron is commonly in the stainless steel, the source may also come from the process equipment. As precipitated compounds, they would be present in 1 to 10s of ppm. Centrifugal contactors in the MCU can pass a small quantity of fine solids with no noticeable process effect. The nature of the sintered metal filters allows a portion of fine particles to pass, especially when new or after an effective cleaning until a filter cake forms. Since the centrifugal contactors would allow micron and sub-micron particles to pass to the coalescer, the qualitative detection of these elements in the solids on the coalescer is not conclusive that the dissolved salt solution feed to ARP is precipitating compounds containing these elements after the ARP filters. The analytical result does support the simulated result that the feed solution is super saturated or includes suspended very fine particles.

A few subtle operational details were revealed by the process simulation. First, higher salt relative to hydroxide concentration in the LWPT sample suggests that mixing in the LWPT is not always homogeneous, or that the real volume of the heels relative to the batch size are larger than were input to the simulation. Simulated heel size was based on best estimate from operational tank level data but may have varied more than expected.

Second, a subtle revelation relates to the source of sodium oxalate solids found downstream of the cross-flow filter. At the end of a process cycle (40 batches in the simulated cycle), the accumulated solids in the LWPT undergo washing and are transferred out of the 512-S facility to the LPPP and subsequently to DWPF. The cross-flow filter is then cleaned with oxalic acid by first flushing the surge tank and then circulating 0.5 M oxalic acid through the filter using the surge tank. Spent filter cleaning material is transferred into the LWPT. The surge tank is flushed with dilute sodium hydroxide in an attempt to neutralize residual acid in the filter system, sending all the spent solutions to the LWPT. The accumulated spent solutions in the LWPT, neutralized by the sodium hydroxide content of the heel at the start of the cleaning cycle, are transferred to the LPPP. The LWPT is prepared for the next process cycle by adding a heel to the tank with a free hydroxide concentration about the same as the feed solution. The source of most of the sodium oxalate comes from the LWPT during solids washing, not because of filter cleaning as one may suspect. The apparent operational effect is as if the sodium oxalate solids passed through the cross-flow filter. The changes in solubility through the course of washing cause solids to pass through the cross-flow and guard filter as dissolved solids which then precipitate when mixed with the higher salt

contented in the LWHT. The material balance resulting from the steady-state simulation of the solids washing operation shows a substantial fraction of the precipitated solids in the LWPT transfer with the wash solution. Figure 5-5 shows the amount of solids predicted in the LWHT through an entire ARP cycle. At the start of the cycle, about 600 ppm precipitated sodium oxalate is progressively diluted and reduced with each successive batch. At the end of the guard filter cleaning, no solids are present at the time of the last transfer out of the tank, but form at the time of the last caustic addition that adjusts the hydroxide concentration back to operating levels. Figure 5-5 shows significant sodium oxalate solids are predicted to form at the caustic neutralization steps, step “lwht heel fw45” – “lwht heel fw47” on the x-axis. Sodium oxalate is predicted to precipitate to form 2.7 wt% solids slurry. Subsequent water flushing is expected to reduce the slurry to zero, but the final caustic addition causes additional solids formation. Secondary filter cleaning is no longer routinely performed. An extra rinse and transfer of the LWHT would eliminate the risk of sodium oxalate solids at the start of the cycle.

The simulation also predicts a very small amount of sodium aluminosilicate and iron oxide solids starting in batch 11 and continuing through batch 40.

The OLI public component database does not include MST so the study evaluated the change in solubility of titanium based on the calculated composition. Small amounts of titanium oxide solids were predicted to form with the sodium oxalate solids.

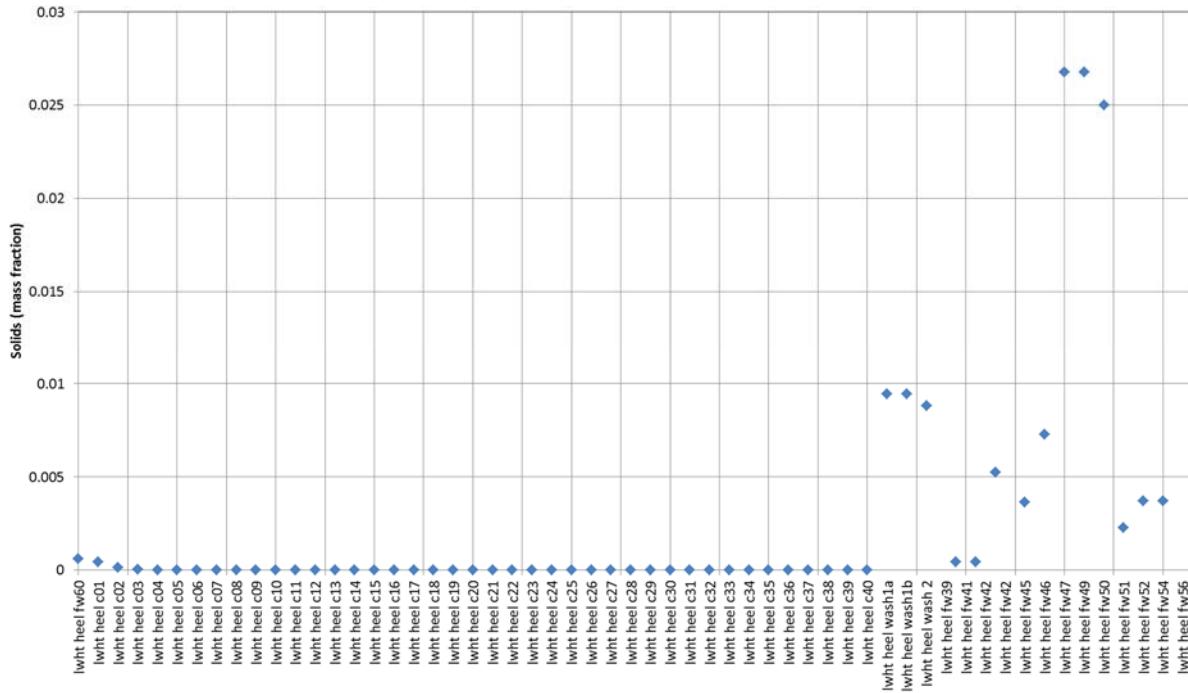


Figure 5-5: Predicted Solids Concentration in LWHT during One Complete ARP Cycle with Guard Filter Cleaning (Martino, Herman, Pike, & Peters, 2014)

This evaluation only considered the DFLAW feed stream compositions and did not trace the consequences through an entire process cycle, so the risk of precipitation related to all the changes to chemistry throughout the process could not be compared. The primary risk associated the DFLAW feed stream is related to gibbsite formation and not sodium oxalate as is the case for SRS feed stream. Only one SRS feed batch was evaluated at high level of detail because the qualifying steps of preparing a feed batch incorporate solids evaluation and mitigation actions. Consequently, the conditions and types of solids formed in SRS facilities is dominantly solids other than gibbsite, most notably sodium oxalate and sodium aluminosilicates.

Regardless, the results of the DFLAW evaluation suggest that there is a significant risk of precipitation of gibbsite throughout the downstream process. Most of the feed batches will be near or above the calculated saturation level, small fluctuation in temperature and composition may initiate precipitation analogous to the problems with sodium oxalate in the ARP-MCU.

It is worth noting that all batches present a risk of sodium oxalate and sodium aluminosilicate precipitation and generally at a lower mass concentration than the predicted gibbsite precipitate.

5.3 Accuracy of the Simulated Results with Analytical Results

Few simulations of high level waste processing have any analytical data much less adequate data to validate simulation results. This section will discuss two instances where analytical data was compared to OLI simulations where the simulation was believed to capture the real conditions. A simulation performed with idealized, simplified, or non-verifiable conditions is not considered an accurate representation of operating conditions for validation purposes.

The extensive evaluation of the ARP flowsheet discussed in the previous section included a comparison to analytical data. The simulation started with an estimate of the feed as a composite of several analytical results from the feed tank to determine a best estimate. Only a few downstream analytical results were available for comparison. Data was from samples only after several ARP batches into a process cycle and at the end of the cycle. The first analytical result shown in Table 5-1 is a comparison demonstrating relative accuracy after 96 simulation steps representing 32 successive equilibrium calculations and 16 ARP batches. The simulation matches very well with the analytical data except for oxalate where the sample is more than 2½ times the simulation estimate. This stream is practically identical for batch 5 to the end of the cycle and represents the feed composition to MCU from ARP.

**Table 5-1: Simulation of LWHT at the End of ARP Batch 16,
Compared with Analytical Results**
(Martino, Herman, Pike, & Peters, 2014)

Stream	LWHT heel c16		LWHT
Phase	Liquid	Solid	sample
Units	M	mass frac.	M
OH^{-1}	2.27E+00		2.23E+00
NO_3^{-1}	2.61E+00		2.57E+00
NO_2^{-1}	5.68E-01		6.10E-01
CO_3^{2-}	2.89E-01		2.84E-01
SO_4^{2-}	6.91E-02		6.57E-02
$\text{C}_2\text{O}_4^{2-}$	4.36E-04		1.17E-03
PO_4^{3-}	4.34E-03		2.49E-03
HCOO^{-1}	7.65E-03		< 1.16E-02
Cl^{-1}	3.00E-03		< 1.47E-02
Al(OH)_4^{-1}	1.91E-01		1.98E-01
Na^{+1}	6.44E+00		6.57E+00
Fe_2O_3		0.001	
$\text{Na}_2\text{C}_2\text{O}_4$		0.796	
$\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}\text{CO}_3 \cdot 1\text{H}_2\text{O}$		0.203	
Mass fraction solids in total stream	1.03E-10		

The second analytical result shown in Table 5-2 is a comparison demonstrating relative accuracy after 289 simulation steps representing 109 successive equilibrium calculations and a complete ARP process cycle. Compared with sample the analytical results from LWPT, the simulation of the post filter cleaning and pH adjustment solution shows the same total sodium, but 33% higher concentration of hydroxide and about 1/5th the concentration of other salt components except for carbonate which is about 1/12th. The simulation assumes perfect mixing and exact heels. The higher salt relative to hydroxide concentration in the actual (LWPT-3) sample suggests that mixing in the tank is not always homogeneous, or that the volume of the heels relative to the batch size are actually larger than simulated. One might also consider the relative ratio of anions to nitrate because nitrate does not appear in any of the precipitates or added to the process other than the feed; thus, nitrate can be treated as an inert component from the feed. The relative ratios compare reasonably well although oxalate is again notably higher in the sample data than the simulation result.

Earlier work identified that OLI consistently underestimates the solubility of sodium oxalate in mixed electrolyte solutions with chemistry consistent with soluble high-level waste (Pike, Badheka, & Ketusky, 2004). The second evaluation was performed as part of developing an integrated process flowsheet that evaluated all downstream effects associated with a method of tank heel or residual cleaning. The evaluation compared simulated solution solubility to three different

**Table 5-2: Simulation of LWPT at the End of Filter Cleaning and Adjustment,
Compared with Analytical Results**
(Martino, Herman, Pike, & Peters, 2014)

Stream	LWPT heel fw34				LWPT-3 sample
	Phase	Liquid	Solid	Ratio to NO ₃ ⁻¹	
		Units	M	mass fraction	
OH ⁻¹		2.26E+00		89.0	1.70E+00
NO ₃ ⁻¹		2.54E-02		1.00	1.25E-01
NO ₂ ⁻¹		5.55E-03		0.219	2.90E-02
CO ₃ ⁻²		4.05E-03		0.159	4.90E-02
SO ₄ ⁻²		6.74E-04		0.0265	3.30E-03
C ₂ O ₄ ⁻²		1.12E-02		0.441	3.34E-02
PO ₄ ⁻³		4.24E-05		0.00167	<5.47E-04
HCOO ⁻¹		7.47E-05		0.00294	<1.15E-02
Cl ⁻¹		2.93E-05		0.00115	<1.47E-02
Al(OH) ₄ ⁻¹		1.05E-02		0.413	<9.07E-03
Na ⁺¹		2.35E+00			2.24E+00
CuO			0.033		
Fe ₂ O ₃			0.011		
Na ₂ C ₂ O ₄			0.478		
Na ₈ Al ₆ Si ₆ O ₂₄ CO ₃ ·1H ₂ O			0.159		
MST			0.319		
Mass fraction solids in total stream		0.0067		~ 0.0007	

laboratory solubility tests for solubility in simulated waste solution by three different experimentalists from 1978, 1980, and 1984 (Wiley, 1978), (Fowler, 1980), (Kilpatrick, 1984). Again, the measured solubility was consistently higher by up to a factor of 2 in the multiple component system (see Figure 5-6 and Figure 5-7) whereas the simulation of the single component of sodium oxalate in water was very good. The discrepancy was resolved by applying an empirical correlation, Kilpatrick's equation 3, with total sodium concentration that provides a good fit to all the available multicomponent data at the time.

The evaluations discussed in this section focused only on accuracy of the simulation concentrations in the aqueous phase and did not verify accuracy of simulated solids compositions. Analytical data would need to identifying chemical species and concentration of the solid phase. Only qualitative data was available from the analytical data to support that the solids are consistent with the simulation results from all the ARP samples. No analytical data was gathered regarding the solids in the sodium oxalate solubility tests. Sodium oxalate was added in excess of solubility and the observable solids were presumed to be sodium oxalate, i.e., no verification if any other species formed.

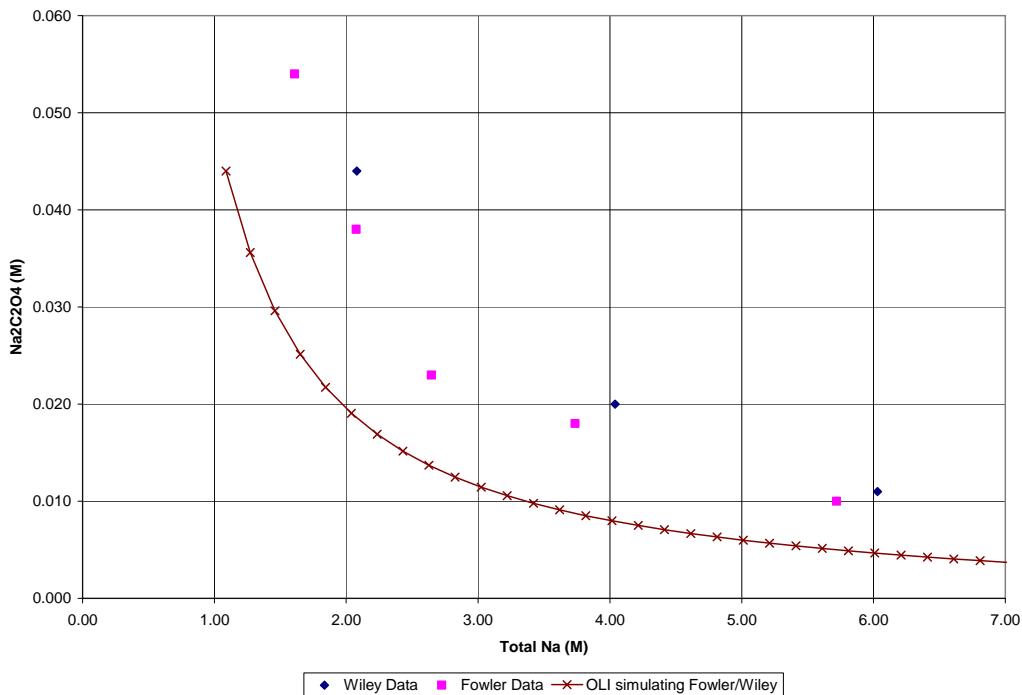


Figure 5-6: Oxalate Solubility in Simple NaNO₃-NaOH Simulated Waste

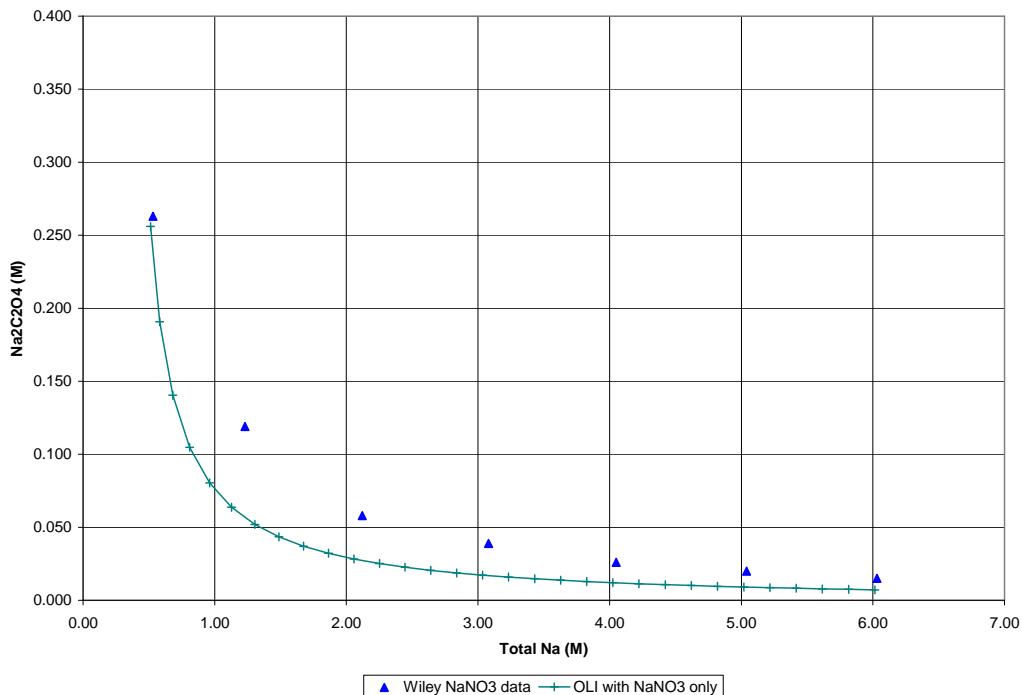


Figure 5-7: Oxalate Solubility in Simple NaNO₃ Simulated Waste

6.0 Conclusions

Simulation indicates that all 65 unique batch compositions are unlikely to precipitate any gibbsite solids above 30°C and at atmospheric pressures. Below 30°C, the risk of precipitation increases significantly with the decrease in temperature for 57 of the 65 compositions such that the solutions may be supersaturated relative to gibbsite solubility by as much as 30% of the aluminum at 25°C. Supersaturation increases to as much as 47% of the aluminum at 20°C.

Although the task request focused only on the risk of precipitating gibbsite, the risk of other solid precipitation is as significant as or more significant than the risk of gibbsite precipitation. Most notably sodium aluminosilicates and sodium oxalates are significant risks for all batches. For some batches, the risk of precipitating aluminum as sodium aluminosilicates is much greater than precipitating gibbsite. This risk cannot be readily mitigated with a higher free hydroxide concentration. These risks may be mitigated by either reformulating the batch or designing the process to tolerate the solids loading.

The simulation results show many other solids inconsistently identified to precipitate at very low concentrations. Most of these are at trace levels that may or may not be present in the real waste. However, a few batches show a significant amount of a precipitating fluoride-phosphate double salt, $\text{Na}_7\text{F}(\text{PO}_4)_2 \cdot 19\text{H}_2\text{O}$.

The Hanford simulated results are compared to operational history process and equivalent simulation work of ARP-MCU process at the SRS. The following items are conclusions related to specific questions from the TOC's task request:

1. Differences in Hanford and Savannah River Waste compositions that will result in different specific interactions between dissolved ions.

The composition of the calculated precipitates from simulating the DFLAW feed batches are compared to simulation and operating experience of the SRP-MCU process at SRS. Fundamentally, the feed solutions for both Hanford and SRS are formed from blends of waste that have been stored for decades as concentrated and precipitated electrolyte salts. The SRS batch preparation, at least in part, mitigates the risk of precipitating solids by evaluating blends and adjusting free hydroxide concentrations when viable to reduce risk of precipitating gibbsite, but other solids are not as readily mitigated. Allowing the process to reach low temperatures below 20°C resulted in precipitating sodium oxalate and sodium aluminosilicates and completely plugging the process. At other times, precipitated solids caused reduction in operational efficiency. The solids in ARP-MCU are predominately sodium oxalate and sodium aluminosilicates because most of the risk of gibbsite precipitation is mitigated by batch formulation and addition of sodium hydroxide to adjust the free hydroxide concentration. The DFLAW batches show risk of gibbsite as well as sodium oxalate and sodium aluminosilicates. Hanford wastes have a unique risk of precipitating a significant amount of a fluoride-phosphate double salt that is probably a result of the generally higher phosphate content of the Hanford waste and some batches with high fluoride content.

2. Difference in the impact of gibbsite precipitation on the two facilities.

Gibbsite precipitation is largely mitigated in the SRS process by batch planning preparation because the centrifugal contactors in the MCU can be plugged with high solids loading. Low loadings can pass through the contactors as demonstrated by the fact that the coalescer media has plugged occasionally. Ion exchange columns are sensitive to solids load as the media bed physically acts like a filter bed. In addition, precipitation on CST ion exchange media can cause formation of particle to particle bridging such that the media does not flow out of the column while liquid flow through the column is still viable. Some laboratory test work exists on compatibility of CST media with SRS waste; however, the work identified does not addresses the impact of solids loading on CST columns. It is noted that CST is a non-elutable resin which is replaced completely upon loading; therefore, processing issues caused by solids buildup must occur faster than loading of the column with cesium.

3. Differences in the relative cost impact of adding NaOH to stabilize gibbsite.

The typical batch requires about 70% increase in free hydroxide to mitigate the risk of gibbsite precipitation at 20°C. Each batch would need to be assessed as prepared and adjusted based on the actual composition. Such a large addition of sodium would result in a total increase of about 15% of the sodium that would be vitrified as low-level waste based on the feed vector provided. At SRS, the primary impact of the sodium additions on cost is due to the increased volume from the sodium hydroxide additions. Since the volume increase in the batch is smaller than the increase in sodium concentrations, the increase in mission length is less. In addition, the cost of grouting the treated supernatant at SRS is much less than the cost of LAW vitrification at Hanford further reducing the cost impact of the hydroxide addition.

It should be noted that the Integrated Solubility Model may underpredict the amount of aluminum in the salt feed vector provided. Thus, the sodium addition could be higher than the 15% determined by this study.

4. Determine if ARP-MCU added acid at any location in their process that could have initiated gibbsite precipitation.

Oxalic acid is added during the ARP-MCU during acid cleaning of the crossflow filter where the spent acid is subsequently neutralized with concentrated sodium hydroxide before removal from ARP-MCU process tanks. Simulation of the process identified that significant amount of sodium oxalate will precipitate and transfer with the spent solution as well remain in the tank heel at the start of normal an operating cycle. Operating experience has realized the risk of precipitating sodium oxalate during a normal ARP-MCU process cycle as well as from increased risk during atypical low temperature excursions that occur during cold weather. No risk of gibbsite precipitation was identified as a result of adding oxalic acid during filter cleaning.

5. Determine if any of the ARP feeds that caused gibbsite precipitation issues originated from high temperature aluminum leaching processes.

High temperature (~90°C) aluminum dissolution was performed as a demonstration for sludge batch preparation in 1982. The leachate was processed through the evaporator system such that the aluminum was mixed with other salt waste that was indistinguishable from typical precipitated salt. Part of that salt waste has been processed through ARP-MCU as feed origin

material from Tank 41 dissolved salt solution. The batch blend evaluation and chemical adjustments mitigated risk of precipitating aluminum during processing.

Low temperature (55-80°C) aluminum dissolution was performed during three sludge batch preparations. The leached aluminum has been stored with the intent of maintaining free hydroxide concentration to avoid reprecipitation. None of the leach solution has been processed. The general plan is to blend the waste into salt solution batches with low aluminum content to avoid reprecipitation such that as much of the aluminum as possible ultimately is processed into grout at the salt stone facility.

7.0 References

- Anderson, K. A., Britton, M. D., Colby, J. M., Cree, L. H., Fountain, M. S., Nelson, D. W., . . . Stone, M. E. (2017). *One System River Protection Project Integrated Flowsheet*. Richland, Washington: Washington River Protection Solutions, LLC., RPP-RPT-57991, Rev. 2, 24590-WTP-RPT-MGT-14-023, Rev. 2, September 2017.
- Bernards, J. K., Hohl, T. M., Jasper, R. T., Orcutt, S. L., Reaksecker, S. D., Smalley, C. S., . . . Wells, M. N. (2017). *River Protection Project System Plan*. Richland, Washington: Washington River Protection Solutions, LLC., ORP-11242, Rev. 8 , October 2017.
- Fondeur, F. F., & Fink, S. D. (2012). *Identification and Characterization of the Solids found in Extraction Contactor SEP-401 in June 2012*. Aiken, SC: Savannah River National Laboratory, SRNL-STI-2012-00595, Rev. 0, June 2012.
- Fowler, J. R. (1980). *Effect of Temperature on Sodium Oxalate Solubility*. Aiken, SC: DPST-80-265, February 22, 1980.
- Kilpatrick, L. L. (1984). *Solubiity of Sodium Oxalate and Sodium Tetraphenylborate in DWPF Supernate*. Aiken, SC: DPST-84-341, February 28, 1984.
- Martino, C., Herman, D., Pike, J., & Peters, T. (2014). *Actinide Removal Process Sample Analysis, Chemical Modeling, and Filtration Evaluation*. Aiken, SC: Savanah River National Laboratory., SRNL-STI-2013-00700, Rev. 0, June 2014.
- Peters, T. B., Fondeur, F. F., & Fink, S. D. (2010). *Results from Analysis of Actinide Removal Process Guard Filter*. Aiken, SC: Savannah River National Laboratory, SRNL-STI-2009-00456 Rev. 1, January 27, 2010.
- Peters, T. B., Fondeur, F. F., & Fink, S. D. (2011). *Results from Analysis of the First and Second Strip Effluent Coalescer Elements from the Radioactive Operations of the Modular Caustic-Side Solvent Extraction Unit*. Aiken, SC: Savannah River National Laboratory, SRNL-STI-2010-00088, Rev. 0, June 2011.
- Peters, T. B., Fondeur, F. F., & Fink, S. D. (2012). *Results of Analyses of Macrobatch 3 Decontaminated Salt Solution (DSS) Coalscer and Pre-filters*. Aiken, SC: Savannah River National Laboratory, SRNL-STI-2011-00513, Rev. 0, June 2012.

Pike, J. A., Badheka, N. P., & Ketusky, E. T. (2004). *Flowsheet for SRS Waste Tank Heel Removal Using Oxalic Acid*. Aiken, SC: Westinghouse Savannah River Company, WSRC-TR-2004-00317, Rev. 0, November 3, 2004.

Wiley, J. R. (1978). *Sodium Oxalate Solubility in Simulated SRP Waste Solutions*. Aiken, SC: DPST-78-480, August 23, 1978.

Wilmarth, W. R., Bush, S. R., Campbell, S. E., Harmon, H. D., Hobbs, D. T., Jain, V., . . . Taylor-Pashow, K. M. (2013). *Salt Integrated Project Chemistry Team Report*. Aiken, SC: Savannah River National Laboratory, SRNL-STI-2013-00354/SRR-STI-2013-00375, Rev. 0, June 2013.

Appendix A: Initial Composition Vector

This appendix contains the specific feed compositions provided as input to this evaluation.

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Liquid Volume (kgal)	Solid Volume (kgal)	Total Volume (kgal)	Liquid Mass (kg)	Solid Mass (kg)	Total Mass (kg)	106-Ru Liquid (kMoles)	113m-Cd Liquid (kMoles)	113m-Cd Solid (kMoles)	125-Sb Liquid (kMoles)	126-Sn Liquid (kMoles)	126-Sn Solid (kMoles)	129-I Liquid (kMoles)	134-Cs Liquid (kMoles)	137-Cs Liquid (kMoles)	137-Cs Solid (kMoles)	137m-Ba Liquid (kMoles)	137m-Ba Solid (kMoles)	14-C Liquid (kMoles)	14-C Solid (kMoles)	151-Sm Liquid (kMoles)	151-Sm Solid (kMoles)	152-Eu Liquid (kMoles)	152-Eu Solid (kMoles)	154-Eu Liquid (kMoles)	154-Eu Solid (kMoles)	155-Eu Liquid (kMoles)	155-Eu Solid (kMoles)	226-Ra Liquid (kMoles)	226-Ra Solid (kMoles)	227-Ac Liquid (kMoles)				
Feb-21	67.1	00:00.0	67.1	3.224E+05	0	3.224E+05	2.17E-14	0	9.65E-08	0	1.88E-09	00:00.0	00:10.5	0	0.001467835	0	1.57E-10	0	0.003232538	0	4.92E-10	0	5.56E-06	0	0.000239594	0	5.00E-09	0	2.32E-08	0	5.85E-09	0	6.12E-11	0	1.71E-11
Mar-21	108.7	00:00.0	108.7	5.219E+05	0	5.219E+05	3.52E-14	0	1.56E-07	0	3.04E-09	00:00.0	00:17.0	0	0.002376539	0	2.54E-10	0	0.005233733	0	7.97E-10	0	9.00E-06	0	0.000387921	0	8.09E-09	0	3.75E-08	0	9.47E-09	0	9.92E-11	0	2.76E-11
May-21	4.7	00:00.0	4.7	2.257E+04	0	2.257E+04	1.52E-15	0	6.76E-09	0	1.32E-10	00:00.0	8.51E-06	0	0.000102763	0	1.10E-11	0	0.000226309	0	3.45E-11	0	3.89E-07	0	1.68E-05	0	3.50E-10	0	1.62E-09	0	4.10E-10	0	1.19E-12		
Jun-21	174.2	00:00.0	174.2	8.365E+05	0	8.365E+05	5.64E-14	0	2.50E-07	0	4.88E-09	00:00.0	00:27.2	0	0.00380882	0	4.07E-10	0	0.008387972	0	1.28E-09	0	1.44E-05	0	0.000621711	0	1.30E-08	0	6.02E-08	0	1.52E-08	0	1.59E-10	0	4.43E-11
Jul-21	82.0	00:00.0	82.0	3.940E+05	0	3.940E+05	2.65E-14	0	1.18E-07	0	2.30E-09	00:00.0	00:12.8	0	0.001793884	0	1.92E-10	0	0.003950581	0	6.02E-10	0	6.79E-06	0	0.000292814	0	6.10E-09	0	2.83E-08	0	7.49E-11	0	2.09E-11		
Aug-21	104.8	00:00.0	104.8	5.033E+05	0	5.033E+05	3.39E-14	0	1.51E-07	0	2.93E-09	00:00.0	00:16.4	0	0.00229157	0	2.45E-10	0	0.005046609	0	7.69E-10	0	8.68E-06	0	0.000374051	0	7.80E-09	0	3.62E-08	0	9.13E-09	0	2.66E-11		
Sep-21	180.5	00:00.0	180.5	8.669E+05	0	8.669E+05	5.84E-14	0	2.59E-07	0	5.05E-09	00:00.0	00:28.2	0	0.003947137	0	4.22E-10	0	0.008692581	0	1.32E-09	0	1.49E-05	0	0.000644288	0	1.34E-08	0	6.24E-08	0	1.57E-08	0	1.65E-10	0	4.59E-11
Oct-21	102.7	00:00.0	102.7	4.930E+05	0	4.930E+05	3.32E-14	0	1.48E-07	0	2.87E-09	00:00.0	00:16.1	0	0.002446664	0	2.40E-10	0	0.004943311	0	7.53E-10	0	8.50E-06	0	0.000363935	0	7.64E-09	0	3.55E-08	0	8.95E-09	0	9.37E-11	0	2.61E-11
Nov-21	77.9	00:00.0	77.9	3.739E+05	0	3.739E+05	2.52E-14	0	1.12E-07	0	2.18E-09	00:00.0	00:12.2	0	0.001702472	0	1.82E-10	0	0.003749269	0	5.71E-10	0	6.45E-06	0	0.000277893	0	5.79E-09	0	2.69E-08	0	6.78E-09	0	7.10E-11	0	1.98E-11
Dec-21	153.7	00:00.0	153.7	7.396E+05	0	7.396E+05	3.65E-14	0	2.10E-07	0	3.24E-09	00:00.0	00:18.4	0	0.003746366	0	2.65E-10	0	0.006950979	0	1.06E-09	0	1.07E-05	0	0.000528645	0	1.05E-08	0	6.42E-08	0	1.40E-08	0	1.36E-10	0	3.96E-11
Jan-22	82.1	00:00.0	82.1	3.964E+05	0	3.964E+05	2.78E-15	0	9.57E-08	0	4.74E-10	00:00.0	4.37E-05	0	0.002407935	0	3.03E-11	0	0.003159777	0	4.81E-10	0	5.63E-06	0	0.00025906	0	4.39E-09	0	4.25E-08	0	6.98E-09	0	6.85E-11	0	2.22E-11
Feb-22	193.2	00:00.0	193.2	9.323E+05	0	9.323E+05	6.55E-15	0	2.25E-07	0	1.11E-09	00:00.0	00:08.9	0	0.00566391	0	7.12E-11	0	0.007432382	0	1.13E-09	0	8.54E-06	0	0.000609358	0	1.03E-08	0	1.64E-08	0	1.61E-10	0	5.22E-11		
Mar-22	97.8	00:00.0	97.8	4.719E+05	0	4.719E+05	3.31E-15	0	1.14E-07	0	5.64E-10	00:00.0	5.20E-05	0	0.002866977	0	3.60E-11	0	0.003762148	0	5.73E-10	0	4.33E-06	0	0.000308447	0	5.23E-09	0	5.06E-08	0	8.31E-09	0	8.16E-11	0	2.64E-11
Apr-22	128.1	00:00.0	128.1	6.184E+05	0	6.184E+05	4.34E-15	0	1.49E-07	0	7.39E-10	00:00.0	6.82E-05	0	0.00375132	0	4.72E-11	0	0.004930241	0	7.51E-10	0	5.67E-06	0	4.04E-04	0	6.85E-09	0	1.09E-08	0	1.07E-10	0	3.46E-11		
May-22	177.7	00:00.0	177.7	8.575E+05	0	8.575E+05	6.02E-15	0	2.07E-07	0	1.02E-09	00:00.0	9.45E-05	0	0.00520959	0	6.55E-11	0	0.006836207	0	1.04E-09	0	7.86E-06	0	0.000560479	0	9.50E-09	0	9.20E-08	0	1.51E-08	0	1.48E-10	0	4.80E-11
Jun-22	74.5	00:00.0	74.5	3.595E+05	0	3.595E+05	2.52E-15	0	8.68E-08	0	4.30E-10	00:00.0	3.96E-05	0	0.002184041	0	2.74E-11	0	0.002865975	0	4.37E-10	0	3.29E-06	0	0.000234972	0	3.98E-09	0	3.86E-08	0	6.33E-09	0	6.21E-11	0	2.01E-11
Jul-22	129.8	00:00.0	129.8	6.266E+05	0	6.266E+05	4.40E-15	0	1.51E-07	0	7.49E-10	00:00.0	6.919E-05	0	0.003807647	0	4.78E-11	0	0.004995346	0	7.61E-10	0	6.94E-09	0	6.72E-08	0	1.10E-08	0	1.08E-08	0	3.51E-11				
Aug-22	68.3	00:00.0	68.3	3.298E+05	0	3.298E+05	2.58E-15	0	8.03E-08	0	4.27E-10	00:00.0	3.69E-05	0	0.002031386	0	2.80E-11	0	0.002687259	0	4.09E-10	0	3.19E-06	0	0.000217153	0	3.72E-09	0	5.73E-09	0	1.91E-11				
Sep-22	136.6	00:00.0	136.6	6.674E+05																															

