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Hanford Waste Simulants Created to Support the Research and Development on the River Protection Project – Waste Treatment Plant

Westinghouse Savannah River Company
Savannah River Site
Aiken, SC 29808

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SAVANNAH RIVER TECHNOLOGY CENTER

Russell E. Eibling and Charles A. Nash

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APPROVALS

____ Date: ________________

Russell E. Eibling, Co-author (ITD/WTT/SRTC)

____ Date: ________________

Charles A. Nash, Co-author (WPT/WTT/SRTC)

____ Date: ________________

Steve T. Wach, RPP Pretreatment Manager (EP Group/SRTC)

____ Date: ________________

Harold F. Sturm, Jr., RPP Program Manager (WPTS/SRTC)

____ Date: ________________

T. Bond Calloway, Jr., Technical Reviewer (ITS/SRTC)

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1.0 Executive Summary

The development of nonradioactive waste simulants to support the River Protection Project –Waste Treatment Plant (RPP-WTP) bench and pilot-scale testing is crucial to the design of the facility. The report documents the simulants developed to support the SRTC programs and the strategies used to produce the simulants. The approved simulants for waste envelopes A, B, and C and the basis for their recipes is included. Additional simulants including sludge simulants, simulants of entrained solids, and simulants to support pretreatment mixing studies are discussed.

At the direction of RPP-WTP, the waste simulants were based upon specific waste characterization samples and did not involve averaging over multiple samples from multiple tanks, collected and analyzed at different times. This decision was made by the RPP-WTP team because most of the available sample analysis data is for grab samples for the Hanford site waste tanks. Grab samples are usually obtained from a single location within the tank waste and these samples may not represent the tank contents as a whole. An additional source of characterization information for Hanford site tank waste is the best basis inventory (BBI) for tank wastes. The BBI inventory is based on multiple, tank sampling events, waste processing information, and process chemistry knowledge. However, the BBI inventory did not list separate compositions for the liquid and solid phases present in each tank and therefore the BBI inventory could not be used effectively to prepare simulants under this task. The advantages and challenges of this approach are discussed along with recommendations for specific analyses that could improve the waste simulants.

The envelope A simulant that was developed as a part of this study and approved by the customer is based on the whole-tank composite analysis for waste stored in tank 241-AN-105. Additional envelope A simulants prepared or calculated include simulants of whole-tank composite compositions for wastes stored in tanks 241-AW-101, 241-AN-104, 241-AN-103 and a composite-dilution-based simulant of 241-AN-105. The envelope B simulant that was approved by the customer was based on the Best Basis Inventory (adjusted for liquid fraction only) for Tank 241-AZ-101, since no analysis of the present, tank liquid fraction was available in 1999. An additional B envelope simulant that was developed is based on the liquid fraction of waste in tank 241-AZ-102. The approved envelope C simulant is based on the liquid fraction of waste in tank 241-AN-107. Entrained solids simulants were created for envelopes A and C based upon analysis of the suspended solids in the waste stored in tanks 241-AN-105 and 241-AN-107 respectively.

The envelope D simulant was developed based upon tank 241-AZ-101 sludge that had not been caustic washed to reduce the aluminum level. Unlike the supernate simulants which assume that the supernate phase is homogeneous, the sludge simulant is based upon multiple samples and therefore make use of averaging. The AZ-101 sludge simulant is based on averaging two separate core samples due to the heterogeneous nature of the settled sludge.

The formulation and testing of Hanford waste simulants to support development of the RPP-WTP was conducted in accordance with the quality assurance requirements of 10-CFR830.120 as implemented in the Savannah River Site quality assurance plan (BNF-003-98-0008).[29]

2.0 Introduction and Background

The River Protection Project –Waste Treatment Plant (RPP-WTP) will process the radioactive wastes currently stored in the single and double–shell tanks (SST and DST) at the Department of Energy Hanford site to produce suitable waste forms for long term storage. As part of the research and development on the processes planned for the waste treatment plant, nonradioactive simulants will be required for much of the testing. This report documents the simulants developed to support the Savannah River Technology Center programs in support of the RPP-WTP. The research described in this report was conducted under task plan BNF-003-98-011, rev 0.[1] Additional simulants described in this report were also developed under task plan BNF-003-98-0079A.[2]

The RPP-WTP will vitrify both high-level wastes (HLW) and low activity wastes (LAW) using separate vitrification systems. The pretreatment processes include ultrafiltration using crossflow filter technology, ^{90}Sr and transuranic (TRU) removal by precipitation (Sr/TRU process), ^{137}Cs and ^{99}Tc removal by ion exchange, evaporation, HLW sludge washing/leaching, and waste and glass former blending. Development of these processes requires testing for lab through pilot scale test with nonradioactive simulants and lab-scale tests with the actual radioactive wastes. Therefore, development of simulants that duplicate the waste chemistry and, in some cases, the physical properties is required to support the overall program.

To aid in planning and designing the RPP-WTP, the waste to be processed was categorized as being part of four different waste envelopes: Envelope A, Envelope B, Envelope C and Envelope D. Each envelope, as it relates to the actual tank waste identified as candidate feed to the RPP-WTP, is described below. The request for proposals for design and construction of the RPP-WTP describes a much broader composition range for Envelopes A, B, C and D wastes. However for this task, simulants were prepared based on actual tank waste compositions that comply with the broader definition of the waste envelopes.

> Envelope A – Also known as Double Shell Slurry Feed and Double-Shell Slurry. The waste was generated by evaporating the low organic content, waste supernates stored in single shell tanks and the supernate produced by the Hanford B plant. Envelope A can be generally characterized as an alkaline ([OH^-}>1 Molar), high sodium (>8 Molar) supernate. The envelope contains ^{137}Cs and ^{99}Tc at concentrations that require removal prior to LAW vitrification. Sr/TRU removal is not required for this waste. The majority of the LAW supernate to be vitrified in the initial phase of the RPP-WTP will be envelope A. The Hanford tanks that have been classified as envelope A include 241-AW-101, 241-AN-103, 241-AN-104, 241-AN-105 and 241-AP-105.

Envelope B – Sometimes referred to as the supernate phase from Neutralized Current Acid Waste (NCAW). The envelope contains higher 137Cs concentrations than envelope A. The LAW glass specifications will require 137Cs and 99Tc removal. Sr/TRU removal is not required for this waste. The envelope B is expected to be high in glass limiting constituents such as sulfate, phosphate, and halides. Only a small part of the LAW waste to be vitrified in the initial phase is envelope B. The tanks with supernate in the envelope are 241-AZ-101 and 241-AZ-102.

Envelope C – Also known as Complex Concentrate. The C waste was produced from evaporation of wastes derived from high organic content single-shell tank waste and waste generated during the Cs/Sr separation and encapsulation process conducted at the Hanford B plant. The waste is characterized by the high organic carbon content due to the presence of organic complexing agents and their decomposition products. Due to the complexing agents, the concentration of ^{90}Sr and TRU will require removal using the Sr/TRU precipitation and filtration process. Removal of ^{137}Cs and ^{99}Tc by ion exchange will also be required. The tanks within the C envelope are 241-AN-102 and 241-AN-107.

Envelope D – Envelope D is composed of insoluble compounds referred to as sludge, primarily insoluble transition metal hydroxides with most of the long half-life radionuclides, slurried with the supernate from the same tank. For example, the slurry from tank 241-AZ-101 would be composed of the B envelope supernate and the D envelope sludge. As such, the tank could be described as a B/D tank. Similarly, there could by A/D and C/D tanks. The D envelope waste will require washing using crossflow filtration and possibly caustic leaching to meet glass specifications. Tanks with solids that are in the D envelope include 241-AZ-101, 241-AZ-102, 241-AY-101 (planned mixture of tank 241-C-104 sludge and tank 241-AY-101 sludge), and 241-AY-102 (contains mixture of tank 241-C-106 sludge and tank 241-AY-102 sludge).

There are four basic kinds of waste simulants. These are (1) supernates, (2) sludges, (3) entrained solids, and (4) miscellaneous simulants that represent intermediate process streams. Each of these types of simulant can represent portions of each of the waste envelopes. For example, A, B, and C waste envelopes are all supernates but with differing compositions and each can have a different composition of entrained solids. Sludge simulants such as the D envelope material can represent washed or caustic leached sludge depending on the sludge composition.

3.0 Discussion

The Strategy Used in Waste Simulants

The development of processes for safe and efficient disposal of radioactive waste requires detailed testing of proposed processes. However, the difficulty of handling radioactive waste makes detailed testing very difficult and expensive. The use of nonradioactive waste simulants eliminates most of the handling problems and allows less expensive detailed studies to proceed. Waste simulants are usually based upon the average composition for a type of waste determined by averaging over multiple samples collected at various times. The advantage of averaging is that a bad result will not seriously bias the simulant and that the impact of spatial distribution within the waste tank can be minimized. The disadvantage of averaging is that the amount of time-dependent waste components such as hydroxide, carbonate, nitrate and nitrite can be seriously under or over represented.

The waste simulants described in this report were not based upon averaging waste compositions. Instead, at the direction of the customer, waste simulants were based upon specific waste samples that were as well characterized as possible. The resulting simulant can represent a specific tank and can be traced back to a specific sample and sample analysis. Using this approach, the time-dependent waste compounds will be correctly simulated. The disadvantage of this approach is that a bad analysis can seriously impact the waste simulant. Therefore, reviewing the quality and reasonableness of the analysis is important to the application of the data. The waste simulant will only be as good or complete, as the analysis is good or complete. The application that the simulant will be used for must also be considered. The simulants described in this report were developed to support the pretreatment process planned for the RPP-WTP. The strategy used for the supernate simulants, entrained solids simulants and sludge simulants will be separately discussed.

Supernate Simulants

Supernate simulants must represent the aqueous phase of the waste present within the Hanford waste tanks. Since many of these supernates are at saturation as indicated by the presence of floating and settled crystallized salts (tank 241-AN-105 and others), production of the simulant will be bounded by the solubility of the various salts present.[3] The steps required in creating the supernate simulant are:

1. Calculate the carbonate concentration from the measured total inorganic carbon (TIC) value. The TIC measurement is obtained by measuring the carbon dioxide released upon treating a sample with acid and therefore directly measures the carbonate concentration.

2. If sulfate and/or phosphate measurements by ion chromatography are not available, calculate sulfate from sulfur and phosphate from phosphorus.

3. Calculate the borate concentration from the boron value and the metasilicate concentration from the silicon value.

4. Convert the chromium concentration to chromate and add as sodium chromate.

5. Calculate the charge balance between anions and cations. If the charge balance is extremely unbalanced (>~30 %), it may be better to find a more complete analysis of a different sample from the same tank.

6. Adjust either the hydroxide/carbonate or the sodium concentration to obtain the required balance. Usually the best choice is to raise or lower the free hydroxide content. Adjusting the hydroxide value is based upon the difficulty of accurately measuring the free hydroxide level. Depending on the other anions present, titration methods can suffer from interference from aluminate, carbonate, organic anions, and phosphate anions. If TIC has not been measured, the carbonate concentration can also be used to assist in charge balancing since carbonate is expected to be present in all of the supernates.

7. Determine if the transition metals plus aluminum content is low enough to permit the use of the metal nitrate, which are generally very soluble, as the source for the metal ion. For example, in envelope A waste the aluminum content would place too much nitrate in the supernate if the aluminum is added as the nitrate.

8. If required, calculate the aluminum as aluminum trihydroxide with an appropriate amount of sodium hydroxide to convert the compound to sodium aluminate.

9. If cesium and strontium concentrations are available from a spectroscopy method, add them as the nitrate salts. If the only concentration values available are for the radionuclides, ^{137}Cs and ^{90}Sr, use the specific activity to calculate a mass concentration. Then adjust the cesium concentration to reflect that ^{137}Cs is ¼ to 1/3 of the total cesium based upon expected fission product yields and ^{90}Sr is typically 1/10 of the total strontium based upon prior experience with strontium isotopics from caustic-neutralized wastes.

10. Since all of the isotopes of technetium are radioactive, a substitute for technetium (rhenium) can be used if needed. Convert the ^{99}Tc value to a molar concentration using the specific activity and then convert to sodium perrhenate (assuming pertechnetate is the primary ^{99}Tc species).

11. Calculate all of the measured anions as sodium salts except boron, which can be added as boric acid.

12. Create the recipe paying close attention to the sequence of compound addition to prevent unwanted destruction of some of the acid-reactive anions such as carbonate and nitrite. The initial test solution should be made up in a volumetric flask to insure that the proper volume of simulant is produced.

13. The sequence of addition used in this study was to mix the acidic compounds such as the transition metal nitrates together and dissolve in water. Of particular concern are compounds such as ferric nitrate or ferric chloride, which must be complexed before addition to the basic mixture. Combining the acidic metals with the complexing agents at this step assures that the metal will be soluble after the caustic is added. The complexing agents can be added as the free acids (adjusting the sodium hydroxide addition appropriately) or as the sodium salts.

14. In a separate container, mix the strong base with the aluminum species to generate the aluminate anion. The aluminum species chosen must be of known aluminum content. For example, Aluminum trihydroxide or Aluminum nitrate with known water contents can be used. Sodium aluminate can also be used if the precise aluminum content is known, however, the water content in the commercial forms of sodium aluminate usually varies. Next, dissolve the other nonreactive salts in the caustic mixture.

15. Blend the acidic and basic solutions together to produce an alkaline solution. The solution at this point must be alkaline to prevent destruction of two of the remaining anions that will be added in step 16.

16. Add the residual sodium nitrate and the reactive salts, sodium carbonate and sodium nitrite to the alkaline solution. Continuous agitation may be necessary to completely dissolve the final salt additions. Heat may also be used to aid in the final dissolution. To some extent, this addition sequence mimics the process by which the waste was originally generated.

17. Finally, measure the density of the simulant solution for use in calculating the water additions for very large batches of simulant where preparation by a volumetric approach is not feasible.

The resulting simulant solution should be low in insoluble solids since it is designed to represent the supernate phase of the tank waste. A trace of insoluble solids can form due to trace contaminants in the reagent chemicals used in preparation. The choice of the reagents can be critical to preparation of a good simulant. Particular attention must be placed on purity and the water of hydration, which is common with many of the metal salts. If excessive insoluble solids are observed, additional focus must be placed on the possible need for trace levels of complexing agents (e.g., EDTA, gluconate, etc.). Matching the measured total organic carbon value (TOC) was not a goal of the above procedure. The more complete the organic analysis is, the better the match with the TOC can be. However, artificially increasing the concentration of a measured organic species to aid in matching the TOC can introduce spurious chemical properties and was therefore not undertaken in this study.

Entrained Solids Simulants

The entrained solid simulant is used for pilot studies of the crossflow filtration processes of the RPP-WTP. The simulant should duplicate the chemical composition and the physical properties of the actual entrained solids where possible. Because of the filtration studies, particle size is an important parameter for the simulant. The customer requested that the simulant be based upon specific solids characterization data, which should include particle size information. If particle size information is not available, the most conservative approach will be to use particles in the range that will be a challenge to the filtration system, less than 10 micron. The wastes requiring an entrained solids simulant will generally be the A and C envelopes. The B envelope waste is expected to have entrained solids that are sludge particles from envelope D. Therefore, a separate B entrained solids simulant was not developed. The steps required in creating the entrained solids simulant are:

1. Calculate the moles of each element or anion detected in the washed solids for that waste.

2. If a TOC measurement is available on the solids, convert the TOC value from moles of carbon to moles of oxalate. This assumes that the insoluble form of organic carbon is oxalate. Research on the solubility of organic complexing agents indicated that oxalate is the major insoluble organic species in Hanford waste.[4]

3. The transition metals and aluminum and silicon are calculated as the insoluble oxides.

4. Alkali metals and alkaline earth's are calculated as the most insoluble salts possible based on the measured anions. For example, if oxalate is present use sodium oxalate or calcium oxalate. Other candidate compounds could be calcium phosphate or calcium sulfate depending on the measured anions present.

5. Calculate the mass of each compound, the total mass of the suggested compounds and the percent the compound makes up of the simulant solids and of the actual solids from the waste. If the percent of the actual solids is greater than 80%, the simulant will probably match, within analytical error, the actual waste solid from an analysis, point of view. If the percent of the actual is less than 80, alternate insoluble species such as different oxidation states for the transition metals, should be considered.

6. Since the simulant is produced by mixing solids together, the particle size of the solids should be specified to match the measured particle size range of the actual entrained solids. This will insure that the simulant properly tests the filtration process.

As with all simulants, the simulant can only be as good as the analytical data it is generated from and the **simulant results should always be confirmed by actual waste tests**.

Envelope D Simulants

The envelope D waste is primarily insoluble transition metal oxides and hydroxides that were generated by addition of sodium hydroxide to nitric acid process waste streams. As such, the best way to generate a simulant, which has the correct chemical and physical properties, is to simulate the original waste stream and then the waste storage process. Unfortunately, the parameters of temperature, time and radiation are not easily simulated in a rapid fashion. Therefore, no effort was made to duplicate these parameters. Rapid mixing and shearing can be used to insure that the precipitated metal oxides and hydroxides produce fine particles instead of large gelatinous flocks. Unlike the supernate simulants, the envelope D simulant can be produced from multiple source compounds as long as sufficient washing is included to remove the unwanted associated anion. The process used to generate the envelope D simulant uses the following steps:

1. Calculate the grams/liter of each metal and anion present in the washed D waste. If the waste simulant is to represent caustic leached envelope D waste either start with an analysis of the waste after caustic leaching or assume a leaching factor for aluminum and reduce the aluminum content by that factor.

2. Calculate the mass of each transition metal to be added based upon the use of nitrate salts. Aluminum should be added as the oxide (preferably boehmite, AlOOH), boron as boric acid, molybdenum as either sodium or potassium molybdate, and silicon and titanium as the oxide. The anions will be added as sodium salts.

3. Calculate the amount of potassium permanganate and manganous nitrate necessary to produce the required hydrated manganese dioxide.

4. Generate the hydrated MnO_2 solids by mixing potassium permanganate and manganous nitrate according to the following stoichiometry:

$$3Mn(NO_3)_2 + 2KMnO_4 + 2H_2O \longrightarrow 2KNO_3 + 5MnO_2 + 4HNO_3$$

5. Add to the hydrated MnO_2 solids the transition metal nitrates that form precipitates in caustic solutions, for example Fe, Ni, Cr, etc. The amphoteric metals such as aluminum and other compounds such as silica and titania will not be added until step 10.

6. Precipitate the metals with sodium hydroxide until a stable pH >10 is achieved.

7. Add a sodium carbonate solution to convert some of the more soluble hydroxides into less soluble carbonates. Allow at least 18 hours (overnight or over a weekend) for the solids to settle.

8. Decant the supernate and wash the precipitated solids. Note that the final wash should be with inhibited water, 0.01 molar in sodium hydroxide and 0.01 molar in sodium nitrite.

9. The washing should continue until the nitrate concentration in the supernate is less than 1000 mg/liter.

10. Add the additional insoluble compounds (Al_2O_3, SiO_2, and TiO2) in a controlled particle size form to assist in duplicating the actual waste particles size. Mix thoroughly and then add the soluble salts that remain followed by additional mixing.

If desired, additional heat treatment can be used to represent some of the waste thermal history. Additional shearing may also be useful in reducing the simulated sludge particle size. As with all simulants, the simulant can only be as good as the analytical data it is generated from and the **simulant results should always be confirmed by actual waste tests**.

Appendix G lists the analytical methods used to measure the concentration of species in simulant test recipes.

Envelope A Simulants

The following simulants were calculated and/or prepared to support SRTC research: Approved A Envelope simulant based upon AN-105 supernate, an AN-105 whole tank composite simulant, an AW-101 simulant, an AN-104 whole tank composite simulant, and a preliminary simulant based upon AN-103. The source of each of these simulants and the specific issues in the preparation of these simulants will be described individually.

Approved A Simulant - AN-105 Simulant

The waste retrieval scenario that the envelope A simulant was based on was the supernate from tank 241-AN-105 was decanted from the solids within the waste tank without any effort to dissolve the solids or dilute the waste. The AN-105 simulant produced to support SRTC testing of filtration, ion exchange and evaporation was based primarily on the initial privatization sample from AN-105 with some supplementary results from another recent AN-105 sample.[5,6] The initial privatization sample was spiked with potassium chromate and cesium hydroxide for use as an envelope B sample even though AN-105 is clearly envelope A material. The measured TOC value of 3.6 grams/Liter carbon suggested that measurable levels of organic compounds such as formate, oxalate, acetate and glycolate should be present in the waste. However, organic speciation data was not available for the 241-AN-105 waste at the time the simulant was being prepared. Since a very similar waste, tank AW-101, was also sampled and analyzed during the initial privatization studies, the values for these organic compounds were taken from that waste analysis.[7] The cesium concentration was based upon the ^{137}Cs concentration of 1.79E+07 becquerels/mL making up 1/3 of the total cesium. The composition basis used for the AN-105 simulant is listed in Table 1.

Table 1 Approved Envelope A Simulant Based on Tank 241-AN-105

Component	Moles/Liter	mg/Liter
Aluminum	1.47E+00	39700
Ammonium	6.65E-03	120
Boron	4.72E-03	51
Cadmium	2.94E-05	3
Calcium	9.98E-04	40
Carbonate	2.09E-01	12540
Cesium	1.22E-04	16
Chromium	2.60E-02	1350
Hydroxide	3.42E+00	58100
Lead	2.56E-04	53
Magnesium	2.22E-04	5
Molybdenum	8.55E-04	82
Potassium	1.92E-01	7500
Selenium	1.25E-05	1
Silicon	7.51E-03	211
Silver	1.51E-04	16
Sodium	1.07E+01	246000
Tin	1.83E-04	22
Zinc	1.54E-04	10
TIC	2.09E-01	2510
TOC	2.99E-01	3590
Chloride	2.56E-01	9090
Fluoride	1.00E-02	190
Formate	6.40E-02	2880
Nitrate	2.66E+00	165000
Nitrite	2.41E+00	111000
Oxalate	6.93E-03	610
Phosphate	6.00E-03	570
Sulfate	8.03E-03	771
Acetate	3.51E-02	2070
Glycolate	1.53E-02	1150

The charge balance for the simulant initially had 0.55 moles/Liter of excess negative ions, which indicates a closure of about 95 %. The excess negative charge was balanced by allowing the sodium to increase by 0.55 moles/Liter from the measured 10.1 moles/Liter to 10.7 moles/Liter. Appendix A details the computations performed to transform Table 1 data into the compounds listed in Table 2.

Table 2 AN-105 Simulant Composition

Compounds	Formula	Grams/Liter
Boric Acid	H_3BO_3	0.292
Cadmium Nitrate	$Cd(NO_3)_2\bullet 4H_2O$	0.009
Calcium Nitrate	$Ca(NO_3)_2\bullet 4H_2O$	0.236
Cesium Nitrate	$CsNO_3$	0.024
Lead nitrate	$Pb(NO_3)_2$	0.085
Magnesium Nitrate	$Mg(NO_3)_2\bullet 6H_2O$	0.057
Potassium Nitrate	KNO_3	19.221
Silver Nitrate	$AgNO_3$	0.026
Zinc Nitrate	$Zn(NO_3)_2\bullet 6H_2O$	0.046
Glycolic Acid	$HOCH_2COOH$, 70 wt%	1.665
Sodium Chloride	$NaCl$	14.984
Sodium Fluoride	NaF	0.420
Sodium Chromate	Na_2CrO_4	4.205
Sodium Sulfate	Na_2SO_4	1.140
Potassium Molybdate	K_2MoO_4	0.204
Ammonium Acetate	CH_3COONH_4	0.513
Aluminum Trihydroxide	$Al(OH)_3$	114.77
Sodium Hydroxide	$NaOH$	196.68
Selenium dioxide	SeO_2	0.001
Sodium meta-silicate	$Na_2SiO_3\bullet 9H_2O$	2.135
Sodium Acetate	$NaCH_3COO\bullet 3H_2O$	3.865
Sodium Formate	$HCOONa$	4.351
Sodium Oxalate	$Na_2C_2O_4$	0.929
Sodium Phosphate	$Na_3PO_4\bullet 12H_2O$	2.281
Sodium Carbonate	Na_2CO_3	22.149
Sodium Nitrate	$NaNO_3$	209.70
Sodium Nitrite	$NaNO_2$	166.48
Water	H_2O	669.37

Testing the AN-105 simulant gave a density of 1.44 g/mL at 20 C. The simulant produced just a small amount of solids but did require several hours of mixing to dissolve the added compounds. On days when the temperature was cooler, more solids would crystallize out. When the temperature rose the solids would redissolve suggesting that the solution is saturated in some of the waste components and is correctly reflecting the AN-105 conditions (floating crystallized salts).[3] Simulant preparation was performed at 20-22 C. Table 3 gives an analysis of some of the waste components in a test batch of the AN-105 simulant.

Table 3 Analytical results on AN-105 Simulant

Component	Units	Found	Planned	% of Target
Al	mg/Liter	35700	39700	90
B	mg/Liter	48	51	94
Ca	mg/Liter	<1	40	<2
Cd	mg/Liter	10	10	100
Cr	mg/Liter	1450	1350	107
K	mg/Liter	8380	7500	112
Mg	mg/Liter	<1	5	<20
Mo	mg/Liter	89	82	109
Na	mg/Liter	257000	246000	104
Pb	mg/Liter	46	53	87
Si	mg/Liter	129	211	61
Zn	mg/Liter	19	12	158
Chloride	mg/Liter	9200	9090	101
Fluoride	mg/Liter	<100	190	<50
Formate	mg/Liter	2980	2880	103
Nitrate	mg/Liter	172000	165000	104
Nitrite	mg/Liter	120000	111000	108
Oxalate	mg/Liter	<100	610	<16
Phosphate	mg/Liter	<100	570	<18
Sulfate	mg/Liter	950	825	115

The results are typical for attempts at measuring a saturated solution, note the high sodium nitrate and nitrite levels measured. Low level of phosphate and fluoride may indicate some formation of the insoluble fluorophosphate double salt, which has been observed in other simulant waste supernates.[8] It is also interesting to note that the alkaline earth metals (Ca and Mg) which form relatively insoluble salts with oxalate, phosphate and fluoride are lower than targeted as are the appropriate anions. The low silicon result could also be due to formation of an aluminosilicate. Other A simulant formulations also had difficulty with lower than planned phosphate concentrations, however, at lower sodium concentrations a higher concentration of phosphate was achieved (see AW-101 and AN-104 simulants).

Relatively large volumes of simulant are required for the pilot ion exchange and crossflow filtration studies. To assist in producing the diluted supernate simulant, a series of diluted AN-105 simulants were prepared volumetrically so that the density of the diluted simulant could be measured. Table 4 lists the measured densities and the weight percent solids calculated for these dilutions as a function of the sodium ion concentration. The weight percent solids value represents the solids with no waters of hydration and is a theoretical (computed) value. This should be used as a guide since measuring the weight percent solids by oven or microwave drying may lead to varying levels of dehydration and possibly some decomposition and therefore a different value.

Table 4 AN-105 Simulant Density and Percent Solids

Na Concentration, Molar	Density, g/mL	Wt % Anhydrous Solids
2.0	1.111	12.89
4.5	1.205	26.63
5.01	1.228	29.06
5.49	1.248	31.37
6.02	1.265	33.91
8.0	1.35	42.26
10.7	1.44	52.72

The densities listed in table 4 were measured at 20 to 22 C (ambient lab temperatures). The sodium concentration versus the density can be fit empirically to the following simple equation to allow predictions of densities (Y, gm/mL) for different sodium concentrations (X, Na molarity) when the supernate is diluted:

$$Y^2 = 1.007 + 0.10029X \quad (1).$$

Besides the measured values, at infinite dilution, the sodium concentration would be zero and the density would be that of water, 0.997 g/mL This assumption was also included in the data set that was fitted. Figure 1 display the fitted curve versus the measured and assumed data point.

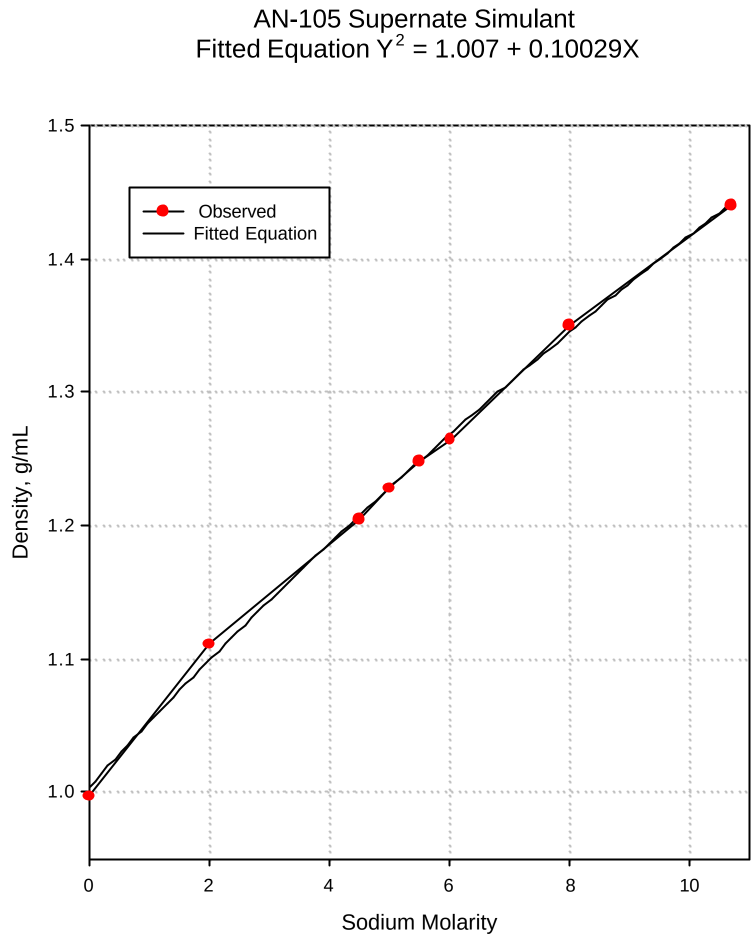


Figure 1 AN-105 Simulant Density as a Function of the Na Concentration

The r^2 value for the fit is 0.998. The relationship can be used for this specific ratio of compounds across the range measured but should not be extended to other simulant recipes.

The weight percent solids (anhydrous) can also plotted and fitted to a curve. Note that the assumption is made that at 0.0 Molar Na (X, Na molarity), the weight percent solid (Y, wt %) is also 0.0. Figure 2 demonstrates that the power law curve,

$$Y = 7.917X^{0.803} \qquad (2)$$

provides a good fit to the results, r^2 is 0.999.

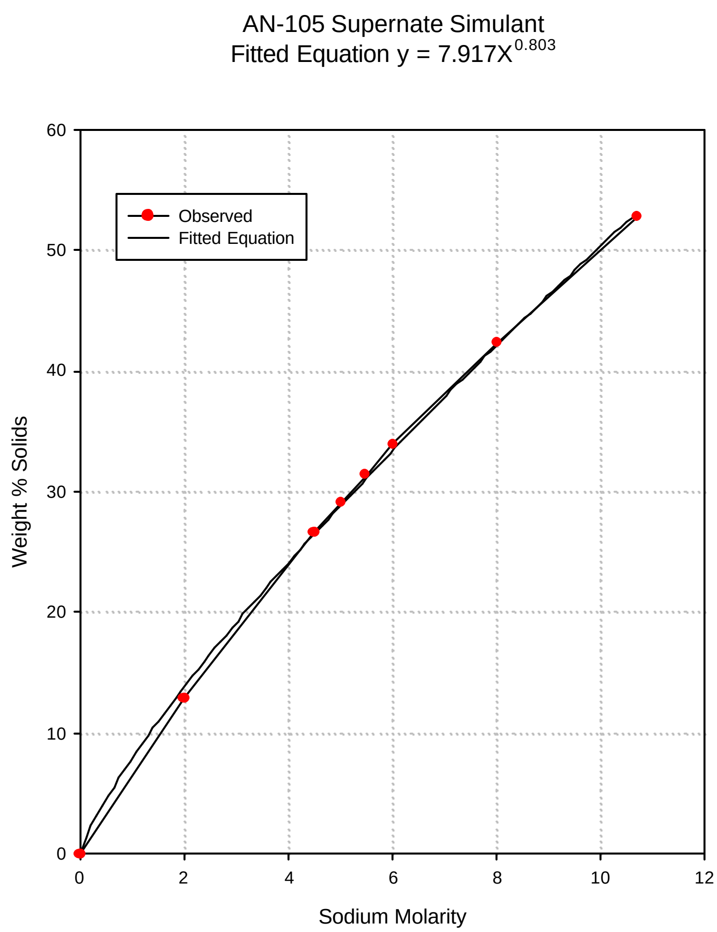


Figure 2 AN-105 Simulant Weight Percent Solids (Anhydrous) as a Function of Na Molarity

As mentioned previously, the relationship given by equation (2) is only for the composition specified for the approved AN-105 simulant. Actual measurements of weight percent solids can differ from this curve due to waters of hydration or due to actual compound decomposition. As such the curve should be used as a guide. For example, equation 2 or figure 2 can be used to estimate the Na concentration after dilution based upon a total solids measurement.

AN-105 Whole Tank Composite Simulant

Another simulant based upon tank 241-AN-105 was created to support the mixing of process heels and process solutions study.[9] The retrieval scenario that the simulant was based upon was one in which the entire tank is mixed and then water is added to achieve 50 % dilution by volume.[10] This scenario produces a supernate which is more of a whole tank composite and contains relatively higher levels of the less soluble anions due to dissolution. Table 5 gives the analytical basis of the simulant.

Table 5 AN-105 Fifty Volume % Dilution Whole Tank Composite Simulant

Component	Moles/Liter	mg/Liter
Aluminum	7.84E-01	21150
Boron	3.05E-03	33
Carbonate	4.51E-01	27054
Chromium	1.64E-02	854
Hydroxide	2.03E+00	34600
Molybdenum	5.42E-04	52
Potassium	1.28E-01	5010
Silicon	3.60E-03	101
Sodium	7.24E+00	166500
TIC	4.51E-01	5415
TOC	1.72E-01	2070
Chloride	1.65E-01	5840
Fluoride	2.38E-02	453
Nitrate	2.17E+00	134500
Nitrite	1.73E+00	79800
Oxalate	6.24E-03	549
Phosphate	1.37E-02	1305
Sulfate	3.85E-02	3695

The planned density for the simulant was 1.32 grams/mL. Equation (1) predicts a density of 1.316 despite the relative change in some of the concentrations. The charge balance showed excess negative ions by 0.62 moles/Liter. The charge balance for the planned simulant was obtained by reducing the hydroxide concentration by 0.62 moles/Liter. Note the significantly higher levels of carbonate, fluoride, phosphate and sulfate despite the solution being more dilute in sodium, nitrate and nitrite. The higher levels of the less soluble anions demonstrate dissolution of some of the crystallized salts in the waste due to the planned retrieval method.