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	227-Ac Solid (kMoles)	228-Ra Liquid (kMoles)	228-Ra Solid (kMoles)	229-Th Liquid (kMoles)	229-Th Solid (kMoles)	231-Pa Liquid (kMoles)	231-Pa Solid (kMoles)	232-Th Liquid (kMoles)	232-U Liquid (kMoles)	232-U Solid (kMoles)	233-U Liquid (kMoles)	234-U Liquid (kMoles)	235-U Liquid (kMoles)	236-U Liquid (kMoles)	236-U Solid (kMoles)	237-Np Liquid (kMoles)	237-Np Solid (kMoles)	238-Pu Liquid (kMoles)	238-Pu Solid (kMoles)	238-U Liquid (kMoles)	238-U Solid (kMoles)	239-Pu Liquid (kMoles)	240-Pu Liquid (kMoles)	240-Pu Solid (kMoles)	241-Am Liquid (kMoles)	241-Am Solid (kMoles)	241-Pu Liquid (kMoles)	241-Pu Solid (kMoles)					
Feb-21	0	1.02E-11	0	5.80E-09	0	4.68E-08	0	0.024879434	0	7.20E-11	0	4.50E-06	0	0.000141237	0	4.56E-06	0	0.000149165	0	4.95E-09	0	0.019943326	0	1.09E-05	0	6.41E-07	0	4.09E-07	0	1.03E-08	0		
Mar-21	0	1.66E-11	0	9.40E-09	0	7.58E-08	0	0.040281755	0	1.17E-10	0	7.29E-06	0	2.51E-06	0	0.000228674	0	7.39E-06	0	0.000241509	0	8.02E-09	0	0.03228981	0	1.76E-05	0	1.04E-06	0	6.62E-07	0	1.67E-08	0
May-21	0	7.17E-13	0	4.06E-10	0	3.28E-09	0	0.001741802	0	5.04E-12	0	3.15E-07	0	1.09E-07	0	9.89E-06	0	3.19E-07	0	1.04E-05	0	3.47E-10	0	0.001396226	0	7.61E-07	0	4.49E-08	0	2.86E-08	0	7.20E-10	0
Jun-21	0	2.66E-11	0	1.51E-08	0	1.21E-07	0	0.06455855	0	1.87E-10	0	1.17E-05	0	4.03E-06	0	0.000366489	0	1.18E-05	0	0.000387061	0	1.29E-08	0	0.0051750062	0	2.82E-05	0	1.66E-06	0	1.06E-06	0	2.67E-08	0
Jul-21	0	1.25E-11	0	7.09E-09	0	5.72E-08	0	0.03040589	0	8.80E-11	0	5.50E-06	0	1.90E-06	0	0.00017261	0	5.57E-06	0	0.000182298	0	6.06E-09	0	0.024373328	0	1.33E-05	0	7.83E-07	0	5.00E-07	0	1.26E-08	0
Aug-21	0	1.60E-11	0	9.06E-09	0	7.31E-08	0	0.038841541	0	1.12E-10	0	7.02E-06	0	2.42E-06	0	0.000220498	0	7.12E-06	0	0.000232874	0	7.74E-09	0	0.031135336	0	1.70E-05	0	1.00E-06	0	6.39E-07	0	1.61E-08	0
Sep-21	0	2.75E-11	0	1.56E-08	0	1.26E-07	0	0.066902991	0	1.94E-10	0	1.21E-05	0	4.17E-06	0	0.000379798	0	1.23E-05	0	0.000401117	0	1.33E-08	0	0.053629363	0	2.92E-05	0	1.72E-06	0	1.10E-06	0	2.77E-08	0
Oct-21	0	1.57E-11	0	8.88E-09	0	7.16E-08	0	0.038464505	0	1.10E-10	0	6.88E-06	0	2.37E-06	0	0.000215984	0	6.98E-06	0	0.000228108	0	7.58E-09	0	0.030498036	0	1.66E-05	0	9.80E-07	0	6.26E-07	0	1.57E-08	0
Nov-21	0	1.19E-11	0	6.73E-09	0	5.43E-08	0	0.028856485	0	8.35E-11	0	5.22E-06	0	1.80E-06	0	0.000163814	0	5.29E-06	0	1.73E-04	0	5.75E-09	0	0.023131326	0	1.26E-05	0	7.44E-07	0	4.74E-07	0	1.19E-08	0
Dec-21	0	1.62E-11	0	1.41E-08	0	1.06E-07	0	0.039276595	0	1.44E-10	0	7.45E-06	0	2.80E-06	0	0.000261035	0	8.23E-06	0	2.42E-04	0	9.75E-09	0	0.036850363	0	2.06E-05	0	1.21E-06	0	7.29E-07	0	1.86E-08	0
Jan-22	0	9.19E-13	0	8.41E-09	0	5.60E-08	0	0.002237539	0	5.40E-11	0	9.51E-07	0	7.03E-07	0	5.73E-05	0	2.05E-06	0	2.41E-05	0	3.49E-09	0	0.010339562	0	6.41E-06	0	3.73E-07	0	1.69E-07	0	4.49E-09	0
Feb-22	0	2.16E-12	0	1.98E-08	0	1.32E-07	0	0.005263108	0	1.27E-10	0	2.24E-06	0	1.65E-06	0	0.000172474	0	4.82E-06	0	5.67E-05	0	8.22E-09	0	0.024320573	0	1.51E-05	0	8.78E-07	0	3.97E-07	0	1.06E-08	0
Mar-22	0	1.09E-12	0	1.00E-08	0	6.67E-08	0	0.02664098	0	6.43E-11	0	1.13E-06	0	8.37E-07	0	2.44E-06	0	2.87E-05	0	4.16E-09	0	0.012310668	0	7.63E-06	0	4.44E-07	0	2.01E-07	0	5.35E-09	0		
Apr-22	0	1.43E-12	0	1.31E-08	0	8.74E-08	0	0.03491262	0	8.42E-11	0	1.48E-06	0	1.10E-06	0	1.14E-04	0	3.76E-05	0	5.45E-09	0	0.016132956	0	1.00E-05	0	5.82E-07	0	2.63E-07	0	7.01E-09	0		
May-22	0	1.99E-12	0	1.82E-08	0	1.21E-07	0	0.004840957	0	1.17E-10	0	2.06E-06	0	1.52E-06	0	0.00015864	0	4.43E-06	0	5.21E-05	0	7.56E-09	0	0.022369742	0	1.39E-05	0	8.08E-07	0	3.65E-07	0	9.72E-09	0
Jun-22	0	8.34E-13	0	7.63E-09	0	5.08E-08	0	0.02029489	0	4.90E-11	0	8.62E-07	0	6.65E-05	0	1.86E-06	0	2.19E-05	0	3.17E-09	0	0.009378171	0	5.81E-06	0	3.39E-07	0	1.53E-07	0	4.08E-09	0		
Jul-22	0	1.45E-12	0	1.33E-08	0	8.85E-08	0	0.03537365	0	8.53E-11	0	1.50E-06	0	1.11E-06	0	3.24E-06	0	3.81E-05	0	5.52E-09	0	0.016345994	0	1.01E-05	0	5.90E-07	0	2.67E-07	0	7.10E-09	0		
Aug-22	0	7.03E-13	0	6.79E-09	0	4.88E-08	0	0.001710853	0	4.38E-11	0	7.91E-07	0	6.14E-07	0	1.83E-06	0	2.34E-05	0	2.85E-09	0	0.00888053	0	5.28E-06	0	3.07E-07	0	3.85E-09	0				
Sep-22	0	1.05E-13	0	9.27E-09	0	1.45E-07	0	0.000255866	0	6.53E-11	0	1.61E-06	0	1.76E-04	0	1.18E-04	0	4.65E-09	0	9.52E-06	0	5.56E-07	0	1.53E-07	0	1.02E-08	0						
Oct-22	0	6.31E-14	0	5.57E-09	0	8.72E-08	0	0.000153722	0	3.92E-11	0	9.67E-07	0	1.12E-06	0	0.000105662	0	3.90E-06	0	2.80E-09	0	0.014331406	0	5.72E-06	0	3.34E-07	0	9.17E-08	0	6.12E-09	0		
Nov-22	0	1.06E-13	0	9.32E-09	0	1.46E-07	0	0.000257287	0	6.56E-11	0	1.62E-06	0	1.87E-06	0	0.000176848	0	6.53E															

Initial Composition Vector (continued)

Appendix A: Initial Composition Vector (continued)

4. Initial Composition Vector (continued)

Transfer Date Range	CdO Solid (kMoles)	Ce+3 Liquid (kMoles)	Ce+3 Solid (kMoles)	Ce2O3 Liquid (kMoles)	Ce2O3 Solid (kMoles)	CH2Cl2 Liquid (kMoles)	CH2Cl2 Solid (kMoles)	CHCl3 Liquid (kMoles)	CHCl3 Solid (kMoles)	CHO2- Solid (kMoles)	Cl- Liquid (kMoles)	CN- Solid (kMoles)	CN- Liquid (kMoles)	Co+3 Solid (kMoles)	Co+3 Liquid (kMoles)	CO3-2 Liquid (kMoles)	CO3-2 Solid (kMoles)	CoO Liquid (kMoles)	CoO Solid (kMoles)	Cr2O3 Liquid (kMoles)	Cr2O3 Solid (kMoles)	CrO4-2 Liquid (kMoles)	CrO4-2 Solid (kMoles)	CrOOH Liquid (kMoles)	CrOOH Solid (kMoles)	Cs+ Liquid (kMoles)	Cs+ Solid (kMoles)	Cs2O Liquid (kMoles)	Cs2O Solid (kMoles)	Cu+2 Liquid (kMoles)	Cu+2 Solid (kMoles)	CuO Liquid (kMoles)	CuO Solid (kMoles)									
Feb-21	0	0	0	0	0	0	0	0	0	0	19.0209706	0	0	0	0	139.1986348	0	0	0	0	0	2.562372547	0	0	0	0.017286597	0	0	0	0	0	0	0	0	0	0						
Mar-21	0	0	0	0	0	0	0	0	0	0	0	30.79644411	0	0	0	0	225.3735135	0	0	0	0	0	4.148682241	0	0	0	0.027988357	0	0	0	0	0	0	0	0	0	0					
May-21	0	0	0	0	0	0	0	0	0	0	0	1.331652437	0	0	0	0	9.745254596	0	0	0	0	0	0.179390932	0	0	0	0.001210229	0	0	0	0	0	0	0	0	0	0					
Jun-21	0	0	0	0	0	0	0	0	0	0	0	49.3566815	0	0	0	0	361.2004259	0	0	0	0	0	6.648988024	0	0	0	0.044856232	0	0	0	0	0	0	0	0	0	0					
Jul-21	0	0	0	0	0	0	0	0	0	0	0	23.24608986	0	0	0	0	170.1187621	0	0	0	0	0	3.131551158	0	0	0	0.021126461	0	0	0	0	0	0	0	0	0	0					
Aug-21	0	0	0	0	0	0	0	0	0	0	0	29.69536291	0	0	0	0	217.3156178	0	0	0	0	0	4.000352259	0	0	0	0.026987675	0	0	0	0	0	0	0	0	0	0					
Sep-21	0	0	0	0	0	0	0	0	0	0	0	51.14906714	0	0	0	0	374.3174029	0	0	0	0	0	6.8904572	0	0	0	0.046485184	0	0	0	0	0	0	0	0	0	0					
Oct-21	0	0	0	0	0	0	0	0	0	0	0	29.08753763	0	0	0	0	212.867451	0	0	0	0	0	3.918470275	0	0	0	0.026435273	0	0	0	0	0	0	0	0	0	0					
Nov-21	0	0	0	0	0	0	0	0	0	0	0	22.06152951	0	0	0	0	161.4499519	0	0	0	0	0	2.971975445	0	0	0	0.020049911	0	0	0	0	0	0	0	0	0	0					
Dec-21	0	0.020955118	0	0	0	0	0	0	0	0	0	49.03116363	0	0	0	0	293.3745999	0	0	0	0	0	5.162668327	0	0.000268676	0	0.037171647	0	0	0	0	0.007695989	0	0	0	0	0	0	0	0	0	0
Jan-22	0	0.033371567	0	0	0	0	0	0	0	0	0	31.973291	0	0	0	0	129.7684058	0	0	0	0	0	2.010109772	0	0.000427874	0	0.017291521	0	0	0	0	0.012261794	0	0	0	0	0	0	0	0	0	0
Feb-22	0	0.078496132	0	0	0	0	0	0	0	0	0	75.20815735	0	0	0	0	305.239425	0	0	0	0	0	4.728152498	0	0.001006439	0	0.040672874	0	0	0	0	0.02884202	0	0	0	0	0	0	0	0	0	0
Mar-22	0	0.039733432	0	0	0	0	0	0	0	0	0	38.0691138	0	0	0	0	154.5071016	0	0	0	0	0	2.393311867	0	0.000509443	0	0.02058793	0	0	0	0	0.014599349	0	0	0	0	0	0	0	0	0	0
Apr-22	0	0.052070097	0	0	0	0	0	0	0	0	0	49.88903179	0	0	0	0	202.4793575	0	0	0	0	0	3.136401137	0	0.000667618	0	0.026980189	0	0	0	0	0.019132239	0	0	0	0	0	0	0	0	0	0
May-22	0	0.072199704	0	0	0	0	0	0	0	0	0	69.17546806	0	0	0	0	280.7551846	0	0	0	0	0	4.34889211	0	0.00092571	0	0.037410372	0	0	0	0	0.026528508	0	0	0	0	0	0	0	0	0	0
Jun-22	0	0.030268618	0	0	0	0	0	0	0	0	0	29.00007532	0	0	0	0	117.7023018	0	0	0	0	0	1.823206265	0	0.00038809	0	0.015683724	0	0	0	0	0.0112167	0	0	0	0	0	0	0	0	0	0
Jul-22	0	0.052757692	0	0	0	0	0	0	0	0	0	50.54782563	0	0	0	0	205.1531349	0	0	0	0	0	3.177817895	0	0.000676434	0	0.027336468	0	0	0	0	0.019384884	0	0	0	0	0	0	0	0	0	0
Aug-22	0	0.025598311	0	0	0	0	0	0	0	0	0	26.29800746	0	0	0	0	109.5738502	0	0	0	0	0	1.775978271	0	0.000328209	0	0.014705724	0	0	0	0	0.009405648	0	0	0	0	0	0	0	0	0	0
Sep-22	0	0.005722425	0	0	0	0	0	0	0	0	0	46.69589335	0	0	0	0	255.5956975	0	0	0	0	0	5.789214062	0	0.036502609	0	0	0	0	0.002102604	0	0	0	0	0	0	0	0	0	0		
Oct-22	0	0.003437989	0	0	0	0	0	0	0	0	0	28.05453536	0	0	0	0	153.5599291	0	0	0	0	0	3.47811528	0	0.041E-05	0	0.021930487	0	0	0	0	0.001263228	0	0	0	0	0	0	0	0	0	0
Nov-22	0	0.005754209	0	0	0	0	0	0	0	0	0	46.9552523	0	0	0	0	257.0153305	0	0	0	0	0	5.821368591	0	0.738E-05	0	0.036705352	0	0	0	0	0.002114283	0	0	0	0	0	0	0	0	0	0
Dec-22	0	0.007065444	0	0	0	0	0	0	0	0	0	57.65513363	0	0	0	0	308.00807886	0	0.906E-05	0	0	0	7.147907158	0	0.045695648	0	0	0	0	0.02596073	0	0	0	0	0	0	0	0	0	0		
Jan-23	0	0.003436726	0	0	0	0	0	0	0	0	0	28.04422913	0	0	0	0	153.5035265	0	0	0	0	0	3.476837768	0	0.441E-05	0	0.021922432	0	0	0	0	0.001262765	0	0	0	0	0	0	0	0	0	0
Feb-23	0	0.004760281	0	0	0	0	0	0	0	0	0	38.84464029	0	0	0	0	212.6209012	0	0	0	0	0	4.815839716	0	0.610E-05	0	0.030365212	0	0	0	0	0.001749081	0</									

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	F-Liquid (kMoles)	F-Solid (kMoles)	Fe+3 Liquid (kMoles)	Fe+3 Solid (kMoles)	Fe2O3 Liquid (kMoles)	Fe2O3 Solid (kMoles)	H+ Liquid (kMoles)	H+ Solid (kMoles)	H2O Liquid (kMoles)	H2O Solid (kMoles)	H2O2 Liquid (kMoles)	H2O2 Solid (kMoles)	HCl Liquid (kMoles)	HCl Solid (kMoles)	HF Liquid (kMoles)	HF Solid (kMoles)	Hg+2 Liquid (kMoles)	Hg+2 Solid (kMoles)	K+ Liquid (kMoles)	K+ Solid (kMoles)	K2O Liquid (kMoles)	K2O Solid (kMoles)	La+3 Liquid (kMoles)	La+3 Solid (kMoles)	La2O3 Liquid (kMoles)	La2O3 Solid (kMoles)	Li+ Liquid (kMoles)	Li+ Solid (kMoles)	Li2O Liquid (kMoles)	Li2O Solid (kMoles)	MnO Liquid (kMoles)	MnO Solid (kMoles)	Mg+2 Liquid (kMoles)	Mg+2 Solid (kMoles)	MgO Liquid (kMoles)	MgO Solid (kMoles)	
Feb-21	3.703019851	0	0.111486501	0	0	0	0	0	12520.38824	0	0	0	0	0	3.32E-05	0	21.13142166	0	0	0	0.00245003	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mar-21	5.99547974	0	0.180505394	0	0	0	0	0	20271.49112	0	0	0	0	0	5.37E-05	0	34.21342999	0	0	0	0.003969984	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
May-21	0.259247307	0	0.007805156	0	0	0	0	0	876.5486188	0	0	0	0	0	2.32E-06	0	1.479404481	0	0	0	0.000171664	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jun-21	9.608803632	0	0.289219426	0	0	0	0	0	32488.60574	0	0	0	0	0	8.61E-05	0	54.83253342	0	0	0	0.006362594	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-21	4.525569911	0	0.136250945	0	0	0	0	0	15301.5362	0	0	0	0	0	4.06E-05	0	25.8253342	0	0	0	0.002996665	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-21	5.781120252	0	0.174051691	0	0	0	0	0	19546.71401	0	0	0	0	0	5.18E-05	0	32.99017953	0	0	0	0.003820844	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sep-21	9.957746897	0	0.299797031	0	0	0	0	0	33668.42798	0	0	0	0	0	8.93E-05	0	56.82425613	0	0	0	0.006593651	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Oct-21	5.6672788274	0	0.170489808	0	0	0	0	0	19146.61832	0	0	0	0	0	5.08E-05	0	32.31491366	0	0	0	0.003749689	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nov-21	4.294958623	0	0.12930795	0	0	0	0	0	14521.80966	0	0	0	0	0	3.85E-05	0	24.50934246	0	0	0	0.002843962	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Dec-21	8.1171193278	0	0.197201143	0	0	0	0	0	28634.45621	0	0	0	0	0	0.000107778	0	56.53120726	0	0	0	0.004738048	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jan-22	3.950168337	0	0.043788031	0	0	0	0	0	15249.82535	0	0	0	0	0	9.12E-05	0	38.80179501	0	0	0	0.00160445	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Feb-22	9.291530585	0	0.102997592	0	0	0	0	0	35870.42541	0	0	0	0	0	0.000214435	0	91.26903828	0	0	0	0.003766896	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mar-22	4.703217678	0	0.052135662	0	0	0	0	0	18157.01056	0	0	0	0	0	0.000108543	0	46.19886362	0	0	0	0.00190674	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Apr-22	6.163499825	0	0.068323043	0	0	0	0	0	23794.5039	0	0	0	0	0	1.42E-04	0	60.54295321	0	0	0	0.002498755	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
May-22	8.546226897	0	0.0947355823	0	0	0	0	0	32993.1427	0	0	0	0	0	0.000197234	0	83.94805384	0	0	0	0.003464741	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jun-22	3.582874448	0	0.03971654	0	0	0	0	0	13831.86866	0	0	0	0	0	8.27E-05	0	35.19393303	0	0	0	0.001452539	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-22	6.244889981	0	0.069225261	0	0	0	0	0	24108.71473	0	0	0	0	0	1.44E-04	0	61.34243411	0	0	0	0.002531752	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-22	3.156094056	0	0.034071269	0	0	0	0	0	12673.56651	0	0	0	0	0	7.00E-05	0	31.45715237	0	0	0	0.001321411	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sep-22	3.06913965	0	0.018738111	0	0	0	0	0	25313.06855	0	0	0	0	0	1.68E-05	0	46.04194432	0	0	0	0.002437495	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Oct-22	2.168207751	0	0.011257713	0	0	0	0	0	15207.89688	0	0	0	0	0	1.01E-05	0	27.661164601	0	0	0	0.001464428	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nov-22	3.628958642	0	0.018842187	0	0	0	0	0	25452.80962	0	0	0	0	0	1.69E-05	0	46.29767109	0	0	0	0.002451034	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Dec-22	4.455903977	0	0.023135581	0	0	0	0	0	31253.89075	0	0	0	0	0	2.07E-05	0	56.84770676	0	0	0	0.003009561	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jan-23	2.167411369	0	0.011253578	0	0	0	0	0	15202.31102																												

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Mn+4 Liquid (kMoles)	Mn+4 Solid (kMoles)	MnO2 Liquid (kMoles)	MnO2 Solid (kMoles)	MnO4-Liquid (kMoles)	MnO4-Solid (kMoles)	Mo+6 Liquid (kMoles)	Mo+6 Solid (kMoles)	MoO3 Liquid (kMoles)	MoO3 Solid (kMoles)	Na+ Liquid (kMoles)	Na+ Solid (kMoles)	Na2O Liquid (kMoles)	Na2O Solid (kMoles)	Nd2O3 Liquid (kMoles)	Nd+3 Liquid (kMoles)	Nd+3 Solid (kMoles)	NH3 Liquid (kMoles)	NH3 Solid (kMoles)	NH4+ Liquid (kMoles)	NH4+ Solid (kMoles)	Ni+2 Liquid (kMoles)	Ni+2 Solid (kMoles)	NiO Liquid (kMoles)	NiO Solid (kMoles)	NO2-Liquid (kMoles)	NO2-Solid (kMoles)	NO3-Liquid (kMoles)	NO3-Solid (kMoles)	O(BOUND) Liquid (kMoles)	O(BOUND) Solid (kMoles)	OH(BOUND) Liquid (kMoles)	OH(BOUND) Solid (kMoles)		
Feb-21	0.006287233	0	0	0	0	0	0	0	0	0	1432.282367	0	0	0	0	0	0	0	0	0	0	0	0	0	0	284.7640906	0	494.5199373	0	0.040190353	0	1.150012005	0		
Mar-21	0.010179524	0	0	0	0	0	0	0	0	0	2318.977553	0	0	0	0	0	0	0	0	0	0	0	0	0	0	800.6665869	0	0.065071336	0	1.861959685	0				
May-21	0.000440167	0	0	0	0	0	0	0	0	0	100.2736582	0	0	0	0	0	0	0	0	0	0	0	0	0	0	19.93624842	0	0.002813715	0	0.080511995	0				
Jun-21	0.016314466	0	0	0	0	0	0	0	0	0	3716.566631	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2658.26075	0	0	0	738.9218363	0	0.1283.208074	0	0.104288183	0
Jul-21	0.007683813	0	0	0	0	0	0	0	0	0	1750.434576	0	0	0	0	0	0	0	0	0	0	0	0	0	0	348.0186043	0	0.049117818	0	0.405463631	0				
Aug-21	0.00981557	0	0	0	0	0	0	0	0	0	2236.065949	0	0	0	0	0	0	0	0	0	0	0	0	0	0	444.5710575	0	0.062744807	0	1.795388078	0				
Sep-21	0.016906925	0	0	0	0	0	0	0	0	0	3851.533578	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2754.79536	0	0	0	1329.8075404	0	0.302483685	0		
Oct-21	0.009614658	0	0	0	0	0	0	0	0	0	2190.296601	0	0	0	0	0	0	0	0	0	0	0	0	0	0	435.4712689	0	0	0	756.2372915	0	0.051460503	0		
Nov-21	0.007292266	0	0	0	0	0	0	0	0	0	1661.236977	0	0	0	0	0	0	0	0	0	0	0	0	0	0	330.2844802	0	0	0	573.5704249	0	0.046614901	0		
Dec-21	0.012132958	0	0	0	0	0	0	0	0	0	3300.727095	0	0	0	0	0	0	0	0	0	0	0	0	0	0	677.6895116	0	0	0	117.97396	0	0.07162631	0		
Jan-22	0.000408086	0	0	0	0	0	0	0	0	0	1784.427386	0	0	0	0	0	0	0	0	0	0	0	0	0	0	388.9274862	0	0.016639347	0	1.105579657	0				
Feb-22	0.009598941	0	0	0	0	0	0	0	0	0	4197.305082	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3076.17081	0	0	0	914.8297809	0	0.039138838	0		
Mar-22	0.004858824	0	0	0	0	0	0	0	0	0	1662.80122	0	0	0	0	0	0	0	0	0	0	0	0	0	0	463.0715638	0	0	0	692.4894413	0	0.136344354	0		
Apr-22	0.006367419	0	0	0	0	0	0	0	0	0	2784.265617	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2040.56566	0	0	0	606.8486933	0	0.025962592	0		
May-22	0.008828979	0	0	0	0	0	0	0	0	0	3021.47965	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	282.942121	0	0	0	841.4483285	0	0.035999385	0	
Jun-22	0.003701414	0	0	0	0	0	0	0	0	0	1266.070896	0	0	0	0	0	0	0	0	0	0	0	0	0	0	352.7642961	0	0	0	527.530412	0	0.01509219	0		
Jul-22	0.006451502	0	0	0	0	0	0	0	0	0	2207.85245	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	206751.171	0	0	0	614.8622426	0	0.026305433	0	
Aug-22	0.003365403	0	0	0	0	0	0	0	0	0	1071.26167	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	104.982816	0	0	0	320.5995184	0	0.014677114	0	
Sep-22	0.006167929	0	0	0	0	0	0	0	0	0	2394.77352	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	124.311155	0	0	0	484.552416	0	0.047360889	0
Oct-22	0.003705644	0	0	0	0	0	0	0	0	0	1746.07534	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	351.1945954	0	0	0	750.5765323	0	0.028454058	0
Nov-22	0.006202187	0	0	0	0	0	0	0	0	0	2922.421871	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	126.250095	0	0	0	0.047623942	0	0.901450221	0
Dec-22	0.007615504	0	0	0	0	0	0	0	0	0	3588.356843	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	154.216834	0	0	0	0.0584762	0	1.10687292	0
Jan-23	0.003704283	0	0	0	0	0	0	0	0	0	1438.23299	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	351.3008456	0	0	0	0.028443607	0	0.538395074	0
Feb-23	0.005130879	0	0	0	0	0	0	0	0	0	0.01992126	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	486.2682068	0	0	0	1039.257179	0	0.039397827	0
Mar-23	0.008014112	0	0	0	0	0	0	0	0	0	0.031115762	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1623.524697	0	0	0	0.0161536941	0	1	

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	OH-Liquid (kMoles)	OH-Solid (kMoles)	P2O5 Liquid (kMoles)	P2O5 Solid (kMoles)	Pb+2 Liquid (kMoles)	PbO Liquid (kMoles)	PbO Solid (kMoles)	Pd+2 Liquid (kMoles)	Pd+2 Solid (kMoles)	PdO Liquid (kMoles)	PdO Solid (kMoles)	PO4-3 Liquid (kMoles)	PO4-3 Solid (kMoles)	Pr+3 Liquid (kMoles)	Pr+3 Solid (kMoles)	Pr2O3 Liquid (kMoles)	Pr2O3 Solid (kMoles)	Pu+4 Liquid (kMoles)	Pu+4 Solid (kMoles)	Rb+ Liquid (kMoles)	Rb+ Solid (kMoles)	Rh+3 Liquid (kMoles)	Rh+3 Solid (kMoles)	Rb2O Liquid (kMoles)	Rb2O Solid (kMoles)	Rh2O3 Liquid (kMoles)	Rh2O3 Solid (kMoles)	Ru+3 Liquid (kMoles)	Ru+3 Solid (kMoles)	RuO2 Liquid (kMoles)	RuO2 Solid (kMoles)	Sb+5 Liquid (kMoles)	Sb+5 Solid (kMoles)
Feb-21	279.125899	0	0	0	0.024988914	0	0	0	0	0	4.663443478	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Mar-21	451.9267354	0	0	0	0.040459013	0	0	0	0	0	7.550489693	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
May-21	19.54152032	0	0	0	0.001749466	0	0	0	0	0	0.326486277	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
Jun-21	724.2915404	0	0	0	0.064842636	0	0	0	0	0	12.10069474	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Jul-21	341.1280038	0	0	0	0.03053969	0	0	0	0	0	5.699331987	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Aug-21	435.7687651	0	0	0	0.039012461	0	0	0	0	0	7.280524712	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Sep-21	750.5941547	0	0	0	0.067197393	0	0	0	0	0	12.54041072	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Oct-21	426.8491478	0	0	0	0.038213927	0	0	0	0	0	7.13150884	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0004E+00	0	0			
Nov-21	323.7450068	0	0	0	0.0289853467	0	0	0	0	0	5.408908853	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Dec-21	728.8940284	0	0	0	0.057246486	0	0	0	0	0.000262276	9.876976503	0	0.000429179	0	0	0	0	0.001551217	0	0.000203425	0	0	0	0	0	0	0	0.016954434	0	0			
Jan-22	484.1398193	0	0	0	0.030589658	0	0	0	0	0.000417681	4.424458657	0	0.000683479	0	0	0	0	0.002470353	0	0.000323959	0	0	0	0	0	0	0.000187655	0	0.027000374				
Feb-22	1138.786896	0	0	0	0.071952564	0	0	0	0	0.000982463	10.40714963	0	0.001607671	0	0	0	0	0.00581073	0	0.000762013	0	0	0	0	0	0	0.000441401	0	0.03509901				
Mar-22	576.4349169	0	0	0	0.036421187	0	0	0	0	0.000497307	5.267925415	0	0.000813776	0	0	0	0	0.002941294	0	0.000385718	0	0	0	0	0	0	0.0002343	0	0.03214762				
Apr-22	755.4097541	0	0	0	0.047729447	0	0	0	0	0.000651713	6.903541277	0	0.001066442	0	0	0	0	0.003854524	0	0.000505478	0	0	0	0	0	0	2.93E-04	0	0.04212904				
May-22	1047.44112	0	0	0	0.066181016	0	0	0	0	0.000903657	9.572358533	0	0.001478714	0	0	0	0	0.005344632	0	0.000700889	0	0	0	0	0	0	0.000405994	0	0.058415566				
Jun-22	439.123612	0	0	0	0.027745375	0	0	0	0	0.000378844	4.013064386	0	0.000619928	0	0	0	0	0.002240655	0	0.000293837	0	0	0	0	0	0	0.000170207	0	0.02448983				
Jul-22	765.3850797	0	0	0	0.048359723	0	0	0	0	0.000660319	6.994703817	0	0.001080525	0	0	0	0	0.003905424	0	0.000512153	0	0	0	0	0	0	0.000296668	0	0.042685362				
Aug-22	392.7384256	0	0	0	0.024085762	0	0	0	0	0.00032039	3.743907175	0	0.000524276	0	0	0	0	0.001894932	0	0.000248499	0	0	0	0	0	0	1.44E-04	0	0.020711163				
Sep-22	580.0491591	0	0	0	0.019697713	0	0	0	0	7.16E-05	8.900212035	0	1.17E-04	0	0	0	0	0.00423606	0	5.56E-05	0	0	0	0	0	0	3.22E-05	0	0.004629198				
Oct-22	348.4890732	0	0	0	0.018342324	0	0	0	0	4.30E-05	5.347178933	0	7.04E-05	0	0	0	0	0.00254499	0	3.34E-05	0	0	0	0	0	0	0.002781619	0	0.004655634				
Nov-22	583.2708757	0	0	0	0.019807118	0	0	0	0	7.20E-05	8.94645709	0	0.000117851	0	0	0	0	0.000425959	0	5.59E-05	0	0	0	0	0	0	0.0024E-05	0	0.004655634				
Dec-22	716.1831454	0	0	0	0.024320645	0	0	0	0	8.84E-05	8.98093731	0	0.000144707	0	0	0	0	0.00523024	0	6.86E-05	0	0	0	0	0	0	3.97E-05	0	0.005716532				
Jan-23	348.3610732	0	0	0	0.018129888	0	0	0	0	4.30E-05	5.345214914	0	7.04E-05	0	0	0	0	0.00254406	0	3.34E-05	0	0	0	0	0	0	0.002780598	0	0.003851463				
Feb-23	482.5221088	0	0	0	0.016385821	0	0	0	0	5.96E-05	7.403767443	0	9.75E-05	0	0	0	0	0.00352383	0	4.62E-05	0	0	0	0	0	0	0.002632121	0	0.003851463				
Mar-23	753.6693468	0	0	0	0.025593628	0	0	0	0	9.31E-05	11.56422156	0	0.000152821	0	0	0	0	0.0005504	0	7.22E-05	0	0	0	0	0	0	0.006015744	0	0.00258629				
Apr-23	316.7937707	0	0	0	0.01075903	0	0	0	0	3.91E-05	8.806049613	0	6.40E-05	0	0	0	0	0.00231353	0														

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Sb2O3 Liquid (kMoles)	Sb2O3 Solid (kMoles)	Se+6 Liquid (kMoles)	Se+6 Solid (kMoles)	SeO2 Liquid (kMoles)	SeO2 Solid (kMoles)	Si+4 Liquid (kMoles)	Si+4 Solid (kMoles)	SiO2 Liquid (kMoles)	SiO2 Solid (kMoles)	SO4-2 Liquid (kMoles)	SO4-2 Solid (kMoles)	Sr+2 Liquid (kMoles)	Sr+2 Solid (kMoles)	SrO Liquid (kMoles)	SrO Solid (kMoles)	Ta+5 Liquid (kMoles)	Ta+5 Solid (kMoles)	Ta2O5 Liquid (kMoles)	Ta2O5 Solid (kMoles)	Tc+7 Liquid (kMoles)	Tc+7 Solid (kMoles)	Te+6 Liquid (kMoles)	Te+6 Solid (kMoles)	TeO2 Liquid (kMoles)	TeO2 Solid (kMoles)	Th+4 Liquid (kMoles)	Th+4 Solid (kMoles)	ThO2 Liquid (kMoles)	ThO2 Solid (kMoles)	Ti+4 Liquid (kMoles)	Ti+4 Solid (kMoles)	TiO2 Liquid (kMoles)	TiO2 Solid (kMoles)	Tl2O Liquid (kMoles)
Feb-21	0	0	0	0	0	0	0.292728964	0	0	0	12.07472637	0	0.002916421	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Mar-21	0	0	0	0	0	0	0.473951165	0	0	0	19.54992957	0	0.004721914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
May-21	0	0	0	0	0	0	0.020493867	0	0	0	0.845347965	0	0.000204178	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
Jun-21	0	0	0	0	0	0	0.759589537	0	0	0	31.33217732	0	0.007567693	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Jul-21	0	0	0	0	0	0	0.357752711	0	0	0	14.75687966	0	0.003564244	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Aug-21	0	0	0	0	0	0	0.457005744	0	0	0	18.85095083	0	0.004553089	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Sep-21	0	0	0	0	0	0	0.787173996	0	0	0	32.47000391	0	0.007842513	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Oct-21	0	0	0	0	0	0	0.447651434	0	0	0	18.4650965	0	0.004459993	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Nov-21	0	0	0	0	0	0	0.339522562	0	0	0	14.00490741	0	0.003382619	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Dec-21	0	0	0	0	0	0	0.651357657	0	0	0	25.005326747	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Jan-22	0	0	0	0	0	0	0.327685288	0	0	0	10.55076354	0	0.001413144	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Feb-22	0	0	0	0	0	0	0.77077674	0	0	0	24.81735809	0	0.003323978	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Mar-22	0	0	0	0	0	0	0.390154319	0	0	0	12.56213239	0	0.001682542	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Apr-22	0	0	0	0	0	0	0.1077665	0	0	0	16.46429497	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
May-22	0	0	0	0	0	0	0.149427596	0	0	0	0.708950247	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Jun-22	0	0	0	0	0	0	0.062645226	0	0	0	0.297216509	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Jul-22	0	0	0	0	0	0	0.109189577	0	0	0	0.518043383	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Aug-22	0	0	0	0	0	0	0.05297936	0	0	0	0.279856383	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Sep-22	0	0	0	0	0	0	0.011843376	0	0	0	0.719043846	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Oct-22	0	0	0	0	0	0	0.007115409	0	0	0	0.431996012	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Nov-22	0	0	0	0	0	0	0.011909157	0	0	0	0.723037569	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Dec-22	0	0	0	0	0	0	0.014622944	0	0	0	0.887799034	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Jan-23	0	0	0	0	0	0	0.007112796	0	0	0	0.43183734	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Feb-23	0	0	0	0	0	0	0.00985208	0	0	0	0.598146808	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Mar-23	0	0	0	0	0	0	0.015388333	0	0	0	0.934267893	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Apr-23	0	0	0	0	0	0	0.006468258	0	0	0	0.3927057	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
May-23	0	0	0	0	0	0	0.005518258	0	0	0	0.668297079	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Jun-23	0	0	0	0	0	0	0.002348477	0	0	0	0.705721887	0	0	0</																					