The planned simulant composition based upon the reported density of 1.32 grams/mL is shown in Table 6.

Table 6 Planned AN-105 Fifty Volume % Dilution Whole Tank Composite Simulant Composition

Compounds	Formula	Grams/Liter
Boric Acid	H_3BO_3	0.189
Potassium Nitrate	KNO_3	12.845
Sodium Chloride	NaCl	9.627
Sodium Fluoride	NaF	1.000
Sodium Chromate	Na_2CrO_4	2.659
Sodium Sulfate	Na_2SO_4	5.464
Potassium Molybdate	K_2MoO_4	0.129
Aluminum Trihydroxide	$Al(OH)_3$	61.142
Sodium Hydroxide	NaOH	113.098
Sodium meta-silicate	$Na_2SiO_3 \bullet 9H_2O$	1.022
Sodium Oxalate	$Na_2C_2O_4$	0.836
Sodium Phosphate	$Na_3PO_4 \bullet 12H_2O$	5.223
Sodium Carbonate	Na_2CO_3	47.784
Sodium Nitrate	$NaNO_3$	173.561
Sodium Nitrite	$NaNO_2$	119.686
Water	H_2O	762.19

A test solution of this simulant was not prepared since computation of a similar simulant representing the envelope A tank AN-104 indicated that the AN-104 simulant was more conservative for the mixing study planned (see the simulant described below).

AN-104 Whole Tank Composite Simulant

The AN-104 whole tank composite simulant is based upon a retrieval scenario in which the entire tank is mixed and then water is added to achieve 50 % dilution by volume.[11] The resulting supernate is 7.61 molar in sodium ion and contains substantially higher levels of phosphate, sulfate and carbonate due to dissolution of salts within the solids present in AN-104. The simulant was created to support the mixing of process heels and process solutions study.[9] Just as in the AN-105 simulant previously described, the AN-104 simulant is a whole tank composite based simulant due to the dissolution of crystallized salts. Due to the addition of water in the presence of the crystallized salts in AN-104, the supernate is likely saturated with carbonates, phosphates and sulfates salts. Table 7 gives the analytical basis for the simulant.

Table 7 AN-104 Fifty Volume % Dilution Whole Tank Composite Simulant

Component	Moles/Liter	mg/Liter
Aluminum	8.60E-01	23200
Boron	3.05E-03	33
Carbonate	6.24E-01	37421
Chromium	4.77E-03	248
Hydroxide	2.48E+00	42100
Molybdenum	5.21E-04	50
Potassium	1.28E-01	5010
Silver	1.21E-04	13
Silicon	5.45E-03	153
Sodium	7.61E+00	175000
TIC	6.24E-01	7490
TOC	1.56E-01	1870
Chloride	1.44E-01	5100
Fluoride	2.66E-02	506
Nitrate	1.65E+00	102000
Nitrite	1.40E+00	64500
Oxalate	6.24E-03	549
Phosphate	3.09E-02	2930
Sulfate	7.41E-02	7120

The oxalate concentration used in the AN-104 simulant was taken from the AN-105 simulant previously described due to the AN-104 measurement being reported as a less than value (<1000 mg/Liter) while oxalate was expected to be present. The TOC value of 1.87 grams/liter also suggested that some oxalate should be added. The charge balance from the analytical data had an excess level of negative ions by 0.37 moles/liter out of 7.72 moles/liter (balance of 95 %). Therefore, the hydroxide concentration was reduced by 0.37 moles/liter. The AN-104 simulant composition based upon the reported density of 1.31 grams/mL is shown in Table 8.

Table 8 AN-104 Fifty Volume % Dilution Whole Tank Composite Simulant Composition

Compounds	Formula	Grams/Liter
Boric Acid	H_3BO_3	0.189
Potassium Nitrate	KNO_3	10.367
Silver Nitrate	$AgNO_3$	0.020
Sodium Chloride	$NaCl$	8.407
Sodium Fluoride	NaF	1.118
Sodium Chromate	Na_2CrO_4	0.773
Sodium Sulfate	Na_2SO_4	10.528
Potassium Molybdate	K_2MoO_4	0.124
Aluminum Trihydroxide	$Al(OH)_3$	67.068
Sodium Hydroxide	$NaOH$	119.053
Sodium meta-silicate	$Na_2SiO_3 \bullet 9H_2O$	1.548
Sodium Oxalate	$Na_2C_2O_4$	0.836
Sodium Phosphate	$Na_3PO_4 \bullet 12H_2O$	11.727
Sodium Carbonate	Na_2CO_3	66.095
Sodium Nitrate	$NaNO_3$	131.086
Sodium Nitrite	$NaNO_2$	96.738
Water	H_2O	776.77

The measured density of the simulant was 1.333 grams/mL at ambient lab temperatures (20 to 22 C). The weight percent total solids using the microwave oven technique was 39.55 %. A day or two after the simulant was prepared, the lab temperature dropped to 8 C and white solids were observed to have crystallized from the simulant. Upon heating to 45 C the solids dissolved. The residual fine solids were filtered and collected. The supernate was submitted for analysis and the solids were submitted for characterization by x-ray diffraction and by scanning electron microscopy with energy dispersive analysis. The analytical results for the supernate are shown in Table 9 while the solids characterization is shown in figures 3 and 4.

Table 9 Analytical Results on AN-104 Simulant

Component	Units	Found	Planned	% of Target
Al	mg/Liter	17650	23200	76
B	mg/Liter	32	33	97
Ag	mg/Liter	1.4	13	11
Cr	mg/Liter	212	248	85
K	mg/Liter	3960	4050	98
Na	mg/Liter	182760	175000	104
Si	mg/Liter	144	153	94
Mo	mg/Liter	49	50	98
Chloride	mg/Liter	5031	5100	99
Fluoride	mg/Liter	103	506	20
Nitrate	mg/Liter	99490	102000	98
Nitrite	mg/Liter	64040	64500	99
Oxalate	mg/Liter	250	549	46
Phosphate	mg/Liter	2017	2930	69
Sulfate	mg/Liter	7072	7120	99
TIC	mg/Liter	13070	7490	175
TOC	mg/Liter	779	150	520

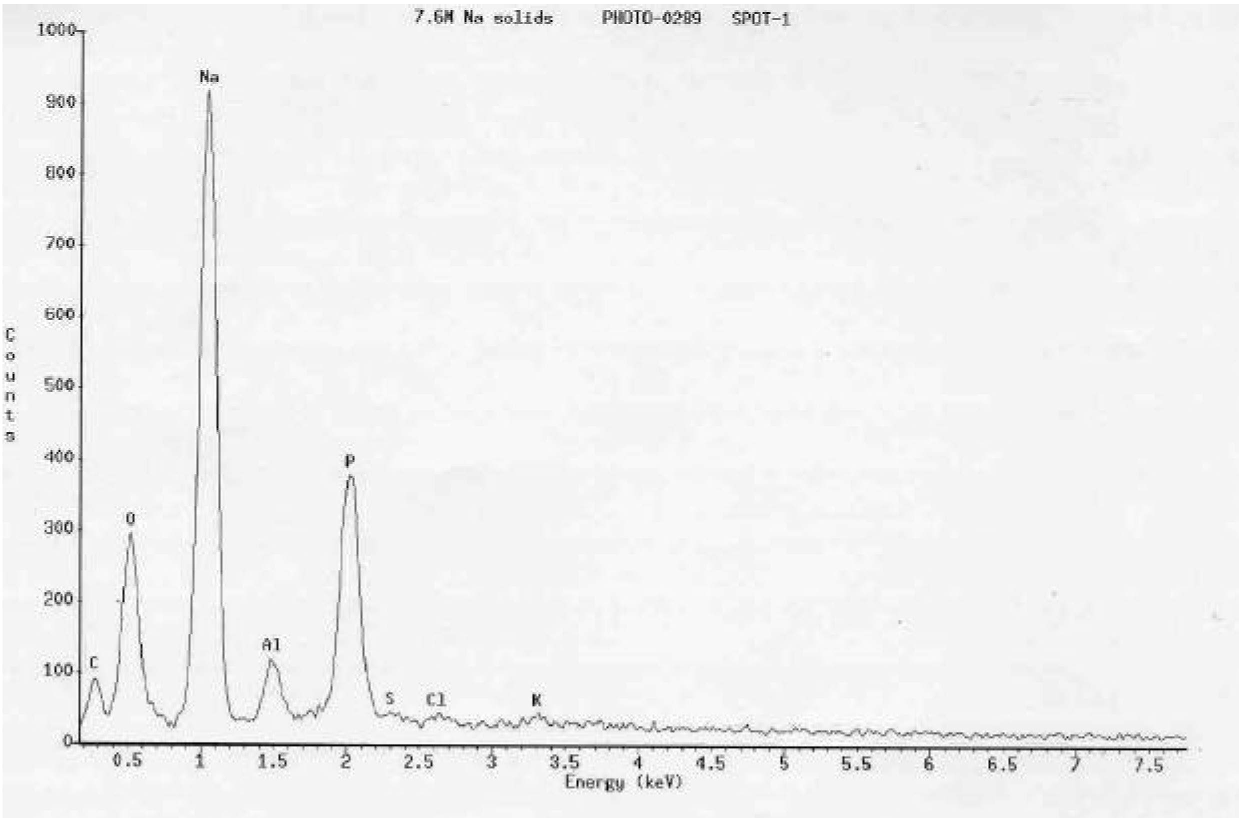


Figure 3 Scanning Electron Microscope – Energy Dispersive Spectra of Solids from AN-104 Simulant

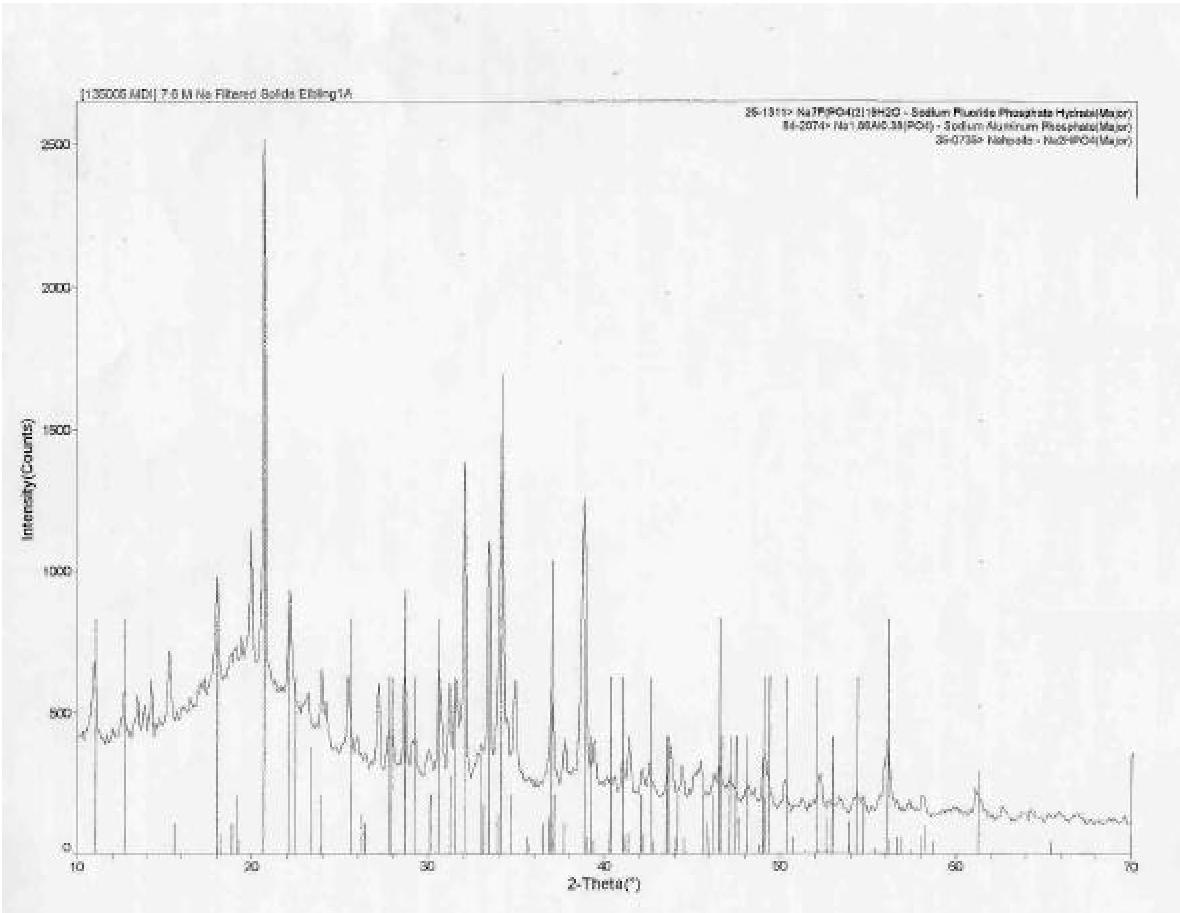


Figure 4 X-ray Diffraction Analysis of Solids from AN-104 simulant

The low results shown for fluoride and phosphate are confirmed by the presence of fluorophosphate double salt detected by XRD in figure 4. The low result for silver may be due to photoreduction of the silver ion since dark particles were observed in the simulant shortly after makeup. The low aluminum result was traced to the aluminum trihydroxide that was used. The aluminum source was only 80% pure due to absorbed water, therefore, the aluminum measured was actually very close to the amount added.

The high TIC result was probably due to carbon dioxide absorption, leading to the production of carbonate.

AW-101 Simulant

The AW-101 simulant was based on supernate samples that were obtained from five equally spaced elevations in the liquid phase of waste stored in Hanford tank 241-AW-101 as diluted with de-ionized water to a sodium concentration of 6.46 molar.[12] The waste simulant is a high hydroxide, high aluminate, envelope A tank. The simulant was created to support the mixing of process heels and process solutions study.[9] The analytical basis for the AW-101 simulant is given in table 10.

Table 10 Basis for AW-101 Simulant

Component	Moles/Liter	mg/Liter
Aluminum	6.06E-01	16350
Carbonate	1.79E-01	10767
Cesium	8.13E-05	11
Chromium	1.08E-03	56
Hydroxide	3.05E+00	51872
Iron	8.42E-05	5
Lead	1.98E-04	41
Nickel	8.18E-05	5
Potassium	5.88E-01	23000
Silicon	4.63E-03	130
Sodium	6.46E+00	148500
Zinc	2.14E-04	14
Zirconium	8.33E-05	8
TIC	1.79E-01	2155
TOC	1.30E-01	1560
Chloride	9.31E-02	3300
Fluoride	4.37E-02	830
Nitrate	1.98E+00	123000
Nitrite	1.36E+00	62750
Phosphate	2.05E-02	1950
Sulfate	1.93E-02	1850

The charge balance for the analytical information has an excess of negative ions by 0.56 moles/Liter, which is a 92 % balance. The hydroxide was reduced by 0.56 moles/Liter so as not to increase the sodium concentration. The analytical information does not show any organic species despite the measured TOC. The AW-101 simulant composition based upon the reported density of 1.32 grams/mL is shown in Table 11.

Table 11 Diluted AW-101 Simulant Composition

Compounds	Formula	Grams/Liter
Cesium Nitrate	$CsNO_3$	0.016
Ferric Nitrate	$Fe(NO_3)_3 \bullet 9H_2O$	0.034
Lead Nitrate	$Pb(NO_3)_2$	0.066
Nickel Nitrate	$Ni(NO_3)_2 \bullet 6H_2O$	0.024
Zinc Nitrate	$Zn(NO_3)_2 \bullet 6H_2O$	0.064
Zirconyl Nitrate	$ZrO(NO_3)_2 \bullet xH_2O$, x~1	0.021
Potassium Nitrate	KNO_3	59.473
Sodium Chloride	NaCl	5.440
Sodium Fluoride	NaF	1.834
Sodium Chromate	Na_2CrO_4	0.175
Sodium Sulfate	Na_2SO_4	2.736
Aluminum Trihydroxide	$Al(OH)_3$	47.266
Sodium Hydroxide	NaOH	123.773
Sodium meta-silicate	$Na_2SiO_3 \bullet 9H_2O$	1.315
Sodium Phosphate	$Na_3PO_4 \bullet 12H_2O$	7.805
Sodium Carbonate	Na_2CO_3	19.017
Sodium Nitrate	$NaNO_3$	118.473
Sodium Nitrite	$NaNO_2$	94.114
Water	H_2O	833.12

The measured density of the simulant was 1.31 grams/mL. The weight percent solids based on microwave drying was 36.0 %. The analytical results for the simulant are shown in Table 12.

Table 12 Analytical Results for AW-101 Simulant

Component	Units	Found	Planned	% of Target
Al	mg/Liter	12150	16350	74
Cr	mg/Liter	45	56	81
Cs	mg/Liter	11.8	11	107
K	mg/Liter	22730	23000	99
Na	mg/Liter	138670	148500	93
Pb	mg/Liter	28	41	68
Si	mg/Liter	125	130	96
Zn	mg/Liter	15	14	109
Chloride	mg/Liter	2570	3300	78
Fluoride	mg/Liter	112	830	13
Nitrate	mg/Liter	105344	123000	86
Nitrite	mg/Liter	59905	62750	95
Phosphate	mg/Liter	799	1950	41
Sulfate	mg/Liter	2403	1850	130
TIC	mg/Liter	9620	2155	446
TOC	mg/Liter	<200		

The simulant generated solids over a week period which were filtered from the feed. The solids were not analyzed. However, it is reasonable to assume that species similar to what was detected in the AN-104 simulant would form in the AW-101 simulant. The low levels of fluoride and phosphate confirm that the insoluble fluorophosphate salt has formed. The source material for aluminum is the reason the aluminum is below target (see AN-104 simulant).

Preliminary AN-103 Simulant

A preliminary tank AN-103 supernate simulant was prepared to support ion exchange studies for the RPP-WTP. The simulant was based upon the analytical characterization of the actual AN-103 sample shipped to SRTC for characterization and active process studies.[13] The Hanford site 222-S Analytical Laboratory prepared the AN-103 waste sample by mixing fractions of a core sample to represent a composite of the AN-103 tank contents. The as received supernate was assumed to be diluted by a factor of 2.276 to a diluted sodium concentration of 5.25 molar. Table 13 lists the basis for the AN-103 supernate simulant.

Table 13 Basis for Preliminary AN-103 Simulant

Component	Moles/Liter	mg/Liter
Aluminum	1.59E+00	42870
Boron	2.78E-03	30
Cadmium	1.16E-05	1
Carbonate	4.76E-01	28578
Chromium	3.27E-03	170
Copper	2.68E-05	2
Hydroxide	3.18E+00	54150
Lead	3.91E-04	81
Molybdenum	8.13E-04	78
Nickel	2.90E-05	2
Potassium	2.76E-01	10790
Silicon	1.02E-02	286
Sodium	1.19E+01	274570
Silver	9.27E-06	1
Zirconium	2.85E-05	3
TIC	4.76E-01	5720
TOC	7.13E-02	856
Chloride	1.40E-01	4960
Fluoride	1.93E-02	367
Formate	6.00E-02	2700
Nitrate	3.57E+00	221650
Nitrite	2.36E+00	108600
Oxalate	1.34E-02	1180
Phosphate	1.57E-02	1490
Sulfate	1.76E-02	1690

The assumption was made that everything would remain in solution at the undiluted concentration. The reality is that some of the species were insoluble in the as received sample and dissolved during dilution.

Oxalate, for example, would not be expected to be soluble at the concentration shown in Table 13 when sodium is nearly 12 molar. The other species that might not be in solution include carbonate, phosphate, fluoride and sulfate. The charge balance for AN-103 had an excess of 0.194 moles/liter of cations (balance is 98 %). Th hydroxide level was increased by 0.194 moles/liter to create the final simulant. The AN-103 simulant composition is shown in Table 14 based upon a density of 1.49 grams/mL.

Table 14 Preliminary AN-103 Simulant Composition

Compounds	Formula	Grams/Liter
Boric Acid	H_3BO_3	0.172
Cadmium Nitrate	$Cd(NO_3)_2 \bullet 4H_2O$	0.004
Copper Nitrate	$Cu(NO_3)_2 \bullet 2.5H_2O$	0.006
Lead Nitrate	$Pb(NO_3)_2$	0.066
Nickel Nitrate	$Ni(NO_3)_2 \bullet 6H_2O$	0.008
Zirconyl Nitrate	$ZrO(NO_3)_2 \bullet xH_2O$, x~1	0.007
Potassium Molybdate	K_2MoO_4	0.194
Potassium Nitrate	KNO_3	27.736
Sodium Chloride	NaCl	8.175
Sodium Fluoride	NaF	0.811
Sodium Chromate	Na_2CrO_4	0.530
Sodium Sulfate	Na_2SO_4	2.499
Aluminum Trihydroxide	$Al(OH)_3$	123.93
Sodium Hydroxide	NaOH	199.02
Sodium meta-silicate	$Na_2SiO_3 \bullet 9H_2O$	2.894
Sodium Phosphate	$Na_3PO_4 \bullet 12H_2O$	5.964
Sodium Formate	NaHCOO	4.079
Sodium Oxalate	$Na_2C_2O_4$	1.796
Sodium Carbonate	Na_2CO_3	50.476
Sodium Nitrate	$NaNO_3$	280.415
Sodium Nitrite	$NaNO_2$	162.881
Water	H_2O	613.30

The AN-103 simulant will require additional testing if further work is planned requiring this simulant.

Envelope B Simulants

The following simulants were calculated and/or prepared to support SRTC research: Approved B Envelope simulant based upon AZ-101 supernate and an AZ-102 simulant. The source of each of these simulants and the specific issues in the preparation of these simulants will be described individually.

Approved B Simulant – AZ-101 Best Basis Inventory Simulant

Tank 241-AZ-101 was a NCAW receiver and the supernate in this tank has not been concentrated by processing through an evaporator. As an envelope B waste, the supernate contains higher ^{137}Cs

concentrations than envelope A. The LAW glass specifications will require ^{137}Cs and ^{99}Tc removal. Sr/TRU removal is not required for this waste. The envelope B is expected to be high in glass limiting constituents such as sulfate. A simulant of envelope B is necessary to support ion exchange studies, evaporation and sulfate removal studies. [Note: Sulfate removal studies were conducted in calendar year 1999, but removal of sulfate from LAW solutions is no longer part of the reference flowsheet for treatment of Hanford site wastes.] A well-characterized sample of AZ-101 supernate was not available for creating a simulant. Therefore, the customer directed that the Best Basis Inventory of 10-1-1998 be used to develop a composition for the simulant. The Best Basis Inventory is a mass based inventory of the waste components.

The spreadsheets used to calculate the envelope B simulant composition and recipe are shown in Appendix B. The inventory information was converted from mass to concentration by using the reported density for AZ-101 supernate of 1.2 grams/mL.[14] The supernate volume is 3.03E+06 liters or 8.00E+05 gallons. The inventory contains only a few of the major waste compounds and, therefore, the simulant will be a simple simulant, without many trace species. Table 15 specifies the analytical information the simulant is based upon.

Table 15 Basis for the B Envelope Approved Simulant

Component	Moles/Liter	mg/Liter
Aluminum	3.95E-01	10670
Ammonium	1.84E-02	313
Cesium	2.81E-04	37
Chromium	1.40E-02	730
Potassium	1.18E-01	4624
Sodium	4.74E+00	108990
Zirconium	3.37E-05	3.1
Chloride	5.63E-03	200
Fluoride	9.54E-02	1813
Nitrate	1.22E+00	75632
Nitrite	1.41E+00	65063
Phosphate	1.58E-02	1503
Sulfate	1.84E-01	17670

The charge balance based upon the inventory is very poor with an excess of positive charge of 1.30 moles/Liter out of 4.78 moles/liter (balance of 72 %). The reason for the poor charge balance is the absence of a value for hydroxide and for carbonate. The ratio of carbonate and hydroxide to the sum of carbonate and hydroxide was fixed based upon a previously reported AZ-101 composition.[15] This ratio was then applied to supply the 1.3 moles/Liter needed for charge balancing the simulant (for details see Table 43). Also missing from the inventory is any organic carbon containing species. Therefore, no organic species was included in the formulation. Note that oxalate or formate would have reduced the amount of both hydroxide and carbonate the formulation requires since they would have reduced the charge imbalance. Table 16 gives the composition of the Envelope B Simulant based upon the calculated hydroxide and carbonate results.

Table 16 Composition of Envelope B Simulant Based on Tank AZ-101

Compounds	Formula	Grams/Liter
Ammonium Nitrate	NH_4NO_3	1.470
Cesium Nitrate	$CsNO_3$	0.055
Zirconyl Nitrate	$ZrO(NO_3)_2 \bullet xH_2O$, x~1	0.008
Potassium Nitrate	KNO_3	11.956
Sodium Chloride	NaCl	0.329
Sodium Fluoride	NaF	4.008
Sodium Chromate	Na_2CrO_4	2.274
Sodium Sulfate	Na_2SO_4	26.128
Aluminum Trihydroxide	$Al(OH)_3$	30.839
Sodium Hydroxide	NaOH	37.205
Sodium Phosphate	$Na_3PO_4 \bullet 12H_2O$	6.015
Sodium Carbonate	Na_2CO_3	40.757
Sodium Nitrate	$NaNO_3$	92.027
Sodium Nitrite	$NaNO_2$	97.583
Water	H_2O	845.93

By comparison with some of the previous simulants, the Envelope B simulant is a simple simulant with a sodium concentration of 4.74 molar. Since the B simulant is already at low sodium concentration (compared to envelopes A and C), dilutions of the B simulant were not made to determine the density. The RPP-WTP processes will probably not need to dilute the envelope B feed. Table 17 gives the analytical results for the approved B simulant after the simulant has equilibrated for more than thirty days.

Table 17 Analytical Results for Envelope B Simulant

Component	Units	Found	Planned	% of Target
Al	mg/Liter	7752	10670	73
Cr	mg/Liter	648	730	89
Cs	mg/Liter	41	37	111
K	mg/Liter	4690	4624	101
Na	mg/Liter	104670	108990	96
Zr	mg/Liter	0.3	3	10
Chloride	mg/Liter	180	200	90
Fluoride	mg/Liter	760	1813	42
Nitrate	mg/Liter	60330	75630	80
Nitrite	mg/Liter	61770	65060	95
Phosphate	mg/Liter	1318	1503	88
Sulfate	mg/Liter	15740	17670	89
TIC	mg/Liter	8466	4620	183

The weight percent solids concentration determined by microwave drying was 29.84 %. The measured aluminum level in Table 17 matches the starting reagent aluminum concentration (80 %) quite well. The high TIC level indicates that ingrowth of carbonate has occurred due to carbon dioxide reaction with the free hydroxide. A better simulant of AZ-101 must wait on availability of a well-characterized sample of AZ-101 supernate.

AZ-102 Simulant

Tank 241-AZ-102 supernate is also a B envelope waste. The simulant for this waste was developed to support the pretreatment mixing studies. The AZ-102 simulant is based upon the recently completed analysis of a B Envelope sample obtained from Hanford tank 241-AZ-102 and an earlier core sample.[16,17] To insure that the simulant included all of the trace metals, the recipe used the trace metal values from the core sample for the planned composition. The resulting simulant represents a more complete B envelope simulant than the AZ-101 simulant. The basis for AZ-102 simulant is shown in Table 18.

Table 18 Basis for AZ-102 Supernate Simulant

Component	Moles/Liter	mg/Liter
Aluminum	2.80E-02	755
Barium	5.75E-06	0.8
Boron	7.77E-04	8.4
Cadmium	1.73E-05	1.9
Calcium	2.69E-03	108
Carbonate	5.11E-01	30660
Chromium	1.94E-02	1010.5
Copper	4.95E-05	3.1
Hydroxide	1.09E-01	1860
Iron	2.01E-04	11.2
Lanthanum	1.27E-05	1.8
Lead	2.88E-05	6
Magnesium	3.68E-05	0.9
Manganese	1.38E-05	0.8
Molybdenum	6.05E-04	58
Neodymium	3.80E-05	5.5
Nickel	3.68E-05	2.2
Potassium	8.10E-02	3167
Silicon	1.99E-02	559
Sodium	2.65E+00	60900
Silver	6.44E-05	6.9
Strontium	2.30E-06	0.2
Zinc	4.60E-06	0.3
Zirconium	4.72E-05	4.3
TIC	5.11E-01	6135
TOC	5.03E-01	6038
Chloride	7.00E-03	248

Fluoride	5.34E-02	1015
Nitrate	2.73E-01	16930
Nitrite	6.59E-01	30320
Oxalate	3.21E-02	2825
Phosphate	5.00E-03	475
Sulfate	1.72E-01	16520

The charge balance for the analytical data in Table 18 is excellent, 97 %. The cations are in excess by 0.0796 moles/Liter. Therefore, the hydroxide concentration was increased by 0.0796 moles/Liter to provide the balance. Note that the only organic carbon containing species is oxalate and that the oxalate only supplies 13 % of the total TOC. Additional effort to measure organic species in AZ-102 supernate may be useful in improving the waste simulant. Using an expected density of 1.135 grams/mL, Table 19 gives the planned simulant composition.

Table 19 Composition of Tank AZ-102 Supernate Simulant

Compounds	Formula	Grams/Liter
Barium Nitrate	$Ba(NO_3)_2$	0.002
Boric Acid	H_3BO_3	0.048
Cadmium Nitrate	$Cd(NO_3)_2\bullet 4H_2O$	0.005
Calcium Nitrate	$Ca(NO_3)_2\bullet 4H_2O$	0.636
Copper Nitrate	$Cu(NO_3)_2\bullet 2.5H_2O$	0.012
Ferric Nitrate	$Fe(NO_3)_3\bullet 9H_2O$	0.081
Lanthanum Nitrate	$La(NO_3)_3\bullet 6H_2O$	0.005
Lead nitrate	$Pb(NO_3)_2$	0.010
Magnesium Nitrate	$Mg(NO_3)_2\bullet 6H_2O$	0.009
Manganous Chloride	$MnCl_2\bullet 4H_2O$	0.003
Neodymium Nitrate	$Nd(NO_3)_3\bullet 6H_2O$	0.017
Nickel Nitrate	$Ni(NO_3)_2\bullet 6H_2O$	0.011
Potassium Nitrate	KNO_3	8.067
Silver Nitrate	$AgNO_3$	0.011
Zinc Nitrate	$Zn(NO_3)_2\bullet 6H_2O$	0.001
Zirconyl Nitrate	$ZrO(NO_3)_2\bullet xH_2O$, x~1	0.012
Sodium Chloride	NaCl	0.407
Sodium Fluoride	NaF	2.243
Sodium Chromate	Na_2CrO_4	3.148
Sodium Sulfate	Na_2SO_4	24.428
Potassium Molybdate	K_2MoO_4	0.144
Aluminum Trihydroxide	$Al(OH)_3$	2.183
Sodium Hydroxide	NaOH	8.772
Sodium meta-silicate	$Na_2SiO_3\bullet 9H_2O$	5.654
Sodium Oxalate	$Na_2C_2O_4$	4.301
Sodium Phosphate	$Na_3PO_4\bullet 12H_2O$	1.901
Sodium Carbonate	Na_2CO_3	54.153
Sodium Nitrate	$NaNO_3$	15.858
Sodium Nitrite	$NaNO_2$	45.475
Water	H_2O	952.85

The measured density of a test batch of the simulant was 1.118 g/mL and the weight percent total solids was 15.76 %. After allowing the test batch to equilibrate for more than thirty days the composition of the supernate was analyzed and the results versus the planned concentration are shown in Table 20.

Table 20 Analytical Results for the AZ-102 Supernate Simulant

Component	Units	Found	Planned	% of Target
Ag	mg/Liter	<0.3	6.9	<4
Al	mg/Liter	230	755	30
B	Mg/Liter	7.3	8.4	87
Ba	mg/Liter	0.01	0.8	1
Ca	mg/Liter	4.8	108	4
Cd	mg/Liter	0.05	1.9	3
Cr	mg/Liter	865	1010	86
Cu	mg/Liter	0.18	3.1	6
Fe	mg/Liter	0.23	11.2	2
K	mg/Liter	3150	3167	99
La	mg/Liter	<0.06	1.8	<3
Mg	mg/Liter	<0.09	0.9	<10
Mn	mg/Liter	<0.01	0.8	<1
Mo	mg/Liter	58	58	100
Na	mg/Liter	58070	60900	95
Nd	mg/Liter	<0.3	5.5	<5
Ni	mg/Liter	<0.06	2.2	<3
Pb	mg/Liter	<0.6	6	<10
Si	mg/Liter	121	559	22
Sr	mg/Liter	0.05	0.2	25
Zr	mg/Liter	0.43	4.3	10
Chloride	mg/Liter	201	248	81
Fluoride	mg/Liter	1111	1015	109
Nitrate	mg/Liter	15360	16930	91
Nitrite	mg/Liter	31050	30320	102
Oxalate	mg/Liter	2671	2825	95
Phosphate	mg/Liter	375	475	79
Sulfate	mg/Liter	14848	16520	90
TIC	mg/Liter	8946	6135	146
TOC	mg/Liter	1052	771	136
Aluminate	Molar	0.03	0.028	107
Carbonate	Molar	0.464	0.511	91
Free Hydroxide	Molar	0.196	0.109	180

Since the simulant does not contain any complexing agents or other organic ions other than oxalate anion, the result of so many of the trace species missing the target value is not a surprise. Without the aid of a complexing mechanism, the solubility of most of these metals in a sodium hydroxide solution is extremely small. Additionally, a relatively high concentration of oxalate anion would reduce the solubility of Ca, La, Nd and other metals which form insoluble oxalate precipitates. Additional analytical work on the AZ-102 supernate may provide an answer to the solubility problem. The low level of aluminum that was maintained in the solution could be due to depletion of the small amount of hydroxide in this simulant. The depletion mechanism could be due to carbon dioxide absorption since the TIC result suggests an ingrowth in carbonate. This simulant illustrates the possibly delicate balance that can occur with the more dilute simulants due to the conversion of free hydroxide to carbonate. The titration results reported for aluminate, carbonate and free hydroxide also illustrate the difficulty of using titration methods based upon differences between results. A shift in the large carbonate result would produce large swings in both the aluminate and the free hydroxide results.