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Tl2O Solid (kMoles)	Tl+3 Liquid (kMoles)	Tl+3 Solid (kMoles)	TOC Liquid (kMoles)	TOC Solid (kMoles)	V+5 Liquid (kMoles)	V+5 Solid (kMoles)	V2O5 Liquid (kMoles)	V2O5 Solid (kMoles)	W+6 Liquid (kMoles)	W+6 Solid (kMoles)	WO3 Liquid (kMoles)	WO3 Solid (kMoles)	Y+3 Liquid (kMoles)	Y+3 Solid (kMoles)	Y2O3 Liquid (kMoles)	Y2O3 Solid (kMoles)	Zn+2 Liquid (kMoles)	Zn+2 Solid (kMoles)	ZnO Liquid (kMoles)	ZnO Solid (kMoles)	Zr+4 Liquid (kMoles)	Zr+4 Solid (kMoles)	ZrO2 Liquid (kMoles)	ZrO2 Solid (kMoles)	
Feb-21	0	0	0	37.20108846	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Mar-21	0	0	0	60.23148165	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
May-21	0	0	0	2.604437026	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Jun-21	0	0	0	96.53147116	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Jul-21	0	0	0	45.46454877	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Aug-21	0	0	0	58.07799433	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Sep-21	0	0	0	100.03700711	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Oct-21	0	0	0	56.88921367	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Nov-21	0	0	0	43.14779346	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Dec-21	0	0.008414569	0	104.1426295	0	0.002449095	0	0	0.000738067	0	0	0.002651519	0	0	0	0.014095942	0	0	0	0	0	0	0	0	0	
Jan-22	0	0.013400419	0	75.66884899	0	0.003900248	0	0	0.00117539	0	0	0.004222613	0	0	0	0.022448152	0	0	0	4.00E-06	0	0	0	0	0	
Feb-22	0	0.031520278	0	177.9872058	0	0.009174108	0	0	0.002764736	0	0	0.009932371	0	0	0	0.052802229	0	0	0	9.41E-06	0	0	0	0	0	
Mar-22	0	0.015955039	0	90.09415243	0	0.00464378	0	0	0.001399463	0	0	0.0050276	0	0	0	0.026726707	0	0	0	4.76E-06	0	0	0	0	0	
Apr-22	0	0.020908851	0	118.0671044	0	0.006085608	0	0	0.001833977	0	0	0.006588599	0	0	0	0.035026148	0	0	0	6.24E-06	0	0	0	0	0	
May-22	0	0.028991935	0	163.710277	0	0.008438223	0	0	0.002542968	0	0	0.009135663	0	0	0	0.048566792	0	0	0	8.65E-06	0	0	0	0	0	
Jun-22	0	0.012154424	0	68.6330208	0	0.003537596	0	0	0.001061	0	0	0.003829987	0	0	0	0.020360882	0	0	0	3.63E-06	0	0	0	0	0	
Jul-22	0	0.021184956	0	119.6262024	0	0.00616597	0	0	0.001858195	0	0	0.006675602	0	0	0	0.035488675	0	0	0	6.32E-06	0	0	0	0	0	
Aug-22	0	0.010279053	0	60.99438771	0	0.002991761	0	0	0.000901606	0	0	0.003239038	0	0	0	0.017219293	0	0	0	3.07E-06	0	0	0	0	0	
Sep-22	0	0.00297851	0	81.61508125	0	0.000668799	0	0	0	0.000201551	0	0	0	0.000724077	0	0	0	0.003849321	0	0	0	6.86E-07	0	0	0	0
Oct-22	0	0.001380531	0	49.03371305	0	0.000401809	0	0	0.00012109	0	0	0.00043502	0	0	0	0.002312642	0	0	0	4.12E-07	0	0	0	0	0	
Nov-22	0	0.002310614	0	82.0683888	0	0.000672514	0	0	0.000202671	0	0	0.000728099	0	0	0	0.003870701	0	0	0	6.90E-07	0	0	0	0	0	
Dec-22	0	0.002837143	0	100.7696411	0	0.000825762	0	0	0.000248854	0	0	0.000894014	0	0	0	0.004752733	0	0	0	8.47E-07	0	0	0	0	0	
Jan-23	0	0.001380024	0	49.01570298	0	0.000401662	0	0	0.000121046	0	0	0.00043486	0	0	0	0.002311793	0	0	0	4.12E-07	0	0	0	0	0	
Feb-23	0	0.0019115	0	67.89266133	0	0.00055635	0	0	0.000167663	0	0	0.000602334	0	0	0	0.003202112	0	0	0	5.70E-07	0	0	0	0	0	
Mar-23	0	0.002985644	0	106.0440896	0	0.000868984	0	0	0.00026188	0	0	0.000940808	0	0	0	0.005001499	0	0	0	8.91E-07	0	0	0	0	0	
Apr-23	0	0.001254971	0	44.57406572	0	0.000362565	0	0	0.000110077	0	0	0.000395455	0	0	0	0.00210306	0	0	0	3.75E-07	0	0	0	0	0	
May-23	0	0.001261645	0	67.50211074	0	0.00182064	0	0	0.005107988	0	0	0.000869094	0	0	0	0.005862227	0	0	0	2.66E-07	0	0	0	0	0	
Jun-23	0	0.000778381	0	65.98858841	0	0.002684891	0	0	0.008512488	0	0	0.001042053	0	0	0	0.007638354	0	0	0	4.48E-08	0	0	0	0	0	
Jul-23	0	0.000556441	0	47.17058523	0	0.001919239	0	0	0.006084977	0	0	0.000744849	0	0	0	0.005460162	0	0	0	3.21E-08	0	0	0	0	0	
Aug-23	0	0.001262457	0	107.0269008	0	0.004354625	0	0	0.013806406	0	0	0.001690106	0	0	0	0.012388647	0	0	0	7.27E-08	0	0	0	0	0	
Sep-23	0	0.000808258	0	68.52148372	0	0.002787947	0	0	0	0.00883923	0	0	0	0.01082051	0	0	0	0.0070931543	0	0	0	4.66E-08	0	0	0	0
Oct-23	0	0.000554837	0	47.037247495	0	0.001913815	0	0	0.00606778	0	0	0.000742785	0	0	0	0.005444689	0</									

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Liquid Volume (kgal)	Solid Volume (kgal)	Total Volume (kgal)	Liquid Mass (kg)	Solid Mass (kg)	Total Mass (kg)	106-Ru Liquid (kMoles)	106-Ru Solid (kMoles)	113m-Cd Liquid (kMoles)	113m-Cd Solid (kMoles)	125-Sb Liquid (kMoles)	126-Sn Liquid (kMoles)	126-Sn Solid (kMoles)	129-I Liquid (kMoles)	134-Cs Liquid (kMoles)	137-Cs Liquid (kMoles)	137-Cs Solid (kMoles)	137m-Ba Liquid (kMoles)	137m-Ba Solid (kMoles)	14-C Liquid (kMoles)	14-C Solid (kMoles)	151-Sm Liquid (kMoles)	151-Sm Solid (kMoles)	152-Eu Liquid (kMoles)	152-Eu Solid (kMoles)	154-Eu Liquid (kMoles)	154-Eu Solid (kMoles)	155-Eu Liquid (kMoles)	155-Eu Solid (kMoles)	226-Ra Liquid (kMoles)	226-Ra Solid (kMoles)	227-Ac Liquid (kMoles)			
Sep-28	98.6	00:00.0	98.6	4.709E+05	0	4.709E+05	3.93E-17	0	7.12E-08	0	9.46E-11	00:00.0	00:21.2	0	0.001321643	0	3.93E-12	0	0.002472062	0	3.77E-10	0	3.63E-05	0	0.000185096	0	2.14E-09	0	9.89E-09	0	1.38E-09	0	4.35E-11	0	7.79E-11
Oct-28	132.3	00:00.0	132.3	6.336E+05	0	6.336E+05	8.95E-17	0	1.03E-07	0	1.82E-10	00:00.0	00:27.0	0	0.002173105	0	8.11E-12	0	0.003108151	0	4.73E-10	0	7.10E-05	0	3.94E-09	0	1.43E-08	0	2.57E-09	0	8.15E-11	0	8.41E-11		
Nov-28	117.8	00:00.0	117.8	5.641E+05	0	5.641E+05	7.97E-17	0	9.13E-08	0	1.62E-10	00:00.0	00:24.0	0	0.001934983	0	7.22E-12	0	0.00276757	0	4.22E-10	0	6.32E-05	0	0.000314631	0	3.51E-09	0	1.28E-08	0	7.26E-11	0	7.49E-11		
Dec-28	129.2	00:00.0	129.2	6.186E+05	0	6.186E+05	8.74E-17	0	1.00E-07	0	1.78E-10	00:00.0	00:26.3	0	0.002121789	0	7.92E-12	0	0.003054755	0	4.62E-10	0	6.93E-05	0	0.000345006	0	3.85E-09	0	1.40E-08	0	2.50E-09	0	7.96E-11	0	8.21E-11
Jan-29	132.9	00:00.0	132.9	6.365E+05	0	6.365E+05	4.55E-17	0	9.81E-08	0	1.42E-10	00:00.0	00:27.1	0	0.002183333	0	5.82E-12	0	0.003051427	0	4.65E-10	0	7.13E-05	0	0.000352282	0	3.76E-09	0	1.33E-08	0	2.23E-09	0	8.19E-11	0	8.64E-11
Feb-29	127.2	00:00.0	127.2	6.091E+05	0	6.091E+05	4.35E-17	0	9.39E-08	0	1.36E-10	00:00.0	00:25.9	0	0.00208924	0	5.57E-12	0	0.002919923	0	4.45E-10	0	6.82E-05	0	3.37E-04	0	3.60E-09	0	1.27E-08	0	7.83E-11	0	8.26E-11		
Mar-29	141.2	00:00.0	141.2	6.761E+05	0	6.761E+05	4.83E-17	0	1.04E-07	0	1.51E-10	00:00.0	00:28.8	0	0.002319169	0	6.18E-12	0	0.003241271	0	4.94E-10	0	7.57E-05	0	3.99E-09	0	1.41E-08	0	2.36E-09	0	8.70E-11	0	9.17E-11		
Apr-29	142.6	00:00.0	142.6	6.831E+05	0	6.831E+05	4.88E-17	0	1.05E-07	0	1.53E-10	00:00.0	00:29.1	0	0.002343196	0	6.25E-12	0	0.003274852	0	4.99E-10	0	7.65E-05	0	3.78E-04	0	4.04E-09	0	1.43E-08	0	2.39E-09	0	8.79E-11	0	9.27E-11
May-29	134.1	00:00.0	134.1	6.383E+05	0	6.383E+05	2.28E-17	0	6.76E-08	0	7.79E-11	00:00.0	00:37.4	0	0.00208636	0	3.15E-12	0	0.003129688	0	4.77E-10	0	4.16E-05	0	2.17E-04	0	2.16E-09	0	1.13E-08	0	5.24E-11	0	3.11E-10		
Jun-29	163.1	00:00.0	163.1	7.728E+05	0	7.728E+05	6.31E-18	0	5.31E-08	0	3.37E-11	00:00.0	00:54.8	0	0.002906465	0	1.29E-12	0	0.003854141	0	5.87E-10	0	2.23E-05	0	1.36E-04	0	1.11E-09	0	1.18E-10	0	3.57E-11	0	2.00E-10		
Jul-29	159.4	00:00.0	159.4	7.554E+05	0	7.554E+05	6.17E-18	0	5.19E-08	0	3.29E-11	00:00.0	00:53.6	0	0.002840985	0	1.26E-12	0	0.003767331	0	5.74E-10	0	2.18E-05	0	1.33E-04	0	1.08E-09	0	1.15E-08	0	3.49E-11	0	1.96E-10		
Aug-29	165.3	00:00.0	165.3	7.835E+05	0	7.835E+05	6.40E-18	0	5.39E-08	0	3.41E-11	00:00.0	00:55.6	0	0.002946705	0	1.31E-12	0	0.003907522	0	5.95E-10	0	2.26E-05	0	1.38E-04	0	1.12E-09	0	1.20E-08	0	3.62E-11	0	2.03E-10		
Sep-29	164.3	00:00.0	164.3	7.785E+05	0	7.785E+05	6.36E-18	0	5.35E-08	0	3.39E-11	00:00.0	00:55.2	0	0.00292784	0	1.30E-12	0	0.003882507	0	5.91E-10	0	2.25E-05	0	0.000137167	0	1.11E-09	0	1.19E-08	0	3.59E-11	0	2.02E-10		
Oct-29	174.9	00:00.0	174.9	8.289E+05	0	8.289E+05	6.77E-18	0	5.70E-08	0	3.61E-11	00:00.0	00:58.8	0	0.003117533	0	1.39E-12	0	0.004134051	0	6.30E-10	0	2.40E-05	0	0.000146054	0	1.19E-09	0	1.27E-08	0	8.35E-10	0	2.15E-10		
Nov-29	116.6	00:00.0	116.6	5.534E+05	0	5.534E+05	4.30E-18	0	3.74E-08	0	2.31E-11	00:00.0	00:37.5	0	0.002034738	0	8.83E-13	0	0.002641444	0	4.02E-10	0	1.58E-05	0	9.29E-09	0	7.55E-10	0	8.07E-09	0	5.31E-10	0	1.37E-10		
Dec-29	235.2	00:00.0	235.2	1.144E+06	0	1.144E+06	7.87E-19	0	5.50E-08	0	1.11E-11	00:00.0	00:10.3	0	0.002483103	0	2.19E-12	0	0.001067672	0	1.63E-10	0	2.48E-05	0	2.25E-05	0	1.76E-10	0	2.09E-09	0	1.27E-10	0	4.15E-11		
Jan-30	179.1	00:00.0	179.1	8.713E+05	0	8.713E+05	3.04E-19	0	3.98E-08	0	6.55E-12	00:00.0	00:9.07E-05	0	0.001891277	0	1.19E-13	0	0.00079467	0	1.21E-10	0	1.89E-05	0	1.70E-05	0	1.47E-09	0	1.71E-11	0	3.26E-11				
Feb-30	160.9	00:00.0	160.9	7.826E+05	0	7.826E+05	2.73E-19	0	3.58E-08	0	6.88E-12	00:00.0	00:55.6	0	0.001698743	0	1.07E-13	0	0.000713772	0	1.09E-10	0	1.69E-05	0	1.53E-04	0	1.32E-09	0	7.50E-11	0	1.54E-11				
Mar-30	180.4	00:00.0	180.4	8.774E+05	0	8.774E+05	3.06E-19	0	4.01E-08	0	6.59E-12	00:00.0	00:9.14E-05	0	0.001904593																				

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	227-Ac Solid (kMoles)	228-Ra Liquid (kMoles)	228-Ra Solid (kMoles)	229-Th Liquid (kMoles)	229-Th Solid (kMoles)	231-Pa Liquid (kMoles)	231-Pa Solid (kMoles)	232-Th Liquid (kMoles)	232-U Liquid (kMoles)	232-U Solid (kMoles)	233-U Liquid (kMoles)	234-U Liquid (kMoles)	235-U Liquid (kMoles)	236-U Liquid (kMoles)	236-U Solid (kMoles)	237-Np Liquid (kMoles)	237-Np Solid (kMoles)	238-Pu Liquid (kMoles)	238-Pu Solid (kMoles)	238-U Liquid (kMoles)	238-U Solid (kMoles)	239-Pu Liquid (kMoles)	239-Pu Solid (kMoles)	240-Pu Liquid (kMoles)	240-Pu Solid (kMoles)	241-Am Liquid (kMoles)	241-Am Solid (kMoles)	241-Pu Liquid (kMoles)	241-Pu Solid (kMoles)				
Sep-28	0	2.26E-12	0	2.76E-09	0	2.08E-07	0	0.005595577	0	3.95E-11	0	1.67E-06	0	1.52E-06	0	0.000166522	0	4.60E-06	0	3.59E-05	0	3.72E-08	0	0.022931666	0	2.55E-04	0	1.61E-05	0	5.26E-06	0	8.90E-08	0
Oct-28	0	3.03E-12	0	4.74E-09	0	2.16E-07	0	0.00772045	0	6.06E-11	0	2.14E-06	0	2.91E-06	0	0.000321916	0	6.28E-06	0	5.03E-05	0	3.57E-08	0	0.04530478	0	1.74E-04	0	1.10E-05	0	5.26E-06	0	6.81E-08	0
Nov-28	0	2.70E-12	0	4.22E-09	0	1.92E-07	0	0.006874469	0	5.40E-11	0	1.90E-06	0	2.59E-06	0	0.000286642	0	5.60E-06	0	4.47E-05	0	3.18E-08	0	0.040340439	0	1.55E-04	0	9.76E-06	0	4.68E-06	0	6.06E-08	0
Dec-28	0	2.96E-12	0	4.63E-09	0	2.11E-07	0	0.00753814	0	5.92E-11	0	2.09E-06	0	2.84E-06	0	0.000314315	0	6.14E-06	0	4.91E-05	0	3.48E-08	0	0.044234956	0	1.70E-04	0	1.07E-05	0	5.13E-06	0	6.65E-08	0
Jan-29	0	3.06E-12	0	4.76E-09	0	2.17E-07	0	0.007756789	0	6.03E-11	0	2.15E-06	0	2.92E-06	0	0.000323432	0	6.31E-06	0	5.05E-05	0	4.45518026	0	1.75E-04	0	1.10E-05	0	5.28E-06	0	6.52E-08	0		
Feb-29	0	2.93E-12	0	4.56E-09	0	2.08E-07	0	0.007422503	0	5.77E-11	0	2.05E-06	0	2.79E-06	0	3.09E-04	0	6.04E-06	0	4.83E-05	0	3.40E-08	0	0.043556383	0	1.68E-04	0	1.05E-05	0	5.05E-06	0	6.24E-08	0
Mar-29	0	3.25E-12	0	5.06E-09	0	2.30E-07	0	0.008239375	0	6.41E-11	0	2.28E-06	0	3.10E-06	0	0.000343554	0	6.71E-06	0	5.36E-05	0	3.78E-08	0	0.048349912	0	1.17E-05	0	5.61E-06	0	6.93E-08	0		
Apr-29	0	3.29E-12	0	5.11E-09	0	2.33E-07	0	0.008324739	0	6.47E-11	0	2.30E-06	0	3.13E-06	0	0.000347113	0	6.78E-06	0	5.42E-05	0	3.82E-08	0	0.048850841	0	1.18E-05	0	5.66E-06	0	7.00E-08	0		
May-29	0	1.80E-12	0	2.50E-09	0	3.41E-07	0	0.004441305	0	3.25E-11	0	1.28E-06	0	1.64E-06	0	0.000182219	0	3.87E-06	0	6.29E-05	0	1.89E-08	0	0.025554573	0	9.55E-05	0	6.00E-06	0	3.21E-06	0	3.55E-08	0
Jun-29	0	9.98E-13	0	9.05E-10	0	5.29E-07	0	0.00225362	0	1.32E-11	0	7.24E-07	0	7.88E-07	0	8.76E-05	0	2.39E-06	0	8.77E-05	0	7.19E-09	0	0.012134844	0	4.06E-05	0	2.55E-06	0	1.93E-06	0	1.49E-08	0
Jul-29	0	9.75E-13	0	8.84E-10	0	5.17E-07	0	0.00220286	0	1.29E-11	0	7.08E-07	0	7.70E-07	0	8.56E-05	0	2.33E-06	0	8.57E-05	0	7.03E-09	0	0.011861523	0	3.97E-05	0	2.49E-06	0	1.89E-06	0	1.46E-08	0
Aug-29	0	1.01E-12	0	9.17E-10	0	5.37E-07	0	0.002284834	0	1.34E-11	0	7.34E-07	0	7.99E-07	0	8.88E-05	0	2.42E-06	0	7.29E-09	0	0.012302916	0	4.12E-05	0	2.58E-06	0	1.96E-06	0	1.52E-08	0		
Sep-29	0	1.01E-12	0	9.11E-10	0	5.33E-07	0	0.002270206	0	1.33E-11	0	7.30E-07	0	7.94E-07	0	8.82E-05	0	2.40E-06	0	8.83E-05	0	7.24E-09	0	0.012224155	0	4.09E-05	0	2.57E-06	0	1.95E-06	0	1.51E-08	0
Oct-29	0	1.07E-12	0	9.71E-10	0	5.68E-07	0	0.002417291	0	1.42E-11	0	7.77E-07	0	8.45E-07	0	9.40E-05	0	2.56E-06	0	7.71E-09	0	0.013016147	0	4.36E-05	0	2.73E-06	0	2.07E-06	0	1.60E-08	0		
Nov-29	0	6.83E-13	0	6.17E-10	0	3.62E-07	0	0.001541036	0	9.06E-12	0	5.00E-07	0	6.29E-05	0	1.68E-06	0	6.87E-05	0	4.93E-09	0	0.008749023	0	2.80E-05	0	1.75E-06	0	1.32E-06	0	1.02E-08	0		
Dec-29	0	2.57E-13	0	1.45E-10	0	1.25E-07	0	0.00487539	0	3.28E-12	0	3.36E-07	0	1.13E-06	0	1.37E-04	0	2.47E-06	0	3.63E-04	0	1.89E-09	0	0.020314287	0	1.91E-05	0	1.08E-06	0	4.41E-08	0	3.98E-09	0
Jan-30	0	1.91E-13	0	1.10E-10	0	9.50E-08	0	0.000371338	0	2.48E-12	0	2.56E-07	0	8.60E-07	0	1.04E-04	0	1.88E-06	0	2.77E-04	0	1.43E-09	0	0.01547255	0	1.45E-05	0	8.25E-07	0	2.89E-09	0		
Feb-30	0	1.71E-13	0	9.91E-11	0	8.54E-08	0	0.000333556	0	2.22E-12	0	2.30E-07	0	7.73E-07	0	9.37E-05	0	1.69E-06	0	2.49E-04	0	1.28E-09	0	0.01389743	0	1.31E-05	0	7.41E-07	0	2.59E-09	0		
Mar-30	0	1.92E-13	0	1.11E-10	0	9.57E-08	0	0.000373953	0	2.49E-12	0	2.58E-07	0	1.05E-04	0	1.90E-06	0	2.79E-04	0	1.44E-09	0	0.015581489	0	1.46E-05	0	8.31E-07	0	2.91E-09	0				
Apr-30	0	1.87E-13	0	1.08E-10	0	9.34E-08	0	0.000364796	0	2.43E-12	0	2.52E-07	0	8.45E-07	0	1.02E-04	0	2.72E-04	0	1.40E-09	0	0.015199977	0	1.43E-05	0	8.10E-07	0	3.29E-07	0	2.84E-09	0		
May-30	0	2.14E-13	0	1.37E-10	0	1.61E-07	0	0.000808356	0	1.13E-11	0	8.12E-07	0	1.27E-06	0	1.34E-04	0	2.71E-06															

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	242-Cm Liquid (kMoles)	242-Cm Solid (kMoles)	242-Pu Liquid (kMoles)	242-Pu Solid (kMoles)	243-Am Liquid (kMoles)	243-Am Solid (kMoles)	243-Cm Liquid (kMoles)	243-Cm Solid (kMoles)	244-Cm Liquid (kMoles)	244-Cm Solid (kMoles)	3-H Liquid (kMoles)	3-H Solid (kMoles)	59-Ni Liquid (kMoles)	59-Ni Solid (kMoles)	60-Co Liquid (kMoles)	60-Co Solid (kMoles)	63-Ni Liquid (kMoles)	63-Ni Solid (kMoles)	79-Se Liquid (kMoles)	79-Se Solid (kMoles)	90-Sr Liquid (kMoles)	90-Y Liquid (kMoles)	90-Y Solid (kMoles)	93-Zr Liquid (kMoles)	93m-Nb Solid (kMoles)	99-Tc Liquid (kMoles)	Ag+ Liquid (kMoles)	Ag+ Solid (kMoles)	Ag2O Liquid (kMoles)	Ag2O Solid (kMoles)	Al(OH)3 Liquid (kMoles)	Al(OH)3 Solid (kMoles)	Al2O3 Liquid (kMoles)				
Sep-28	7.53E-11	0	2.33E-07	0	5.00E-08	0	2.12E-10	0	2.15E-09	0	8.29E-09	0	6.90E-05	0	5.18E-10	0	4.48E-06	0	0.000119496	0	2.12E-05	0	5.40E-09	0	0.011380002	0	1.22E-07	0	0.018774056	0	0.006446949	0	0	0	0	0	0
Oct-28	4.22E-11	0	3.09E-07	0	3.32E-08	0	1.36E-10	0	1.38E-09	0	7.99E-09	0	9.26E-05	0	7.85E-10	0	4.05E-06	0	0.000132656	0	2.24E-05	0	5.69E-09	0	0.019534314	0	2.02E-07	0	0.025847133	0	0.007804571	0	0	0	0	0	0
Nov-28	3.76E-11	0	2.75E-07	0	2.95E-08	0	1.21E-10	0	1.23E-09	0	7.12E-09	0	8.24E-05	0	6.99E-10	0	3.61E-06	0	0.00011812	0	2.00E-05	0	5.07E-09	0	0.017393812	0	1.79E-07	0	0.023014893	0	0.006949374	0	0	0	0	0	0
Dec-28	4.12E-11	0	3.02E-07	0	3.24E-08	0	1.33E-10	0	1.34E-09	0	7.80E-09	0	9.04E-05	0	7.66E-10	0	3.96E-06	0	0.000129524	0	2.19E-05	0	5.56E-09	0	0.019073032	0	1.97E-07	0	0.02523678	0	0.007620275	0	0	0	0	0	0
Jan-29	4.22E-11	0	3.11E-07	0	3.33E-08	0	1.33E-10	0	1.33E-09	0	7.59E-09	0	9.30E-05	0	6.91E-10	0	4.05E-06	0	0.000113328	0	2.20E-05	0	5.58E-09	0	0.019626252	0	2.03E-07	0	0.025968708	0	0.007841307	0	0	0	0	0	0
Feb-29	4.04E-11	0	2.97E-07	0	3.19E-08	0	1.28E-10	0	1.27E-09	0	7.26E-09	0	8.90E-05	0	6.61E-10	0	3.87E-06	0	0.000127537	0	2.10E-05	0	5.34E-09	0	0.01878044	0	1.94E-07	0	0.024849562	0	0.007503378	0	0	0	0	0	0
Mar-29	4.49E-11	0	3.30E-07	0	3.54E-08	0	1.42E-10	0	1.41E-09	0	8.06E-09	0	9.88E-05	0	7.34E-10	0	4.30E-06	0	0.000141572	0	2.33E-05	0	5.93E-09	0	0.020847291	0	2.15E-07	0	0.027584341	0	0.008329151	0	0	0	0	0	0
Apr-29	4.53E-11	0	3.33E-07	0	3.57E-08	0	1.43E-10	0	1.43E-09	0	8.14E-09	0	9.98E-05	0	7.42E-10	0	4.34E-06	0	0.000143039	0	2.36E-05	0	5.99E-09	0	0.021063238	0	2.18E-07	0	0.027870129	0	0.008415445	0	0	0	0	0	0
May-29	2.69E-11	0	1.63E-07	0	2.23E-08	0	7.86E-11	0	8.22E-09	0	5.74E-05	0	5.28E-10	0	3.02E-06	0	0.000150998	0	1.79E-05	0	4.56E-09	0	0.017088199	0	1.78E-07	0	0.02419664	0	0.011980854	0	0	0	0	0	0		
Jun-29	1.82E-11	0	5.81E-08	0	1.66E-08	0	4.45E-11	0	4.45E-10	0	1.05E-08	0	3.60E-05	0	4.85E-10	0	2.69E-06	0	0.000199034	0	1.79E-05	0	4.54E-09	0	0.018260802	0	1.91E-07	0	0.027566733	0	0.018357885	0	0	0	0	0	0
Jul-29	1.78E-11	0	5.68E-08	0	1.63E-08	0	4.26E-11	0	4.25E-10	0	1.03E-08	0	3.52E-05	0	4.74E-10	0	2.63E-06	0	0.000194551	0	1.75E-05	0	4.44E-09	0	0.017849501	0	1.87E-07	0	0.026945827	0	0.017944397	0	0	0	0	0	0
Aug-29	1.84E-11	0	5.90E-08	0	1.69E-08	0	4.41E-11	0	4.41E-10	0	1.07E-08	0	3.65E-05	0	4.92E-10	0	2.72E-06	0	0.000201797	0	1.81E-05	0	4.61E-09	0	0.018513721	0	1.94E-07	0	0.027948541	0	0.018612148	0	0	0	0	0	0
Sep-29	1.83E-11	0	5.86E-08	0	1.68E-08	0	4.39E-11	0	4.38E-10	0	1.06E-08	0	3.63E-05	0	4.89E-10	0	2.71E-06	0	0.000200499	0	1.80E-05	0	4.58E-09	0	0.018395198	0	1.93E-07	0	0.027769618	0	0.018492995	0	0	0	0	0	0
Oct-29	1.95E-11	0	6.24E-08	0	1.79E-08	0	4.67E-11	0	4.67E-10	0	1.13E-08	0	3.86E-05	0	5.21E-10	0	2.88E-06	0	0.000213489	0	1.92E-05	0	4.87E-09	0	0.019587007	0	2.05E-07	0	0.029568788	0	0.019691114	0	0	0	0	0	0
Nov-29	1.25E-11	0	3.97E-08	0	1.14E-08	0	2.99E-11	0	2.99E-09	0	6.73E-05	0	3.32E-10	0	2.02E-06	0	0.000142247	0	1.32E-05	0	3.35E-09	0	0.012623529	0	1.32E-07	0	0.019500063	0	0.012534733	0	0	0	0	0	0		
Dec-29	8.06E-12	0	1.04E-08	0	3.99E-09	0	1.38E-11	0	1.39E-10	0	2.29E-08	0	7.54E-05	0	1.15E-10	0	7.63E-06	0	0.000284044	0	4.19E-05	0	1.06E-08	0	0.009310524	0	8.78E-08	0	0.031441175	0	0.003247167	0	0	0	0	0	0
Jan-30	6.11E-12	0	7.93E-09	0	3.04E-09	0	1.03E-11	0	1.02E-10	0	1.65E-08	0	5.74E-05	0	7.71E-11	0	5.77E-06	0	0.000216344	0	3.11E-05	0	7.91E-09	0	0.007091437	0	6.73E-08	0	0.023947361	0	0	0	0	0	0		
Feb-30	5.49E-12	0	7.12E-09	0	2.73E-09	0	9.22E-12	0	9.13E-11	0	1.48E-08	0	5.16E-05	0	6.93E-11	0	5.18E-06	0	0.00019432	0	2.80E-05	0	7.10E-09	0	0.006369522	0	0	0	0	0	0						
Mar-30	6.15E-12	0	7.98E-09	0	3.06E-09	0	1.03E-11	0	1.02E-10	0	1.66E-08	0	5.78E-05	0	7.76E-11	0</td																					

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Al2O3 Solid (kMoles)	Al(OH)4-Liquid (kMoles)	Al(OH)4-Solid (kMoles)	Al+3 Liquid (kMoles)	Al+3 Solid (kMoles)	AlOOH Liquid (kMoles)	AlOOH Solid (kMoles)	As+5 Liquid (kMoles)	As+5 Solid (kMoles)	As2O5 Liquid (kMoles)	As2O5 Solid (kMoles)	B+3 Liquid (kMoles)	B+3 Solid (kMoles)	B2O3 Liquid (kMoles)	B2O3 Solid (kMoles)	BaO Liquid (kMoles)	BaO Solid (kMoles)	Ba+2 Liquid (kMoles)	Ba+2 Solid (kMoles)	Be+2 Liquid (kMoles)	Be+2 Solid (kMoles)	BeO Liquid (kMoles)	BeO Solid (kMoles)	Bi+3 Liquid (kMoles)	Bi+3 Solid (kMoles)	Bi2O3 Liquid (kMoles)	Bi2O3 Solid (kMoles)	C2O4-2 Liquid (kMoles)	C2O4-2 Solid (kMoles)	Ca+2 Liquid (kMoles)	Ca+2 Solid (kMoles)	CaO Liquid (kMoles)	CaO Solid (kMoles)	Cd+2 Liquid (kMoles)	Cd+2 Solid (kMoles)	CdO Liquid (kMoles)
Sep-28	0	55.49328538	0	0	0	0	0	0.026412601	0	0	0	0.372560282	0	0	0	0.00216375	0	0.010719286	0	0	0	0.027326877	0	0	0	0	3.936280641	0	0	0	0.02555725	0	0			
Oct-28	0	66.14597247	0	0	0	0	0	0.044942281	0	0	0	0.515343365	0	0	0	0.002981269	0	0.010231454	0	0	0	0.040301166	0	0	0	0	4.522714937	0	0	0	0.03569322	0	0			
Nov-28	0	58.89792588	0	0	0	0	0	0.040017661	0	0	0	0.458873823	0	0	0	0.002654592	0	0.009110326	0	0	0	0.035885104	0	0	0	0	4.027131497	0	0	0	0.03178208	0	0			
Dec-28	0	64.58400662	0	0	0	0	0	0.043881017	0	0	0	0.503174086	0	0	0	0.00291087	0	0.009989849	0	0	0	0.039349497	0	0	0	0	4.415915898	0	0	0.517529666	0	0				
Jan-29	0	66.45731694	0	0	0	0	0	0.045153821	0	0	0	0.51776905	0	0	0	0.002995302	0	0.010279612	0	0	0	0.040490861	0	0	0	0	4.54400304	0	0	0.532541024	0	0				
Feb-29	0	63.59327529	0	0	0	0	0	0.043207874	0	0	0	0.495455297	0	0	0	0.002866216	0	0.009836603	0	0	0	0.038745868	0	0	0	0	4.348174882	0	0	0.509590659	0	0				
Mar-29	0	70.59193252	0	0	0	0	0	0.047963048	0	0	0	0.49981846	0	0	0	0.003181653	0	0.010919154	0	0	0	0.043009983	0	0	0	0	4.826706384	0	0	0.565672852	0	0				
Apr-29	0	71.32330007	0	0	0	0	0	0.048459969	0	0	0	0.555679931	0	0	0	0.003214617	0	0.01032282	0	0	0	0.043455588	0	0	0	0	4.876713465	0	0	0.571533505	0	0				
May-29	0	63.93377747	0	0	0	0	0	0.028715216	0	0	0	0.599798063	0	0	0	0.002874169	0	0.0120116	0	0	0	0.026001999	0	0	0	0	3.711629906	0	0	0.365238873	0	0				
Jun-29	0	74.86435889	0	0	0	0	0	0.01926094	0	0	0	0.801544926	0	0	0	0.003538544	0	0.01439597	0	0	0	0.017813145	0	0	0	0	3.702519611	0	0	0.284202234	0	0				
Jul-29	0	73.17813566	0	0	0	0	0	0.018827112	0	0	0	0.783491159	0	0	0	0.003282702	0	0.01407172	0	0	0	0.017411927	0	0	0	0	3.619125126	0	0	0.277800945	0	0				
Aug-29	0	75.90125603	0	0	0	0	0	0.01952771	0	0	0	0.812646599	0	0	0	0.003404859	0	0.01459536	0	0	0	0.018059863	0	0	0	0	3.758300872	0	0	0.288138533	0	0				
Sep-29	0	75.41534607	0	0	0	0	0	0.019402697	0	0	0	0.807444141	0	0	0	0.003380361	0	0.014501922	0	0	0	0.017944246	0	0	0	0	3.297769438	0	0	0.286293907	0	0				
Oct-29	0	80.30144062	0	0	0	0	0	0.02065978	0	0	0	0.859757743	0	0	0	0.003602247	0	0.015441489	0	0	0	0.019106838	0	0	0	0	3.971417949	0	0	0.30484264	0	0				
Nov-29	0	51.76382583	0	0	0	0	0	0.013145066	0	0	0	0.547383425	0	0	0	0.002992613	0	0.009828661	0	0	0	0.012229698	0	0	0	0	2.774100363	0	0	0.203964731	0	0				
Dec-29	0	38.5927041	0	0	0	0	0	0.003161007	0	0	0	0.145302927	0	0	0	0.000576016	0	0.025111739	0	0	0	0.005510446	0	0	0	0	10.3010972	0	0	0.438896551	0	0				
Jan-30	0	29.39446277	0	0	0	0	0	0.002407608	0	0	0	0.110671215	0	0	0	0.000438728	0	0.001913088	0	0	0	0.004197078	0	0	0	0	7.845918685	0	0	0.334289307	0	0				
Feb-30	0	26.40207896	0	0	0	0	0	0.002162511	0	0	0	0.099404782	0	0	0	0.000394065	0	0.001718333	0	0	0	0.003079811	0	0	0	0	0.020508431	0	0	0.004042814	0	0				
Mar-30	0	29.60142235	0	0	0	0	0	0.00244559	0	0	0	0.111450426	0	0	0	0.000441817	0	0.001926557	0	0	0	0.004226629	0	0	0	0	7.901159972	0	0	0.336642961	0	0				
Apr-30	0	28.87663304	0	0	0	0	0	0.02365194	0	0	0	0.108721568	0	0	0	0.000430999	0	0.001879386	0	0	0	0.00412314	0	0	0	0	7.707700476	0	0	0.328400275	0	0				
May-30	0	37.11285099	0	0	0	0	0	0.005811239	0	0	0	0.381371005	0	0	0	0.001232749	0	0.003523762	0	0	0	0.0109066	0	0	0	0	5.934576553	0	0	0.324728786	0	0				
Jun-30	0	72.40550077	0	0	0	0	0	0.014290956	0	0	0	0.101549952	0	0	0	0.003128447	0	0.008055842	0	0	0	0.027254076	0	0	0	0	7.345694469	0	0	0.529799321	0	0				
Jul-30	0	62.67755022	0	0	0	0	0	0.012370912	0	0	0	0.86698796	0	0	0	0.002708128	0	0.006973509	0	0	0	0.023592389														