Envelope C Simulants

As previously mentioned, the C waste was produced in the Hanford B plant during the Cs/Sr separation and encapsulation process. The waste is characterized by the high organic carbon content due to the presence of organic complexing agents and their decomposition products. Due to the complexing agents, the concentration of ^{90}Sr and TRU will require removal using the Sr/TRU precipitation and filtration process. Removal of ^{137}Cs and ^{99}Tc by ion exchange will also be required. The tanks within the C envelope are 241-AN-102 and 241-AN-107. Currently, only a simulant for AN-107 has been developed.

Approved C Simulant – AN-107 Simulant

The supernate within tank AN-107 is known as complex concentrate since it contains high levels of complexed metals. A successful simulant must have sufficient complexing agents present to duplicate the soluble metal concentrations observed within the waste. The AN-107 simulant will be used for testing the following processes: ion exchange, Sr/TRU precipitation, pilot-scale crossflow filtration, low-pressure evaporation, sulfate removal (no longer included in RPP-WTP reference flowsheet) and low activity waste vitrification. The analytical basis for the simulant composition for all but one component come from recent waste samples.[18,19] One waste component, sodium gluconate, is based upon process knowledge and history.

Initial tests of the C simulant were not successful at preventing the precipitation of metals upon the addition of sodium hydroxide. The tests varied the order of addition of both the complexing agents and the aluminum. The oxidation state of iron was also tested by using Fe(II) instead of Fe(III) in the formulation. Finally, the test mixture was heated to 80 C to determine if temperature could aid in generating the metal complexes.

The Hanford B plant consumption of sodium gluconate was greater than 4500 kilograms. per year. After reviewing the negative results with the customer and reviewing the Hanford B plant process history, sodium gluconate was added to the simulant formulation at 0.2 moles/Liter prior to the addition of the sodium hydroxide. The gluconate (sequestering agent) prevented the precipitation of the strontium and iron from test solutions under precipitation treatment, thus it was considered to be much too high.

The final gluconate concentration for this simulant is not based upon a measured concentration since a method for analyzing for gluconate in the C waste stream has not yet been developed. The current concentration used, 0.018 molar, was agreed to based upon the results of iron precipitation tests from the Sr/TRU precipitation program.[27] Those tests varied the gluconate level and correlated it with iron solubility. Nonradioactive Cells Filter work also examined the role of gluconate in complexing metals and found that gluconate is a powerful complexant in these alkaline solutions.[28] Since the soluble iron:gluconate molar ratio was at least 1:1 and possibly 2:1 or more, the 0.018 M level was chosen. It is approximately half of the iron concentration in the real waste. The analytical basis for the AN-107 simulant is listed in Table 21. Similar to the A envelope simulant, the Cs value is based upon the measured ^{137}Cs value and the assumption that ^{137}Cs is 1/3 of the total cesium. The Sr concentration is based on ^{90}Sr making up 10 % of the total Sr in the waste. The bases for the organic compounds that are in the AN-107 simulant are listed in Table 22. Gluconate ion is not listed in Table 22 since it is not based on an analytically measured value.

Table 21 Analytical Basis for Approved C Simulant based on AN-107

Component	Moles/Liter	mg/Liter
Aluminum	1.43E-02	386
Ammonium	1.22E-03	22
Barium	5.42E-05	7
Boron	3.24E-03	35
Cadmium	5.70E-04	64
Calcium	1.47E-02	591
Carbonate	1.40E+00	83936
Cesium	1.40E-04	18.6
Cerium	3.77E-04	53
Chromium	3.38E-03	176
Copper	4.74E-04	30
Hydroxide	2.00E-02	340
Iron	3.03E-02	1690
Lanthanum	3.24E-04	46
Lead	1.87E-03	388
Magnesium	1.03E-03	25
Manganese	1.02E-02	563
Molybdenum	3.73E-04	36
Neodymium	6.65E-04	96
Nickel	9.03E-03	530
Potassium	4.63E-02	1810
Selenium	6.33E-06	1
Silver	1.33E-04	14
Sodium	8.48E+00	195000
Zinc	6.93E-04	45
Zirconium	7.67E-04	70
TIC	1.40E+00	16800
TOC	3.36E+00	40400

Chloride	5.16E-02	1830
Fluoride	7.00E-03	133
Nitrate	3.71E+00	230000
Nitrite	1.33E+00	61000
Phosphate	1.17E-02	1110
Sulfate	8.59E-02	8250

Table 22 Organic Basis for Approved C Simulant from AN-107

Component	Moles/Liter	mg/Liter
Acetate	1.86E-02	1100
Ethylenediaminetetraacetate (EDTA)	1.95E-02	5620
Formate	2.31E-01	10400
Glycolate	2.48E-01	18600
n-Hydroxyethylenediamine triacetate (HEDTA)	7.78E-03	2140
Oxalate	9.38E-03	826
Nitrilotriacetate (NTA)	2.98e-03	561
Citrate	4.49e-02	8495
Iminodiacetate (IDA)	4.54e-02	5947

The charge balance based on tables 21 and 22 shows an excess of negative ions by 0.31 mole/Liter compared to a total of 9.04 moles/Liter (balance is 96 %). Since the hydroxide level is very low, 0.02 moles/Liter (important characteristic of AN-107 supernate), the hydroxide could not be reduced by 0.31 moles/Liter. Therefore, the Na ion concentration was increased by 0.31 moles/Liter to balance the anions. The sodium gluconate level was set to 0.018 moles/Liter. Based upon a volumetric preparation of the simulant, the density of the undiluted AN-107 simulant is 1.429 g/mL. Appendix C details the computations performed to transform the data in Tables 21 and 22 into the compounds listed in Table 23.

Table 23 Approved C Simulant based on Tank AN-107 Supernate

Compounds	Formula	Grams/Liter
Aluminum Nitrate	$Al(NO_3)_3 \bullet 9H_2O$	5.367
Ammonium Acetate	NH4CH3COO	0.094
Barium Nitrate	$Ba(NO_3)_2$	0.014
Boric Acid	H_3BO_3	0.200
Cadmium Nitrate	$Cd(NO_3)_2 \bullet 4H_2O$	0.176
Calcium Nitrate	$Ca(NO_3)_2 \bullet 4H_2O$	3.482
Cerium Nitrate	$Ce(NO_3)_3 \bullet 6H_2O$	0.164
Cesium Nitrate	$CsNO_3$	0.027
Copper Nitrate	$Cu(NO_3)_2 \bullet 2.5H_2O$	0.110
Disodium EDTA	$C_{10}H_{14}N_2Na_2O_8 \bullet 2H_2O$	7.259
Ferric Nitrate	$Fe(NO_3)_3 \bullet 9H_2O$	12.226
HEDTA Acid	$C_{10}H_{18}N_2O_7$	2.164
Lanthanum Nitrate	$La(NO_3)_3 \bullet 6H_2O$	0.142
Lead nitrate	$Pb(NO_3)_2$	0.620
Magnesium Nitrate	$Mg(NO_3)_2 \bullet 6H_2O$	0.264
Manganous Chloride	$MnCl_2 \bullet 4H_2O$	2.028
Neodymium Nitrate	$Nd(NO_3)_3 \bullet 6H_2O$	0.291
Nickel Nitrate	$Ni(NO_3)_2 \bullet 6H_2O$	2.626
Potassium Nitrate	KNO_3	4.605
Silver Nitrate	$AgNO_3$	0.023
Strontium Nitrate	$Sr(NO_3)_2$	0.016
Zinc Nitrate	$Zn(NO_3)_2 \bullet 6H_2O$	0.206
Zirconyl Nitrate	$ZrO(NO_3)_2 \bullet xH_2O$, x~1	0.191
Glycolic Acid	$HOCH_2COOH$, 70 wt%	26.928
Sodium Gluconate	$C_6H_{11}O_7Na$	3.927
Citric Acid	$C_6H_8O_7 \bullet H_2O$	9.440
Nitrilotriacetic Acid	$C_6H_9NO_6$	0.570
Iminodiacetic Acid	$C_4H_7NO_4$	6.038
Sodium Chloride	NaCl	1.819
Sodium Fluoride	NaF	0.294
Sodium Chromate	Na_2CrO_4	0.548
Sodium Sulfate	Na_2SO_4	12.199
Potassium Molybdate	K_2MoO_4	0.089
Sodium Hydroxide	NaOH	25.263
Sodium Oxalate	$Na_2C_2O_4$	1.257
Sodium Acetate	$NaCH_3COO \bullet 3H_2O$	2.369
Sodium Formate	NaHCOO	15.712
Sodium Phosphate	$Na_3PO_4 \bullet 12H_2O$	4.443
Sodium Carbonate	Na_2CO_3	148.250
Sodium Nitrate	$NaNO_3$	294.672
Sodium Nitrite	$NaNO_2$	91.489
Water	H_2O	726.96

Testing the AN-107 simulant gave a density of 1.44 g/mL at 20 C. The simulant produced a solution with a deep brown color and just a small amount of solids but did require several hours of mixing to dissolve the added compounds. The inorganic and organic analytical results for the AN-107 simulant are listed in Tables 24 and Table 25 respectively.

Table 24 Inorganic Analytical Results for AN-107 Simulant

Component	Units	Found	Planned	% of Target
Al	mg/L	194	386	50
B	mg/L	38	35	108
Ba	mg/L	0.17	7	2
Ca	mg/L	138	591	23
Ce	mg/L	50.2	53	95
Cr	mg/L	148	176	84
Cs	mg/L	22.3	18.6	120
Cu	mg/L	32	30	106
Fe	mg/L	1623	1690	96
K	mg/L	1921	1810	106
La	mg/L	40	46	88
Mg	mg/L	20	25	79
Mn	mg/L	564	563	100
Mo	mg/L	36	36	100
Na	mg/L	188170	195000	96
Na	mg/L	201400	195000	103
Nd	mg/L	84.4	96	88
Ni	mg/L	501	530	95
P	mg/L	420	362	116
Pb	Mg/L	364	388	94
Sr	mg/L	1.3	6.6	20
Zn	mg/L	44	45	98
Zr	mg/L	45	70	64
Chloride	mg/L	1330	1100	121
Fluoride	mg/L	3430	133	2579
Formate	mg/L	11232	10400	108
Nitrate	mg/L	213930	230000	93
Nitrite	mg/L	57090	61000	94
Oxalate	mg/L	335	826	41
Phosphate	mg/L	1500	1110	135
Sulfate	mg/L	7280	8250	88
TIC	mg/L	16100	16800	96
TOC	mg/L	15800	12450	127

Table 25 Organic Analytical Results for AN-107 Simulant

Component	Units	Found	Planned	% of Target
EDTA	mg/L	1088	5620	19
HEDTA	mg/L	3231	2140	151
Glycolate	mg/L	18864	18600	101
Citrate	mg/L	8952	8495	105
Formate	mg/L	12374	10400	119
Acetate	mg/L	964	1100	88
Iminodiacetic Acid	mg/L	8251	5947	139

The exceptionally high fluoride result listed in Table 24 was obtained by ion chromatography, which has known interference's for fluoride due to weak organic acid anions such as acetate and glycolate. An alternative analytical technique such as capillary electrophoresis may be necessary to properly measure the fluoride content. The low aluminum result is probably due to the extremely low hydroxide concentration of the AN-107 simulant (pH~12). Any shift in free hydroxide due to CO_2 absorption would cause a drop in soluble aluminum. The organic analytical results, which are more than 30 % off from the target value, were for new methods recently implemented at SRTC. These methods require measuring a recovery and adjusting the results for the recovery. If the recovery measurement does not reproduce the sample measurement, the adjustment can introduce substantial errors. Additional testing should clarify the source of the problems.

Several features make this an interesting simulant. The first is the extremely high organic content of the waste and of the simulant. Any attempt to match the TOC of the waste would introduce excess levels of organic compounds beyond what can be measured. The actual waste has a much longer list of organic compounds, most of which can act as complexing agents. The compounds used in the simulant are most of the major compounds, especially those that were originally used in the process. Iminodiacetate ion was added to represent the typical decomposition products of the starting complexing agents. Second, very high carbonate level in the simulant led to the formation of tabular crystal over a 36 day period which were identified as the monohydrate of sodium carbonate.[9] Third, turbidity measurements during the simulant pretreatment mixing study demonstrated that over extended periods, more than 60 days, the simulant slowly begins to produce additional fine solids.[9] Currently, these solids have not been conclusively identified. Finally, the lower than planned levels of some of the +2 cations may be an indication that some additional complexing agent or a higher level of gluconate ion may be necessary to prevent precipitation of these ions by oxalate, which was also lower than planned.

Relatively large volumes of simulant are required for the pilot ion exchange and Sr/TRU precipitation/crossflow filtration studies. To assist in producing the diluted supernate simulant, a series of diluted AN-107 simulants were prepared volumetrically so that the density of the diluted simulant could be measured. Table 26 lists the measured densities and the weight percent solids calculated for these dilutions as a function of the sodium ion concentration. The densities listed in table 4 were measured at 20 to 22 C (ambient lab temperatures). The weight percent solids value represents the solids with no waters of hydration and is a theoretical (computed) value. This should be used as a guide since measuring the weight percent solids by oven or microwave drying may lead to varying levels of dehydration and possibly some decomposition and therefore a different value.

Table 26 An-107 Simulant Density and Weight Percent Solids

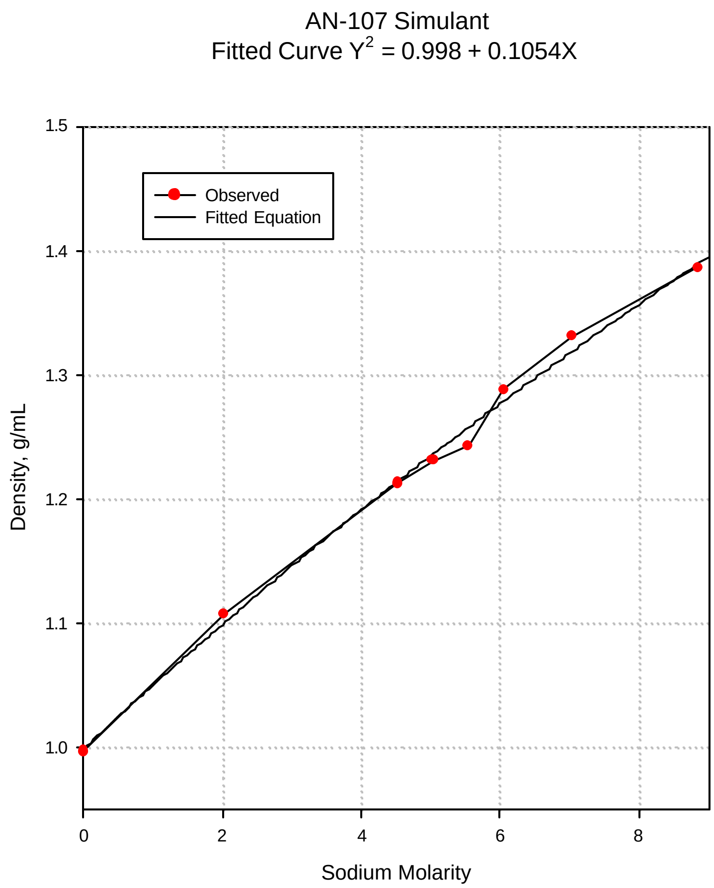
Na Concentration, Molar	Density, g/mL	Wt % Anhydrous Solids
2.03	1.108	13.85
4.53	1.213	28.22
5.04	1.231	30.97
5.55	1.243	33.75
6.06	1.288	35.54
7.04	1.331	40.02
8.85	1.386	48.28

The sodium concentration (X, molarity) versus the density (Y, gm/L) can be fit empirically to the following simple equation to allow predictions of densities for different sodium concentrations when the supernate is diluted:

$$Y^2 = 0.998 + 0.1054X \quad (3),$$

Besides the measured values, at infinite dilution, the sodium concentration would be zero and the density would be that of water, 0.997 g/mL. This assumption was also included in the data set that was fitted. Figure 5 display the fitted curve versus the measured and assumed data point.

Figure 5 Envelope C Simulant Density as a Function of Na Concentration



The r2 value for the fit is 0.995. The relationship can be used for this specific ratio of compounds across the range of measured concentrations but should not be extended to other simulant recipes except as a very crude estimate.

The weight percent solids (anhydrous) can also be calculated for a specific sodium concentration and then also plotted and fitted to a curve. Note that the assumption is made that at 0.0 Molar Na (X), the weight percent solids (Y) is also 0.0. Figure 6 demonstrates that the polynomial listed as equation (4),

$$Y = 0.1637 + 6.99X - 0.179X^2 \qquad (4),$$

provides a good fit to the results without forcing an intercept at the origin.

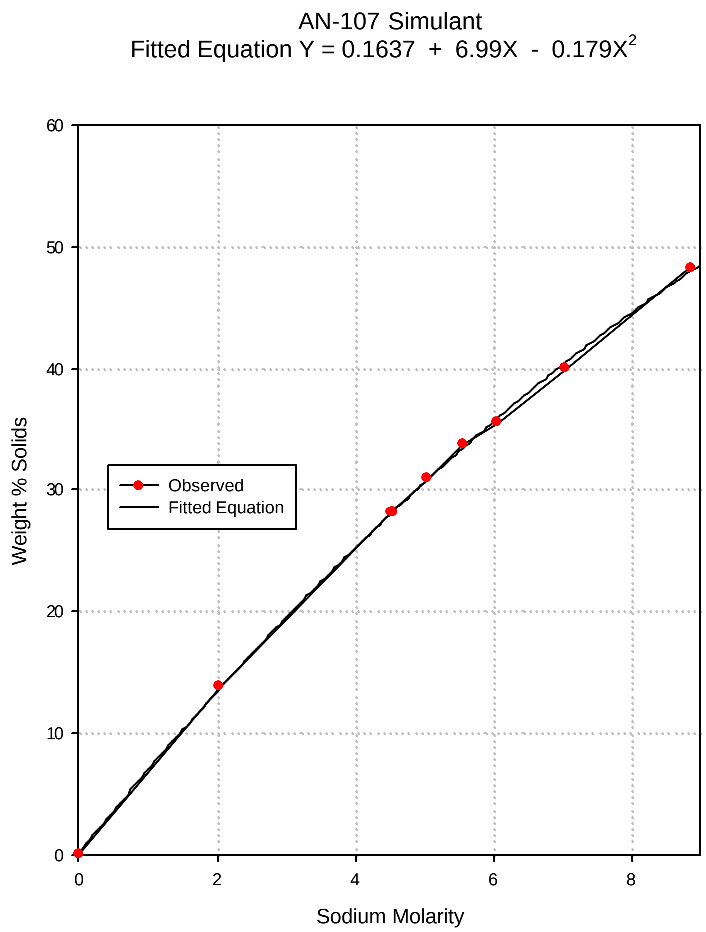


Figure 6 AN-107 Simulant Weight % Solids (Anhydrous) as a Function of the Na Concentration

As mentioned previously, the relationship given by equation (4) is only for the composition specified for the approved AN-107 simulant. Actual measurements of weight percent solids can differ from this curve due to waters of hydration or due to actual compound decomposition. As such the curve should be used as a guide. For example, equation 4 or figure 6 can be used to estimate the Na concentration after dilution based upon a total solids measurement.

Envelope D Simulant

The envelope D simulant represents the insoluble solids from than Hanford waste tanks that will be processed and vitrified as high activity waste. The waste is often referred to as sludge and is usually high in iron, aluminum, zirconium, manganese and nickel oxides or hydroxides. Substantial amounts of insoluble carbonates can also be present. The majority of the long term radionuclides and transuranics are present in envelope D. The initial tanks planned to be processed in the RPP-WTP that contain envelope D waste are 241-AZ-101 and 241-AZ-102. The initial work on envelope D simulant formulation focused on tank AZ-101.

AZ-101 Sludge Simulant

Unlike the other simulants described in this report, research and formulation work on the AZ-101 sludge simulant is still in progress. The information described in this section maybe superceded by later information obtained from the High Level Waste Mixing Study.[20] However, the formulated composition of the AZ-101 sludge simulant will not change. For comparisons with other sludge simulants refer to the High Level Waste Mixing Study.[20]

Tank 241-AZ-101 served as a receiver for neutralized current acid waste and contains about 35,000 gallons of insoluble sludge solids. Because of the layered nature of the settled sludge solids, sampling of the sludge solids uses a core sampling approach. The insoluble portion of the core samples are combined and blended to represent the total, insoluble layer in the tank. However, different core samples from different locations within a tank often show shifts in waste composition due to the three dimensional variation within a settled sludge layer. The AZ-101 sludge simulant target composition is based on averaging the results from two separate AZ-101 core samples.[21,14] The target composition for the AZ-101 sludge blend is shown in Table 27. Appendix D displays the spreadsheets used to calculate the values given in Table 27 and defines how the recipe for generating sludge is formed. Since the sludge is generated by reacting the metals listed in Table 27 with sodium hydroxide and sodium carbonate, a separate table defining the final sludge composition such as has been listed for the supernate simulants will not be included.

Table 27 Blended AZ-101 Solids Composition

Component	Grams/Liter	micrograms/gram of solids
Aluminum	8.970	57907
Barium	0.328	2114
Boron	0.124	803
Cadmium	3.454	22295
Calcium	1.400	9036
Cerium	0.436	2817
Chromium	0.347	2238
Copper	0.152	979
Iron	44.150	285023
Lanthanum	1.784	11520
Lead	0.505	3258
Magnesium	0.249	1610
Manganese	1.027	6630
Molybdenum	0.022	144
Neodymium	1.192	7696
Nickel	2.719	17552
Potassium	0.986	6365
Silver	0.346	2235
Sodium	12.853	82976
Silicon	2.182	14084
Strontium	0.234	1508
Titanium	0.042	274
Zinc	0.134	865
Zirconium	14.772	95366
TIC	1.109	7161
Chloride	0.039	255
Fluoride	0.215	1390
Nitrate	3.909	25238
Nitrite	5.567	35942
Phosphate	0.260	1678
Sulfate	1.406	9078

The initial simulated sludge work was based upon a blend of caustic leached sludge from both tanks AZ-101 and AZ-102. Since the composition of the blended sludge was similar to the AZ-101 simulant and the preparation of the sludge was identical, the physical properties of the blended AZ-101/AZ-102 sludge simulant will be discussed. For example, the aluminum in the AZ-101/AZ-102 sludge simulant was added post precipitation of the metal cations and sludge washing just as is called for in the AZ-101 simulant recipe. Results for an AZ-101 sludge simulant prepared in the same manner are expected to be similar.

A sludge simulant must not only match the chemical composition for the waste, it must also compare favorably with the physical properties of the waste. Amongst the physical properties important for the operation of the RPP-WTP are particle size and rheology. A particle size analysis for the AZ-101/AZ-102 simulant blend after sludge washing is shown in Figure 7. A comparison of the median particle size is listed in Table 28.

Table 28 Sludge Particle Size Comparisons

Sludge	*Median Particle Size, micrometers*
AZ-101 Core 1	9.0
AZ-101 Core 2	5.4
NCAW Simulant[22]	25.6
RFP Simulant[22]	12.4
SRTC AZ-101/AZ-102 Blend	16

The particle size is in the mid range of the previous simulants and not much larger than observed for the actual sludge. Since particle size is expected to be sensitive to the amount of shear, additional shearing is planned during the HLW blending studies.[20]

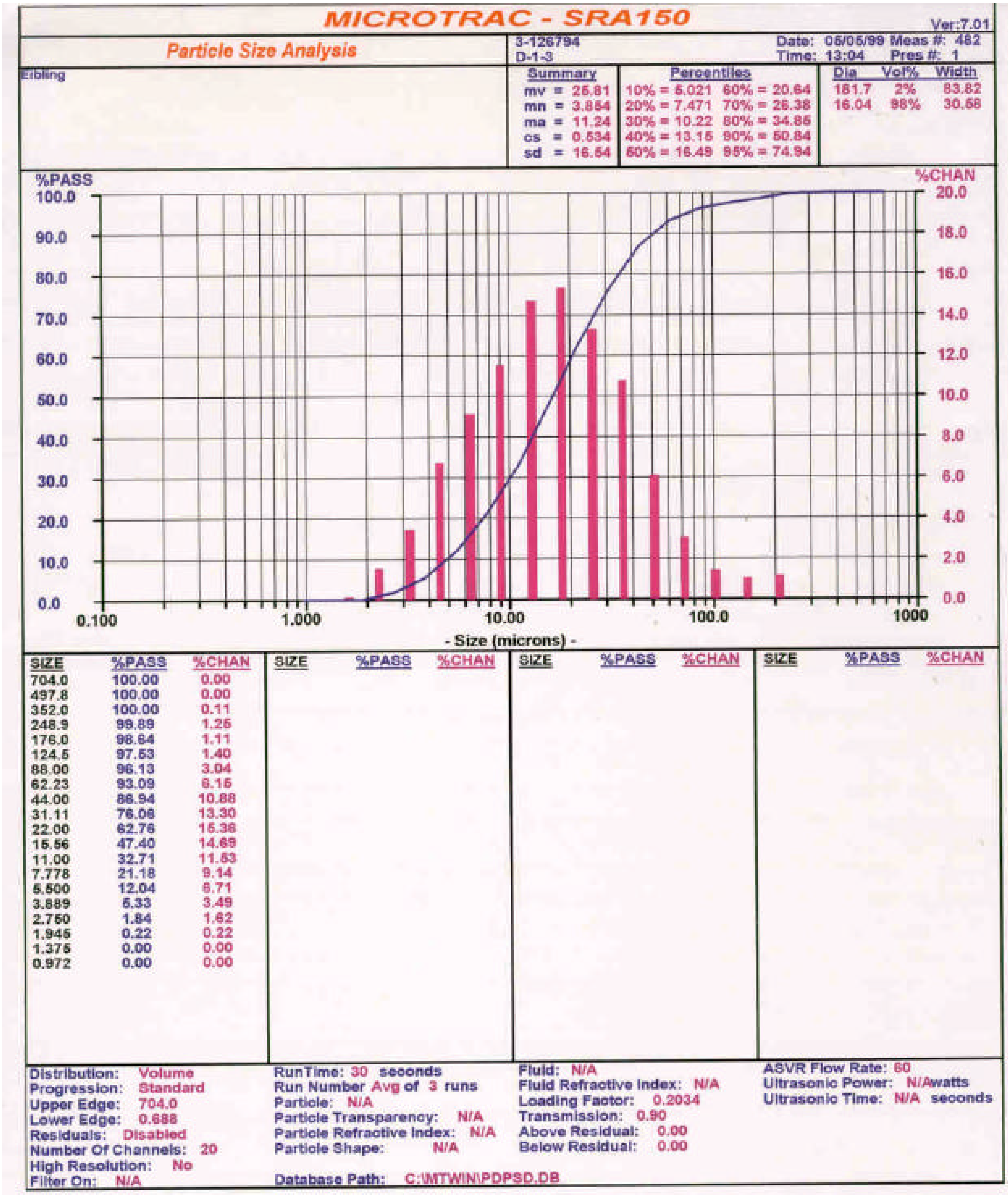


Figure 7 Particle Size analysis for Blended AZ-101/AZ-102 Sludge

The fluid properties of the simulated sludge was studied using a Haake rheometer with a M5 measuring head. The sample was run using the MV1 geometry (concentric cylinders) at 298 K after verifying correct rheometer operation with a known viscosity oil. The instrument was operated in the dynamic flow curve operation with the shear ranging from zero seconds^{-1} to 350 seconds^{-1}. Figure 8 compares the flow curve for the blend simulant to information from the core samples.

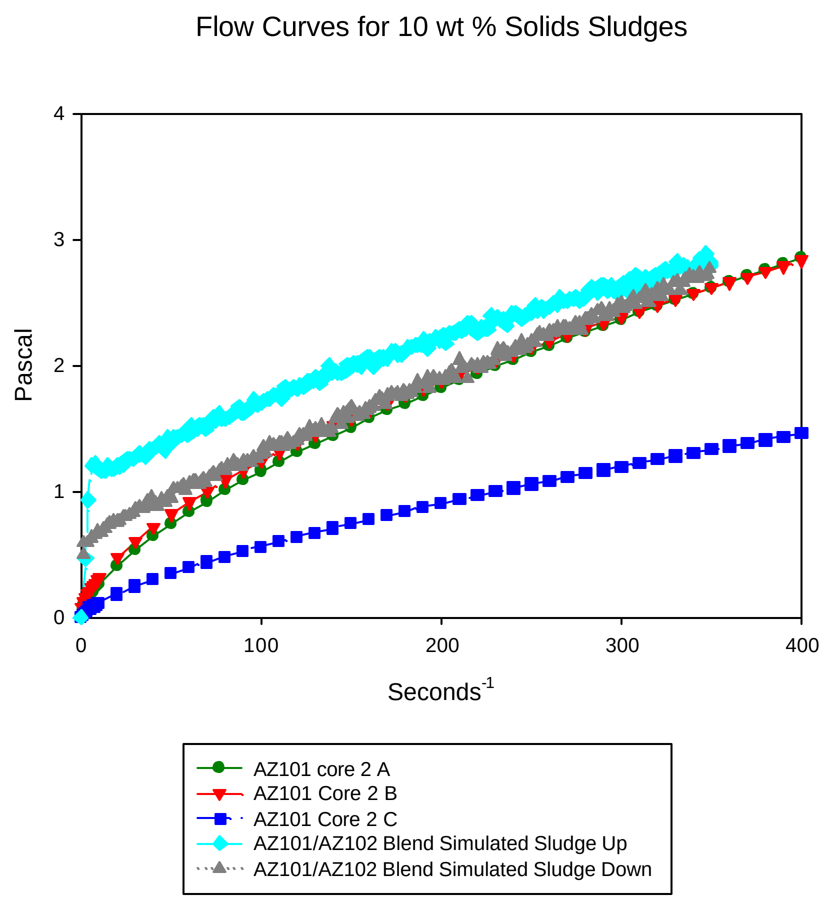


Figure 8 Rheology of AZ-101 sludge Compared to the AZ-101/AZ-102 Blend Simulant

The Blend simulant down curve indicates that the sludge is thixotropic (shear thinning). The data shown for the AZ-101 core 2 sample is actually produced from the power law model to which the data was fit. Applying a Bingham model to the core 2A curve and to the up curve for the Blend simulant gives a yield stress of 0.5 and 1.2 Pascal respectively while the consistency (slope of the curve) would appear to be very similar. Additional tests with the Blend simulant have indicated that the yield stress may increase with aging. Unfortunately, when the Blend simulant was completed the SRTC rheometer was inoperable. The curve shown above is for the Blend simulant after 3 months of aging. This suggests that the initial yield stress of the Blend simulant may have been even closer to that of the actual waste.

Additional physical property data shall be obtained for the AZ-101 simulant in the near future. The additional studies planned are particle size before and after pumping through a high shear pump, rheology as a function of weight percent solids, and the effect of pH on rheological properties. The physical properties information for the AZ-101 sludge simulant will be compared to the physical properties analytical results for actual AZ-101 sludge that were recently obtained during a test of mixer pumps in tank 241-AZ-101 (HNF-7078, AZ-101 Results of Retrieval Testing of Sludge from Tank 241-AZ-101).

Entrained Solids Simulants

An entrained solids simulant is designed to represent the insoluble solids observed in decanted supernate from the Hanford waste tanks. These simulants are need for pilot crossflow filtration studies and must duplicate the expected particle size range. Two different simulants were formulated based on entrained solids in Tank AN-105 supernate and entrained solids in Tank AN-107 supernate.

AN-105 Entrained Solids Simulant

The entrained solids in Tank 241-AN-105 supernate are expected to be primarily composed of corrosion products and insoluble precipitated solids. The compositional basis for the waste simulant is derived from dilution studies of solids from AN-105.[6] These studies also reported that the particle size of the washed solids had two maxima, one near 5 micrometers and a narrower distribution near 50 micrometers. Since the 50-micrometer material is expected to be easy to filter due to its size, the simulant will be composed primarily of particles of 5 micrometer and less in size. As expected, the number density is weighted to the finer particles. The elemental composition of the solids is listed in Table 29.

Table 29 Basis for Envelope A Entrained Solids from AN-105 Supernate

Component	Grams/100 grams of Sample
TOC	0.065
Al	0.025
Ca	0.008
Cr	0.103
Fe	0.004
Mn	0.001
Na	0.092
Ni	0.002
Si	0.013
Solids	0.57

The strategy described for producing an entrained solids simulant was used to convert the information in Table 29 into compounds, which could be obtained in the desired particle size range. Appendix E contains the spreadsheet used to calculate compounds and estimate the mass balance. Table 30 gives the formulation for the entrained solids in terms of grams of the compound per 100 grams of entrained solids.

Table 30 Envelope A Entrained Solids Formulation Based on Tank AN-105

Compound	*Formula*	*Grams/100 grams of solids*
Aluminum oxide	Al_2O_3	9.2
Calcium Oxalate	CaC_2O_4	5.0
Chromic Oxide	Cr_2O_3	26.0
Ferric Oxide	Fe_2O_3	1.1
Manganese Dioxide	MnO_2	0.3
Sodium Oxalate	$Na_2C_2O_4$	52.4
Nickel oxide	NiO	0.5
Silica	SiO_2	5.4

This combination of solids calculated to be 90 % of the measured, washed solids mass giving reasonable agreement with the goal. Using other species such as AlOOH or FeOOH did not improve the balance. Using other insoluble sodium species such as sodium aluminosilicate did not measurably improve the balance since the ratio of sodium to either Al or Si was so high. As mentioned above, the recommended particle size range was less than 5 micrometers

AN-107 Entrained Solids Simulant

The entrained solids in C envelope will experience the precipitation of strontium carbonate and manganese dioxide before being processed through a crossflow filter. Since the presence of the unwashed entrained solids may have an impact on the precipitation product, the entrained solids must represent the unwashed solids in the AN-107 supernate. While washed solids were used in the basis for the AN-105 entrained solid, the AN-107 solids must be based on unwashed solids. However, an unwashed AN-107 solids analysis was not available. Instead, an analysis of washed solids and the wash waters from washing those solids was used to reassemble the composition of the unwashed solids.[23] Appendix F displays the spreadsheets used to calculate the mass of each species in the wash water at each stage of the wash. These amounts were then summed to produce a composition for the unwashed solids as shown in Table 31.