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	CdO Solid (kMoles)	Ce+3 Liquid (kMoles)	Ce+3 Solid (kMoles)	Ce2O3 Liquid (kMoles)	Ce2O3 Solid (kMoles)	CH2Cl2 Liquid (kMoles)	CH2Cl2 Solid (kMoles)	CHCl3 Liquid (kMoles)	CHCl3 Solid (kMoles)	CHO2- Liquid (kMoles)	CHO2- Solid (kMoles)	Cl- Liquid (kMoles)	Cl- Solid (kMoles)	CN- Liquid (kMoles)	CN- Solid (kMoles)	Co+3 Liquid (kMoles)	Co+3 Solid (kMoles)	CO3-2 Liquid (kMoles)	CO3-2 Solid (kMoles)	CoO Liquid (kMoles)	CoO Solid (kMoles)	Cr2O3 Liquid (kMoles)	Cr2O3 Solid (kMoles)	CrO4-2 Liquid (kMoles)	CrO4-2 Solid (kMoles)	CrOOH Liquid (kMoles)	CrOOH Solid (kMoles)	Cs+ Liquid (kMoles)	Cs+ Solid (kMoles)	Cs2O Liquid (kMoles)	Cs2O Solid (kMoles)	Cu+2 Liquid (kMoles)	Cu+2 Solid (kMoles)	CuO Liquid (kMoles)	CuO Solid (kMoles)		
Sep-28	0	0.041763805	0	0	0	0	0	0	0	0	0	29.94905622	0	2.02E-03	0	0.004566749	0	174.782845	0	0	0	0	0	2.038812951	0	0.000145268	0	0.015535436	0	0	0	0	0.006370127	0	0	0	0
Oct-28	0	0.075991235	0	0	0	0	0	0	0	0	0	37.77280562	0	5.04E-03	0	0.006762301	0	206.372726	0	0	0	0	0	4.018809491	0	9.28E-05	0	0.019532696	0	0	0	0	0.088342523	0	0	0	0
Nov-28	0	0.067664379	0	0	0	0	0	0	0	0	0	33.63379239	0	4.49E-03	0	0.006021312	0	183.7591174	0	0	0	0	0	3.578442265	0	8.27E-05	0	0.017392371	0	0	0	0	0.007428378	0	0	0	0
Dec-28	0	0.074196784	0	0	0	0	0	0	0	0	0	36.88084152	0	4.92E-03	0	0.006602617	0	201.4994565	0	0	0	0	0	3.923909636	0	9.07E-05	0	0.019071452	0	0	0	0	0.008145524	0	0	0	0
Jan-29	0	0.076348921	0	0	0	0	0	0	0	0	0	37.95059957	0	5.07E-03	0	0.006794131	0	207.344108	0	0	0	0	0	4.037725746	0	9.33E-05	0	0.019624635	0	0	0	0	0.008381791	0	0	0	0
Feb-29	0	0.073058591	0	0	0	0	0	0	0	0	0	36.31508218	0	0.004847211	0	0.006501331	0	198.4084153	0	0	0	0	0	3.863716093	0	8.93E-05	0	0.018778892	0	0	0	0	0.00802057	0	0	0	0
Mar-29	0	0.08109939	0	0	0	0	0	0	0	0	0	40.31168105	0	0.005380663	0	0.007216825	0	220.2439393	0	0	0	0	0	4.28893125	0	9.91E-05	0	0.020845574	0	0	0	0	0.008903261	0	0	0	0
Apr-29	0	0.081939164	0	0	0	0	0	0	0	0	0	40.72933013	0	0.005436409	0	0.007291595	0	222.5257761	0	0	0	0	0	4.333566713	0	1.00E-04	0	0.021061544	0	0	0	0	0.08995503	0	0	0	0
May-29	0	0.042756022	0	0	0	0	0	0	0	0	0	36.49810518	0	0.003092298	0	0.005031925	0	137.0294105	0	0	0	0	0	2.940842023	0	5.63E-05	0	0.020128176	0	0	0	0	0.007446597	0	0	0	0
Jun-29	0	0.02012338	0	0	0	0	0	0	0	0	0	42.72694347	0	0.0018837	0	0.004424819	0	99.54385074	0	0	0	0	0	2.523161575	0	3.34E-05	0	0.024787606	0	0	0	0	0.008117902	0	0	0	0
Jul-29	0	0.019670127	0	0	0	0	0	0	0	0	0	41.76457411	0	0.001841272	0	0.004325156	0	97.30175374	0	0	0	0	0	2.466330611	0	3.26E-05	0	0.024229297	0	0	0	0	0.007935057	0	0	0	0
Aug-29	0	0.020402096	0	0	0	0	0	0	0	0	0	43.31872634	0	0.001909789	0	0.004486104	0	100.9225673	0	0	0	0	0	2.558102831	0	3.38E-05	0	0.025130923	0	0	0	0	0.008230338	0	0	0	0
Sep-29	0	0.020271485	0	0	0	0	0	0	0	0	0	43.0414055	0	0.001897563	0	0.004457385	0	100.2764742	0	0	0	0	0	2.541731556	0	3.36E-05	0	0.02497038	0	0	0	0	0.008177648	0	0	0	0
Oct-29	0	0.021584856	0	0	0	0	0	0	0	0	0	45.83002065	0	0.002020505	0	0.004746175	0	106.7732996	0	0	0	0	0	2.706408128	0	3.58E-05	0	0.026587825	0	0	0	0	0.008707471	0	0	0	0
Nov-29	0	0.013725468	0	0	0	0	0	0	0	0	0	29.42940005	0	0.001293057	0	0.00303869	0	71.25075675	0	0	0	0	0	1.777982727	0	2.28E-05	0	0.01698244	0	0	0	0	0.00554422	0	0	0	0
Dec-29	0	0.002981445	0	0	0	0	0	0	0	0	0	17.5758171	0	0.0006020547	0	0.001466103	0	146.3030476	0	0	0	0	0	2.605963656	0	6.95E-06	0	0.006866658	0	0	0	0	0.001488066	0	0	0	0
Jan-30	0	0.002270843	0	0	0	0	0	0	0	0	0	13.38677124	0	0.000458935	0	0.00111667	0	111.4329661	0	0	0	0	0	1.948454482	0	5.30E-06	0	0.005230049	0	0	0	0	0.001133398	0	0	0	0
Feb-30	0	0.002039669	0	0	0	0	0	0	0	0	0	12.02398541	0	0.001002992	0	0.001088959	0	100.0889859	0	0	0	0	0	1.782794438	0	4.76E-06	0	0.004697625	0	0	0	0	0.001801807	0	0	0	0
Mar-30	0	0.002286831	0	0	0	0	0	0	0	0	0	14.38102438	0	0.000462166	0	0.001214532	0	112.2175397	0	0	0	0	0	1.99882938	0	5.33E-06	0	0.02566872	0	0	0	0	0.001141378	0	0	0	0
Apr-30	0	0.002230838	0	0	0	0	0	0	0	0	0	13.15094219	0	0.00045985	0	0.001096998	0	109.469899	0	0	0	0	0	1.949888145	0	5.20E-06	0	0.005137913	0	0	0	0	0.001113432	0	0	0	0
May-30	0	0.004469617	0	0	0	0	0	0	0	0	0	2																									

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	F- Liquid (kMoles)	F- Solid (kMoles)	Fe+3 Liquid (kMoles)	Fe+3 Solid (kMoles)	Fe2O3 Liquid (kMoles)	Fe2O3 Solid (kMoles)	H+ Liquid (kMoles)	H+ Solid (kMoles)	H2O Liquid (kMoles)	H2O Solid (kMoles)	H2O2 Liquid (kMoles)	H2O2 Solid (kMoles)	HCl Liquid (kMoles)	HCl Solid (kMoles)	HF Liquid (kMoles)	HF Solid (kMoles)	Hg+2 Liquid (kMoles)	Hg+2 Solid (kMoles)	K+ Liquid (kMoles)	K+ Solid (kMoles)	K2O Liquid (kMoles)	K2O Solid (kMoles)	La+3 Liquid (kMoles)	La+3 Solid (kMoles)	La2O3 Liquid (kMoles)	La2O3 Solid (kMoles)	Li+ Liquid (kMoles)	Li+ Solid (kMoles)	Li2O Liquid (kMoles)	Li2O Solid (kMoles)	MnO Liquid (kMoles)	MnO Solid (kMoles)	Mg+2 Liquid (kMoles)	Mg+2 Solid (kMoles)	MgO Liquid (kMoles)	MgO Solid (kMoles)
Sep-28	3.868736777	0	0.076912978	0	0	0	0	0	18522.38586	0	0	0	0	0.008618101	0	30.53879057	0	0	0	0.001915463	0	0	0	0.069754963	0	0	0	0	0.077362882	0	0	0	0			
Oct-28	5.872326474	0	0.155445924	0	0	0	0	0	24674.43077	0	0	0	0	0.004817544	0	33.33002579	0	0	0	0.003999125	0	0	0	0.082176204	0	0	0	0	0.15976515	0	0	0	0			
Nov-28	5.228857276	0	0.138412698	0	0	0	0	0	21970.6921	0	0	0	0	0.004289654	0	29.67783699	0	0	0	0.003560915	0	0	0	0.07317162	0	0	0	0	0.1422558638	0	0	0	0			
Dec-28	5.733657813	0	0.151775256	0	0	0	0	0	24091.77068	0	0	0	0	0.004703783	0	32.54297315	0	0	0	0.003090469	0	0	0	0.080235702	0	0	0	0	0.155992468	0	0	0	0			
Jan-29	5.899967104	0	0.156177597	0	0	0	0	0	24790.57159	0	0	0	0	0.004840222	0	33.48690789	0	0	0	0.004017949	0	0	0	0.082563002	0	0	0	0	0.160517153	0	0	0	0			
Feb-29	5.645702378	0	0.149446974	0	0	0	0	0	23722.19819	0	0	0	0	0.004631626	0	32.04375756	0	0	0	0.003844791	0	0	0	0.07900487	0	0	0	0	0.153599513	0	0	0	0			
Mar-29	6.267031214	0	0.165894124	0	0	0	0	0	26332.90715	0	0	0	0	0.005141352	0	35.57028257	0	0	0	0.004267924	0	0	0	0.087699626	0	0	0	0	0.170503664	0	0	0	0			
Apr-29	6.331960777	0	0.16761287	0	0	0	0	0	26605.72918	0	0	0	0	0.005194619	0	35.9388084	0	0	0	0.004312141	0	0	0	0.088608238	0	0	0	0	0.172270167	0	0	0	0			
May-29	6.003355132	0	0.112282084	0	0	0	0	0	24731.93451	0	0	0	0	0.00310549	0	38.64046165	0	0	0	0.002098119	0	0	0	0.193880639	0	0	0	0	0.192450528	0	0	0	0			
Jun-29	7.349137724	0	0.094442755	0	0	0	0	0	29821.39925	0	0	0	0	0.00212345	0	51.5145889	0	0	0	0.000732823	0	0	0	0.338679383	0	0	0	0	0.262451096	0	0	0	0			
Jul-29	7.183607864	0	0.092315554	0	0	0	0	0	29149.71065	0	0	0	0	0.002075622	0	30.35428915	0	0	0	0.000716317	0	0	0	0.331051066	0	0	0	0	0.256539723	0	0	0	0			
Aug-29	7.45092581	0	0.09575082	0	0	0	0	0	30234.4359	0	0	0	0	0.002152861	0	52.22808369	0	0	0	0.000742973	0	0	0	0.343370209	0	0	0	0	0.266086134	0	0	0	0			
Sep-29	7.403225954	0	0.095137835	0	0	0	0	0	30040.87897	0	0	0	0	0.002139078	0	51.8937263	0	0	0	0.000738217	0	0	0	0.341171998	0	0	0	0	0.264382685	0	0	0	0			
Oct-29	7.882874512	0	0.1610170133	0	0	0	0	0	31987.20134	0	0	0	0	0.002277667	0	55.2558756	0	0	0	0.000786045	0	0	0	0.363276234	0	0	0	0	0.281511809	0	0	0	0			
Nov-29	5.163097669	0	0.073675587	0	0	0	0	0	21302.87647	0	0	0	0	0.001480844	0	35.28068256	0	0	0	0.00049975	0	0	0	0.231195599	0	0	0	0	0.179210971	0	0	0	0			
Dec-29	6.88387783	0	0.37704742	0	0	0	0	0	42164.66429	0	0	0	0	0.00158931	0	13.29184236	0	0	0	0.000114143	0	0	0	0.057784327	0	0	0	0	0.046807079	0	0	0	0			
Jan-30	5.243164358	0	0.287181389	0	0	0	0	0	32115.07677	0	0	0	0	0.001210512	0	10.12384529	0	0	0	0.869-05	0	0	0	0.044011926	0	0	0	0	0.035651011	0	0	0	0			
Feb-30	4.709405521	0	0.09575082	0	0	0	0	0	28845.73191	0	0	0	0	0.00108728	0	9.093228365	0	0	0	0.781-05	0	0	0	0.039531471	0	0	0	0	0.032021705	0	0	0	0			
Mar-30	5.280080258	0	0.289203366	0	0	0	0	0	32341.19156	0	0	0	0	0.001219035	0	10.19512493	0	0	0	0.875-05	0	0	0	0.044321804	0	0	0	0	0.035902022	0	0	0	0			
Apr-30	5.150797764	0	0.282122326	0	0	0	0	0	31549.31914	0	0	0	0	0.001189187	0	9.945497816	0	0	0	0.854-05	0	0	0	0.043236587	0	0	0	0	0.035022963	0	0	0	0			
May-30	6.052725626	0	0.170421396	0	0	0	0	0	27046.8567	0	0	0	0	0.001281734	0	13.82014193	0	0	0	0.00039655	0	0	0	0.08202065	0	0	0	0	0.110287068	0	0	0	0			
Jun-30	11.20415137	0	0.127693602	0	0	0	0	0	38379.37788	0	0	0	0	0.002237772	0	28.06836371	0	0	0	0.001079285	0	0	0	0.188153932	0	0	0	0	0.284727616	0	0	0	0			
Jul-30	9.698831614	0	0.110537488	0	0	0	0	0	33222.96454	0	0	0	0	0.001937119	0	24.29751011																				

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Mn+4 Liquid (kMoles)	Mn+4 Solid (kMoles)	MnO2 Liquid (kMoles)	MnO2 Solid (kMoles)	MnO4-Liquid (kMoles)	MnO4-Solid (kMoles)	Mo+6 Liquid (kMoles)	Mo+6 Solid (kMoles)	MoO3 Liquid (kMoles)	MoO3 Solid (kMoles)	Na+ Liquid (kMoles)	Na+ Solid (kMoles)	Na2O Liquid (kMoles)	Na2O Solid (kMoles)	Nd2O3 Liquid (kMoles)	Nd3 Liquid (kMoles)	NH3 Liquid (kMoles)	NH3 Solid (kMoles)	NH4+ Liquid (kMoles)	NH4+ Solid (kMoles)	Ni+2 Liquid (kMoles)	Ni+2 Solid (kMoles)	NiO Liquid (kMoles)	NiO Solid (kMoles)	NO2-Liquid (kMoles)	NO2-Solid (kMoles)	NO3-Liquid (kMoles)	NO3-Solid (kMoles)	O(BOUND) Liquid (kMoles)	O(BOUND) Solid (kMoles)	OH(BOUND) Liquid (kMoles)	OH(BOUND) Solid (kMoles)
Sep-28	0.076498621	0	0	0	0	0	0.062177017	0	0	0	2091.55421	0	0	0	0	0.016441956	0	0	0	0.118150133	0	0	0	382.3485824	0	633.1421421	0	0.035134046	0	0.733462884	0	
Oct-28	0.050660132	0	0	0	0	0	0.081834375	0	0	0	2806.963918	0	0	0	0	0.019475505	0	0	0	0.144365132	0	0	0	494.3222804	0	1019.094842	0	0.074802896	0	1.537673435	0	
Nov-28	0.04510897	0	0	0	0	0	0.072867248	0	0	0	2499.386533	0	0	0	0	0.017341447	0	0	0	0.1285461	0	0	0	440.1561568	0	907.4259584	0	0.066606254	0	1.370151067	0	
Dec-28	0.049463848	0	0	0	0	0	0.079901945	0	0	0	2740.68049	0	0	0	0	0.019015612	0	0	0	0.140956105	0	0	0	482.6493924	0	995.0300155	0	0.073036506	0	1.502427195	0	
Jan-29	0.050898586	0	0	0	0	0	0.082219564	0	0	0	2820.176101	0	0	0	0	0.019567175	0	0	0	0.145044648	0	0	0	496.6490207	0	1023.89165	0	0.075154988	0	1.546006287	0	
Feb-29	0.048705063	0	0	0	0	0	0.078676233	0	0	0	2698.637914	0	0	0	0	0.018723909	0	0	0	0.13879381	0	0	0	475.2454561	0	979.7660599	0	0.071916112	0	1.479379667	0	
Mar-29	0.054065221	0	0	0	0	0	0.087334821	0	0	0	2995.63237	0	0	0	0	0.020784539	0	0	0	0.154068543	0	0	0	527.5478423	0	0.079830726	0	1.642190454	0	1.642190454	0	
Apr-29	0.054625364	0	0	0	0	0	0.088239653	0	0	0	3026.668478	0	0	0	0	0.020999877	0	0	0	0.15566477	0	0	0	533.0135005	0	1098.8606664	0	0.080657812	0	1.659204365	0	
May-29	0.040245483	0	0	0	0	0	0.097458106	0	0	0	2848.606441	0	0	0	0	0.0281645	0	0	0	0.088172501	0	0	0	535.1283277	0	1128.174112	0	0.039710011	0	0.96001874	0	
Jun-29	0.038619208	0	0	0	0	0	0.132031482	0	0	0	3467.82699	0	0	0	0	0.042091437	0	0	0	0.053139796	0	0	0	682.5526119	0	1460.71304	0	0.041705628	0	0.609773691	0	
Jul-29	0.03774936	0	0	0	0	0	0.129057643	0	0	0	3389.718655	0	0	0	0	0.041143382	0	0	0	0.05194289	0	0	0	667.1789936	0	1427.812361	0	0.014374402	0	0.596039324	0	
Aug-29	0.039154098	0	0	0	0	0	0.1353860163	0	0	0	3515.857587	0	0	0	0	0.042674418	0	0	0	0.0538758	0	0	0	692.0062005	0	1480.944419	0	0.014909306	0	0.618219267	0	
Sep-29	0.038903438	0	0	0	0	0	0.133003208	0	0	0	3493.349525	0	0	0	0	0.042401222	0	0	0	0.053530894	0	0	0	687.5760669	0	1471.463605	0	0.014813858	0	0.614261508	0	
Oct-29	0.041423958	0	0	0	0	0	0.14162037	0	0	0	3719.680596	0	0	0	0	0.04514836	0	0	0	0.056999114	0	0	0	732.1235211	0	1566.79845	0	0.015773635	0	0.654058975	0	
Nov-29	0.026544188	0	0	0	0	0	0.090165317	0	0	0	2479.470282	0	0	0	0	0.028738411	0	0	0	0.036807206	0	0	0	485.4529587	0	1072.77879	0	0.010033293	0	0.416342681	0	
Dec-29	0.013694657	0	0	0	0	0	0.0239202	0	0	0	4990.72339	0	0	0	0	0.007384342	0	0	0	0.02992257	0	0	0	881.6472338	0	3214.908351	0	0.002299849	0	0.107442423	0	
Jan-30	0.010430653	0	0	0	0	0	0.018219025	0	0	0	3801.227106	0	0	0	0	0.005624347	0	0	0	0.022790781	0	0	0	671.5141476	0	2448.662411	0	0.017517	0	0.081858813	0	
Feb-30	0.009368802	0	0	0	0	0	0.016364311	0	0	0	3414.25863	0	0	0	0	0.005051783	0	0	0	0.020470658	0	0	0	603.153379	0	2199.386286	0	0.01573375	0	0.073525509	0	
Mar-30	0.010504092	0	0	0	0	0	0.018347301	0	0	0	3827.990661	0	0	0	0	0.005663947	0	0	0	0.02951246	0	0	0	676.2421224	0	2465.902873	0	0.001764033	0	0.082431561	0	
Apr-30	0.0102469	0	0	0	0	0	0.017898068	0	0	0	3734.262506	0	0	0	0	0.005525265	0	0	0	0.022389286	0	0	0	659.6843687	0	2405.525367	0	0.001720841	0	0.080416741	0	
May-30	0.011294076	0	0	0	0	0	0.058763558	0	0	0	3180.328072	0	0	0	0	0.014812602	0	0	0	0.033858274	0	0	0	594.9002484	0	1833.032064	0	0.004232972	0	0.364612164	0	
Jun-30	0.020035588	0	0	0	0	0	0.152754638	0	0	0	4479.304517	0	0	0	0	0.037116674	0	0	0	0.017414758	0	0	0	891.0689477	0	2234.890464	0	0.010412423	0	0.098762035	0	
Jul-30	0.017343732	0	0	0	0	0	0.132231479	0	0	0	3877.493158	0	0	0	0	0.032129909	0	0	0	0.061870298	0	0	0	771.3504931	0	1934.62455	0	0.009013475</td				

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	OH-Liquid (kMoles)	OH-Solid (kMoles)	P2O5 Liquid (kMoles)	P2O5 Solid (kMoles)	Pb+2 Liquid (kMoles)	Pb+2 Solid (kMoles)	PbO Liquid (kMoles)	PbO Solid (kMoles)	Pd+2 Liquid (kMoles)	Pd+2 Solid (kMoles)	PdO Liquid (kMoles)	PdO Solid (kMoles)	PO4-3 Liquid (kMoles)	PO4-3 Solid (kMoles)	Pr+3 Solid (kMoles)	Pr2O3 Liquid (kMoles)	Pr2O3 Solid (kMoles)	Pu+4 Liquid (kMoles)	Pu+4 Solid (kMoles)	Rb+ Liquid (kMoles)	Rb+ Solid (kMoles)	Rh+3 Liquid (kMoles)	Rh+3 Solid (kMoles)	Rb2O Liquid (kMoles)	Rb2O Solid (kMoles)	Rh2O3 Liquid (kMoles)	Rh2O3 Solid (kMoles)	Ru+3 Liquid (kMoles)	Ru+3 Solid (kMoles)	RuO2 Liquid (kMoles)	RuO2 Solid (kMoles)	Sb+5 Liquid (kMoles)	Sb+5 Solid (kMoles)
Sep-28	508.5376189	0	0	0	0.056268798	0	0	0.014183303	0	0	0	17.4886511	0	0.009633976	0	0	0	0	0.020665695	0	0.0041231	0	0	0	0	0.009670247	0	0	0	0.026037475	0		
Oct-28	617.8808049	0	0	0	0.050926827	0	0	0.027709112	0	0	0	26.04085108	0	0.017951871	0	0	0	0	0.035846383	0	0.008498602	0	0	0	0	0.022887787	0	0	0	0.039862861	0		
Nov-28	550.1755661	0	0	0	0.045346441	0	0	0	0.024672844	0	0	0	23.1873848	0	0.015984767	0	0	0	0.03191846	0	0.007567355	0	0	0	0	0.020379823	0	0	0	0.035494826	0		
Dec-28	603.2902156	0	0	0	0.049724245	0	0	0	0.027054791	0	0	0	25.42592444	0	0.017527957	0	0	0	0	0.03499909	0	0.008297917	0	0	0	0	0.022347317	0	0	0	0.038921542	0	
Jan-29	620.7891266	0	0	0	0.051166536	0	0	0	0.027839537	0	0	0	26.16342354	0	0.018036369	0	0	0	0.036015109	0	0.008538605	0	0	0	0	0.022995518	0	0	0	0.040050492	0		
Feb-29	594.0356253	0	0	0	0.048961465	0	0	0	0.026639766	0	0	0	25.03588578	0	0.017259074	0	0	0	0	0.034463003	0	0.008170625	0	0	0	0	0.022004505	0	0	0	0.038324478	0	
Mar-29	659.4112756	0	0	0	0.054349842	0	0	0	0.029571563	0	0	0	27.79117055	0	0.019158494	0	0	0	0	0.038255775	0	0.009069831	0	0	0	0	0.024426175	0	0	0	0.042542218	0	
Apr-29	666.2431046	0	0	0	0.054912933	0	0	0	0.029877939	0	0	0	28.0791091	0	0.019356986	0	0	0	0	0.038655213	0	0.009163799	0	0	0	0	0.024679243	0	0	0	0.042982976	0	
May-29	604.2979515	0	0	0	0.062556545	0	0	0	0.014630248	0	0	0	20.29779849	0	0.00950118	0	0	0	0	0.019106844	0	0.004739657	0	0	0	0	0.012969339	0	0	0	0.034305296	0	
Jun-29	714.5214175	0	0	0	0.086258262	0	0	0	0.005276809	0	0	0	19.01516431	0	0.003467401	0	0	0	0	0.007213161	0	0.00216031	0	0	0	0	0.006257706	0	0	0	0.036049385	0	
Jul-29	698.4277473	0	0	0	0.084315406	0	0	0	0.005157956	0	0	0	18.58687224	0	0.003389302	0	0	0	0	0.00705694	0	0.002111652	0	0	0	0	0.006116759	0	0	0	0.035274194	0	
Aug-29	724.417785	0	0	0	0.087452969	0	0	0	0.005349895	0	0	0	19.27853089	0	0.003515426	0	0	0	0	0.007031306	0	0.002190231	0	0	0	0	0.006344377	0	0	0	0.036548682	0	
Sep-29	719.7801567	0	0	0	0.086893106	0	0	0	0.005315645	0	0	0	19.15511224	0	0.003492922	0	0	0	0	0.007266249	0	0.002176209	0	0	0	0	0.006303761	0	0	0	0.036314702	0	
Oct-29	766.4140858	0	0	0	0.092522835	0	0	0	0.005660041	0	0	0	20.39615527	0	0.003719224	0	0	0	0	0.007737023	0	0.002317204	0	0	0	0	0.006712176	0	0	0	0.0386675	0	
Nov-29	494.7309243	0	0	0	0.058987893	0	0	0	0.003597336	0	0	0	14.14720158	0	0.002364483	0	0	0	0	0.004922056	0	0.001478065	0	0	0	0	0.00482496	0	0	0	0.024855828	0	
Dec-29	395.2307065	0	0	0	0.01882136	0	0	0	0.000711442	0	0	0	48.988494602	0	0.000493622	0	0	0	0	0.001155191	0	0.000500094	0	0	0	0	0.001559549	0	0	0	0.015840041	0	
Jan-30	301.0308441	0	0	0	0.01433545	0	0	0	0.000541876	0	0	0	37.31284925	0	0.000375972	0	0	0	0	0.000879861	0	0.000380901	0	0	0	0	0.001187844	0	0	0	0.012064702	0	
Feb-30	270.3856225	0	0	0	0.012876087	0	0	0	0.000486713	0	0	0	35.51436629	0	0.000373697	0	0	0	0	0.00079029	0	0.000342125	0	0	0	0	0.00106692	0	0	0	0.010836504	0	
Mar-30	303.1503322	0	0	0	0.014436382	0	0	0	0.000545691	0	0	0	37.57556034	0	0.000378619	0	0	0	0	0.000886056	0	0.000383583	0	0	0	0	0.00196207	0	0	0	0.02149647	0	
Apr-30	295.7277118	0	0	0	0.014082908	0	0	0	0.00053233	0	0	0	36.65552467	0	0.000369348	0	0	0	0	0.00864361	0	0.000374191	0	0	0	0	0.001166918	0	0	0	0.01852164	0	
May-30	369.7702334	0	0	0	0.023817816	0	0	0	0.000958515	0	0	0	29.54360688	0	0.000988855	0	0	0	0	0.004001846	0	0.003909926	0	0	0	0	0.01330263	0	0	0	0.01039928	0	
Jun-30	710.4229683	0	0	0	0.052561262	0	0	0	0.02162394	0	0	0	38.91750102	0	0.002477145	0	0	0	0	0.01088827	0	0.011282338	0	0	0	0	0.038614365	0	0	0	0.015137671	0	
Jul-30	614.9749784	0	0	0	0.04549946	0	0	0	0.001871868	0	0	0	33																				

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Sb2O3 Liquid (kMoles)	Sb2O3 Solid (kMoles)	Se+6 Liquid (kMoles)	Se+6 Solid (kMoles)	SeO2 Liquid (kMoles)	SeO2 Solid (kMoles)	Si+4 Liquid (kMoles)	Si+4 Solid (kMoles)	SiO2 Liquid (kMoles)	SiO2 Solid (kMoles)	SO4-2 Liquid (kMoles)	SO4-2 Solid (kMoles)	Sr+2 Liquid (kMoles)	Sr+2 Solid (kMoles)	SrO Liquid (kMoles)	SrO Solid (kMoles)	Ta+5 Liquid (kMoles)	Ta+5 Solid (kMoles)	Ta2O5 Liquid (kMoles)	Ta2O5 Solid (kMoles)	Tc+7 Liquid (kMoles)	Tc+7 Solid (kMoles)	Te+6 Liquid (kMoles)	Te+6 Solid (kMoles)	TeO2 Liquid (kMoles)	TeO2 Solid (kMoles)	Th+4 Liquid (kMoles)	Th+4 Solid (kMoles)	Ti+4 Liquid (kMoles)	Ti+4 Solid (kMoles)	TiO2 Liquid (kMoles)	TiO2 Solid (kMoles)	Tl2O Liquid (kMoles)		
Sep-28	0	0	0.033423364	0	0	0	2.230283181	0	0	0	25.85929248	0	0.00345758	0	0	0	0.003481938	0	0	0	0	0.008963407	0	0	0	0	0.532E-06	0	0	0	0.00484202	0	0	0	0
Oct-28	0	0	0.059455108	0	0	0	1.900301713	0	0	0	22.63675336	0	0.00753343	0	0	0	0.006810986	0	0	0	0	0.017599818	0	0	0	0	9.37E-06	0	0	0	0.008765739	0	0	0	0
Nov-28	0	0	0.059240223	0	0	0	1.692073232	0	0	0	20.15629632	0	0.006707943	0	0	0	0.006064662	0	0	0	0	0.015671291	0	0	0	0	8.35E-06	0	0	0	0.00780522	0	0	0	0
Dec-28	0	0	0.05805114	0	0	0	1.855428136	0	0	0	22.10221083	0	0.007355536	0	0	0	0.006650152	0	0	0	0	0.017184217	0	0	0	0	9.15E-06	0	0	0	0.008558746	0	0	0	0
Jan-29	0	0	0.059734959	0	0	0	1.9092463	0	0	0	22.74330298	0	0.007568889	0	0	0	0.006843045	0	0	0	0	0.017682659	0	0	0	0	9.42E-06	0	0	0	0.00886999	0	0	0	0
Feb-29	0	0	0.057160624	0	0	0	1.826965504	0	0	0	21.76315858	0	0.0072427	0	0	0	0.006548137	0	0	0	0	0.016920608	0	0	0	0	9.01E-06	0	0	0	0.008427453	0	0	0	0
Mar-29	0	0	0.063451346	0	0	0	2.0280293	0	0	0	24.15826854	0	0.008039784	0	0	0	0.007268782	0	0	0	0	0.018782779	0	0	0	0	1.00E-05	0	0	0	0.009354923	0	0	0	0
Apr-29	0	0	0.064108733	0	0	0	2.049040693	0	0	0	24.40856023	0	0.008123081	0	0	0	0.00734409	0	0	0	0	0.018977378	0	0	0	0	1.01E-05	0	0	0	0.009451845	0	0	0	0
May-29	0	0	0.082915942	0	0	0	2.708519926	0	0	0	18.18222816	0	0.004507635	0	0	0	0.003598001	0	0	0	0	0.009320885	0	0	0	0	4.96E-06	0	0	0	0.010135197	0	0	0	0
Jun-29	0	0	0.121918238	0	0	0	4.022023562	0	0	0	17.68383062	0	0.002572338	0	0	0	0.001301006	0	0	0	0	0.034132151	0	0	0	0	1.81E-06	0	0	0	0.01348991	0	0	0	0
Jul-29	0	0	0.119172187	0	0	0	3.931432663	0	0	0	17.28552512	0	0.002514399	0	0	0	0.001271703	0	0	0	0	0.03335492	0	0	0	0	1.77E-06	0	0	0	0.013186067	0	0	0	0
Aug-29	0	0	0.1253606848	0	0	0	4.077729973	0	0	0	17.92875776	0	0.002607966	0	0	0	0.001319025	0	0	0	0	0.03459613	0	0	0	0	1.83E-06	0	0	0	0.01367675	0	0	0	0
Sep-29	0	0	0.122815533	0	0	0	4.051624877	0	0	0	17.81398019	0	0.00259127	0	0	0	0.001310581	0	0	0	0	0.03437465	0	0	0	0	1.82E-06	0	0	0	0.013589193	0	0	0	0
Oct-29	0	0	0.130772644	0	0	0	4.314126122	0	0	0	18.96813244	0	0.002759156	0	0	0	0.001395493	0	0	0	0	0.03660175	0	0	0	0	1.94E-06	0	0	0	0.014469625	0	0	0	0
Nov-29	0	0	0.08939706	0	0	0	2.844924517	0	0	0	12.7881914	0	0.001857463	0	0	0	0.000886967	0	0	0	0	0.002326859	0	0	0	0	1.24E-06	0	0	0	0.009211382	0	0	0	0
Dec-29	0	0	0.262752643	0	0	0	4.58099706	0	0	0	31.11073691	0	0.00441795	0	0	0	0.000176897	0	0	0	0	0.00482482	0	0	0	0	3.43E-07	0	0	0	0.002405477	0	0	0	0
Jan-30	0	0	0.200127795	0	0	0	3.489155546	0	0	0	23.69575855	0	0.003364969	0	0	0	0.000134735	0	0	0	0	0.00367487	0	0	0	0	2.61E-07	0	0	0	0.001832152	0	0	0	0
Feb-30	0	0	0.179754598	0	0	0	3.135956247	0	0	0	21.28350816	0	0.003024214	0	0	0	0.000121019	0	0	0	0	0.00303076	0	0	0	0	2.35E-07	0	0	0	0.001645637	0	0	0	0
Mar-30	0	0	0.201536848	0	0	0	3.513721879	0	0	0	23.86259487	0	0.003388661	0	0	0	0.000135683	0	0	0	0	0.003070074	0	0	0	0	2.63E-07	0	0	0	0.001845052	0	0	0	0
Apr-30	0	0	0.196602229	0	0	0	3.427688579	0	0	0	23.27832046	0	0.003305369	0	0	0	0.000132361	0	0	0	0	0.00361013	0	0	0	0	2.57E-07	0	0	0	0.001799876	0	0	0	0
May-30	0	0	0.12081198	0	0	0	3.347521707	0	0	0	18.11010647	0	0.001857463	0	0	0	0.000108697	0	0	0	0	0.002326859	0	0	0	0	1.24E-06	0	0	0	0.009211382	0	0	0	0
Jun-30	0	0	0.095171631	0	0	0	5.403564564	0	0	0	22.74871838	0	0.004686543	0	0	0	0.00086462	0	0	0	0	0.02541827	0	0	0	0	8.36E-08	0	0	0	0.014486531</td				

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Tl2O Solid (kMoles)	Tl+3 Liquid (kMoles)	Tl+3 Solid (kMoles)	TOC Liquid (kMoles)	TOC Solid (kMoles)	V+5 Liquid (kMoles)	V+5 Solid (kMoles)	V2O5 Liquid (kMoles)	V2O5 Solid (kMoles)	W+6 Liquid (kMoles)	W+6 Solid (kMoles)	WO3 Liquid (kMoles)	WO3 Solid (kMoles)	Y+3 Liquid (kMoles)	Y+3 Solid (kMoles)	Y2O3 Liquid (kMoles)	Y2O3 Solid (kMoles)	Zn+2 Liquid (kMoles)	Zn+2 Solid (kMoles)	ZnO Liquid (kMoles)	ZnO Solid (kMoles)	Zr+4 Liquid (kMoles)	Zr+4 Solid (kMoles)	ZrO2 Liquid (kMoles)	ZrO2 Solid (kMoles)	
Sep-28	0	0.010548455	0	52.61208805	0	0.01205347	0	0	0.023584001	0	0	0	0.004854989	0	0	0	0.019948844	0	0	0	0.021867996	0	0	0	0	
Oct-28	0	0.018297057	0	73.61546813	0	0.020095463	0	0	0.053042913	0	0	0	0.01216427	0	0	0	0.021776845	0	0	0	0.010833854	0	0	0	0	
Nov-28	0	0.016292129	0	65.54894007	0	0.017893472	0	0	0.047230655	0	0	0	0.010831351	0	0	0	0.019390613	0	0	0	0.009646717	0	0	0	0	
Dec-28	0	0.017864992	0	71.87711819	0	0.019620931	0	0	0.051790362	0	0	0	0.011877024	0	0	0	0.021262608	0	0	0	0.010578024	0	0	0	0	
Jan-29	0	0.01838318	0	73.96197099	0	0.020190051	0	0	0.053292583	0	0	0	0.012221526	0	0	0	0.021879347	0	0	0	0.010884848	0	0	0	0	
Feb-29	0	0.01759094	0	70.7745091	0	0.019319942	0	0	0.050995888	0	0	0	0.011694828	0	0	0	0.020936435	0	0	0	0.010415755	0	0	0	0	
Mar-29	0	0.019526883	0	78.56348564	0	0.021446167	0	0	0.056608159	0	0	0	0.012981883	0	0	0	0.023240562	0	0	0	0.011562044	0	0	0	0	
Apr-29	0	0.019729191	0	79.37744246	0	0.02166836	0	0	0.057194648	0	0	0	0.013116382	0	0	0	0.023481345	0	0	0	0.011681833	0	0	0	0	
May-29	0	0.009767963	0	54.787877435	0	0.035963703	0	0	0.029847721	0	0	0	0.007280064	0	0	0	0.01967265	0	0	0	0.00946184	0	0	0	0	
Jun-29	0	0.003714572	0	48.18976726	0	0.058247808	0	0	0	0.014053771	0	0	0	0.004156918	0	0	0	0.021693816	0	0	0	0.010094532	0	0	0	0
Jul-29	0	0.003630906	0	47.10435483	0	0.056935851	0	0	0	0.013737228	0	0	0	0.004063288	0	0	0	0.02120519	0	0	0	0.009867166	0	0	0	0
Aug-29	0	0.00376602	0	48.85721212	0	0.050905456	0	0	0	0.014248421	0	0	0	0.004214492	0	0	0	0.021994283	0	0	0	0.010234345	0	0	0	0
Sep-29	0	0.003741911	0	48.54443461	0	0.0586765	0	0	0	0.014157204	0	0	0	0.004187512	0	0	0	0.021853478	0	0	0	0.010168826	0	0	0	0
Oct-29	0	0.009384346	0	51.689586222	0	0.0624781	0	0	0	0.015074437	0	0	0	0.004485817	0	0	0	0.022369346	0	0	0	0.010827656	0	0	0	0
Nov-29	0	0.002533228	0	33.11637437	0	0.039770385	0	0	0	0.009619152	0	0	0	0.002850949	0	0	0	0.014808154	0	0	0	0.006934612	0	0	0	0
Dec-29	0	0.000536454	0	16.8548673	0	0.01025904	0	0	0	0.003397872	0	0	0	0.001229794	0	0	0	0.003666785	0	0	0	0.003435512	0	0	0	0
Jan-30	0	0.000408595	0	12.83765367	0	0.007813885	0	0	0	0.002588018	0	0	0	0.000936683	0	0	0	0.002792838	0	0	0	0.002616687	0	0	0	0
Feb-30	0	0.000566999	0	11.53076851	0	0.007018424	0	0	0	0.002324555	0	0	0	0.000841328	0	0	0	0.002508525	0	0	0	0.002350306	0	0	0	0
Mar-30	0	0.000411472	0	12.9280406	0	0.007868901	0	0	0	0.00260624	0	0	0	0.000943278	0	0	0	0.002812502	0	0	0	0.00263511	0	0	0	0
Apr-30	0	0.000401397	0	12.6149819	0	0.007676231	0	0	0	0.002542426	0	0	0	0.0009180182	0	0	0	0.002743638	0	0	0	0.00250759	0	0	0	0
May-30	0	0.000811726	0	31.52992061	0	0.020853695	0	0	0	0.028118496	0	0	0	0.011939722	0	0	0	0.005387217	0	0	0	0.002774101	0	0	0	0
Jun-30	0	0.001898916	0	77.8412247	0	0.052394429	0	0	0	0.018134121	0	0	0	0.034757543	0	0	0	0.0124935	0	0	0	0.004847678	0	0	0	0
Jul-30	0	0.001643789	0	67.38296426	0	0.045355041	0	0	0	0.070412714	0	0	0	0.030087737	0	0	0	0.010814952	0	0	0	0.004196375	0	0	0	0
Aug-30	0	0.001659167	0	68.0133485	0	0.045779349	0	0	0	0.071071442	0	0	0	0.030369215	0	0	0	0.010916128	0	0	0	0.004235633	0	0	0	0
Sep-30	0	0.001596389	0	65.43992487	0	0.044047194	0	0	0	0.068382309	0	0	0	0.029220134	0	0	0	0.010503094	0	0	0	0.004075369	0	0	0	0
Oct-30	0	0.001655275	0	67.85381637	0	0.045671969	0	0	0	0.070904737	0	0	0	0.030297981	0	0	0	0.010890523	0	0	0	0.004225698	0	0	0	0
Nov-30	0	0.022581258	0	62.62839745	0	0.012454542	0	0	0	0.019054893	0	0	0	0.008191659	0	0	0	0.014629426	0	0	0	0.0653886093	0	0	0	0
Dec-30	0	0.024438032	0	64.95144674	0	0.011478754	0	0	0	0.017516021	0	0	0	0.007538314	0	0	0	0.015393666	0	0	0	0.070960557	0	0	0	0
Jan-31	0	0.024490091	0	65.0898099	0	0.011503207	0	0	0	0.017553334	0	0	0	0.007554372	0	0</td										