Table 31 Calculated Basis for the AN-107 Entrained Solids

Component	Milligrams
TOC	55.7
Al	24.7
Ca	0.26
Cr	2.4
Fe	30.3
Mn	17.7
Na	205.4
Si	2.2
TIC	28.5
Fluoride	20.6
Sulfate	11.2
Phosphate	21.0

At this point, the entrained solids strategy can be used to assemble a possible solids composition. The more soluble species such as the fluoride, sulfate, phosphate, oxalate (from the TOC) and the carbonate (from the TIC) will obviously wash from the solids when the Sr/TRU precipitate is washed. After reviewing all of the possible combinations, the composition detailed in Table 32 was chosen as the entrained solids formulation.

Table 32 AN-107 Unwashed Entrained Solids Formulation

Compounds	Formula	grams/100 grams of solids
Aluminum Oxide	Al_2O_3	5.1
Calcium Phosphate, Tribasic	$Ca_3(PO_4)_2$	0.1
Chromic Oxide	Cr_2O_3	0.4
Ferric Oxide	Fe_2O_3	4.8
Manganese Dioxide	MnO_2	3.1
Sodium Aluminosilicate	$Na_2O.Al_2O_3.(SiO_2)_2 \bullet 5H_2O$	1.6
Sodium Oxalate	$Na_2C_2O_4$	34.2
Sodium Carbonate Monohydrate	$Na_2CO_3 \bullet H_2O$	32.3
Sodium Fluoride	NaF	5.0
Sodium Sulfate Decahydrate	$Na_2SO_4 \bullet 10H_2O$	4.1
Sodium Phosphate Dodecahydrate	$Na_3PO_4 \bullet 12H_2O$	9.3

Since these solids will be unwashed, particle size will change as washing proceeds. To insure a conservative basis testing filtration the particles should be less than 5 micrometers as similarly specified for the A envelope entrained solids.

Miscellaneous Simulants

Two miscellaneous simulants were created to support the pretreatment mixing study. Each simulant will be individually described.

C-106 Caustic Leachate Simulant

The C-106 caustic leach simulant is designed to represent the solution obtained when Hanford tank 241-C-106 solids are leached with a 3 molar sodium hydroxide solution at a temperature of at least 85 C. In the planned RPP-WTP process the solids from C-106 could be leached with 3 molar NaOH and the filtrate (leachate) transfer to the low activity waste feed tanks. The simulant is based on leaching studies of the C-106 solids.[24] Since this supernate is similar but more dilute than the envelope A supernates, the supernate simulant strategy can be applied to this simulant. The analytical basis for the C-106 caustic leachate simulant is listed in Table 33.

Table 33 Analytical Basis for C-106 Caustic Leachate Simulant

Component	Moles/Liter	mg/Liter
Aluminum	1.15E-01	3100
Boron	6.20E-03	67
Chromium	1.12E-03	58
Copper	4.41E-05	3
Hydroxide	2.70E+00	45920
Iron	1.79E-04	10
Lead	1.50E-04	31
Silicon	1.05E-02	295
Sodium	4.78E+00	110000
Zirconium	4.49E-05	4
Nitrate	5.40E-03	335
Nitrite	1.49E-01	6850
Oxalate	2.84E-02	2500
Phosphate	3.53E-03	335
Sulfate	1.87E-02	1800

Unlike the other supernates previously simulated, a measure of the carbonate level was not available since TIC was not reported for the leachate solution. The charge balance without carbonate being measured is very poor (1.67 moles/Liter excess positive charge compared to a total charge of 4.79 moles/liter). After confirming that the sludge in C-106 is high in carbonate, carbonate anion was used to balance the charge.[25] The composition calculated for the C-106 caustic leachate is shown in Table 34 based upon a supernate density of 1.18 g/mL.

Table 34 C-106 Caustic Leachate Simulant Composition

Compounds	Formula	Grams/Liter
Boric Acid	H_3BO_3	0.383
Copper Nitrate	$Cu(NO_3)_2 \bullet 2.5H_2O$	0.010
Ferric Nitrate	$Fe(NO_3)_3 \bullet 9H_2O$	0.072
Lead nitrate	$Pb(NO_3)_2$	0.050
Zirconyl Nitrate	$ZrO(NO_3)_2 \bullet xH_2O$, x~1	0.011
Sodium Chromate	Na_2CrO_4	0.181
Sodium Sulfate	Na_2SO_4	2.662
Aluminum Trihydroxide	$Al(OH)_3$	8.962
Sodium Hydroxide	NaOH	113.334
Sodium meta-silicate	$Na_2SiO_3 \bullet 9H_2O$	2.985
Sodium Oxalate	$Na_2C_2O_4$	3.806
Sodium Phosphate	$Na_3PO_4 \bullet 12H_2O$	1.341

Compounds	Formula	Grams/Liter
Sodium Carbonate	Na_2CO_3	88.502
Sodium Nitrate	$NaNO_3$	0.373
Sodium Nitrite	$NaNO_2$	10.274
Water	H_2O	944.55

The analytical results for a test solution used in the pretreatment mixing study is shown as Table 35.

Table 35 Analytical Results for Simulated C-106 Caustic Leachate

Component	Found, mg/L	Planned, mg/L	% of Target
Al	2460	3100	79
B	68	67	101
Cr	49	58	85
Na	105670	110000	96
Pb	26	31	85
Si	303	295	103
Nitrate	241	335	72
Nitrite	6589	6850	96
Oxalate	698	2500	28
Phosphate	303	335	90
Sulfate	1570	1800	87
TIC	3	10029	0

The aluminum result is very close to the amount actually added based upon the purity of the hydrated aluminum trihydroxide used (80 %). The TIC appears to be a bad analytical result. The low level for the oxalate anion my be due to precipitation of sodium oxalate in the C-106 caustic leachate simulant. The leaching of the actual C-106 high-level waste sludge was conducted at ~90 C, which increased the solubility of oxalate. Oxalate probably precipitated in the actual leachate after cooling to ~25 C.

AZ-102 Caustic Leachate Simulant

The AZ-102 caustic leach simulant is designed to represent the solution obtained when Hanford tank 241-AZ-102 solids (envelope D material) are leached with a 3 molar sodium hydroxide solution. In the planned RPP-WTP, process the solids from AZ-102 could be leached with 3 molar NaOH and the filtrate (leachate) transferred to the low activity waste feed tanks. The simulant is based on leaching studies of the AZ-102 solids.[26] Since this supernate is similar but more dilute than the envelope A supernates, the supernate simulant strategy can be applied to this simulant. The analytical basis for the AZ-102 caustic leachate simulant is listed in Table 36.

Table 36 Basis for a AZ-102 Caustic Leachate Simulant

Component	Moles/Liter	mg/Liter
Aluminum	5.71E-2	1540
Chromium	3.73E-03	194
Molybdenum	1.46E-04	14
Potassium	2.31E-02	904
Sodium	2.58E+00	59200
Chloride	6.21E-04	22
Fluoride	7.16E-03	136
Nitrate	9.58E-02	5940
Nitrite	1.72E-01	7930
Phosphate	6.25E-03	594
Sulfate	5.05E-02	4850
TIC	1.95E-01	23.40

The anion that was not measured in the reported AZ-102 caustic leachate is hydroxide. Therefore, hydroxide was used to provide the balance. The composition of the simulant based upon a supernate density of 1.095 g/mL is shown in Table 37.

Table 37 AZ-102 Caustic Leachate Simulant Composition

Compounds	Formula	Grams/Liter
Potassium Nitrate	KNO_3	2.308
Sodium Chloride	NaCl	0.036
Sodium Chromate	Na_2CrO_4	0.604
Sodium Fluoride	NaF	0.301
Sodium Sulfate	Na_2SO_4	7.172
Aluminum Trihydroxide	$Al(OH)_3$	4.452
Sodium Hydroxide	NaOH	72.203
Sodium Phosphate	$Na_3PO_4 \bullet 12H_2O$	2.377
Sodium Carbonate	Na_2CO_3	20.649
Sodium Nitrate	$NaNO_3$	6.202
Sodium Nitrite	$NaNO_2$	11.894
Water	H_2O	965.45

The density of the AZ-102 leachate simulant test batch was 1.112 g/mL and the weight percent total solids were 13.6 %. The analytical results for the AZ-102 leachate simulant is listed in Table 38.

Table 38 Analytical Results for AZ-102 Caustic Leachate Simulant

Component	Found	Planned	% of Target
Al	1195	1540	78
Cr	160	194	82
K	920	904	102
Mo	14	14	99
Na	57070	59200	96
Chloride	117	22	532
Fluoride	100.0	136	74
Nitrate	4515	5940	76
Nitrite	7393	7930	93
Phosphate	770	594	130
Sulfate	4844	4850	100
TIC	<200	2340	<8.5

The aluminum result is very close to the amount actually added, based upon the purity of the hydrated aluminum trihydroxide used (80 %). The TIC and chloride appear to be bad analytical results.

4.0 Conclusion/Summary

The development of nonradioactive waste simulants to support the River Protection Project –Waste Treatment Plant bench and pilot-scale testing is crucial to the design of the facility. The report documents the simulants developed to support the SRTC programs and the strategies used to produce the simulants. The approved simulants for waste envelopes A, B, and C and the basis for their recipes were included. Additional simulants including sludge simulants, simulants of entrained solids, and simulants to support pretreatment mixing studies were discussed.

At the direction of the customer, the waste simulants were based upon specific waste characterization samples and did not involve averaging over multiple samples collected and analyzed at different times. The advantages and challenges of this approach were discussed along with recommendations for specific analyses that could improve the waste simulants. In general, the results of the A and B envelope simulants indicate that low concentrations of complexing agents may need to be analyzed for if trace metals are to be included in the simulant. For the C simulant, a method of analyzing for sodium gluconate either as the anion or as a derivatized organic compound is needed to provide a sounder basis for addition to the waste. At this point, it has definitely been established that some level of gluconate ion must be in the AN-107 waste to allow the level of soluble metals that are measured to be there.

The envelope A simulant that was developed as a part of this study and approved by the customer is based on tank 241-AN-105. Additional envelope A simulants prepared or calculated include simulants of tanks 241-AW-101, 241-AN-104, 241-AN-103 and a composite-dilution based simulant of 241-

AN-105. The envelope B simulant that was approved by the customer was based on the Best Basis Inventory for Tank 241-AZ-101. An additional B envelope simulant that was developed is based on tank 241-AZ-102. Additional characterization work on the B supernates is recommended to measure the low level of complexing agents that must be present. Addition of these complexants should allow the trace species in the simulant to more accurately reflect the actual waste. The approved envelope C simulant is based on tank 241-AN-107. Entrained solids simulants were created for envelopes A and C based upon tanks 241-AN-105 and 241-AN-107 respectively.

The envelope D simulant was developed based upon tank 241-AZ-101 sludge that had not been caustic washed to reduce the aluminum level. Unlike the supernate simulants which assume that the supernate phase is homogeneous, the sludge simulant is based upon multiple samples and therefore make use of averaging. The AZ-101 sludge simulant is based on averaging two separate core samples due to the heterogeneous nature of the settled sludge. Initial results on particle size and rheology are promising. Work on the Envelope D simulant will be continued as part of the physical properties of the High Level Waste studies planned to support the vitrification process.

5.0 References

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Appendixes

Appendix A Envelope A Simulant Spreadsheets

Table 39 AN-105 Analytical Information

Tank AN105 Supernate Composition											
										TOC	Source
Component	**Molecular weight**	**Concentration**	**Units**	**Concentration**	**Units**		**Moles of plus**	**Moles of Minus**	**% Carbon**	**mg/Liter**	
Acetate	59.04462	2070	mg/Liter	3.51E-02	M			3.51E-02	40.68	842	From AW-101
Aluminum	26.98154	39700	mg/Liter	1.47E+00	M			1.47E+00			Part A AN105 Sample
Ammonium	18.03846	120	mg/Liter	6.65E-03	M		6.65E-03				From AW-101
Barium	137.33		mg/Liter	0.00E+00	M		0.00E+00				
Boron	10.81	51	mg/Liter	4.72E-03	M			1.42E-02			DTR-046 report
Bromide	79.904		mg/Liter	0.00E+00	M			0.00E+00			
Cadmium	112.41	3	mg/Liter	2.94E-05	M		5.87E-05				
Calcium	40.08	40	mg/Liter	9.98E-04	M		2.00E-03				Part A AN105 Sample
Carbonate	60.0092	12540	mg/Liter	2.09E-01	M			4.18E-01			Part A AN105 Sample
Cerium	140.12		mg/Liter	0.00E+00	M		0.00E+00				
Cesium	132.9054	16	mg/Liter	1.22E-04	M						
Chloride	35.453	9090	mg/Liter	2.56E-01	M			2.56E-01			Part A AN105 Sample

Tank AN105 Supernate Composition											
										TOC	**Source**
Component	**Molecular weight**	**Concentration**	**Units**	**Concentration**	**Units**		**Moles of plus**	**Moles of Minus**	**% Carbon**	**mg/Liter**	
Chromium	51.996	1350	mg/Liter	2.60E-02	M			5.19E-02			DTR-046 report
Copper	63.546		mg/Liter	0.00E+00	M		0.00E+00				
Ethylenediaminetetraacetic acid	288.20824		mg/Liter	0.00E+00	M			0.00E+00	41.67	0	
Fluoride	18.9984	190	mg/Liter	1.00E-02	M			1.00E-02			less than from DTR-04
Formate	45.01774	2880	mg/Liter	6.40E-02	M			6.40E-02	26.68	768	From AW-101
Glycolate	75.04206	1150	mg/Liter	1.53E-02	M			1.53E-02	32.01	368	From AW-101
Hydroxide	17.00734	58100	mg/Liter	3.42E+00	M			3.42E+00			Part A AN105 Sample
Iron	55.847		mg/Liter	0.00E+00	M		0.00E+00				
Lanthanum	138.9055		mg/Liter	0.00E+00	M		0.00E+00				
Lead	207.2	53	mg/Liter	2.56E-04	M		5.12E-04				Part A AN105 Sample
Magnesium	24.305	5	mg/Liter	2.22E-04	M		4.44E-04				Part A AN105 Sample
Manganese	54.938		mg/Liter	0.00E+00	M		0.00E+00				
Molybdenum	95.94	82	mg/Liter	8.55E-04	M			1.71E-03			DTR-046 report
Neodymium	144.24		mg/Liter	0.00E+00	M		0.00E+00				

Tank AN105 Supernate Composition											
										TOC	**Source**
Component	**Molecular weight**	**Concentration**	**Units**	**Concentration**	**Units**		**Moles of plus**	**Moles of Minus**	**% Carbon**	**mg/Liter**	
n-Hydroxyethylenediaminetriacetic acid	275.23618		mg/Liter	0.00E+00	M			0.00E+00	43.64	0	
Nickel	58.69		mg/Liter	0.00E+00	M		0.00E+00				
Nitrate	62.0049	165000	mg/Liter	2.66E+00	M			2.66E+00			Part A AN105 Sample
Nitrite	46.0055	111000	mg/Liter	2.41E+00	M			2.41E+00			Part A AN105 Sample
Oxalate	88.0196	610	mg/Liter	6.93E-03	M			1.39E-02	27.29	166	From AW-101
Phosphate	94.97136	570	mg/Liter	6.00E-03	M			1.80E-02			Part A AN105 Sample
Potassium	39.0983	7500	mg/Liter	1.92E-01	M		1.92E-01				DTR-046 report
Selenium	78.96	1	mg/Liter	1.25E-05	M			2.51E-05			
Silicon	28.0855	211	mg/Liter	7.51E-03	M			1.50E-02			DTR-046 report
Silver	107.8682	16	mg/Liter	1.51E-04	M		1.51E-04				
Sodium	22.9898	233000	mg/Liter	1.01E+01	M		1.01E+01				Part A AN105 Sample
Sulfate	96.0576	771	mg/Liter	8.03E-03	M			1.61E-02			Part A AN105 Sample
Tin		22	mg/Liter	1.83E-04	M						
TIC	12.011	2510	mg/Liter	2.09E-01	M						Part A AN105 Sample

Tank AN105 Supernate Composition											
										TOC	**Source**
Component	**Molecular weight**	**Concentration**	**Units**	**Concentration**	**Units**		**Moles of plus**	**Moles of Minus**	**% Carbon**	**mg/Liter**	
TOC		3590	mg/Liter	3.59	g/L						Part A AN105 Sample
Uranium			mg/Liter	0.00E+00	ug/mL						
Zinc	65.38	10	mg/Liter	1.54E-04	M		3.09E-04				
Zirconium	91.22		mg/Liter	0.00E+00	M		0.00E+00				
						Total	10.34	1.09E+01	Moles/Liter		
						Balance		5.54E-01			
Additional Organics(based upon PNNL Report on FY1997 Results)											
Nitrilotriacetic Acid	188.11618		mg/Liter	0.00E+00	M			0.00E+00	Moles/Liter		
Citric Acid	189.09618		mg/Liter	0.00E+00	M			0.00E+00	Moles/Liter		
Iminodiacetic Acid	131.08412		mg/Liter	0.00E+00	M			0.00E+00	Moles/Liter		
Source											
Sodium Gluconate	218.14	0	mg/Liter		M		0.00E+00	0.0			
						Total	10.34	10.89		1979	mg/Liter
						Short	0.55			1611	mg/Liter