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Liquid Volume (kgal)	Solid Volume (kgal)	Total Volume (kgal)	Liquid Mass (kg)	Solid Mass (kg)	Total Mass (kg)	106-Ru Liquid (kMoles)	113m-Cd Liquid (kMoles)	113m-Cd Solid (kMoles)	125-Sb Liquid (kMoles)	126-Sn Liquid (kMoles)	126-Sn Solid (kMoles)	129-I Liquid (kMoles)	134-Cs Liquid (kMoles)	134-Cs Solid (kMoles)	137-Cs Liquid (kMoles)	137-Cs Solid (kMoles)	137m-Ba Liquid (kMoles)	137m-Ba Solid (kMoles)	14-C Liquid (kMoles)	14-C Solid (kMoles)	151-Sm Liquid (kMoles)	151-Sm Solid (kMoles)	152-Eu Liquid (kMoles)	152-Eu Solid (kMoles)	154-Eu Liquid (kMoles)	154-Eu Solid (kMoles)	155-Eu Liquid (kMoles)	155-Eu Solid (kMoles)	226-Ra Liquid (kMoles)	226-Ra Solid (kMoles)	227-Ac Liquid (kMoles)			
Mar-37	281.4	00:00:00	281.4	1.353E+06	0	1.353E+06	1.06E-19	0	6.11E-08	0	1.26E-11	0:00:00	0:05:3.5	0	0.005133455	0	2.73E-13	0	0.004638175	0	7.07E-10	0	7.03E-05	0	0.000241772	0	1.77E-09	0	1.24E-08	0	5.61E-10	0	7.54E-11	0	2.07E-10
Apr-37	272.0	00:00:00	272.0	1.308E+06	0	1.308E+06	1.02E-19	0	5.91E-08	0	1.21E-11	0:00:00	0:05:1.7	0	0.004962013	0	2.64E-13	0	0.004483274	0	6.83E-10	0	6.79E-05	0	0.000236989	0	1.71E-09	0	1.20E-08	0	5.42E-10	0	7.29E-11	0	2.00E-10
May-37	90.9	00:00:00	90.9	4.371E+05	0	4.371E+05	3.42E-20	0	1.98E-08	0	4.06E-12	0:00:00	0:01:7.3	0	0.001658429	0	8.81E-14	0	0.001498423	0	2.28E-10	0	2.27E-05	0	7.81E-05	0	5.72E-10	0	4.01E-09	0	1.81E-10	0	2.44E-11	0	6.70E-11
Feb-38	122.0	00:00:00	122.0	5.826E+05	0	5.826E+05	1.59E-20	0	2.06E-08	0	3.32E-12	0:00:00	0:02:4.0	0	0.001930814	0	6.67E-14	0	0.002281168	0	3.47E-10	0	4.00E-05	0	8.94E-05	0	5.07E-10	0	4.59E-09	0	1.81E-10	0	2.65E-11	0	1.21E-10
Mar-38	281.4	00:00:00	281.4	1.344E+06	0	1.344E+06	3.66E-20	0	4.75E-08	0	7.66E-12	0:00:00	0:05:5.5	0	0.004455115	0	1.54E-13	0	0.005263514	0	8.02E-10	0	9.24E-05	0	0.000206296	0	1.17E-09	0	1.06E-08	0	4.18E-10	0	6.12E-11	0	2.79E-10
Apr-38	272.2	00:00:00	272.2	1.301E+06	0	1.301E+06	3.54E-20	0	4.60E-08	0	7.41E-12	0:00:00	0:05:3.7	0	0.004310368	0	1.49E-13	0	0.005092501	0	7.76E-10	0	8.94E-05	0	0.000199593	0	1.13E-09	0	1.02E-08	0	5.92E-11	0	2.70E-10		
May-38	280.9	00:00:00	280.9	1.342E+06	0	1.342E+06	3.65E-20	0	4.74E-08	0	7.64E-12	0:00:00	0:05:5.4	0	0.004447202	0	1.54E-13	0	0.005254165	0	8.00E-10	0	9.22E-05	0	0.000205929	0	1.17E-09	0	1.06E-08	0	4.17E-10	0	6.11E-11	0	2.78E-10
Jun-38	9.2	00:00:00	9.2	4.392E+04	0	4.392E+04	1.20E-21	0	1.55E-09	0	2.50E-13	0:00:00	2.10E-05	0	0.000145562	0	5.03E-15	0	0.000171975	0	2.62E-11	0	3.02E-06	0	6.74E-06	0	3.82E-11	0	1.37E-11	0	2.00E-12	0	9.11E-12		
Aug-39	57.0	00:00:00	57.0	2.700E+05	0	2.700E+05	3.96E-21	0	4.49E-09	0	2.44E-12	0:00:00	6.26E-05	0	0.000272513	0	5.48E-14	0	0.000687755	0	1.05E-10	0	1.45E-05	0	1.71E-05	0	1.05E-05	0	1.21E-09	0	4.00E-11	0	6.03E-12	0	2.22E-11
Sep-39	271.9	00:00:00	271.9	1.289E+06	0	1.289E+06	1.89E-20	0	2.14E-08	0	1.17E-11	0:00:00	0:02:5.8	0	0.002517255	0	2.61E-13	0	0.003280938	0	5.00E-10	0	6.94E-05	0	8.17E-05	0	5.03E-10	0	5.76E-09	0	1.91E-10	0	2.88E-11	0	1.06E-10
Oct-39	281.4	00:00:00	281.4	1.334E+06	0	1.334E+06	1.95E-20	0	2.22E-08	0	1.21E-11	0:00:00	0:02:6.7	0	0.002605174	0	2.71E-13	0	0.00339553	0	5.17E-10	0	7.18E-05	0	8.45E-05	0	5.21E-10	0	5.96E-09	0	1.98E-10	0	2.98E-11	0	1.10E-10
Nov-39	271.9	00:00:00	271.9	1.289E+06	0	1.289E+06	1.89E-20	0	2.14E-08	0	1.17E-11	0:00:00	0:02:5.8	0	0.002517255	0	2.61E-13	0	0.003280938	0	5.00E-10	0	6.94E-05	0	8.17E-05	0	5.03E-10	0	5.76E-09	0	1.91E-10	0	2.88E-11	0	1.06E-10
Dec-39	112.4	00:00:00	112.4	5.327E+05	0	5.327E+05	7.81E-21	0	8.86E-09	0	4.82E-12	0:00:00	0:10:7	0	0.001040638	0	1.08E-13	0	0.00356347	0	2.07E-09	0	2.87E-05	0	2.08E-10	0	7.90E-11	0	1.19E-11	0	4.38E-11				
Mar-40	63.0	00:00:00	63.0	2.991E+05	0	2.991E+05	2.72E-22	0	2.04E-09	0	3.31E-13	0:00:00	2.18E-05	0	0.000464665	0	5.66E-15	0	0.000469055	0	7.14E-11	0	1.82E-05	0	3.57E-06	0	2.28E-11	0	4.09E-10	0	1.11E-11	0	2.66E-12	0	1.38E-11
Apr-40	271.9	00:00:00	271.9	1.291E+06	0	1.291E+06	1.88E-21	0	8.82E-09	0	4.82E-12	0:00:00	9.40E-05	0	0.002006107	0	2.04E-14	0	0.002025128	0	3.08E-10	0	7.86E-05	0	1.54E-05	0	9.85E-11	0	1.77E-09	0	4.80E-11	0	1.15E-11	0	5.98E-11
May-40	281.3	00:00:00	281.3	1.336E+06	0	1.336E+06	1.22E-21	0	9.13E-09	0	1.48E-12	0:00:00	9.73E-05	0	0.002075724	0	2.53E-14	0	0.002095405	0	3.19E-10	0	8.13E-05	0	1.60E-05	0	1.02E-10	0	1.83E-09	0	4.96E-11	0	6.18E-11		
Jun-40	272.4	00:00:00	272.4	1.294E+06	0	1.294E+06	1.18E-21	0	8.84E-09	0	4.83E-12	0:00:00	9.42E-05	0	0.002099795	0	2.45E-14	0	0.002028851	0	3.09E-10	0	7.88E-05	0	1.55E-05	0	1.77E-09	0	4.80E-11	0	1.15E-11	0	5.99E-11		
Jul-40	54.0	00:00:00	54.0	5.264E+05	0	5.264E+05	2.34E-22	0	1.75E-09	0	2.84E-13	0:00:00	1.87E-05	0	0.003998271	0	4.85E-15	0	0.000402048	0	6.12E-11	0	1.56E-05	0	3.51E-10	0	9.52E-12	0	1.19E-11	0	2.28E-12	0			

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	227-Ac Solid (kMoles)	228-Ra Liquid (kMoles)	228-Ra Solid (kMoles)	229-Th Liquid (kMoles)	229-Th Solid (kMoles)	231-Pa Liquid (kMoles)	231-Pa Solid (kMoles)	232-Th Liquid (kMoles)	232-U Liquid (kMoles)	232-U Solid (kMoles)	233-U Liquid (kMoles)	234-U Liquid (kMoles)	235-U Solid (kMoles)	236-U Liquid (kMoles)	236-U Solid (kMoles)	237-Np Liquid (kMoles)	237-Np Solid (kMoles)	238-Pu Liquid (kMoles)	238-Pu Solid (kMoles)	238-U Liquid (kMoles)	238-U Solid (kMoles)	239-Pu Liquid (kMoles)	239-Pu Solid (kMoles)	240-Pu Liquid (kMoles)	240-Pu Solid (kMoles)	241-Am Liquid (kMoles)	241-Am Solid (kMoles)	241-Pu Liquid (kMoles)	241-Pu Solid (kMoles)				
Mar-37	0	8.28E-12	0	9.46E-09	0	4.90E-07	0	0.020806102	0	1.59E-10	0	2.20E-05	0	4.90E-05	0	0.005785735	0	0.000122	0	0.000189957	0	5.71E-08	0	1.08449741	0	0.000264781	0	1.49E-05	0	1.84E-05	0	8.31E-08	0
Apr-37	0	8.01E-12	0	9.15E-09	0	4.74E-07	0	0.020111241	0	1.53E-10	0	2.13E-05	0	4.74E-05	0	0.005592508	0	0.000117925	0	0.000183613	0	5.52E-08	0	0.048232354	0	0.000255938	0	1.44E-05	0	1.78E-05	0	8.03E-08	0
May-37	0	2.68E-12	0	3.06E-09	0	1.58E-07	0	0.006721681	0	5.12E-11	0	7.11E-06	0	1.58E-05	0	0.001869157	0	3.94E-05	0	6.14E-05	0	1.84E-08	0	0.350345557	0	8.55E-05	0	4.80E-06	0	5.94E-08	0	2.69E-08	0
Feb-38	0	3.08E-12	0	2.78E-09	0	2.90E-07	0	0.00736893	0	5.17E-11	0	7.48E-06	0	1.68E-05	0	0.001962999	0	5.02E-05	0	6.86E-05	0	2.40E-08	0	0.317222335	0	8.70E-05	0	5.14E-06	0	8.12E-06	0	3.23E-08	0
Mar-38	0	7.10E-12	0	6.41E-09	0	6.70E-07	0	0.017002901	0	1.19E-10	0	1.73E-05	0	3.87E-05	0	0.004529378	0	0.000115937	0	0.000158212	0	5.54E-08	0	0.731951536	0	0.000200749	0	1.19E-05	0	1.87E-05	0	7.46E-08	0
Apr-38	0	6.87E-12	0	6.20E-09	0	6.48E-07	0	0.016450472	0	1.15E-10	0	1.67E-05	0	3.74E-05	0	0.004382218	0	0.000112171	0	0.000153072	0	5.36E-08	0	0.70817024	0	0.000194227	0	1.15E-05	0	1.81E-05	0	7.22E-08	0
May-38	0	7.08E-12	0	6.40E-09	0	6.69E-07	0	0.0169727	0	1.19E-10	0	1.72E-05	0	3.86E-05	0	0.000452133	0	0.000115731	0	0.000157931	0	5.53E-08	0	0.730651445	0	0.000200393	0	1.18E-05	0	1.87E-05	0	7.44E-08	0
Jun-38	0	2.32E-13	0	2.09E-10	0	2.19E-08	0	0.000555538	0	3.90E-12	0	5.64E-07	0	1.26E-06	0	0.000147989	0	3.79E-06	0	5.17E-06	0	1.81E-09	0	0.023915129	0	6.56E-06	0	3.87E-07	0	6.12E-07	0	2.44E-09	0
Aug-39	0	7.30E-13	0	4.89E-10	0	5.18E-08	0	0.001679887	0	1.29E-11	0	2.10E-06	0	4.31E-06	0	0.000517666	0	9.80E-06	0	2.80E-05	0	5.75E-09	0	0.078149707	0	2.13E-05	0	1.29E-06	0	3.00E-06	0	7.57E-09	0
Sep-39	0	3.48E-12	0	2.33E-09	0	2.47E-07	0	0.008016301	0	6.15E-11	0	1.00E-05	0	2.05E-05	0	0.002470266	0	4.67E-05	0	0.000133687	0	2.74E-08	0	0.372924918	0	0.000101573	0	6.15E-06	0	1.43E-05	0	3.61E-08	0
Oct-39	0	3.61E-12	0	2.41E-09	0	2.56E-07	0	0.008296282	0	6.36E-11	0	1.04E-05	0	2.13E-05	0	0.002556544	0	4.84E-05	0	0.000138356	0	2.84E-08	0	0.385949869	0	0.000105121	0	6.37E-06	0	1.48E-05	0	3.74E-08	0
Nov-39	0	3.48E-12	0	2.33E-09	0	2.47E-07	0	0.008016301	0	6.15E-11	0	1.00E-05	0	2.05E-05	0	0.002470266	0	4.67E-05	0	0.000133687	0	2.74E-08	0	0.372924918	0	0.000101573	0	6.15E-06	0	1.43E-05	0	3.61E-08	0
Dec-39	0	1.44E-12	0	9.64E-10	0	1.02E-07	0	0.003313956	0	2.54E-11	0	4.14E-06	0	0.001021213	0	1.93E-05	0	5.53E-05	0	1.13E-08	0	0.154167954	0	4.20E-05	0	5.91E-06	0	1.49E-05	0	2.33E-08	0		
Mar-40	0	2.53E-13	0	9.41E-11	0	3.51E-08	0	0.000668797	0	7.88E-12	0	1.62E-06	0	2.99E-06	0	5.48E-06	0	3.83E-05	0	2.13E-09	0	0.054779746	0	1.37E-05	0	7.91E-07	0	1.39E-06	0	2.42E-09	0		
Apr-40	0	1.09E-12	0	4.06E-10	0	1.52E-07	0	0.002887505	0	3.40E-11	0	7.01E-06	0	1.29E-05	0	0.001598311	0	2.37E-05	0	0.000165285	0	9.18E-09	0	0.236509382	0	5.93E-05	0	3.41E-06	0	6.00E-06	0	1.04E-08	0
May-40	0	1.13E-12	0	4.21E-10	0	1.57E-07	0	0.002987708	0	3.52E-11	0	7.25E-06	0	1.34E-05	0	0.001653776	0	2.45E-05	0	0.00017021	0	9.50E-09	0	0.244716845	0	6.13E-05	0	3.53E-06	0	6.21E-06	0	1.08E-08	0
Jun-40	0	1.09E-12	0	4.07E-10	0	1.52E-07	0	0.002892813	0	3.41E-11	0	7.02E-06	0	1.29E-05	0	0.000165589	0	2.37E-05	0	0.0001601249	0	9.19E-09	0	0.236944141	0	5.94E-05	0	3.42E-06	0	6.01E-06	0	1.05E-08	0
Jul-40	0	2.17E-13	0	8.07E-11	0	3.01E-08	0	0.000573255	0	6.76E-12	0	1.39E-06	0	2.56E-06	0	3.28E-05	0	1.82E-09	0	0.046954068	0	1.18E-05	0	6.78E-07	0	2.07E-09	0	0.20E-08	0				
Dec-40	0	3.07E-12	0	1.32E-10	0	2.45E-07	0	0.006096891	0	6.16E-11	0	1.61E-06	0	3.42E-06	0	0.004041259	0	9.51E-07	0	1.42E-08	0	0.066611754	0	3.06E-05	0	2.33E-05	0	1.04E-08	0	2.04E-08	0		
Jan-41	0	6.33E-12	0	2.78E-10	0	5.16E-07	0	0.012833156	0	4.91E-11	0	1.30E-05	0	2.70E-06	0	0.000844597	0	2.00E-05	0	0.000182121	0	2.97E-08	0	0.140209011	0	6.44E-05	0	4.20E-06	0				

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	242-Cm Liquid (kMoles)	242-Cm Solid (kMoles)	242-Pu Liquid (kMoles)	242-Pu Solid (kMoles)	243-Am Liquid (kMoles)	243-Am Solid (kMoles)	243-Cm Liquid (kMoles)	243-Cm Solid (kMoles)	244-Cm Liquid (kMoles)	244-Cm Solid (kMoles)	3-H Liquid (kMoles)	3-H Solid (kMoles)	59-Ni Liquid (kMoles)	59-Ni Solid (kMoles)	60-Co Liquid (kMoles)	60-Co Solid (kMoles)	63-Ni Liquid (kMoles)	63-Ni Solid (kMoles)	79-Se Liquid (kMoles)	79-Se Solid (kMoles)	90-Sr Liquid (kMoles)	90-Y Liquid (kMoles)	90-Y Solid (kMoles)	93-Zr Liquid (kMoles)	93m-Nb Solid (kMoles)	99-Tc Liquid (kMoles)	99-Tc Solid (kMoles)	Ag+ Liquid (kMoles)	Ag+ Solid (kMoles)	Ag2O Liquid (kMoles)	Ag2O Solid (kMoles)	Al(OH)3 Liquid (kMoles)	Al(OH)3 Solid (kMoles)	Al2O3 Liquid (kMoles)			
Mar-37	1.02E-10	0	2.62E-07	0	1.77E-07	0	5.09E-10	0	4.64E-09	0	5.04E-08	0	0.000308685	0	1.18E-09	0	2.36E-05	0	0.000357136	0	0.00014626	0	3.71E-08	0	0.021084334	0	2.15E-07	0	0.045366198	0	0.006813309	0	0	0	0	0	0
Apr-37	9.89E-11	0	2.54E-07	0	1.71E-07	0	4.92E-10	0	4.49E-09	0	4.87E-08	0	0.000298376	0	1.14E-09	0	2.28E-05	0	0.000141375	0	3.59E-08	0	0.02038018	0	2.08E-07	0	0.043851102	0	0.006585765	0	0	0	0	0	0		
May-37	3.31E-11	0	8.47E-08	0	5.71E-08	0	1.64E-10	0	1.50E-09	0	1.63E-08	0	9.97E-05	0	3.81E-10	0	7.62E-06	0	0.000115377	0	4.73E-05	0	1.20E-08	0	0.006811567	0	6.94E-08	0	0.014656139	0	0.002201128	0	0	0	0	0	0
Feb-38	3.97E-11	0	8.32E-08	0	8.24E-08	0	2.22E-10	0	1.99E-09	0	1.67E-08	0	0.000154311	0	4.79E-10	0	1.15E-05	0	0.000135599	0	8.66E-05	0	2.20E-08	0	0.009540352	0	9.84E-08	0	0.019614419	0	0.003321252	0	0	0	0	0	0
Mar-38	9.16E-11	0	1.92E-07	0	1.90E-07	0	5.12E-10	0	4.59E-09	0	3.85E-08	0	0.000356053	0	1.11E-09	0	2.66E-05	0	0.000312878	0	5.07E-08	0	0.02201319	0	2.27E-07	0	0.045257859	0	0.007663381	0	0	0	0	0	0		
Apr-38	8.87E-11	0	1.86E-07	0	1.84E-07	0	4.95E-10	0	4.44E-09	0	3.72E-08	0	0.000344485	0	1.07E-09	0	2.57E-05	0	0.000193271	0	4.91E-08	0	0.021297975	0	2.20E-07	0	0.04378742	0	0.007414396	0	0	0	0	0	0		
May-38	9.15E-11	0	1.92E-07	0	1.90E-07	0	5.11E-10	0	4.58E-09	0	3.84E-08	0	0.000355421	0	1.10E-09	0	2.66E-05	0	0.000312322	0	5.06E-08	0	0.02197409	0	2.27E-07	0	0.045177473	0	0.00764977	0	0	0	0	0	0		
Jun-38	2.99E-12	0	6.27E-09	0	6.21E-09	0	1.67E-11	0	1.50E-10	0	1.26E-09	0	1.16E-05	0	3.61E-11	0	8.69E-07	0	1.02E-05	0	6.53E-06	0	0.000719239	0	7.42E-09	0	0.001478715	0	0.000250386	0	0	0	0	0	0		
Aug-39	9.56E-12	0	1.65E-08	0	3.35E-08	0	4.67E-11	0	4.14E-10	0	6.71E-09	0	4.62E-05	0	1.06E-10	0	3.72E-06	0	4.88E-05	0	1.76E-05	0	0.002478337	0	2.63E-08	0	0.006397767	0	0.000605249	0	0	0	0	0	0		
Sep-39	4.56E-11	0	7.87E-08	0	1.60E-07	0	2.23E-10	0	1.97E-09	0	3.20E-08	0	0.000220664	0	5.05E-10	0	1.77E-05	0	0.000232988	0	8.38E-05	0	2.13E-08	0	0.011826449	0	1.25E-07	0	0.030529694	0	0.002888205	0	0	0	0	0	0
Oct-39	4.72E-11	0	8.14E-08	0	1.65E-07	0	2.31E-10	0	2.04E-09	0	3.31E-08	0	0.000228371	0	5.23E-10	0	1.84E-05	0	0.000241125	0	8.67E-05	0	2.20E-08	0	0.012239505	0	1.30E-07	0	0.031595989	0	0.00289908	0	0	0	0	0	0
Nov-39	4.56E-11	0	7.87E-08	0	1.60E-07	0	2.23E-10	0	1.97E-09	0	3.20E-08	0	0.000220664	0	5.05E-10	0	1.77E-05	0	0.000232988	0	8.38E-05	0	2.13E-08	0	0.011826449	0	1.25E-07	0	0.030529694	0	0.002888205	0	0	0	0	0	0
Dec-39	1.89E-11	0	3.25E-08	0	6.61E-08	0	9.21E-11	0	8.16E-10	0	1.32E-08	0	9.12E-05	0	2.09E-10	0	7.34E-06	0	9.63E-05	0	8.80E-09	0	0.01262104	0	5.18E-08	0	0.0019399	0	0	0	0	0	0				
Mar-40	4.78E-12	0	3.98E-09	0	1.76E-08	0	1.79E-11	0	1.54E-10	0	6.71E-09	0	3.94E-05	0	4.82E-11	0	3.51E-06	0	5.40E-05	0	1.37E-05	0	3.47E-09	0	0.000227117	0	1.32E-08	0	0.005628855	0	0.00164222	0	0	0	0	0	0
Apr-40	2.06E-11	0	1.72E-08	0	7.78E-08	0	6.65E-10	0	2.90E-08	0	0.000170062	0	2.08E-10	0	1.52E-05	0	0.000230007	0	5.90E-05	0	0.000298031	0	5.70E-08	0	0.024302358	0	0.000709012	0	0	0	0	0	0				
May-40	2.13E-11	0	1.78E-08	0	7.85E-08	0	7.99E-11	0	6.88E-10	0	3.00E-08	0	0.000175963	0	2.15E-10	0	1.57E-05	0	0.000241093	0	6.10E-05	0	1.55E-08	0	0.005481886	0	5.90E-08	0	0.02514571	0	0.000733616	0	0	0	0	0	0
Jun-40	2.07E-11	0	1.72E-08	0	7.60E-08	0	7.74E-11	0	6.66E-10	0	2.90E-08	0	0.000170374	0	2.09E-10	0	1.52E-05	0	0.000233435	0	5.91E-05	0	1.50E-08	0	0.024347031	0	0.000710151	0	0	0	0	0	0				
Jul-40	4.09E-12	0	3.41E-09	0	1.51E-08	0	1.32E-11	0	5.75E-09	0	3.38E-05	0	4.13E-11	0	3.01E-06	0	4.63E-05	0	1.17E-05	0	0.001051815	0	1.13E-08	0	0.004824733	0	0.00014076	0	0	0	0	0	0				
Dec-40	1.90E-11	0	1.34E-08	0	3.54E-07	0	1.09E-09	0	0.000267301	0	1.29E-10	0	2.19E-05	0	0.000111964	0	6.88E-05	0	1.75E-08	0	0.01173485	0	7.96E-08	0	0.001063549	0</											

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Al2O3 Solid (kMoles)	Al(OH)4-Liquid (kMoles)	Al(OH)4-Solid (kMoles)	Al+3 Liquid (kMoles)	Al+3 Solid (kMoles)	AlOOH Liquid (kMoles)	AlOOH Solid (kMoles)	As+5 Liquid (kMoles)	As+5 Solid (kMoles)	As2O5 Liquid (kMoles)	As2O5 Solid (kMoles)	B+3 Liquid (kMoles)	B+3 Solid (kMoles)	B2O3 Liquid (kMoles)	B2O3 Solid (kMoles)	BaO Liquid (kMoles)	BaO Solid (kMoles)	Ba+2 Liquid (kMoles)	Ba+2 Solid (kMoles)	Be+2 Liquid (kMoles)	Be+2 Solid (kMoles)	BeO Liquid (kMoles)	BeO Solid (kMoles)	Bi+3 Liquid (kMoles)	Bi+3 Solid (kMoles)	C2O4-2 Liquid (kMoles)	C2O4-2 Solid (kMoles)	Ca+2 Liquid (kMoles)	Ca+2 Solid (kMoles)	CaO Liquid (kMoles)	CaO Solid (kMoles)	Cd+2 Liquid (kMoles)	Cd+2 Solid (kMoles)	CdO Liquid (kMoles)			
Mar-37	0	103.6163389	0	0.007242988	0	0	0	0.068527928	0	0	0	0.652152289	0	0	0	0	0.005624346	0	0.022924583	0	0	0	0	0.073284003	0	0	0	0	9.520858272	0	1.507221047	0	0	0	0.074650173	0	0
Apr-37	0	100.1558622	0	0.007001094	0	0	0	0.066239299	0	0	0	0.630373247	0	0	0	0	0.00543651	0	0.022158971	0	0	0	0	0.070836536	0	0	0	0	9.202889999	0	0.456884359	0	0	0	0.07215708	0	0
May-37	0	33.4746025	0	0.002339941	0	0	0	0.022138836	0	0	0	0.210686257	0	0	0	0	0.001817018	0	0.007406084	0	0	0	0	0.023675348	0	0	0	0	3.075836779	0	0.486927312	0	0	0	0.024116707	0	0
Feb-38	0	37.35752019	0	0.000891485	0	0	0	0.020153681	0	0	0	0.282475972	0	0	0	0	0.002451266	0	0.007564247	0	0	0	0	0.020517609	0	0	0	0	4.262769253	0	0.704926667	0	0	0	0.028678978	0	0
Mar-38	0	86.19788471	0	0.002056992	0	0	0	0.046502142	0	0	0	0.651778575	0	0	0	0	0.005655994	0	0.017453569	0	0	0	0	0.047341861	0	0	0	0	9.835815941	0	1.626531613	0	0	0	0.066173216	0	0
Apr-38	0	83.39729295	0	0.00199016	0	0	0	0.044991275	0	0	0	0.630602119	0	0	0	0	0.005472229	0	0.016886498	0	0	0	0	0.045803711	0	0	0	0	9.516247717	0	1.573685177	0	0	0	0.064023231	0	0
May-38	0	86.04478011	0	0.002053338	0	0	0	0.046419545	0	0	0	0.650620886	0	0	0	0	0.005645948	0	0.017422568	0	0	0	0	0.047257772	0	0	0	0	9.818345576	0	1.623642569	0	0	0	0.066055679	0	0
Jun-38	0	2.816352518	0	6.72E-05	0	0	0	0.001519369	0	0	0	0.02129563	0	0	0	0	0.0000184799	0	0.000570262	0	0	0	0	0.001546806	0	0	0	0	0.321366645	0	0.005134383	0	0	0	0.00212084	0	0
Aug-39	0	14.51116064	0	4.56E-05	0	0	0	0.004137938	0	0	0	0.048278282	0	0	0	0	0.000500864	0	0.001449323	0	0	0	0	0.006112927	0	0	0	0	2.627809437	0	0.355192479	0	0	0	0.006109959	0	0
Sep-39	0	69.24624023	0	0.000217601	0	0	0	0.019745948	0	0	0	0.230380574	0	0	0	0	0.002390087	0	0.006916066	0	0	0	0	0.029248481	0	0	0	0	12.53972223	0	0.1694953586	0	0	0	0.029156298	0	0
Oct-39	0	71.664767	0	0.000225202	0	0	0	0.020435604	0	0	0	0.238426954	0	0	0	0	0.002473565	0	0.00715762	0	0	0	0	0.030270027	0	0	0	0	12.97769047	0	1.754152333	0	0	0	0.030174624	0	0
Nov-39	0	69.24624023	0	0.000217601	0	0	0	0.019745948	0	0	0	0.230380574	0	0	0	0	0.002390087	0	0.006916066	0	0	0	0	0.029248481	0	0	0	0	0.1694953586	0	0.029156298	0	0	0	0.021053275	0	0
Dec-39	0	28.6265429	0	9.00E-05	0	0	0	0.008163017	0	0	0	0.095239819	0	0	0	0	0.000988067	0	0.002859117	0	0	0	0	0.012091384	0	0	0	0	0.518947822	0	0.700697415	0	0	0	0.0212481	0	0
Mar-40	0	13.60609384	0	1.25E-05	0	0	0	0.000822335	0	0	0	0.012727397	0	0	0	0	0.000182435	0	0.000323992	0	0	0	0	0.007417152	0	0	0	0	0.2846900577	0	0.0376042075	0	0	0	0.01129829	0	0
Apr-40	0	58.4377023	0	5.40E-05	0	0	0	0.003503939	0	0	0	0.054950029	0	0	0	0	0.000787655	0	0.001437682	0	0	0	0	0.032023259	0	0	0	0	12.29138027	0	1.600232449	0	0	0	0.048779919	0	0
May-40	0	60.78232497	0	5.59E-05	0	0	0	0.003673607	0	0	0	0.056856932	0	0	0	0	0.000814989	0	0.001487573	0	0	0	0	0.033134546	0	0	0	0	12.7179217	0	1.65576449	0	0	0	0.050472703	0	0
Jun-40	0	58.8517551	0	5.41E-05	0	0	0	0.003556926	0	0	0	0.055051041	0	0	0	0	0.000781093	0	0.001440325	0	0	0	0	0.030281225	0	0	0	0	12.31397472	0	1.603174053	0	0	0	0.048869588	0	0
Jul-40	0	11.66236615	0	1.07E-05	0	0	0	0.000704859	0	0	0	0.010909197	0	0	0	0	0.000156373	0	0.000285422	0	0	0	0	0.006357559	0	0	0	0	2.440200495	0	0.317693207	0	0	0	0.009684249	0	0
Dec-40	0	27.9805267	0	0.000299111	0	0	0	0.002930203	0	0	0	0.113544154	0	0	0	0	0.00154578	0	0.001874967	0	0	0	0	0.006992997	0	0	0	0	7.269895504	0	0.981797519	0	0	0	0.068706475	0	0
Jan-41	0	57.66930977	0	0.000629589	0	0	0	0.006167692	0	0	0	0.238995562	0	0	0	0	0.003253664	0	0.00394656	0																	

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	CdO Solid (kMoles)	Ce+3 Liquid (kMoles)	Ce+3 Solid (kMoles)	Ce2O3 Liquid (kMoles)	Ce2O3 Solid (kMoles)	CH2Cl2 Liquid (kMoles)	CH2Cl2 Solid (kMoles)	CHCl3 Liquid (kMoles)	CHCl3 Solid (kMoles)	CHO2- Liquid (kMoles)	CHO2- Solid (kMoles)	CN- Liquid (kMoles)	CN- Solid (kMoles)	Co+3 Liquid (kMoles)	Co+3 Solid (kMoles)	CO3-2 Liquid (kMoles)	CoO Liquid (kMoles)	CoO Solid (kMoles)	Cr2O3 Liquid (kMoles)	Cr2O3 Solid (kMoles)	CrO4-2 Liquid (kMoles)	CrO4-2 Solid (kMoles)	CrOOH Liquid (kMoles)	CrOOH Solid (kMoles)	Cs+ Liquid (kMoles)	Cs+ Solid (kMoles)	Cs2O Liquid (kMoles)	Cs2O Solid (kMoles)	Cu+2 Liquid (kMoles)	Cu+2 Solid (kMoles)	CuO Liquid (kMoles)	CuO Solid (kMoles)				
Mar-37	0	0.021649105	0	0	0	0	0	0	0	0	0	85.96981962	0	0.000939006	0	0.024755851	0	461.6036912	0	0	0	16.7505702	0	0.062684657	0	0.035859612	0	0	0	0.037327982	0	0	0	0		
Apr-37	0	0.02092609	0	0	0	0	0	0	0	0	0	83.09868403	0	0.000907646	0	0.023929079	0	446.1875046	0	0	0	16.19115111	0	0.060591177	0	0.034662008	0	0	0	0.036081399	0	0	0	0		
May-37	0	0.006994024	0	0	0	0	0	0	0	0	0	27.7366551	0	0.000303358	0	0.007997699	0	149.1270608	0	0	0	5.411489008	0	0.020251092	0	0.011584913	0	0	0	0.012059289	0	0	0	0		
Feb-38	0	0.008052716	0	0	0	0	0	0	0	0	0	36.41800711	0	0.000108848	0	0.009348786	0	193.0205532	0	0	0	0	0	0.8660957113	0	0.003043887	0	0.018053783	0	0	0	0.021723817	0	0	0	0
Mar-38	0	0.018580652	0	0	0	0	0	0	0	0	0	84.03007377	0	0.000251153	0	0.021571175	0	445.3815776	0	0	0	0	0	19.98409367	0	0.007023394	0	0.014656885	0	0	0	0.0205125036	0	0	0	0
Apr-38	0	0.017976962	0	0	0	0	0	0	0	0	0	81.29991476	0	0.000242993	0	0.020870322	0	430.911014	0	0	0	0	0	19.33480525	0	0.006795202	0	0.040303442	0	0	0	0.048496461	0	0	0	0
May-38	0	0.018547649	0	0	0	0	0	0	0	0	0	83.88081964	0	0.000250707	0	0.02153286	0	444.5904914	0	0	0	0	0	19.94859794	0	0.007010919	0	0.041582894	0	0	0	0.050036004	0	0	0	0
Jun-38	0	0.000670788	0	0	0	0	0	0	0	0	0	2.745523404	0	8.21E-06	0	0.000704779	0	14.55199985	0	0	0	0	0	0.652942386	0	0.000229476	0	0.00136106	0	0	0	0.001637741	0	0	0	0
Aug-39	0	0.01068561	0	0	0	0	0	0	0	0	0	11.16811146	0	4.49E-05	0	0.001757816	0	120.6573339	0	0	0	0	0	6.7416301	0	0.000205282	0	0.005151566	0	0	0	0.003836405	0	0	0	0
Sep-39	0	0.007675942	0	0	0	0	0	0	0	0	0	53.29344415	0	0.000214353	0	0.008388176	0	575.76833	0	0	0	0	0	0.321705857	0	0.000966708	0	0.024582912	0	0	0	0.018307057	0	0	0	0
Oct-39	0	0.007944035	0	0	0	0	0	0	0	0	0	55.15479606	0	0.000221839	0	0.008681145	0	595.8778857	0	0	0	0	0	0.3329419076	0	0.001000472	0	0.0245441506	0	0	0	0.018946458	0	0	0	0
Nov-39	0	0.007675942	0	0	0	0	0	0	0	0	0	53.29344415	0	0.000214353	0	0.008388176	0	575.76833	0	0	0	0	0	0.3217058574	0	0.000966708	0	0.024582912	0	0	0	0.018307057	0	0	0	0
Dec-39	0	0.003173251	0	0	0	0	0	0	0	0	0	22.03162309	0	8.86E-05	0	0.00346769	0	238.0238515	0	0	0	0	0	0.1329938853	0	0.000399639	0	0.010162628	0	0	0	0.007568176	0	0	0	0
Mar-40	0	0.000429261	0	0	0	0	0	0	0	0	0	11.97264335	0	1.29E-05	0	0.000443221	0	113.9037832	0	0	0	0	0	6.177008355	0	0.003831514	0	0	0	0.001278347	0	0	0	0		
Apr-40	0	0.001853319	0	0	0	0	0	0	0	0	0	51.69141255	0	5.58E-05	0	0.00191359	0	491.77506538	0	0	0	0	0	26.66898845	0	0.043977609	0	0.01654241	0	0	0	0.005519213	0	0	0	0
May-40	0	0.001917633	0	0	0	0	0	0	0	0	0	53.48523297	0	5.77E-05	0	0.00197996	0	508.8408801	0	0	0	0	0	27.5944686	0	0.045503742	0	0.017116472	0	0	0	0.005710743	0	0	0	0
Jun-40	0	0.001856726	0	0	0	0	0	0	0	0	0	51.78643353	0	5.59E-05	0	0.001917107	0	492.6790621	0	0	0	0	0	26.71801233	0	0.044058451	0	0.016572819	0	0	0	0.005529358	0	0	0	0
Jul-40	0	0.000637938	0	0	0	0	0	0	0	0	0	10.26226573	0	1.11E-05	0	0.000379904	0	97.63181414	0	0	0	0	0	5.29457859	0	0.008730849	0	0.003284155	0	0	0	0.01095726	0	0	0	0
Dec-40	0	0.002436247	0	0	0	0	0	0	0	0	0	49.1923296	0	0.000122982	0	0.003358865	0	378.1268398	0	0	0	0	0	7.375347488	0	0.000933879	0	0	0	0.01746766	0	0	0	0		
Jan-41	0	0.00512798	0	0	0	0	0	0	0	0	0	41.08542698	0	0.00025886	0	0.00706997	0	795.9074362	0	0	0	0	0	15.52413977	0	0.00993293	0	0.019015132	0	0	0	0.036767134	0	0	0	0
Feb-41	0	0.004635256	0	0	0	0	0	0	0	0	0	37.13771692	0	0.000235987	0	0	0	719.4323445	0	0	0	0	0	14.03249644	0	0.0009033084	0	0	0	0.017188055	0	0	0	0		
Mar-41	0	0.00513710																																		

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	F- Liquid (kMoles)	F- Solid (kMoles)	Fe+3 Liquid (kMoles)	Fe+3 Solid (kMoles)	Fe2O3 Liquid (kMoles)	Fe2O3 Solid (kMoles)	H+ Liquid (kMoles)	H+ Solid (kMoles)	H2O Liquid (kMoles)	H2O Solid (kMoles)	H2O2 Liquid (kMoles)	H2O2 Solid (kMoles)	HCl Liquid (kMoles)	HCl Solid (kMoles)	HF Liquid (kMoles)	HF Solid (kMoles)	Hg+2 Liquid (kMoles)	Hg+2 Solid (kMoles)	K+ Liquid (kMoles)	K+ Solid (kMoles)	K2O Liquid (kMoles)	K2O Solid (kMoles)	La+3 Liquid (kMoles)	La+3 Solid (kMoles)	La2O3 Liquid (kMoles)	La2O3 Solid (kMoles)	Li+ Liquid (kMoles)	Li+ Solid (kMoles)	Li2O Liquid (kMoles)	Li2O Solid (kMoles)	MnO Liquid (kMoles)	MnO Solid (kMoles)	Mg+2 Liquid (kMoles)	Mg+2 Solid (kMoles)	MgO Liquid (kMoles)	MgO Solid (kMoles)
Mar-37	27.2284637	0	3.519275455	0	0	0	0	0	51947.87959	0	0	0	0	0.029514439	0	66.50650952	0	0	0	0.008337706	0	0	0	0.107671394	0	0	0	0	0	0.154365907	0	0	0	0		
Apr-37	26.31911422	0	3.40174215	0	0	0	0	0	50212.97534	0	0	0	0	0.028528744	0	64.28539044	0	0	0	0.008059252	0	0	0	0.10407549	0	0	0	0	0	0.149210546	0	0	0	0		
May-37	8.796508433	0	1.1369475791	0	0	0	0	0	16782.43642	0	0	0	0	0.009535022	0	21.48579069	0	0	0	0.002693604	0	0	0	0.034784641	0	0	0	0	0	0.04986909	0	0	0	0		
Feb-38	27.21224172	0	1.03931691	0	0	0	0	0	22488.06635	0	0	0	0	0.011257946	0	27.10039275	0	0	0	0.002626932	0	0	0	0.045453336	0	0	0	0	0	0.047647809	0	0	0	0		
Mar-38	62.78890199	0	2.398095984	0	0	0	0	0	51888.44817	0	0	0	0	0.025976325	0	62.53082426	0	0	0	0.006061323	0	0	0	0.104877985	0	0	0	0	0	0.10994146	0	0	0	0		
Apr-38	60.74887419	0	2.320181221	0	0	0	0	0	50202.57896	0	0	0	0	0.025132348	0	60.49918148	0	0	0	0.005864389	0	0	0	0.101470472	0	0	0	0	0	0.10636943	0	0	0	0		
May-38	62.67737641	0	2.393836489	0	0	0	0	0	51796.28396	0	0	0	0	0.025930186	0	62.41975708	0	0	0	0.006050557	0	0	0	0.104691701	0	0	0	0	0	0.109746182	0	0	0	0		
Jun-38	2.051508373	0	0.078353241	0	0	0	0	0	1695.256703	0	0	0	0	0.000884727	0	2.043076172	0	0	0	0.000198042	0	0	0	0.003426689	0	0	0	0	0	0.003592129	0	0	0	0		
Aug-39	15.57485553	0	0.217072988	0	0	0	0	0	10590.3398	0	0	0	0	0.002573761	0	8.047816535	0	0	0	0.000488791	0	0	0	0.008107295	0	0	0	0	0	0.010105965	0	0	0	0		
Sep-39	74.32211763	0	1.035857067	0	0	0	0	0	50536.35836	0	0	0	0	0.012281805	0	38.40361575	0	0	0	0.0023232478	0	0	0	0.03867443	0	0	0	0	0	0.048224955	0	0	0	0		
Oct-39	76.91792689	0	1.072035898	0	0	0	0	0	52301.41499	0	0	0	0	0.012710765	0	39.7449185	0	0	0	0.002413963	0	0	0	0.040038659	0	0	0	0	0	0.04990283	0	0	0	0		
Nov-39	74.32211763	0	1.035857067	0	0	0	0	0	50536.35836	0	0	0	0	0.012281805	0	38.40361575	0	0	0	0.002323478	0	0	0	0.03867443	0	0	0	0	0	0.048224955	0	0	0	0		
Dec-39	30.72492141	0	0.428225513	0	0	0	0	0	20891.83796	0	0	0	0	0.005077324	0	15.78163638	0	0	0	0.000964251	0	0	0	0.015993471	0	0	0	0	0	0.019936299	0	0	0	0		
Mar-40	18.68667524	0	0.21795118	0	0	0	0	0	11644.9892	0	0	0	0	0.002037077	0	6.266596156	0	0	0	0.000188557	0	0	0	0.002072094	0	0	0	0	0	0.002065101	0	0	0	0		
Apr-40	80.67897881	0	0.940995569	0	0	0	0	0	50276.77875	0	0	0	0	0.008795001	0	27.0578023	0	0	0	0.000598214	0	0	0	0.008946185	0	0	0	0	0	0.00891599	0	0	0	0		
May-40	83.47873978	0	0.973650452	0	0	0	0	0	52021.50786	0	0	0	0	0.009100209	0	27.99468301	0	0	0	0.000618973	0	0	0	0.00295564	0	0	0	0	0	0.009225396	0	0	0	0		
Jun-40	80.82728576	0	0.942725234	0	0	0	0	0	50369.1993	0	0	0	0	0.008811168	0	27.10551512	0	0	0	0.000599313	0	0	0	0.008962631	0	0	0	0	0	0.008932379	0	0	0	0		
Jul-40	16.01715021	0	0.186815297	0	0	0	0	0	9981.419311	0	0	0	0	0.001746066	0	5.371368133	0	0	0	0.000118763	0	0	0	0.001776081	0	0	0	0	0	0.001770086	0	0	0	0		
Dec-40	88.21932762	0	0.851361476	0	0	0	0	0	25267.88441	0	0	0	0	0.0020212362	0	15.12913245	0	0	0	0.001607072	0	0	0	0.017611632	0	0	0	0	0	0.005255545	0	0	0	0		
Jan-41	185.6901216	0	1.792004318	0	0	0	0	0	51385.58416	0	0	0	0	0.004254703	0	31.84484081	0	0	0	0.003382675	0	0	0	0.03719647	0	0	0	0	0	0.011062234	0	0	0	0		
Feb-41	167.8480103	0	1.619818849	0	0	0	0	0	48075.22554	0	0	0	0	0.003845888	0	28.78501625	0	0	0	0.003057649	0	0	0	0.033622432	0	0	0	0	0	0.009999314	0	0	0	0		
Mar-41	186.0205311	0	1.795192937	0	0	0	0	0	53280.22043	0	0	0	0	0.004262274	0	31.90150423	0	0	0	0.003388694	0	0	0	0.037262555	0	0	0	0	0	0.011081917	0	0	0	0		
Apr-41																																				

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Mn+4 Liquid (kMoles)	Mn+4 Solid (kMoles)	MnO2 Liquid (kMoles)	MnO2 Solid (kMoles)	MnO4-Liquid (kMoles)	MnO4-Solid (kMoles)	Mo+6 Liquid (kMoles)	Mo+6 Solid (kMoles)	MoO3 Liquid (kMoles)	MoO3 Solid (kMoles)	Na+ Liquid (kMoles)	Na+ Solid (kMoles)	Na2O Liquid (kMoles)	Na2O Solid (kMoles)	Nd2O3 Liquid (kMoles)	Nd3 Liquid (kMoles)	NH3 Liquid (kMoles)	NH3 Solid (kMoles)	NH4+ Liquid (kMoles)	NH4+ Solid (kMoles)	Ni+2 Liquid (kMoles)	Ni+2 Solid (kMoles)	NiO Liquid (kMoles)	NiO Solid (kMoles)	NO2-Liquid (kMoles)	NO2-Solid (kMoles)	NO3-Liquid (kMoles)	NO3-Solid (kMoles)	O(BOUND) Liquid (kMoles)	O(BOUND) Solid (kMoles)	OH(BOUND) Liquid (kMoles)	OH(BOUND) Solid (kMoles)
Mar-37	0.221365181	0	0	0	2.032058344	0	0.121329154	0	0	0	5970.330493	0	0	0	0.018823571	0	0.247004896	0	0	0	0.917261937	0	0	0	988.4833467	0	2534.35251	0	0.050496616	0	9.02489354	0
Apr-37	0.213972244	0	0	0	1.964193655	0	0.117277122	0	0	0	5770.939259	0	0	0	0.01819492	0	0.238755669	0	0	0	0.886628123	0	0	0	955.4709508	0	2449.712694	0	0.04881018	0	8.72348904	0
May-37	0.071514893	0	0	0	0.65648281	0	0.039196957	0	0	0	1928.792719	0	0	0	0.006081199	0	0.079798136	0	0	0	0.296333368	0	0	0	319.3423687	0	818.7554563	0	0.016313587	0	2.915608936	0
Feb-38	0.074250951	0	0	0	1.651962503	0	0.049469852	0	0	0	2600.521785	0	0	0	0.008898311	0	0.177941463	0	0	0	0.466160774	0	0	0	406.3052389	0	1067.808552	0	0.022972572	0	5.200341158	0
Mar-38	0.171324939	0	0	0	3.811700366	0	0.114145601	0	0	0	6000.384282	0	0	0	0.020531758	0	0.410570848	0	0	0	1.075608671	0	0	0	937.4993831	0	2463.836947	0	0.053006386	0	11.99914784	0
Apr-38	0.165758548	0	0	0	3.687857227	0	0.11043698	0	0	0	5805.430232	0	0	0	0.019864676	0	0.39723826	0	0	0	1.040661864	0	0	0	907.0397857	0	238.786242	0	0.051284194	0	11.60929239	0
May-38	0.170120632	0	0	0	3.804930028	0	0.113942855	0	0	0	5989.726406	0	0	0	0.02049529	0	0.40984878	0	0	0	1.073698176	0	0	0	935.8341977	0	2459.460682	0	0.052912236	0	11.9783496	0
Jun-38	0.005597718	0	0	0	0.124540085	0	0.003729491	0	0	0	196.0511843	0	0	0	0.000670836	0	0.01341486	0	0	0	0.035143475	0	0	0	30.63101556	0	80.50120268	0	0.001731883	0	0.392049414	0
Aug-39	0.014326305	0	0	0	0.26333142	0	0.010199773	0	0	0	1213.476401	0	0	0	0.001569883	0	0.041998619	0	0	0	0.101504786	0	0	0	172.1577447	0	450.0616339	0	0.00458439	0	1.05192544	0
Sep-39	0.068364121	0	0	0	1.256599055	0	0.048673555	0	0	0	5790.624228	0	0	0	0.007491373	0	0.200414465	0	0	0	0.484373716	0	0	0	82.15246764	0	2147.684008	0	0.021876387	0	5.205760914	0
Oct-39	0.070751838	0	0	0	1.300487625	0	0.05037355	0	0	0	5992.870294	0	0	0	0.00775302	0	0.207414235	0	0	0	0.50129118	0	0	0	850.2176339	0	2222.69503	0	0.022640452	0	5.201293004	0
Nov-39	0.068364121	0	0	0	1.256599055	0	0.048673555	0	0	0	5790.624228	0	0	0	0.007491373	0	0.200414465	0	0	0	0.484373716	0	0	0	82.15246764	0	2147.684008	0	0.021876387	0	5.205760914	0
Dec-39	0.028261873	0	0	0	0.51948072	0	0.020121751	0	0	0	239.856364	0	0	0	0.00309695	0	0.082851766	0	0	0	0.20241124	0	0	0	33.96200474	0	887.8517337	0	0.009043745	0	2.077660244	0
Mar-40	0.006827636	0	0	0	0.096229031	0	0.002832082	0	0	0	1336.070636	0	0	0	0.000491506	0	0.015678861	0	0	0	0.074212395	0	0	0	178.1463533	0	566.318174	0	0.001274889	0	0.384539769	0
Apr-40	0.02947805	0	0	0	0.415465021	0	0.010284542	0	0	0	5768.431951	0	0	0	0.000212205	0	0.06769286	0	0	0	0.32040907	0	0	0	769.1391098	0	2445.056244	0	0.05504284	0	1.660235193	0
May-40	0.030501011	0	0	0	0.429882689	0	0.010641442	0	0	0	5968.610868	0	0	0	0.002195697	0	0.07004197	0	0	0	0.33152806	0	0	0	795.8308728	0	2529.905769	0	0.005695296	0	1.718749478	0
Jun-40	0.029532327	0	0	0	0.416228744	0	0.010303448	0	0	0	5779.035686	0	0	0	0.002125957	0	0.067817295	0	0	0	0.320998057	0	0	0	770.536708	0	2449.550832	0	0.005514402	0	1.663287096	0
Jul-40	0.00585226	0	0	0	0.082842026	0	0.002041784	0	0	0	1145.203402	0	0	0	0.000421291	0	0.013439024	0	0	0	0.065610624	0	0	0	152.6968742	0	485.4155778	0	0.010919262	0	0.329605516	0
Dec-40	0.016691327	0	0	0	1.517259918	0	0.018988603	0	0	0	2706.998791	0	0	0	0.003804833	0	0.04644971	0	0	0	0.470019117	0	0	0	282.0251785	0	900.4886495	0	0.014890484	0	5.340517076	0
Jan-41	0.035113055	0	0	0	3.193633258	0	0.039968652	0	0	0	5697.878025	0	0	0	0.008086668	0	0.097705513	0	0	0	0.989328636	0	0	0	593.6051972	0	1895.410579	0	0.031342516	0	11.24108846	0
Feb-41	0.031757281	0	0	0	2.886771699	0	0.036128128	0	0	0	5150.395083	0	0	0	0.007239152	0	0.083762278	0	0	0	0.894268589	0	0	0	536.5683989	0	173.289278	0	0.028330598	0	10.16098387	0

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	OH- Liquid (kMoles)	OH- Solid (kMoles)	P2O5 Liquid (kMoles)	P2O5 Solid (kMoles)	Pb+2 Liquid (kMoles)	Pb+2 Solid (kMoles)	PbO Liquid (kMoles)	PbO Solid (kMoles)	Pd+2 Liquid (kMoles)	Pd+2 Solid (kMoles)	PdO Liquid (kMoles)	PdO Solid (kMoles)	PO4-3 Liquid (kMoles)	PO4-3 Solid (kMoles)	Pr+3 Solid (kMoles)	Pr2O3 Liquid (kMoles)	Pr2O3 Solid (kMoles)	Pu+4 Liquid (kMoles)	Pu+4 Solid (kMoles)	Rb+ Liquid (kMoles)	Rb+ Solid (kMoles)	Rh+3 Liquid (kMoles)	Rh+3 Solid (kMoles)	Rb2O Liquid (kMoles)	Rb2O Solid (kMoles)	Rh2O3 Liquid (kMoles)	Rh2O3 Solid (kMoles)	Ru+3 Liquid (kMoles)	Ru+3 Solid (kMoles)	RuO2 Liquid (kMoles)	RuO2 Solid (kMoles)	Sb+5 Liquid (kMoles)	Sb+5 Solid (kMoles)
Mar-37	984.2300255	0	0	0	0.204199794	0	0	0	0.049523585	0	0	0	45.6465128	0	0.000134759	0	0	0	0.000608959	0	0.013637257	0	0	0	0	0.001974574	0	0	0	0.019871328	0		
Apr-37	951.359676	0	0	0	0.19738013	0	0	0	0.047869645	0	0	0	44.1220554	0	0.000130258	0	0	0	0.000588621	0	0.013181813	0	0	0	0	0.00190863	0	0	0	0.019207685	0		
May-37	317.9682775	0	0	0	0.065969393	0	0	0	0.015999236	0	0	0	14.74669813	0	4.35E-05	0	0	0	0.000196732	0	0.004405693	0	0	0	0	0.000637912	0	0	0	0.00641969	0		
Feb-38	418.1474529	0	0	0	0.075026333	0	0	0	0.027187329	0	0	0	13.94078705	0	4.90E-05	0	0	0	0.000177259	0	0.007252421	0	0	0	0	0.000240979	0	0	0	0.010498219	0		
Mar-38	964.823836	0	0	0	0.173114038	0	0	0	0.062731418	0	0	0	32.16665208	0	0.000111312	0	0	0	0.000409004	0	0.016734069	0	0	0	0	0.000556029	0	0	0	0.02422335	0		
Apr-38	933.476458	0	0	0	0.167489517	0	0	0	0.060693258	0	0	0	31.2154917	0	0.000109445	0	0	0	0.000395715	0	0.016190375	0	0	0	0	0.000537964	0	0	0	0.023436327	0		
May-38	963.110117	0	0	0	0.172806553	0	0	0	0.062619994	0	0	0	32.10951771	0	0.000112919	0	0	0	0.000408277	0	0.016704346	0	0	0	0	0.000555042	0	0	0	0.024180324	0		
Jun-38	31.52379028	0	0	0	0.005656173	0	0	0	0.00204963	0	0	0	1.050984393	0	3.70E-06	0	0	0	0.000546754	0	0	0	0	0.0018205	0	0	0	0.000719452	0				
Aug-39	135.0163014	0	0	0	0.018922163	0	0	0	0.007278367	0	0	0	5.883639207	0	8.48E-05	0	0	0	4.00E-05	0	0.002120244	0	0	0	0	8.68E-05	0	0	0	0.002161146	0		
Sep-39	644.2883154	0	0	0	0.090295235	0	0	0	0.034731856	0	0	0	28.07631341	0	0.000404725	0	0	0	0.000191114	0	0.010117654	0	0	0	0	0.000414199	0	0	0	0.010312836	0		
Oct-39	666.7910323	0	0	0	0.093448929	0	0	0	0.035949497	0	0	0	29.05691994	0	0.000418861	0	0	0	0.000197789	0	0.010471028	0	0	0	0	0.000428665	0	0	0	0.010673027	0		
Nov-39	644.2883154	0	0	0	0.090295235	0	0	0	0.034731856	0	0	0	28.07631341	0	0.000404725	0	0	0	0.000191114	0	0.010117654	0	0	0	0	0.000414199	0	0	0	0.010312836	0		
Dec-39	266.3501591	0	0	0	0.037328242	0	0	0	0.014358223	0	0	0	11.06680764	0	0.000167314	0	0	0	0.000418266	0	0	0	0	0.000171231	0	0	0	0.004263348	0				
Mar-40	129.1865838	0	0	0	0.014414306	0	0	0	0.002433342	0	0	0	7.634922304	0	1.36E-05	0	0	0	0.000672315	0	0	0	0	0.0025E-05	0	0	0	0.000752174	0				
Apr-40	557.1579749	0	0	0	0.062233194	0	0	0	0.010505857	0	0	0	32.96347407	0	5.88E-05	0	0	0	5.79E-05	0	0.000290263	0	0	0	0	9.70E-05	0	0	0	0.003247481	0		
May-40	577.1153532	0	0	0	0.064392841	0	0	0	0.010870437	0	0	0	34.1073885	0	6.08E-05	0	0	0	5.99E-05	0	0.003003423	0	0	0	0	0.000100354	0	0	0	0.003360177	0		
Jun-40	558.7832393	0	0	0	0.062347594	0	0	0	0.01052517	0	0	0	33.02406869	0	5.89E-05	0	0	0	5.80E-05	0	0.0002908029	0	0	0	0	9.72E-05	0	0	0	0.003253451	0		
Jul-40	110.7313575	0	0	0	0.012355119	0	0	0	0.002085722	0	0	0	6.544219117	0	1.17E-05	0	0	0	1.15E-05	0	0.00057627	0	0	0	0	1.93E-05	0	0	0	0.000644721	0		
Dec-40	261.3289471	0	0	0	0.065005763	0	0	0	0.012417393	0	0	0	11.57292494	0	1.25E-05	0	0	0	0.000128296	0	0.008291333	0	0	0	0	6.14E-05	0	0	0	0.002410793	0		
Jan-41	550.603181	0	0	0	0.136832821	0	0	0	0.065764088	0	0	0	24.35949012	0	2.63E-05	0	0	0	0.000270045	0	0.01745217	0	0	0	0	0.000129266	0	0	0	0.00574404	0		
Feb-41	497.2101352	0	0	0	0.123685183	0	0	0	0.059445119	0	0	0	22.01889854	0	2.37E-05	0	0	0	0.000244098	0	0.015775271	0	0	0	0	0.000116845	0	0	0	0.00486828	0		
Mar-41	551.0419411	0	0	0	0.1307076295	0	0	0	0.065881106	0	0	0	24.4028344	0	2.63E-05	0	0	0	0.000270526	0	0.017483224	0	0	0	0	0.000129496	0	0	0	0.00583433	0		
Apr-41	102.7698114	0	0	0	0.025564851	0	0	0	0.012286885	0	0	0	4.551150289	0	4.90E-06	0	0	0	0.000260637	0	0.003260637	0	0	0	0	0.000948065	0	0	0	0.00094864	0		
Dec-41	122.802545	0	0	0	0.018681567	0	0</																										

Appendix A: Initial Composition Vector (continued)

Transfer Date Range	Sb2O3 Liquid (kMoles)	Sb2O3 Solid (kMoles)	Se+6 Liquid (kMoles)	Se+6 Solid (kMoles)	SeO2 Liquid (kMoles)	SeO2 Solid (kMoles)	Si+4 Liquid (kMoles)	Si+4 Solid (kMoles)	SiO2 Liquid (kMoles)	SiO2 Solid (kMoles)	SO4-2 Liquid (kMoles)	SO4-2 Solid (kMoles)	Sr+2 Liquid (kMoles)	Sr+2 Solid (kMoles)	SrO Liquid (kMoles)	SrO Solid (kMoles)	Ta+5 Liquid (kMoles)	Ta+5 Solid (kMoles)	Ta2O5 Liquid (kMoles)	Ta2O5 Solid (kMoles)	Tc+7 Liquid (kMoles)	Tc+7 Solid (kMoles)	Te+6 Liquid (kMoles)	Te+6 Solid (kMoles)	TeO2 Liquid (kMoles)	TeO2 Solid (kMoles)	Th+4 Liquid (kMoles)	Th+4 Solid (kMoles)	Ti+4 Liquid (kMoles)	Ti+4 Solid (kMoles)	TiO2 Liquid (kMoles)	TiO2 Solid (kMoles)	Tl2O Liquid (kMoles)
Mar-37	0	0	0.172873267	0	0	0	7.379334344	0	0	0	48.48916956	0	0.642507841	0	0	0	0.006985532	0	0	0	0	0.000124484	0	0	0	0	0	0	0	0	0	0	
Apr-37	0	0	0.167099815	0	0	0	7.13286584	0	0	0	46.8697759	0	0.62104995	0	0	0	0.006752236	0	0	0	0	0.000120327	0	0	0	0	0	0	0	0	0	0	
May-37	0	0	0.055848952	0	0	0	2.383989692	0	0	0	15.6650528	0	0.207570493	0	0	0	0.002256767	0	0	0	0	4.02E-05	0	0	0	0	8.16E-06	0	0	0	0	0	
Feb-38	0	0	0.091075532	0	0	0	3.471637839	0	0	0	23.35886938	0	0.494325166	0	0	0	0.0038513473	0	0	0	0	3.12E-05	0	0	0	0	1.13E-05	0	0	0	0	0	
Mar-38	0	0	0.210145591	0	0	0	8.010377473	0	0	0	53.89771911	0	1.140594544	0	0	0	0.008840653	0	0	0	0	7.19E-05	0	0	0	0	2.60E-05	0	0	0	0	0	
Apr-38	0	0	0.203317906	0	0	0	7.75011822	0	0	0	52.14656816	0	1.10353633	0	0	0	0.008553418	0	0	0	0	6.96E-05	0	0	0	0	2.52E-05	0	0	0	0	0	
May-38	0	0	0.209772331	0	0	0	7.996149449	0	0	0	53.80198604	0	1.138568621	0	0	0	0.00882495	0	0	0	0	7.18E-05	0	0	0	0	2.60E-05	0	0	0	0	0	
Jun-38	0	0	0.006866109	0	0	0	0.261723902	0	0	0	1.761005823	0	0.037266765	0	0	0	0.000288852	0	0	0	0	2.35E-06	0	0	0	0	8.50E-07	0	0	0	0	0	
Aug-39	0	0	0.025457295	0	0	0	2.810492057	0	0	0	14.58497606	0	0.097316963	0	0	0	0.001135623	0	0	0	0	0.000837425	0	0	0	0	2.68E-06	0	0	0	0	0	
Sep-39	0	0	0.121480423	0	0	0	13.41147087	0	0	0	69.59848223	0	0.464389719	0	0	0	0.005419113	0	0	0	0	0.003996134	0	0	0	0	1.28E-05	0	0	0	0	0	
Oct-39	0	0	0.125723306	0	0	0	13.87988621	0	0	0	72.02931158	0	0.480609213	0	0	0	0.005608383	0	0	0	0	0.004135705	0	0	0	0	1.33E-05	0	0	0	0	0	
Nov-39	0	0	0.121480423	0	0	0	13.41147087	0	0	0	69.59848223	0	0.464389719	0	0	0	0.005419113	0	0	0	0	0.003996134	0	0	0	0	1.28E-05	0	0	0	0	0	
Dec-39	0	0	0.005202625	0	0	0	5.544303564	0	0	0	28.7716049	0	0.191979697	0	0	0	0.002240273	0	0	0	0	0.00165201	0	0	0	0	5.29E-06	0	0	0	0	0	
Mar-40	0	0	0.01925861	0	0	0	5.353064615	0	0	0	18.66691232	0	0.057704217	0	0	0	0.000357797	0	0	0	0	0.000115153	0	0	0	0	8.21E-07	0	0	0	0	0	
Apr-40	0	0	0.083006894	0	0	0	23.11164045	0	0	0	80.59365319	0	0.249135665	0	0	0	0.001544776	0	0	0	0	0.000497169	0	0	0	0	3.54E-06	0	0	0	0	0	
May-40	0	0	0.085887439	0	0	0	23.91367551	0	0	0	83.39045314	0	0.257781292	0	0	0	0.001598384	0	0	0	0	0.000514422	0	0	0	0	3.67E-06	0	0	0	0	0	
Jun-40	0	0	0.08315948	0	0	0	23.15412869	0	0	0	80.74180329	0	0.249593635	0	0	0	0.001547616	0	0	0	0	0.000498083	0	0	0	0	3.55E-06	0	0	0	0	0	
Jul-40	0	0	0.01647931	0	0	0	4.588341099	0	0	0	16.00021056	0	0.049460757	0	0	0	0.000306683	0	0	0	0	9.87E-05	0	0	0	0	7.04E-07	0	0	0	0	0	
Dec-40	0	0	0.020728666	0	0	0	13.56984694	0	0	0	50.05570898	0	0.560987649	0	0	0	0.00440139	0	0	0	0	0.000443459	0	0	0	0	9.22E-06	0	0	0	0	0	
Jan-41	0	0	0.0568918	0	0	0	28.5627492	0	0	0	105.3607066	0	1.180680471	0	0	0	0.009264349	0	0	0	0	8.15E-05	0	0	0	0	1.94E-05	0	0	0	0	0	
Feb-41	0	0	0.051425328	0	0	0	25.18128575	0	0	0	95.23707994	0	1.067347294	0	0	0	0.00837418	0	0	0	0	7.36E-05	0	0	0	0	1.75E-05	0	0	0	0	0	
Mar-41	0	0	0.056993031	0	0	0	28.612157259	0	0	0	105.5481811	0	1.182690549	0	0	0	0.009280384	0	0	0	0	8.16E-05	0	0	0	0	1.94E-05	0	0	0	0	0	
Apr-41	0	0	0.010629251	0	0	0	5.336456701	0	0	0	19.6842952	0	0.220613122	0	0	0	0.001730884	0	0	0	0	1.52E-05	0	0	0	0	3.63E-06	0	0	0	0	0	
Dec-41	0	0	0.009289304	0	0	0	8.395492045	0	0	0	33.61599977	0	0.167242302	0	0	0	0.00497274	0	0	0	0	1.36E-05	0	0	0	0	1.26E-06	0	0	0	0	0	
Jan-42	0	0	0.031300493	0	0	0	29.91558252	0	0</																								

Appendix A: Initial Composition Vector (continued)

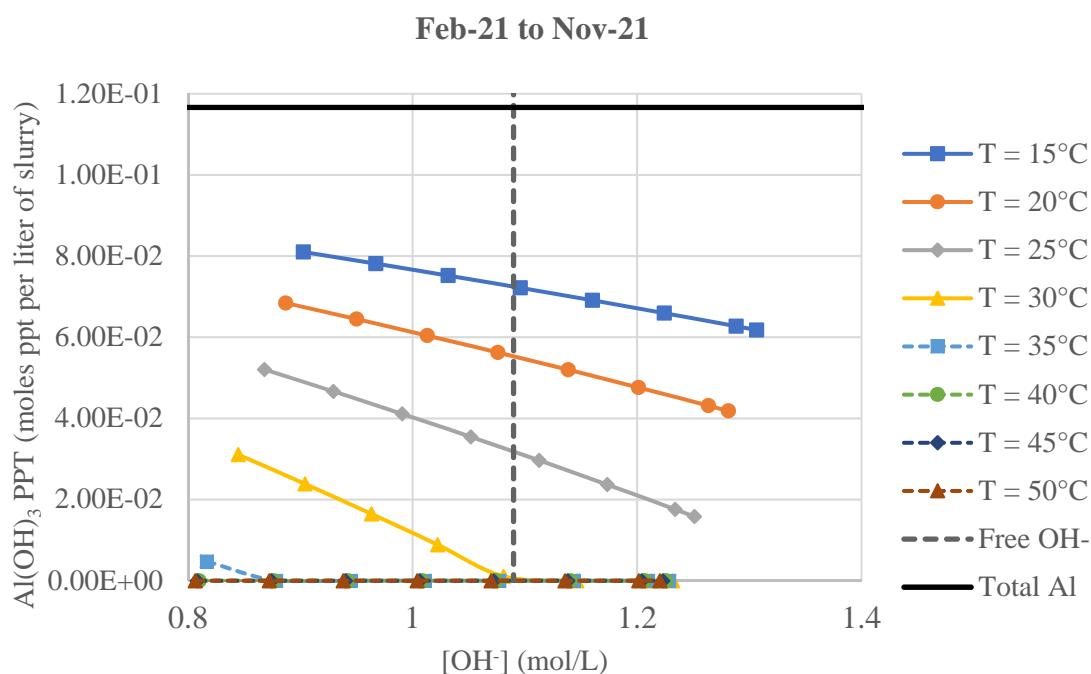
Transfer Date Range	Tl2O Solid (kMoles)	Tl+3 Liquid (kMoles)	Tl+3 Solid (kMoles)	TOC Liquid (kMoles)	TOC Solid (kMoles)	V+5 Liquid (kMoles)	V+5 Solid (kMoles)	V2O5 Liquid (kMoles)	V2O5 Solid (kMoles)	W+6 Liquid (kMoles)	W+6 Solid (kMoles)	WO3 Liquid (kMoles)	WO3 Solid (kMoles)	Y+3 Liquid (kMoles)	Y+3 Solid (kMoles)	Y2O3 Liquid (kMoles)	Y2O3 Solid (kMoles)	Zn+2 Liquid (kMoles)	Zn+2 Solid (kMoles)	ZnO Liquid (kMoles)	ZnO Solid (kMoles)	Zr+4 Liquid (kMoles)	Zr+4 Solid (kMoles)	ZrO2 Liquid (kMoles)	ZrO2 Solid (kMoles)	
Mar-37	0	0.0091376	0	306.0727189	0	0.014274897	0	0	0.00417678	0	0	0.010498649	0	0	0.054523431	0	0	0	0.3791701	0	0	0	0	0	0	0
Apr-37	0	0.008832431	0	295.8508028	0	0.013798158	0	0	0.004037288	0	0	0.010148026	0	0	0.052702511	0	0	0	0.36650695	0	0	0	0	0	0	0
May-37	0	0.0092502	0	98.8807625	0	0.004611691	0	0	0.001349363	0	0	0.003391725	0	0	0.017614502	0	0	0	0.12249582	0	0	0	0	0	0	0
Feb-38	0	0.007368425	0	165.7951953	0	0.005941714	0	0	0.000540189	0	0	0.004579149	0	0	0.021656162	0	0	0	0.383474876	0	0	0	0	0	0	0
Mar-38	0	0.017001734	0	382.5520286	0	0.013709774	0	0	0.00124642	0	0	0.010565823	0	0	0.049968932	0	0	0	0.884821127	0	0	0	0	0	0	0
Apr-38	0	0.016449343	0	370.1228134	0	0.01326434	0	0	0.001205924	0	0	0.010222537	0	0	0.048345428	0	0	0	0.856073058	0	0	0	0	0	0	0
May-38	0	0.016971536	0	381.8725401	0	0.013685423	0	0	0.001244206	0	0	0.010547056	0	0	0.049880177	0	0	0	0.883249509	0	0	0	0	0	0	0
Jun-38	0	0.000555499	0	12.49916251	0	0.000447941	0	0	4.07E-05	0	0	0.000345218	0	0	0.00163264	0	0	0	0.028909853	0	0	0	0	0	0	0
Aug-39	0	0.001257213	0	35.81660917	0	0.001005699	0	0	0.001346318	0	0	0.000962313	0	0	0.004132113	0	0	0	0.06340024	0	0	0	0	0	0	0
Sep-39	0	0.005999331	0	170.9143455	0	0.004799125	0	0	0.006424537	0	0	0.00459209	0	0	0.019718153	0	0	0	0.302541496	0	0	0	0	0	0	0
Oct-39	0	0.006208866	0	176.8837804	0	0.004966742	0	0	0.006648923	0	0	0.004752476	0	0	0.020406839	0	0	0	0.313108203	0	0	0	0	0	0	0
Nov-39	0	0.005999331	0	170.9143455	0	0.004799125	0	0	0.006424537	0	0	0.00459209	0	0	0.019718153	0	0	0	0.302541496	0	0	0	0	0	0	0
Dec-39	0	0.002480136	0	70.65635373	0	0.001983969	0	0	0.002655917	0	0	0.00189838	0	0	0.0080151526	0	0	0	0.125071298	0	0	0	0	0	0	0
Mar-40	0	0.000385059	0	20.44218602	0	0.000308249	0	0	0.000203792	0	0	0.000312574	0	0	0.00195504	0	0	0	0.028308972	0	0	0	0	0	0	0
Apr-40	0	0.001662476	0	88.25832696	0	0.001330852	0	0	0.000879862	0	0	0.001349525	0	0	0.005161539	0	0	0	0.122228262	0	0	0	0	0	0	0
May-40	0	0.001720168	0	91.32111014	0	0.001370736	0	0	0.000910396	0	0	0.001396357	0	0	0.005340657	0	0	0	0.126464299	0	0	0	0	0	0	0
Jun-40	0	0.001665532	0	88.42056654	0	0.00133298	0	0	0.00088148	0	0	0.001352006	0	0	0.005171027	0	0	0	0.122447536	0	0	0	0	0	0	0
Jul-40	0	0.00033005	0	17.52187374	0	0.000264213	0	0	0.000174679	0	0	0.00026792	0	0	0.001024717	0	0	0	0.024264833	0	0	0	0	0	0	0
Dec-40	0	0.00340257	0	137.8846283	0	0.001291579	0	0	0.000163677	0	0	0.00393659	0	0	0.011875787	0	0	0	0.101226542	0	0	0	0	0	0	0
Jan-41	0	0.007161964	0	290.2290699	0	0.002718605	0	0	0.000287687	0	0	0.008286005	0	0	0.024996975	0	0	0	0.213068413	0	0	0	0	0	0	0
Feb-41	0	0.006473803	0	262.3422909	0	0.002457387	0	0	0.000260044	0	0	0.007489841	0	0	0.022595131	0	0	0	0.192595647	0	0	0	0	0	0	0
Mar-41	0	0.007174707	0	290.7454917	0	0.00273442	0	0	0.000288199	0	0	0.008037049	0	0	0.025041454	0	0	0	0.213447538	0	0	0	0	0	0	0
Apr-41	0	0.001338089	0	54.22429242	0	0.000507924	0	0	5.37E-05	0	0	0.001548097	0	0	0.004670253	0	0	0	0.039808155	0	0	0	0	0	0	0
Dec-41	0	0.000280158	0	30.88167959	0	0.000159732	0	0	3.47E-05	0	0	0.000438638	0	0	0.001352876	0	0	0	0.0414536	0	0	0	0	0	0	0
Jan-42	0	0.000998284	0	110.0404157	0	0.000569171	0	0	0.000123592	0	0	0.01562995	0	0	0.004820691	0	0	0	0.147711246	0	0	0	0	0	0	0
Feb-42	0	0.00090076	0	99.29046387	0	0.000513569	0	0	0.000111519	0	0	0.001410304	0	0	0.00439753	0	0	0	0.133281195	0	0	0	0	0	0	0
Mar-42	0	0.000998284	0	110.0404157	0	0.000569171	0	0	0.000123592	0	0	0.001562995	0	0	0.004820691	0	0	0	0.147711246	0	0	0	0	0	0	0
Apr-42	0	0.000203366	0	22.0862646	0	0.000114239	0	0	2.48E-05	0	0	0.000313709	0	0	0.000967563	0	0	0	0.029647195	0	0	0	0	0	0	0
Sep-42	0	0.000417689	0	29.65739713	0	0.000418897	0	0	7.29E-05	0	0	0.0001														

Appendix B: Calculated Gibbsite Precipitation for Each Composition

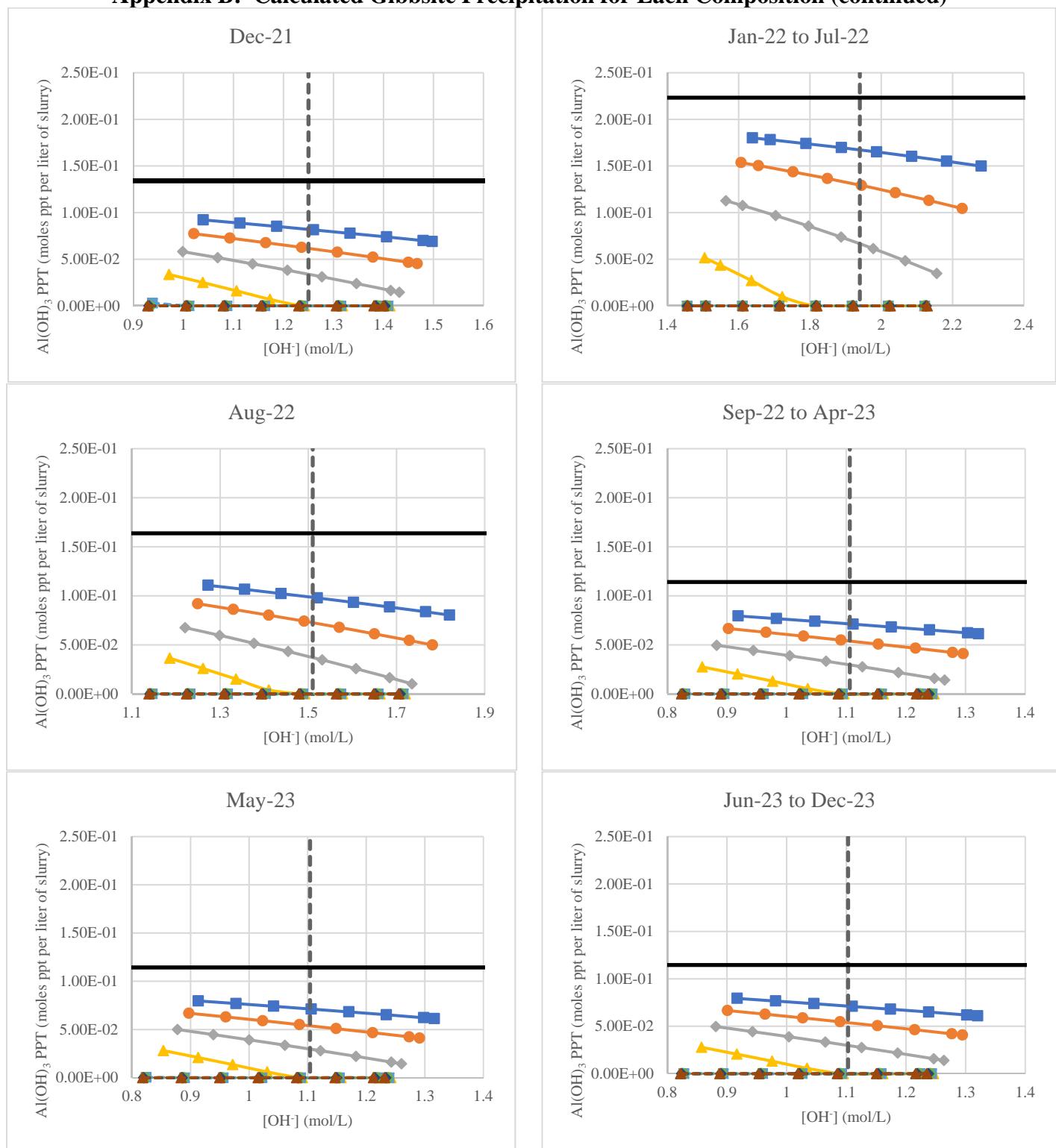
This appendix contains graphical representations of the amount of gibbsite estimated to form at the concentrations for each of the unique compositions in Appendix A. The first graph on this page illustrates the format and legend for all the graphs. The heading identifies the time range corresponding to the monthly compositions provided in Appendix A.

The dotted vertical line represents the free hydroxide ion at the concentration identified for each composition. The solid black horizontal line represents total potential gibbsite if all the aluminum precipitated as gibbsite. Simulated isotherms are plotted for every 5 degrees between 15 and 50°C and roughly plus or minus 20% of the input free hydroxide concentration. The isotherms represent the amount of gibbsite at equilibrium as a function of free hydroxide concentration while simultaneously maintaining constant volumetric concentrations for all other input components. These graphs provide a quick visualization of the simulation results relative to the risk of precipitating gibbsite as well as the expected effect of adjusting the free hydroxide concentration. The approximate fraction of aluminum precipitating as gibbsite is proportional to the distance between the intersection of the dotted line with an isotherm and the solid black line from the x-axis. For example, on the Feb-21 to Nov-21 batch, the 20°C isotherm shows around $\frac{1}{2}$ of the aluminum is expected to precipitate as gibbsite.

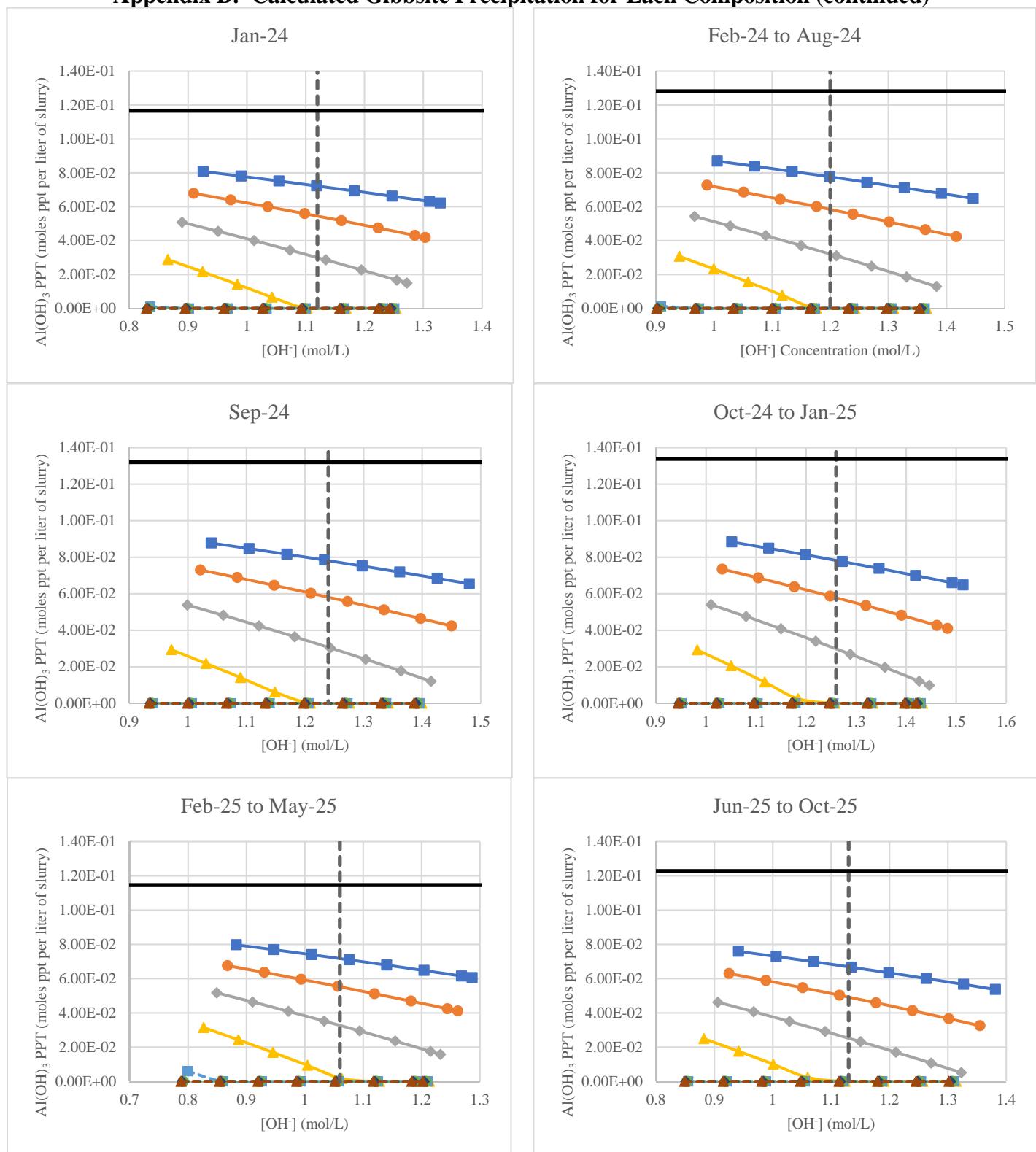
Aluminum in solution is predicted to be in the form of dissolved sodium aluminate. Solid phases are aluminum hydroxide identified as gibbsite and sodium aluminosilicate (multiple possible forms). The aluminosilicates tend to occur with little effect on total gibbsite precipitates formed. The amount of sodium aluminosilicate may be of interest because, once formed, they are much more difficult to remediate in an operating facility. Appendix C provides numerical results for all batches.



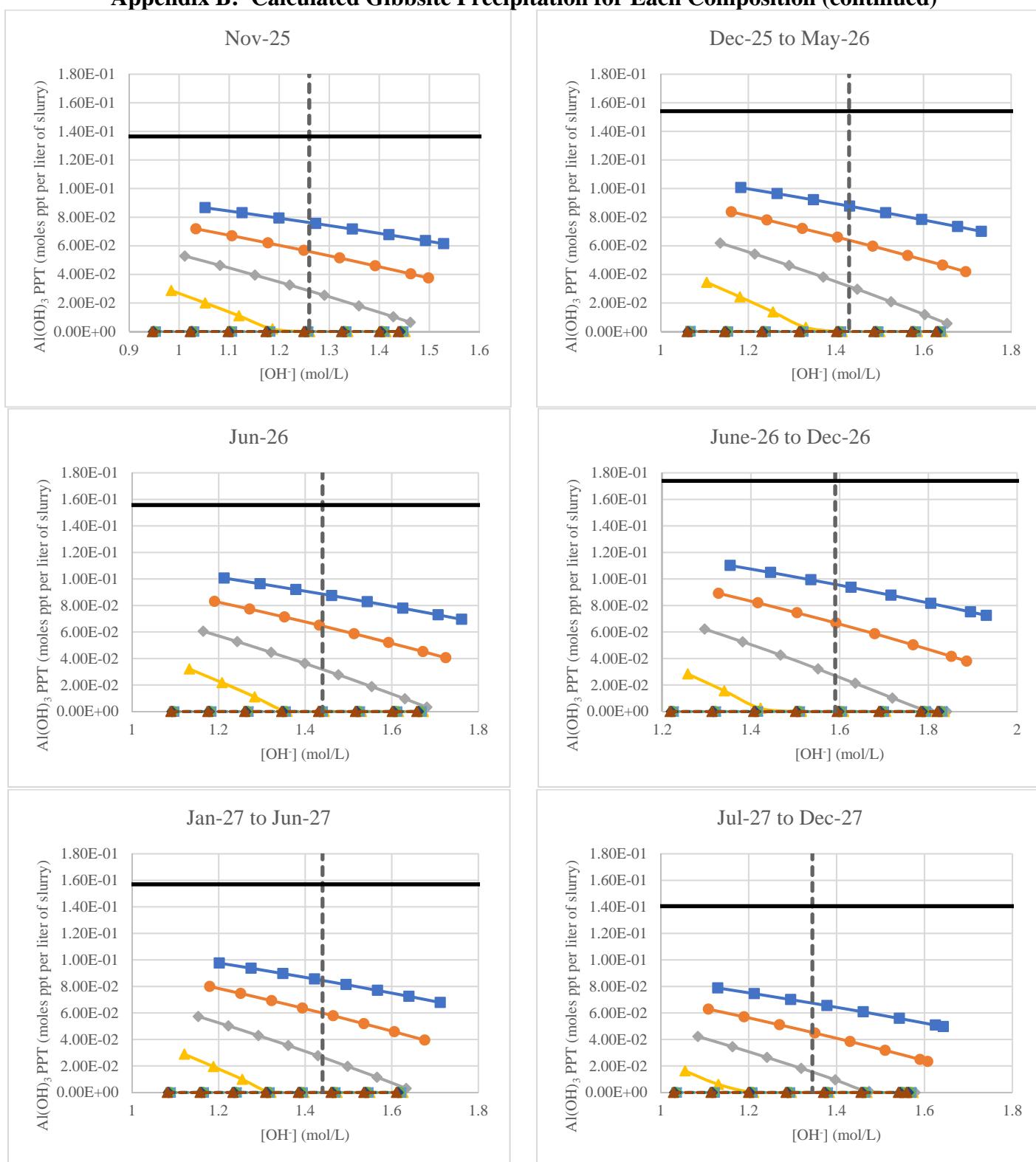
Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)



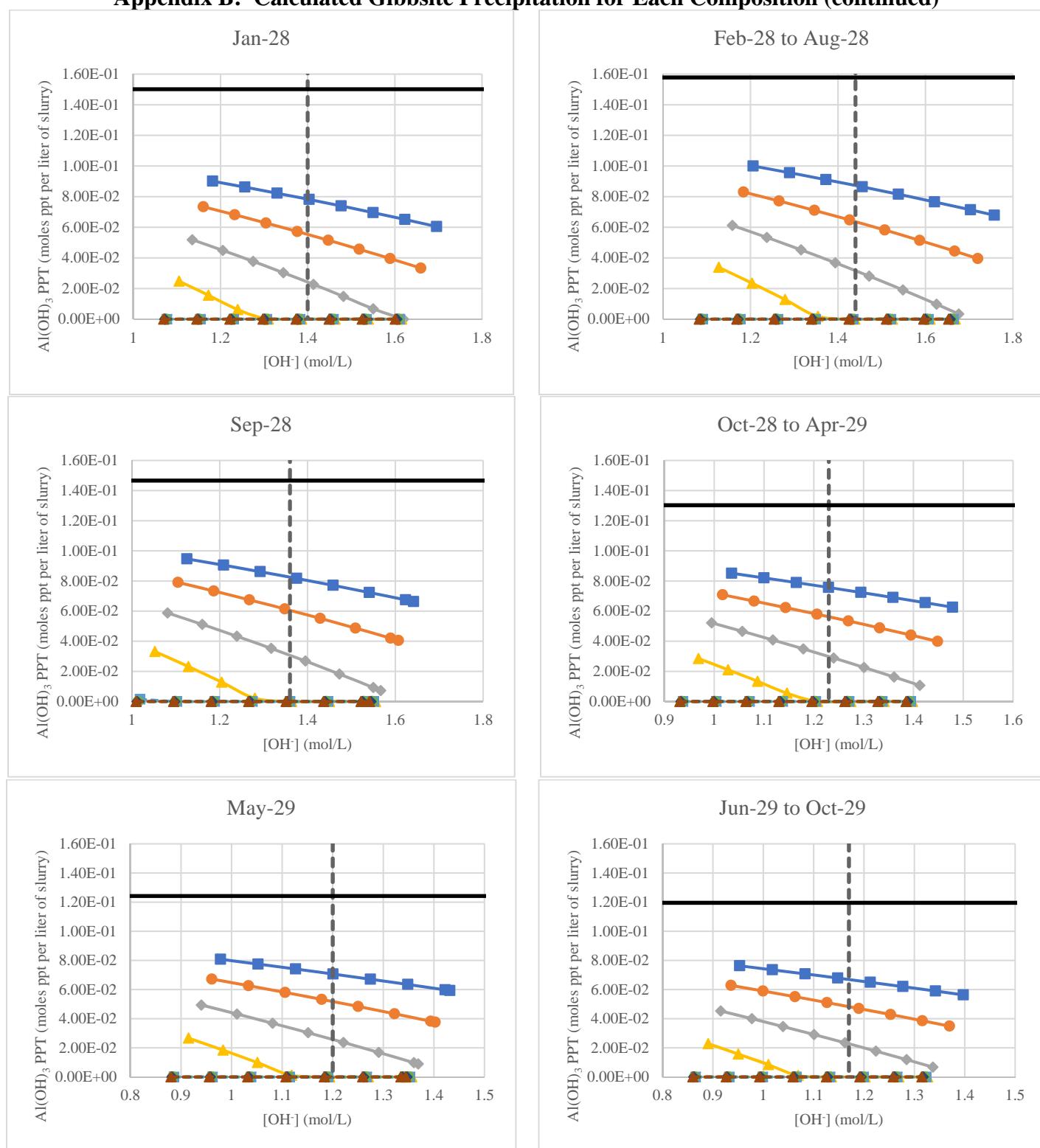
Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)



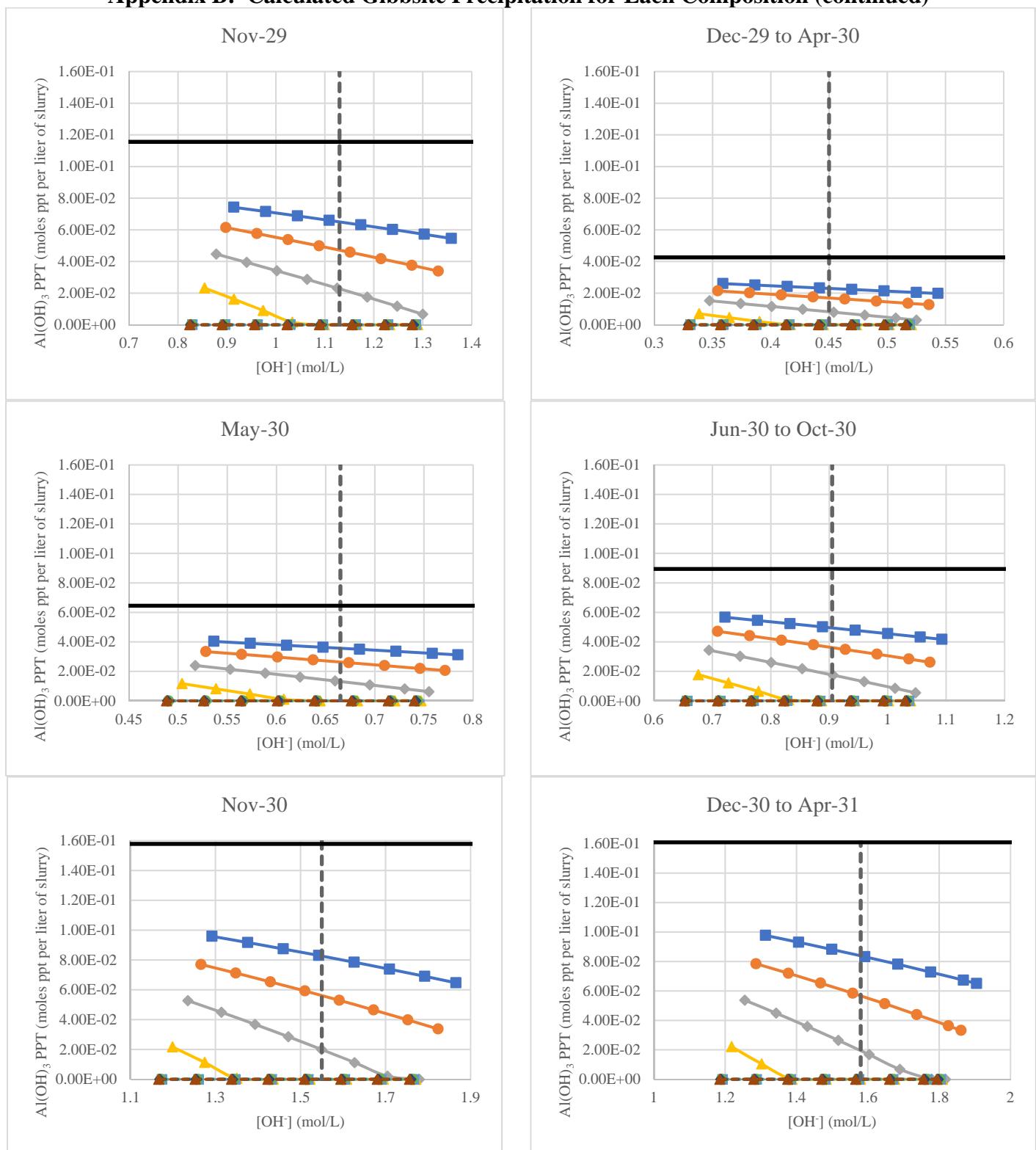
Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)



Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)

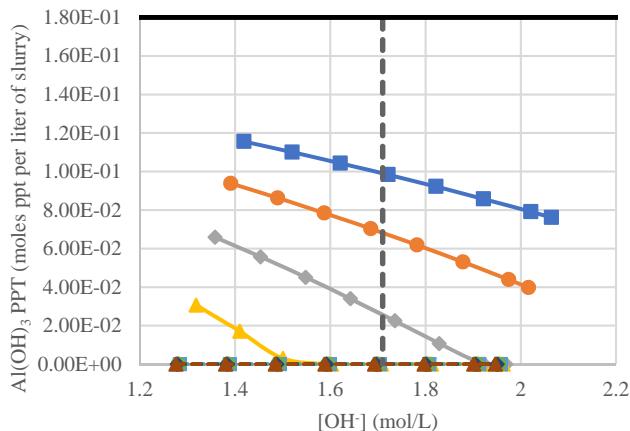


Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)

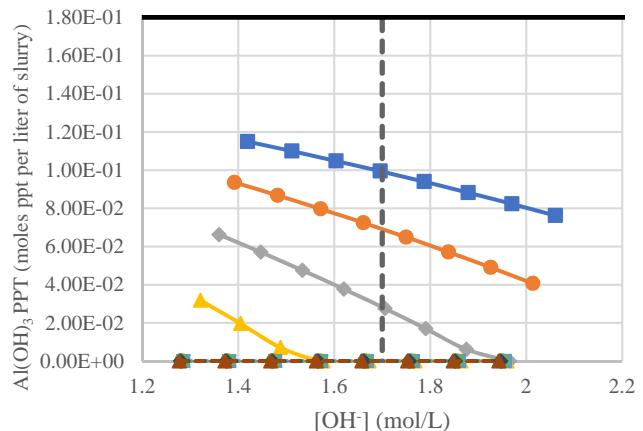


Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)

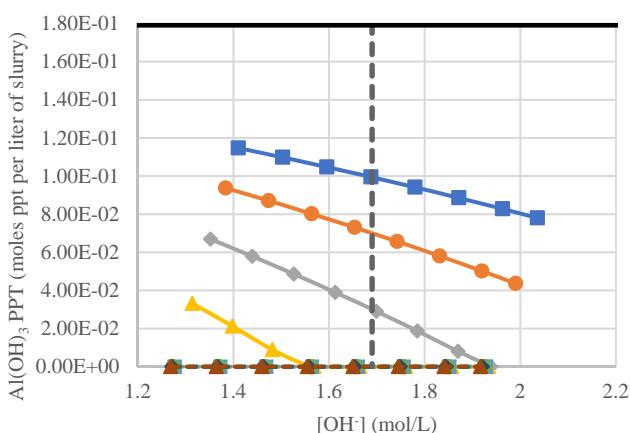
May-31 to Sep-31



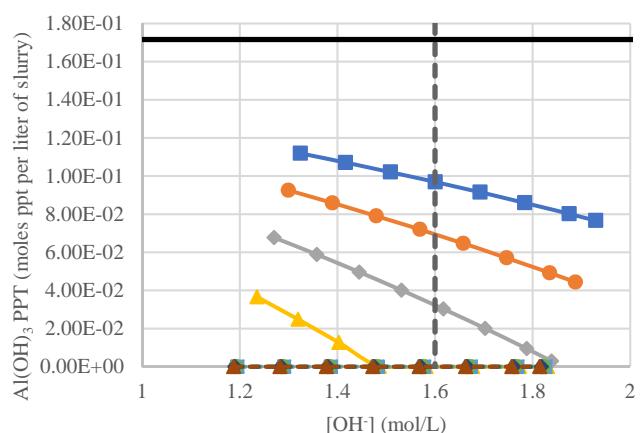
Oct-31



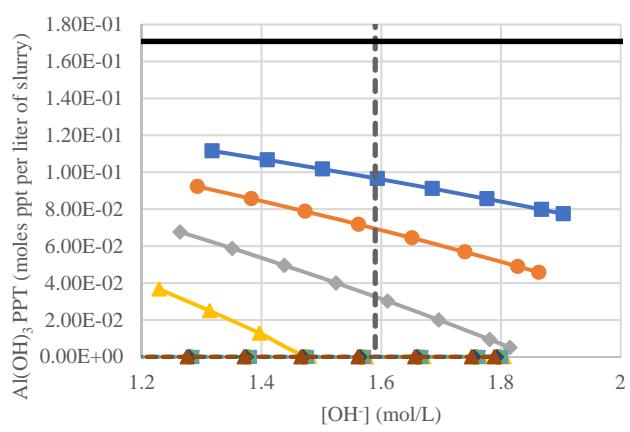
Nov-31 to Mar-32



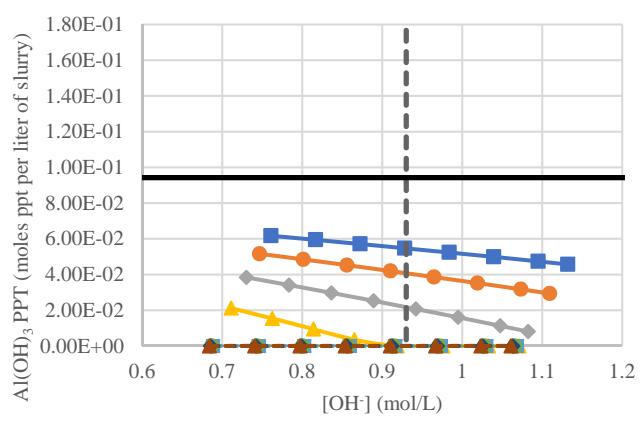
Apr-32



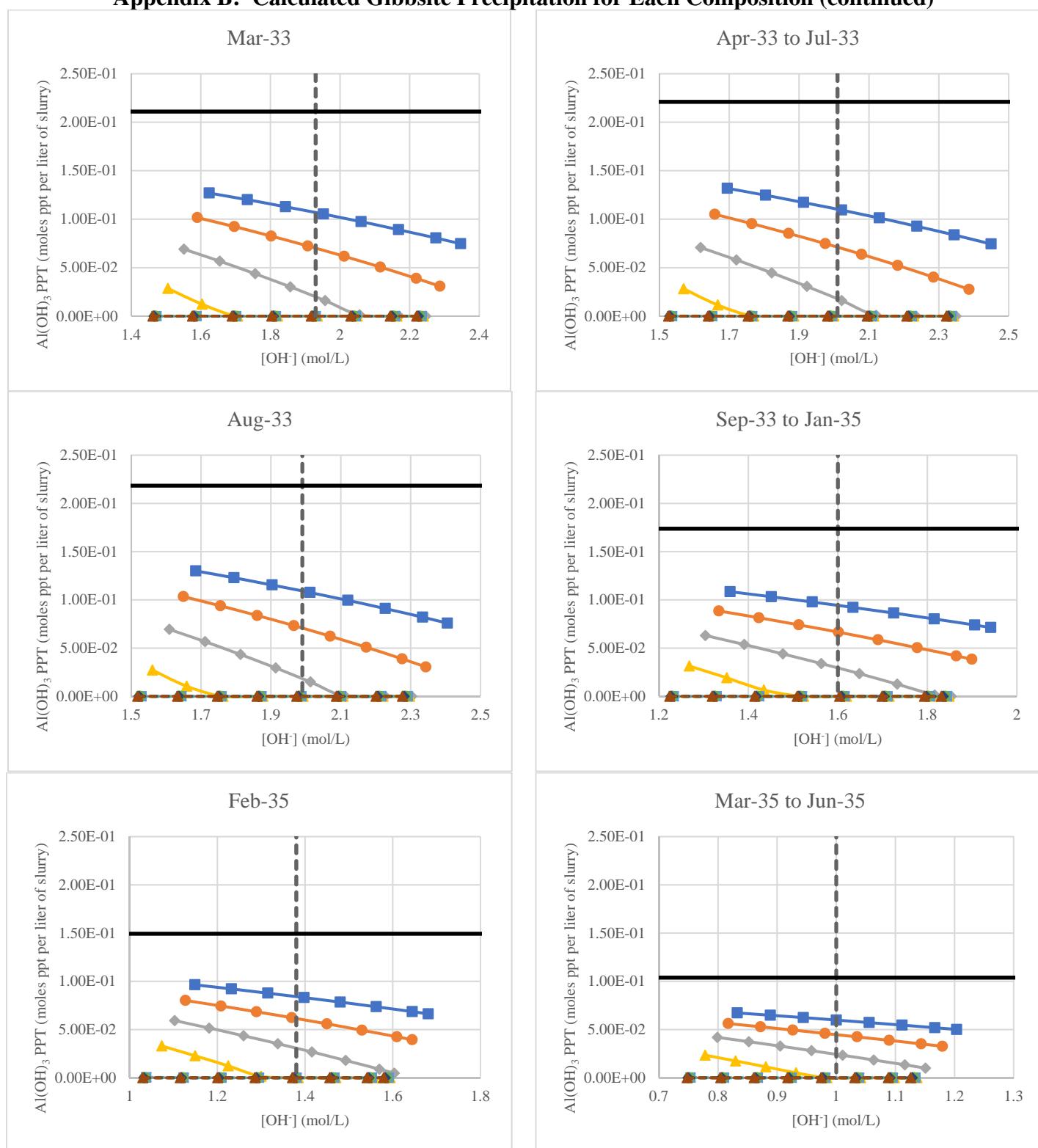
May-32 to Sep-32



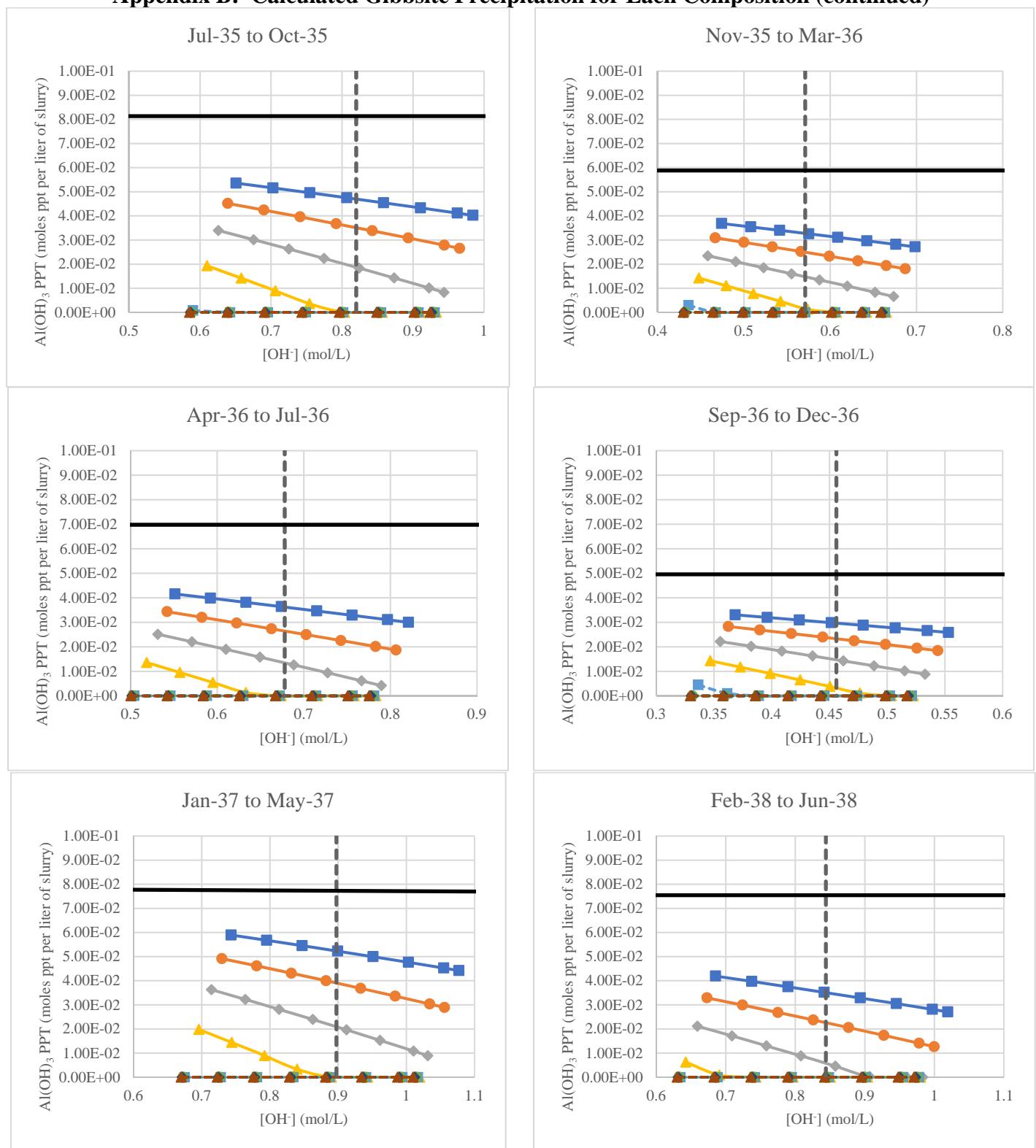
Oct-32 to Feb-33



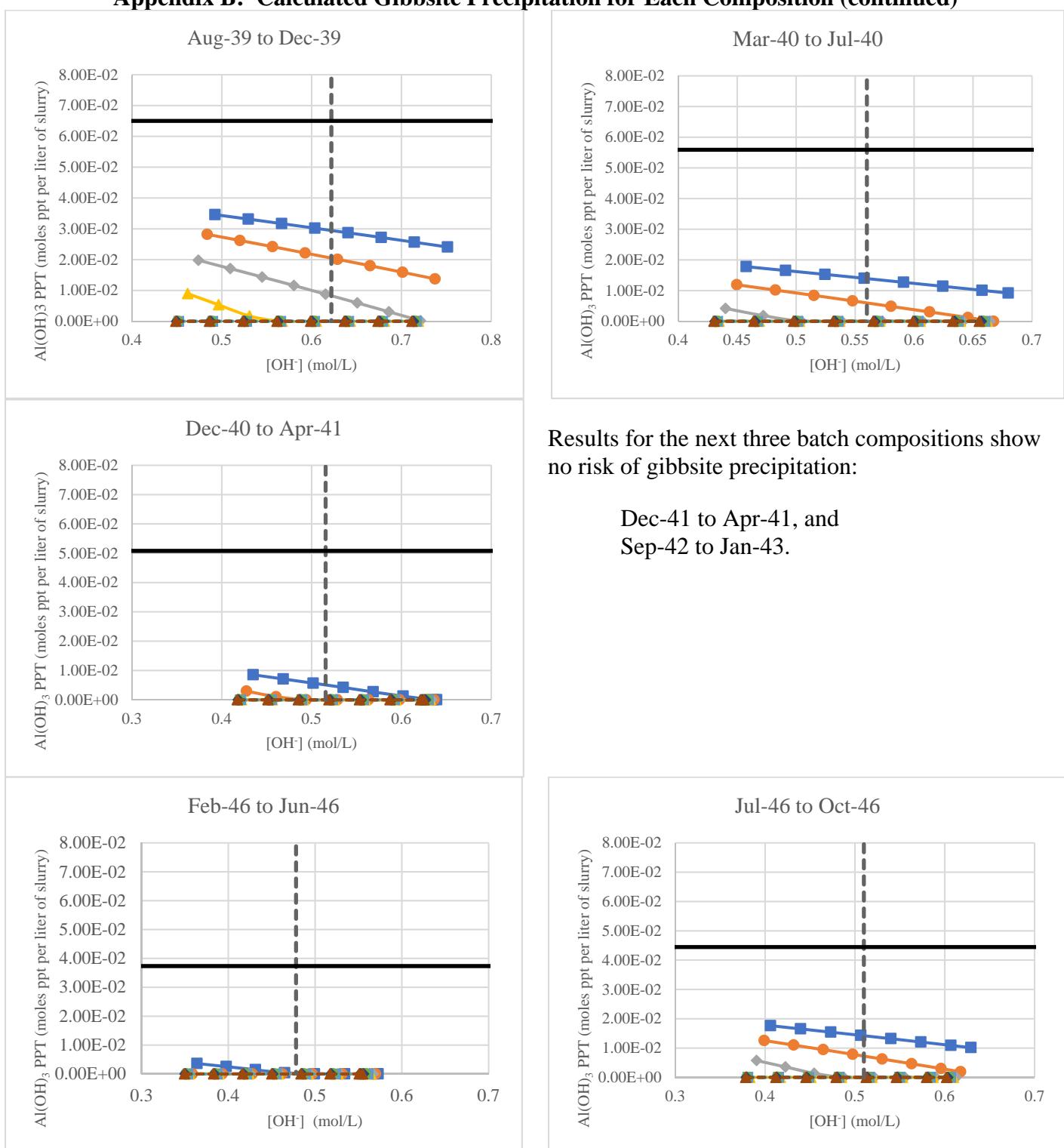
Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)



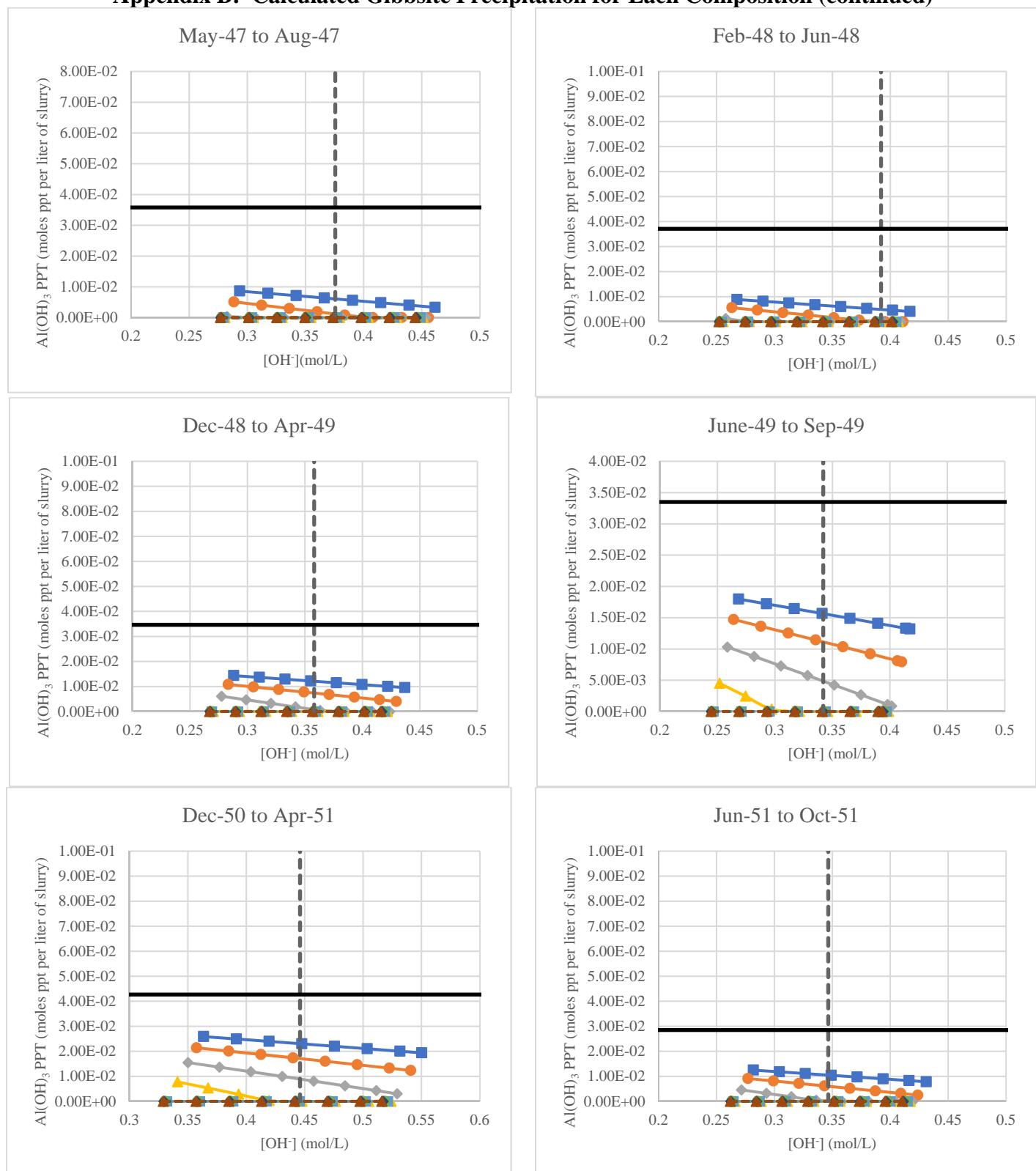
Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)



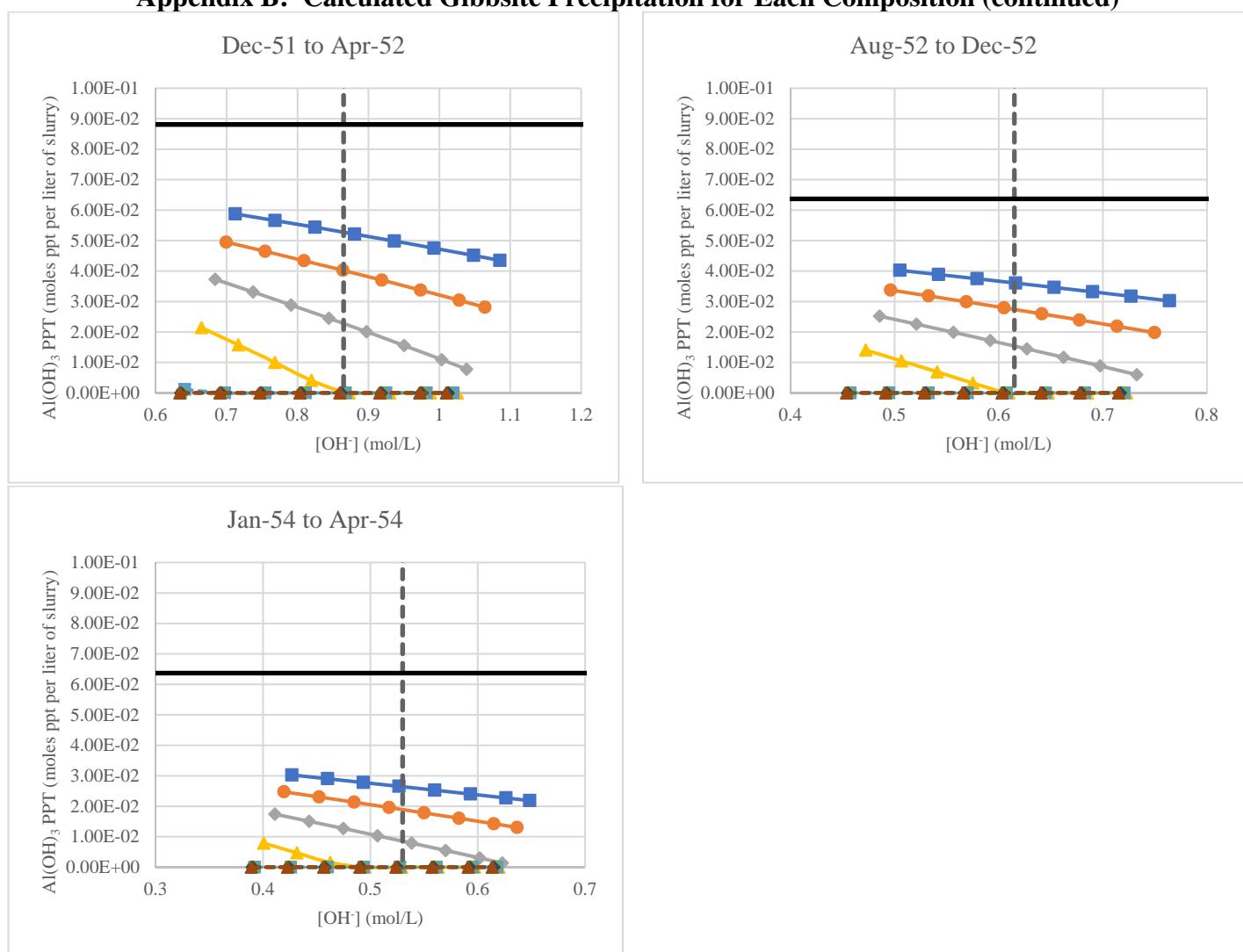
Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)



Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)



Appendix B: Calculated Gibbsite Precipitation for Each Composition (continued)



Appendix C: Calculated Quantities of Precipitates for Each Composition

This appendix contains a table of the solids estimated to form at the concentrations for each of the unique compositions in Appendix A at 25°C and 1 atmosphere pressure. The solids are reported in terms of moles of solid per liter of total slurry. Only solids reported at or above 1E-5 mole solid/L are quantified and qualitatively identified any other solids reported between 1E-5 and 1E-10 mole solid/L. Because the scope of the evaluation intended to focus on the risk precipitating gibbsite, the relative percent of the total aluminum represented by the precipitated gibbsite is also provided.

The units in this table allow for easy interpretation of the amount solids expected for any given amount of feed but introduces a dependency on property estimation for solution and solids densities. The OLI property density estimation is different than the density implied in the physical parameters provided in Appendix A for total volume relative to the molar composition.

Appendix C: Calculated Quantities of Precipitates for Each Composition (Continued)

SRNL-STI-2018-00446

Revision 0

Batch ID	Feb-21 to Nov-21	Dec-21	Jan-22 to Jul-22	Aug-22	Sep-22 to Apr-23	May-23	June23 to Dec23	Jan-24	Feb24 to Aug24	Sep-24	Oct24 to Jan25	Feb25 to May25	Jun25 to Oct25	Nov-25	Dec25 to May26	Jun-26	Jul-26 to Dec-26	Jan-27 to Jun-27	Jul-27 to Dec-27	
Al(OH)₃	3.18E-02	3.39E-02	6.69E-02	3.71E-02	2.97E-02	2.97E-02	2.97E-02	3.00E-02	3.21E-02	3.07E-02	2.98E-02	3.27E-02	2.52E-02	2.85E-02	3.17E-02	3.18E-02	2.72E-02	2.65E-02	1.53E-02	
% of Total Al	27%	25%	30%	23%	26%	26%	26%	26%	25%	23%	22%	29%	21%	21%	21%	20%	16%	17%	11%	
Na[COO]₂	5.75E-03	5.55E-03	1.13E-02	5.07E-03	4.64E-03	4.94E-03	5.14E-03	5.35E-03	6.47E-03	7.14E-03	7.45E-03	7.47E-03	8.79E-03	7.84E-03	6.57E-03	6.66E-03	7.76E-03	1.00E-02	1.04E-02	
NAS	1.80E-04	1.74E-04	1.41E-04	1.67E-04	2.17E-04	2.40E-04	2.55E-04	2.68E-04	3.35E-04	5.78E-04	6.91E-04	2.30E-04	1.73E-03	1.32E-03	7.71E-04	7.58E-04	5.94E-04	1.40E-03	2.49E-03	
Ag[‡]	-	-	-	-	1.46E-05	†	†	†	†	-	1.26E-05	1.46E-05	†	†	†	1.21E-05	1.18E-05	†	†	†
Bi(OH)₃	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
Ca5F(PO₄)₃[‡]	2.63E-04	2.51E-04	2.01E-04	2.18E-04	1.39E-04	1.38E-04	1.38E-04	1.41E-04	1.58E-04	1.57E-04	1.57E-04	2.27E-04	1.18E-04	1.41E-04	1.71E-04	1.67E-04	1.18E-04	3.82E-04	7.67E-04	
Cd(OH)₂	-	-	-	-	-	-	-	-	-	†	†	†	†	-	-	-	-	-	-	
Ce(OH)₃	-	3.55E-05	9.42E-05	9.78E-05	1.07E-05	1.53E-05	1.85E-05	2.54E-05	6.21E-05	4.23E-05	3.32E-05	3.13E-05	1.42E-05	3.64E-05	6.53E-05	6.28E-05	3.27E-05	3.60E-05	2.25E-05	
Co(OH)₂	-	-	1.05E-05	-	-	-	-	-	1.37E-05	†	-	-	-	-	-	-	-	-	-	
Co(OH)₃[‡]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
CoCr₂O₄[‡]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
CoFe₂O₄[‡]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
CuO	-	†	1.19E-05	2.54E-05	-	-	†	†	1.91E-05	1.65E-05	1.53E-05	1.94E-05	†	†	1.93E-05	1.90E-05	1.55E-05	1.52E-05	†	
Fe(OH)₃	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
H₅O₄Ru[‡]	-	-	-	†	†	†	†	†	1.04E-05	†	†	†	†	†	†	†	†	†	†	
La(OH)₃[‡]	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	
Mg(OH)₂[‡]	-	7.80E-05	2.07E-04	2.14E-04	2.37E-05	7.53E-05	1.11E-04	1.54E-04	3.83E-04	2.41E-04	1.75E-04	9.99E-05	5.31E-05	1.09E-04	1.81E-04	1.79E-04	1.61E-04	1.64E-04	1.08E-04	
Mn(OH)₂	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
MnO₂	2.14E-05	1.73E-05	†	1.04E-05	†	1.04E-05	1.15E-05	1.26E-05	1.84E-05	2.32E-05	2.55E-05	2.05E-05	1.84E-04	1.18E-04	3.13E-05	3.11E-05	2.74E-05	2.04E-05	1.85E-04	
Na₂SO₄.NaF	-	-	5.39E-03	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
Na₇F(PO₄)₂.19H₂O	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
Nd(OH)₃[‡]	-	2.07E-05	5.50E-05	5.69E-05	†	†	†	1.32E-05	3.22E-05	2.25E-05	1.81E-05	2.14E-05	†	2.12E-07	3.71E-05	3.63E-05	2.61E-05	2.28E-05	1.45E-05	
Ni(OH)₂	1.73E-04	2.31E-04	2.97E-04	3.36E-04	2.24E-04	2.19E-04	2.16E-04	2.17E-04	2.24E-04	1.92E-04	1.77E-04	2.09E-04	5.18E-05	1.29E-04	2.30E-04	2.23E-04	1.46E-04	1.56E-04	1.80E-04	
NiCr₂O₄[‡]	†	†	-	-	†	†	†	†	†	†	†	-	†	5.92E-05	3.59E-05	†	†	†	4.81E-05	
NiFe₂O₄[‡]	2.17E-04	1.68E-04	6.21E-05	6.52E-05	1.77E-05	4.15E-05	5.82E-05	7.60E-05	1.71E-04	1.59E-04	1.53E-04	2.26E-04	6.09E-05	5.59E-05	4.94E-05	5.31E-05	9.80E-05	8.93E-05	7.48E-05	
NiTiO₃	-	-	1.16E-05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
PbTiO₃	-	†	1.11E-05	2.36E-05	†	†	†	1.14E-05	2.83E-05	1.36E-05	†	2.63E-05	-	-	-	-	-	-	-	
PbZr_{0.3}Ti_{0.7}O₃	-	-	-	†	-	-	-	-	-	1.96E-05	2.87E-05	†	1.51E-05	1.26E-05	-	†	3.40E-05	†	-	
PbZr_{0.6}Ti_{0.4}O₃	-	-	-	-	-	-	-	-	-	-	-	-	-	1.09E-05	4.14E-05	4.09E-05	-	3.37E-05	-	
PbZr_{0.75}Ti_{0.25}O₃[‡]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4.52E-05	
PdO.H₂O	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
Rh₂O₃.H₂O	-	-	-	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	
SrCO₃	1.11E-05	†	†	†	†	†	†	†	†	1.05E-05	1.10E-05	1.12E-05	†	†	†	†	†	†	†	
ThO₂[‡]	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	
Y(OH)₃[‡]	-	†	1.20E-05	1.24E-05	†	†	†	†	†	†	1.05E-05	1.19E-05	†	†	†	†	1.54E-05	1.03E-05	†	
ZnO.Fe₂O₃	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
ZrO₂	-	-	-	-	-	-	-	-	-	-	-	-	-	2.05E-04	1.19E-04	†	-	4.62E-05	1.61E-04	

† = less than 1E-5 but greater than 1E-10 moles precipitated per liter of slurry

‡ This component concentration for each batch composition did not vary as a function of temperature or free hydroxide.

Appendix C: Calculated Quantities of Precipitates for Each Composition (Continued)

SRNL-STI-2018-00446

Revision 0

Batch ID	Jan-28	Feb-28 to Aug-28	Sep-28	Oct-28 to Apr-29	May-29	Jun-29 to Oct-29	Nov-29	Dec-29 to Apr-30	May-30	Jun-30 to Oct-30	Nov-30	Dec-30 to Apr-31	May-31 to Sep-31	Oct-31	Nov-31 to Mar-32	Apr-32	May-32 to Sep-32	Oct-32 to Feb-33	Mar-33			
Al(OH)₃	2.42E-02	3.16E-02	3.07E-02	2.99E-02	2.57E-02	2.28E-02	2.27E-02	8.22E-03	1.31E-02	1.76E-02	2.00E-02	1.94E-02	2.57E-02	2.82E-02	3.01E-02	3.23E-02	3.26E-02	2.18E-02	1.99E-02			
% of Total Al	16%	20%	21%	23%	21%	19%	20%	19%	20%	20%	13%	12%	14%	16%	17%	19%	19%	23%	9%			
Na[COO]₂	1.03E-02	1.02E-02	9.10E-03	7.53E-03	5.89E-03	4.63E-03	4.88E-03	9.38E-03	8.52E-03	7.54E-03	9.01E-03	9.07E-03	6.86E-03	6.35E-03	5.77E-03	6.52E-03	6.60E-03	5.83E-03	7.44E-03			
NAS	1.78E-03	1.22E-03	9.73E-04	6.14E-04	8.68E-04	1.06E-03	1.05E-03	8.38E-04	9.64E-04	1.10E-03	1.29E-03	1.30E-03	4.54E-04	5.01E-04	5.53E-04	4.71E-04	4.62E-04	7.03E-04	1.37E-03			
Ag[‡]	1.27E-05	1.82E-05	1.71E-05	-	2.33E-05	2.94E-05	2.80E-05	-	1.20E-05	2.21E-05	1.07E-05	-	-	1.10E-05	1.83E-05	1.49E-05	1.45E-05	-	2.75E-05			
Bi(OH)₃	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
Ca5F(PO₄)₃[‡]	5.37E-04	3.55E-04	2.96E-04	2.09E-04	1.42E-04	9.09E-05	9.12E-05	9.70E-05	1.13E-04	1.31E-04	1.64E-04	1.66E-04	1.35E-04	1.02E-04	-	-	4.97E-05	4.57E-05	6.18E-05			
Cd(OH)₂	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.80E-05	-			
Ce(OH)₃	5.65E-05	8.36E-05	1.10E-04	1.50E-04	8.31E-05	3.21E-05	3.06E-05	-	-	1.28E-05	-	-	1.13E-05	2.86E-05	4.87E-05	3.77E-05	3.66E-05	-	5.79E-05			
Co(OH)₂	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
Co(OH)₃[‡]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
CoCr₂O₄[‡]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
CoFe₂O₄[‡]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2.98E-05			
CuO	†	†	-	†	†	†	†	-	†	†	†	†	†	†	†	†	†	-	†			
Fe(OH)₃	-	-	-	-	-	-	-	-	3.35E-04	1.49E-04	-	-	-	-	-	-	-	-	-			
H₅O₄Ru[‡]	†	1.23E-05	2.56E-05	4.52E-05	2.52E-05	1.00E-05	†	†	2.32E-05	4.78E-05	1.35E-05	†	†	†	1.85E-05	1.34E-05	1.29E-05	†	†			
La(OH)₃[‡]	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†			
Mg(OH)₂[‡]	1.20E-04	1.29E-04	2.05E-04	3.15E-04	3.74E-04	4.20E-04	4.01E-04	5.17E-05	1.92E-04	3.52E-04	1.01E-04	8.91E-05	7.30E-05	1.57E-04	2.55E-04	2.00E-04	1.95E-04	3.77E-05	3.36E-04			
Mn(OH)₂	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3.00E-04			
MnO₂	2.31E-04	2.68E-04	1.99E-04	9.67E-05	7.51E-05	5.77E-05	3.86E-05	-	-	3.73E-05	3.78E-05	2.59E-05	7.18E-05	1.25E-04	9.22E-05	8.89E-05	2.09E-05	4.78E-05	-			
Na₂SO₄.NaF	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
Na₇F(PO₄)_{2.19H₂O}	-	-	-	-	-	-	-	-	-	-	-	5.28E-03	5.41E-03	-	-	-	-	-	1.42E-03	-		
Nd(OH)₃[‡]	3.26E-05	4.70E-05	4.35E-05	3.84E-05	5.48E-05	6.73E-05	6.43E-05	-	2.58E-05	4.59E-05	2.63E-05	2.54E-05	1.41E-05	2.61E-05	3.99E-05	3.21E-05	3.14E-05	1.57E-05	5.55E-05			
Ni(OH)₂	1.86E-04	1.91E-04	1.56E-04	1.06E-04	4.40E-05	-	-	-	-	-	-	-	4.51E-05	2.58E-05	-	1.66E-05	1.80E-05	4.08E-05	-			
NiCr₂O₄[‡]	6.28E-05	7.46E-05	5.46E-05	2.51E-05	1.83E-05	-	-	-	-	-	-	-	-	1.95E-05	3.55E-05	2.56E-05	2.46E-05	-	-			
NiFe₂O₄[‡]	7.03E-05	6.67E-05	1.02E-04	1.53E-04	1.09E-04	7.55E-05	8.23E-05	3.31E-05	5.89E-05	7.90E-05	9.75E-05	9.83E-05	2.41E-04	1.55E-04	5.37E-05	3.38E-05	3.18E-05	3.32E-05	2.85E-04			
NiTiO₃	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
PbTiO₃	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
PbZr_{0.3}Ti_{0.7}O₃	-	-	-	-	†	1.58E-05	2.24E-05	2.13E-05	†	1.40E-05	2.00E-05	3.17E-05	3.32E-05	†	-	1.91E-05	-	-	†			
PbZr_{0.6}Ti_{0.4}O₃	-	-	-	-	†	2.16E-05	1.48E-05	1.43E-05	†	-	-	†	†	3.92E-05	5.53E-05	2.35E-05	3.42E-05	3.37E-05	-			
PbZr_{0.75}Ti_{0.25}O₃[‡]	4.18E-05	3.91E-05	5.13E-05	-	-	-	-	-	-	-	-	-	-	-	-	-	1.32E-05	1.17E-05	-	7.48E-05		
PdO.H₂O	-	-	-	-	2.11E-05	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
Rh₂O₃.H₂O	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†			
SrCO₃	†	†	†	†	1.46E-05	†	†	†	†	†	†	†	†	1.87E-05	1.26E-05	†	†	†	†			
ThO₂[‡]	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†			
Y(OH)₃[‡]	†	†	†	1.29E-05	2.40E-05	1.42E-05	†	†	†	2.08E-05	4.30E-05	1.22E-05	†	†	†	1.43E-05	1.04E-05	†	†			
ZnO.Fe₂O₃	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.70E-05			
ZrO₂	9.92E-05	5.02E-05	1.63E-05	-	-	-	-	-	-	-	-	-	-	9.60E-04	1.00E-03	7.84E-05	3.14E-05	-	2.84E-05	3.38E-05	1.31E-03	2.07E-04

Appendix C: Calculated Quantities of Precipitates for Each Composition (Continued)

SRNL-STI-2018-00446

Revision 0

Batch ID	Apr-33 to Jul-33	Aug-33	Sep-33 to Jan-35	Feb-35	Mar-35 to Jun-35	Jul-35 to Oct-35	Nov-35 to Mar-36	Apr-36 to Jul-36	Sep-36 to Dec-36	Jan-37 to May-37	Feb-38 to Jun-38	Aug-39 to Dec-39	Mar-40 to Jul-40	Dec-40 to Apr-41	Dec-41 to Apr-42	Sep-42 to Jan-43	Feb-46 to Jun-46	Jul-46 to Oct-46
Al(OH)_3	1.79E-02	1.83E-02	2.94E-02	3.07E-02	2.43E-02	1.87E-02	1.48E-02	1.35E-02	1.47E-02	2.09E-02	5.77E-03	8.31E-03	-	-	-	-	-	-
% of Total Al	8%	8%	17%	21%	23%	23%	25%	19%	30%	22%	8%	13%	-	-	-	-	-	-
$\text{Na}[\text{COO}]_2$	7.55E-03	7.56E-03	7.50E-03	8.30E-03	9.76E-03	9.66E-03	5.08E-03	6.19E-03	1.01E-02	7.18E-03	7.45E-03	9.87E-03	9.54E-03	1.13E-02	1.12E-02	8.95E-03	1.02E-02	6.96E-03
NAS	1.43E-03	1.39E-03	8.25E-04	8.17E-04	8.05E-04	8.52E-04	6.01E-04	1.23E-03	5.90E-04	1.13E-03	1.23E-03	2.12E-03	3.67E-03	4.40E-03	4.59E-03	6.65E-03	3.84E-03	2.38E-03
Ag [‡]	2.93E-05	2.86E-05	1.65E-05	1.30E-05	†	†	-	-	-	-	-	-	-	-	-	-	†	-
Bi(OH)_3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5.83E-05
$\text{Ca5F(PO}_4\text{)}_3^{\ddagger}$	6.32E-05	6.29E-05	5.77E-05	5.66E-05	5.46E-05	8.64E-05	6.95E-04	4.49E-04	3.27E-04	2.80E-04	3.01E-04	3.23E-04	3.05E-04	3.82E-04	2.01E-04	2.27E-04	8.03E-04	7.90E-04
Cd(OH)_2	-	-	-	-	-	5.76E-05	2.01E-04	1.06E-04	7.27E-05	6.14E-05	5.38E-05	2.29E-05	4.24E-05	1.30E-04	3.11E-05	1.91E-05	†	1.49E-05
Ce(OH)_3	6.21E-05	5.97E-05	1.92E-05	1.57E-05	†	†	†	1.43E-05	1.93E-05	2.00E-05	1.71E-05	†	†	†	†	†	†	†
Co(OH)_2	-	-	-	-	-	-	†	-	-	-	-	-	-	-	-	-	†	-
$\text{Co(OH)}_3^{\ddagger}$	-	-	-	-	-	-	2.84E-05	1.65E-05	2.19E-05	-	-	-	-	-	-	-	-	2.30E-05
$\text{CoCr}_2\text{O}_4^{\ddagger}$	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
$\text{CoFe}_2\text{O}_4^{\ddagger}$	3.18E-05	3.06E-05	-	-	-	-	-	-	-	2.30E-05	2.00E-05	†	†	-	†	†	-	-
CuO	†	†	†	-	-	-	1.24E-04	8.04E-05	5.65E-05	2.86E-05	4.06E-05	1.33E-05	†	3.04E-05	†	-	-	†
Fe(OH)_3	-	-	-	-	-	-	-	-	-	1.41E-03	8.87E-05	†	2.68E-04	-	3.07E-04	5.09E-04	-	-
$\text{H}_5\text{O}_4\text{Ru}^{\ddagger}$	†	†	1.61E-05	1.19E-05	†	†	†	†	†	†	†	†	†	†	†	†	†	†
$\text{La(OH)}_3^{\ddagger}$	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†
$\text{Mg(OH)}_2^{\ddagger}$	3.62E-04	3.50E-04	1.53E-04	1.25E-04	7.25E-05	2.88E-05	7.12E-05	3.16E-05	1.98E-05	1.43E-04	1.02E-04	4.60E-05	†	1.02E-05	†	†	†	1.38E-05
Mn(OH)_2	3.22E-04	3.04E-04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
MnO_2	5.15E-05	4.94E-05	7.30E-05	6.10E-05	3.77E-05	2.09E-05	1.37E-02	7.23E-03	4.73E-03	2.09E-03	3.69E-03	1.26E-03	4.22E-04	2.98E-03	5.19E-04	1.07E-04	9.21E-05	4.50E-04
$\text{Na}_2\text{SO}_4\text{NaF}$	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
$\text{Na}_7\text{F(PO}_4\text{)}_2\text{19H}_2\text{O}$	-	-	-	-	2.23E-03	-	-	-	-	-	3.15E-04	-	2.37E-03	2.50E-04	1.15E-02	9.95E-03	2.67E-02	1.50E-02
$\text{Nd(OH)}_3^{\ddagger}$	5.90E-05	5.77E-05	3.60E-05	2.85E-05	1.45E-05	†	1.14E-05	2.65E-05	3.18E-05	1.75E-05	1.90E-05	†	†	†	†	†	†	†
Ni(OH)_2	-	-	2.67E-05	1.97E-05	†	3.09E-05	2.54E-03	1.60E-03	8.44E-04	-	-	-	-	8.63E-05	-	1.54E-05	4.21E-04	-
$\text{NiCr}_2\text{O}_4^{\ddagger}$	-	-	1.95E-05	1.63E-05	1.02E-05	†	-	-	-	-	-	-	-	-	-	-	1.98E-05	-
$\text{NiFe}_2\text{O}_4^{\ddagger}$	3.03E-04	2.93E-04	8.66E-05	6.87E-05	3.53E-05	3.16E-05	1.64E-05	8.73E-05	1.08E-03	8.51E-04	9.97E-04	4.62E-04	3.06E-04	8.29E-04	2.87E-04	1.42E-04	7.42E-04	1.79E-03
NiTiO_3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
PbTiO_3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
$\text{PbZr}_{0.3}\text{Ti}_{0.7}\text{O}_3$	-	-	-	-	-	†	-	-	-	-	-	-	-	-	-	-	-	-
$\text{PbZr}_{0.6}\text{Ti}_{0.4}\text{O}_3$	-	-	-	-	-	1.07E-05	-	-	-	-	-	-	-	-	-	-	-	-
$\text{PbZr}_{0.75}\text{Ti}_{0.25}\text{O}_3^{\ddagger}$	8.02E-05	7.75E-05	3.21E-05	2.69E-05	-	-	2.35E-05	2.49E-05	1.84E-05	5.07E-05	3.62E-05	1.62E-05	†	1.05E-05	†	†	†	†
$\text{PdO.H}_2\text{O}$	-	-	-	-	-	-	-	1.33E-04	1.11E-04	2.68E-05	4.01E-05	2.34E-05	†	5.32E-05	†	-	-	†
$\text{Rh}_2\text{O}_3\text{H}_2\text{O}$	†	†	†	†	†	†	†	1.94E-05	1.55E-05	†	†	†	†	†	†	†	†	†
SrCO_3	†	†	†	†	†	†	†	5.90E-03	2.48E-03	1.29E-03	5.96E-04	1.06E-03	4.43E-04	2.37E-04	1.09E-03	5.51E-04	2.18E-04	1.02E-04
ThO_2^{\ddagger}	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†	†
$\text{Y(OH)}_3^{\ddagger}$	†	†	1.49E-05	1.10E-05	†	†	†	1.93E-05	1.45E-05	†	†	†	†	†	†	†	†	†
$\text{ZnO.Fe}_2\text{O}_3$	7.58E-05	6.94E-05	-	-	-	-	-	-	-	4.98E-05	4.56E-05	1.83E-05	†	-	†	†	-	-
ZrO_2	1.12E-04	1.77E-04	1.26E-03	9.14E-04	2.80E-04	3.68E-04	5.06E-04	1.17E-03	4.66E-04	3.12E-04	7.91E-04	2.75E-04	1.13E-04	1.88E-04	1.34E-04	2.83E-04	7.77E-05	5.89E-05

Appendix C: Calculated Quantities of Precipitates for Each Composition (Continued)

SRNL-STI-2018-00446

Revision 0

Batch ID	May-47 to Aug-47	Feb-48 to Jun-48	Dec-48 to Apr-49	Jun-49 to Sep-49	Dec-50 to Apr-51	Jun-51 to Oct-51	Dec-51 to Apr-52	Aug-52 to Dec-52	Jan-54 to Apr-54
Al(OH)₃	-	-	7.75E-04	4.87E-03	8.91E-03	2.45E-04	2.28E-02	1.54E-02	8.56E-03
% of Total Al	-	-	2%	15%	21%	1%	26%	24%	13%
Na[COO]₂	9.54E-03	1.03E-02	9.22E-03	9.98E-03	1.10E-02	1.12E-02	1.06E-02	9.64E-03	7.54E-03
NAS	3.10E-03	3.39E-03	1.92E-03	1.22E-03	8.33E-04	1.30E-03	8.15E-04	1.07E-03	1.61E-03
Ag[‡]	-	†	†	†	†	†	†	†	†
Bi(OH)₃	6.67E-05	9.37E-05	5.41E-05	†	-	-	-	-	-
Ca5F(PO₄)₃[‡]	5.03E-04	5.73E-04	3.44E-04	2.39E-04	1.57E-04	3.88E-04	2.40E-04	6.15E-04	1.18E-03
Cd(OH)₂	†	†	†	†	-	†	-	-	†
Ce(OH)₃	†	†	†	†	†	†	1.66E-05	†	†
Co(OH)₂	-	-	-	-	-	-	-	-	-
Co(OH)₃[‡]	-	-	-	-	-	-	-	-	-
CoCr₂O₄[‡]	-	†	†	†	†	†	-	†	†
CoFe₂O₄[‡]	†	-	-	-	-	-	1.04E-05	-	-
CuO	-	-	-	-	-	-	-	-	-
Fe(OH)₃	1.77E-03	1.90E-03	1.20E-03	1.02E-03	7.55E-04	1.15E-03	8.26E-04	8.06E-04	1.33E-03
H₅O₄Ru[‡]	†	†	†	†	†	†	†	†	†
La(OH)₃[‡]	†	†	†	†	†	†	†	†	†
Mg(OH)₂[‡]	†	†	†	†	2.31E-05	†	9.84E-05	5.38E-05	†
Mn(OH)₂	-	†	1.55E-05	1.37E-05	1.69E-05	2.82E-05	†	†	1.19E-05
MnO₂	1.05E-04	5.95E-05	3.12E-05	4.72E-05	1.36E-05	1.90E-05	†	3.10E-05	1.75E-05
Na₂SO₄.NaF	-	-	-	-	-	-	-	-	-
Na₇F(PO₄)_{2.19H2O}	2.35E-02	2.03E-02	1.65E-02	1.88E-02	2.06E-02	2.66E-02	2.18E-02	9.21E-03	-
Nd(OH)₃[‡]	†	†	†	†	†	†	1.70E-05	†	†
Ni(OH)₂	-	-	-	-	-	-	-	-	-
NiCr₂O₄[‡]	-	-	-	-	-	-	-	-	-
NiFe₂O₄[‡]	7.33E-04	5.26E-04	2.10E-04	†	8.65E-05	2.32E-04	1.59E-04	2.76E-04	1.86E-04
NiTiO₃	-	-	-	-	-	-	-	-	-
PbTiO₃	-	-	-	-	-	-	-	-	-
PbZr_{0.3}Ti_{0.7}O₃	-	-	-	-	†	-	-	-	-
PbZr_{0.6}Ti_{0.4}O₃	-	-	-	-	†	-	†	-	-
PbZr_{0.75}Ti_{0.25}O₃[‡]	†	†	†	†	-	†	†	1.21E-05	†
PdO.H₂O	-	-	-	-	-	-	-	-	-
Rh₂O₃.H₂O	†	†	†	†	†	†	†	†	†
SrCO₃	8.91E-05	6.43E-05	9.34E-05	5.77E-05	8.36E-05	2.11E-04	1.25E-04	2.81E-04	2.99E-04
ThO₂[‡]	†	†	†	†	†	†	†	†	†
Y(OH)₃[‡]	†	†	†	†	†	†	†	†	†
ZnO.Fe₂O₃	†	†	†	†	†	†	2.24E-05	1.21E-05	†
ZrO₂	2.39E-05	3.82E-05	3.06E-05	2.46E-05	2.56E-05	1.83E-05	2.45E-05	1.54E-05	1.31E-05