Tank AN105 Supernate Composition											
										TOC	**Source**
Component	**Molecular weight**	**Concentration**	**Units**	**Concentration**	**Units**		**Moles of plus**	**Moles of Minus**	**% Carbon**	**mg/Liter**	
Density (average)		1.4									

Table 40 Compound Calculations for AN-105 Simulant

Measured TOC	**3.6**								
							Formula Weight	**Mass Needed**	**Mass of H2O**
Compounds	**Moles**	**Nitrate Moles**	**Contains [Na]**	**Moles of Na Needed**	**Wt % Carbon**	**Formula**	**grams**	**grams**	**grams**
Aluminum Trihydroxide	1.47E+00			1.47E+00		Al(OH)3	78	114.767	
Ammonium Acetate	6.65E-03				31.2	CH3COONH4	77.08	0.513	
Barium Nitrate	0.00E+00	0.00E+00				Ba(NO3)2	261.35	0.000	
Boric Acid	4.72E-03			1.42E-02		H3BO3	61.83	0.292	
Cadmium Nitrate	2.94E-05	5.87E-05				Cd(NO3)2.4H2O	308.47	0.009	2.11E-03
Calcium Nitrate	9.98E-04	2.00E-03				Ca(NO3)2.4H2O	236.15	0.236	7.19E-02
Cerium Nitrate	0.00E+00	0.00E+00				Ce(NO3)3.6H2O	434.23	0.000	0.00E+00
Cesium Nitrate	1.22E-04	1.22E-04				CsNO3	194.91	0.024	
Sodium Chromate	2.60E-02		5.19E-02			Na2CrO4	161.97	4.205	
Copper Nitrate	0.00E+00	0.00E+00				Cu(NO3)2.2.5H2O	232.59	0.000	0.00E+00
Ethylenediaminetetraacetic acid	0.00E+00		0.00E+00	0.00E+00	32.3	Na2EDTA.2H2O	372.24	0.000	
Ferric Nitrate	0.00E+00	0.00E+00				Fe(NO3)3.9H2O	404	0.000	0.00E+00

Measured TOC	**3.6**								
							Formula Weight	**Mass Needed**	**Mass of H2O**
Compounds	**Moles**	**Nitrate Moles**	**Contains [Na]**	**Moles of Na Needed**	**Wt % Carbon**	**Formula**	**grams**	**grams**	**grams**
Lanthanum Nitrate	0.00E+00	0.00E+00				La(NO3)3.6H2O	433.03	0.000	0.00E+00
Lead nitrate	2.56E-04	5.12E-04				Pb(NO3)2	331.2	0.085	
Magnesium Nitrate	2.22E-04	4.44E-04				Mg(NO3)2.6H2O	256.41	0.057	2.40E-02
Manganous Chloride	0.00E+00					MnCl2.4H2O	197.9	0.000	0.00E+00
Potassium Molybdate	8.55E-04					K2MoO4	238.14	0.204	
Neodymium Nitrate	0.00E+00	0.00E+00				Nd(NO3)3.6H2O	438.35	0.000	0.00E+00
n-Hydroxyethylenediaminetriacetic acid	0.00E+00			0	43.2	HEDTA	278.26	0.000	
Nickel Nitrate	0.00E+00	0.00E+00				Ni(NO3)2.6H2O	290.81	0.000	0.00E+00
Potassium Nitrate	1.90E-01	1.90E-01				KNO3	101.1	19.221	
Selenium dioxide	1.25E-05			2.51E-05		SeO2	110.96	0.001	
Sodium meta-silicate	7.51E-03		1.50E-02			Na2SiO3.9H2O	284.2	2.135	1.22E+00
Silver Nitrate	1.51E-04	1.51E-04				AgNO3	169.87	0.026	
Strontium Nitrate		0.00E+00				Sr(NO3)2	211.63	0.000	
Zinc Nitrate	1.54E-04	3.09E-04				Zn(NO3)2.6H2O	297.47	0.046	0.016684001

Measured TOC	**3.6**								
							Formula Weight	**Mass Needed**	**Mass of H2O**
Compounds	**Moles**	**Nitrate Moles**	**Contains [Na]**	**Moles of Na Needed**	**Wt % Carbon**	**Formula**	**grams**	**grams**	**grams**
Zirconyl Nitrate	0.00E+00	0					249.23	0.000	0
Sodium Acetate	2.84E-02		2.84E-02		17.7	NaCH3COO.3H2O	136.08	3.865	1.53E+00
Sodium Bromide	0.00E+00		0.00E+00			NaBr	102.89	0.000	
Sodium Carbonate	2.09E-01		4.18E-01			Na2CO3	105.99	22.149	
Sodium Chloride	2.56E-01		2.56E-01			NaCl	58.44	14.984	
Sodium Fluoride	1.00E-02		1.00E-02			NaF	41.99	0.420	
Sodium Formate	6.40E-02		6.40E-02		17.7	HCOONa	68.01	4.351	
Glycolic Acid	1.53E-02			1.53E-02	31.6	HOCH2COOH, 70 wt%	76.05	1.665	
Sodium Nitrite	2.41E+00		2.41E+00			NaNO2	69	166.480	
Sodium Oxalate	6.93E-03		1.39E-02		17.9	Na2C2O4	134	0.929	
Sodium Phosphate	6.00E-03		1.80E-02			Na3PO4.12H2O	380.12	2.281	1.30E+00
Sodium Sulfate	8.03E-03		1.61E-02			Na2SO4	142.04	1.140	
Sodium Nitrate	2.47E+00	2.47E+00	2.47E+00			NaNO3	84.99	209.702	
Sodium Hydroxide	4.92E+00		4.92E+00			NaOH	40	196.682	

Measured TOC	**3.6**								
							Formula Weight	**Mass Needed**	**Mass of H2O**
Compounds	**Moles**	**Nitrate Moles**	**Contains [Na]**	**Moles of Na Needed**	**Wt % Carbon**	**Formula**	**grams**	**grams**	**grams**
Totals		2.66E+00	10.7					766.468	4.16E+00
Target		2.66E+00	10.1						
		0.00E+00	-0.55						
Sodium Hydroxide Charge balance	4.36E+00								
Difference	-5.54E-01								
Measured Density	1.44	grams/mL							
Total Solution Mass	1440	grams/mL							
% Solids	5.294E+01								
Mass of Water	6.74E+02	grams							

Table 41 AN-105 Simulant Recipe

Complete Envelope A Recipe			
Volume of Feed		1000	mL
In a tared	1000	mL Volumetric Flask add	
	grams	Actual Wt, grams	
Water	200		
Transition Metals and Complexing agents			
Compounds	Formula	Mass Needed	Actual Wt, grams
Boric Acid	H3BO3	0.292	
Cadmium Nitrate	Cd(NO3)2.4H2O	0.009	
Calcium Nitrate	Ca(NO3)2.4H2O	0.236	
Cesium Nitrate	CsNO3	0.024	
Lead nitrate	Pb(NO3)2	0.085	
Magnesium Nitrate	Mg(NO3)2.6H2O	0.057	
Potassium Nitrate	KNO3	19.221	
Silver Nitrate	AgNO3	0.026	
Zinc Nitrate	Zn(NO3)2.6H2O	0.046	
Glycolic Acid	HOCH2COOH, 70 wt%	1.665	

Sodium Chloride	NaCl	14.984	
Sodium Fluoride	NaF	0.420	
Sodium Chromate	Na2CrO4	4.205	
Sodium Sulfate	Na2SO4	1.140	
Potassium Molybdate	K2MoO4	0.204	
Ammonium Acetate	CH3COONH4	0.513	
In a separate container mix the following			
Compounds	Formula	Mass Needed	Actual Wt, grams
Aluminum Trihydroxide	Al(OH)3	114.77	
Sodium Hydroxide	NaOH	196.68	
Selenium dioxide	SeO2	0.001	
Sodium meta-silicate	Na2SiO3.9H2O	2.135	
Sodium Acetate	NaCH3COO.3H2O	3.865	
Sodium Formate	HCOONa	4.351	
Sodium Oxalate	Na2C2O4	0.929	
Sodium Phosphate	Na3PO4.12H2O	2.281	
Add	grams	Actual Wt, grams	
Water	300		
Mix thoroughly. Then add this solution to the volumetric flask.			

Add	Formula	Mass Needed	Actual Wt, grams
Sodium Carbonate	Na2CO3	22.149	
Mix thoroughly.			
Add	Formula	Mass Needed	Actual Wt, grams
Sodium Nitrate	NaNO3	209.70	
Sodium Nitrite	NaNO2	166.48	
Mix thoroughly.			
Mix thoroughly and dilute to the mark.			
Record Final Weight		grams	
The final addition of water would be		173.53	grams based upon
a density of 1.44 g/mL.			

Appendix B Envelope B Simulant Spreadsheets

Table 42 Best Basis Inventory for Tank 241-AZ-101 used in Envelope B Simulant

Inventory based on dst inventory calculations from both nomalized TRAC or BBI as of 10/1/98 where available. File is		
dst_inv_99.csv		
TANK	**AZ-101**	**Concentration**
SOLUBLE	**AZ-101**	**mg/Liter**
106-Ru	0.00E+00	0.0
113m-Cd	0.00E+00	0.0
125-Sb	0.00E+00	0.0
126-Sn	0.00E+00	0.0
129-I	0.00E+00	0.0
134-Cs	0.00E+00	0.0
137m-Ba	0.00E+00	0.0
137-Cs	6.35E+01	21.0
14-C	0.00E+00	0.0
151-Sm	0.00E+00	0.0
152-Eu	0.00E+00	0.0
154-Eu	0.00E+00	0.0
155-Eu	0.00E+00	0.0
226-Ra	0.00E+00	0.0
227-Ac	0.00E+00	0.0
228-Ra	0.00E+00	0.0
229-Th	0.00E+00	0.0
231-Pa	0.00E+00	0.0
232-Th	0.00E+00	0.0
232-U	0.00E+00	0.0
233-U	0.00E+00	0.0
234-U	0.00E+00	0.0
235-U	0.00E+00	0.0
236-U	0.00E+00	0.0
237-Np	0.00E+00	0.0
238-Pu	0.00E+00	0.0
238-U	0.00E+00	0.0
239-Pu	0.00E+00	0.0
240-Pu	0.00E+00	0.0
241-Am	0.00E+00	0.0
241-Pu	0.00E+00	0.0
242-Cm	0.00E+00	0.0
242-Pu	0.00E+00	0.0

Inventory based on dst inventory calculations from both nomalized TRAC or BBI as of 10/1/98 where available. File is		
dst_inv_99.csv		
TANK	**AZ-101**	**Concentration**
SOLUBLE	**AZ-101**	**mg/Liter**
243-Am	0.00E+00	0.0
243-Cm	0.00E+00	0.0
244-Cm	0.00E+00	0.0
3-H	0.00E+00	0.0
59-Ni	0.00E+00	0.0
60-Co	0.00E+00	0.0
63-Ni	0.00E+00	0.0
79-Se	0.00E+00	0.0
90-Sr	3.05E-02	0.0
90-Y	0.00E+00	0.0
93m-Nb	0.00E+00	0.0
93-Zr	0.00E+00	0.0
99-Tc	4.40E+01	14.5
Ag+	0.00E+00	0.0
Al+3	3.23E+04	10667.7
As+5	0.00E+00	0.0
B+3	0.00E+00	0.0
Ba+2	0.00E+00	0.0
Be+2	0.00E+00	0.0
Bi+3	0.00E+00	0.0
Ca+2	0.00E+00	0.0
Cd+2	0.00E+00	0.0
Ce+3	0.00E+00	0.0
Cl-	6.04E+02	199.5
CN-	0.00E+00	0.0
Co+3	0.00E+00	0.0
CO3-2	0.00E+00	0.0
Cr(TOTAL)	2.21E+03	729.9
Cs+	1.13E+02	37.3
Cu+2	0.00E+00	0.0
F-	5.49E+03	1813.2
Fe+3	0.00E+00	0.0
H2O	2.76E+06	911542.7
Hg+2	0.00E+00	0.0
K+	1.40E+04	4623.8
La+3	0.00E+00	0.0
Li+	0.00E+00	0.0
Mg+2	0.00E+00	0.0

Inventory based on dst inventory calculations from both nomalized TRAC or BBI as of 10/1/98 where available. File is

dst_inv_99.csv		
TANK	**AZ-101**	**Concentration**
SOLUBLE	**AZ-101**	**mg/Liter**
Mn+4	0.00E+00	0.0
Mo+6	0.00E+00	0.0
Na+	3.30E+05	108988.8
Nd+3	0.00E+00	0.0
NH3	9.47E+02	312.8
Ni+2	0.00E+00	0.0
NO2-	1.97E+05	65063.0
NO3-	2.29E+05	75631.6
OH-	0.00E+00	0.0
Pb+2	0.00E+00	0.0
Pd+2	0.00E+00	0.0
PO4-3	4.55E+03	1502.7
Pr+3	0.00E+00	0.0
Pu+4	0.00E+00	0.0
Rb+	0.00E+00	0.0
Rh+3	0.00E+00	0.0
Ru+3	0.00E+00	0.0
Sb+5	0.00E+00	0.0
Se+6	0.00E+00	0.0
Si+4	0.00E+00	0.0
SO4-2	5.35E+04	17669.4
Sr+2	0.00E+00	0.0
Ta+5	0.00E+00	0.0
Tc+7	0.00E+00	0.0
Te+6	0.00E+00	0.0
Th+4	0.00E+00	0.0
Ti+4	0.00E+00	0.0
Tl+3	0.00E+00	0.0
TOC	3.57E+03	1179.1
U(TOTAL)	0.00E+00	0.0
V+5	0.00E+00	0.0
W+6	0.00E+00	0.0
Y+3	0.00E+00	0.0
Zn+2	0.00E+00	0.0
Zr+4	9.30E+00	3.1
Total, kg	3.63E+06	
Density, kg/l	1.2	
Volume, liters	3.03E+06	

Inventory based on dst inventory calculations from both nomalized TRAC or BBI as of 10/1/98 where available. File is		
dst_inv_99.csv		
TANK	**AZ-101**	**Concentration**
SOLUBLE	**AZ-101**	**mg/Liter**
Volume, gallons	8.00E+05	

Table 43 Hydroxide and Carbonate Basis for B Envelope Simulant

The basis for Hydroxide and Carbonate

The value for both of these in the BBI is 0 while

I need some to balance the Na+.

I decide to use the following Source.

G. K.Patello and K. D. Wiemers

TWRS Privatization Phase 1 Waste Characterization Data Evaluation for the Request for Proposal

PNNL-11109

Table 2.3	mg/Liter	Mole Wt	Concentration	units	Requires Na+ Moles
Hydroxide	11300	17.00734	0.664419	M	0.664419
TIC	5780	12.011	0.481226	M	0.962451
				Total	1.62687

Sodium that needs to be balanced is 1.30 moles.

I will ratio the OH/(OH+CO3) and CO3/(OH+CO3).

	Moles/Liter	Mole Wt	mg/Liter		Requires Na+ Moles
OH for Na	0.530924	17.00734	9030		0.530924
CO3 for Na	0.384538	12.011	4619		0.769076
				Total	1.3

Table 44 Calculated "Analytical" Data for Envelope B Simulant

Tank AZ101 Supernate Composition								
Component	Molecular weight	**Concentration**	**Units**	**Concentration**	**Units**		Moles of plus	Moles of Minus
Aluminum	26.98154	10667.7	mg/Liter	3.95E-01	Molar			3.95E-01
Ammonia	17.03052	312.8	mg/Liter	1.84E-02	Molar		1.84E-02	
Arsenic	74.9216	0.0	mg/Liter	0.00E+00	Molar			0.00E+00
Barium	137.33	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Boron	10.81	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Cadmium	112.41	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Calcium	40.08	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Carbonate	60.0092	23075.8	mg/Liter	3.85E-01	Molar			7.69E-01
Cesium	132.9054	37.3	mg/Liter	2.81E-04	Molar		2.81E-04	
Chloride	35.453	199.5	mg/Liter	5.63E-03	Molar			5.63E-03

Tank AZ101 Supernate Composition								
Component	Molecular weight	**Concentration**	**Units**	**Concentration**	**Units**		Moles of plus	Moles of Minus
Chromium	51.996	729.9	mg/Liter	1.40E-02	Molar			2.81E-02
Copper	63.546	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Fluoride	18.998	1813.2	mg/Liter	9.54E-02	Molar			9.54E-02
Hydroxide	17.00734	9029.6	mg/Liter	5.31E-01	Molar			5.31E-01
Iron	55.847	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Lanthanum	138.9055	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Lead	207.2	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Lithium	6.941	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Magnesium	24.305	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Manganese	54.938	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Molybdenum	95.94	0.0	mg/Liter	0.00E+00	Molar			0.00E+00
Neodymium	144.24	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	

Tank AZ101 Supernate Composition

Component	Molecular weight	Concentration	Units	Concentration	Units		Moles of plus	Moles of Minus
Nickel	58.69	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Nitrate	62.0049	75631.6	mg/Liter	1.22E+00	Molar			1.22E+00
Nitrite	46.0055	65063.0	mg/Liter	1.41E+00	Molar			1.41E+00
Phosphate	94.97136	1502.7	mg/Liter	1.58E-02	Molar			4.75E-02
Potassium	39.0983	4623.8	mg/Liter	1.18E-01	Molar		1.18E-01	
Rhenium	186.207		mg/Liter	0.00E+00	Molar			0.00E+00
Rhodium	102.9055	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Ruthenium	101.07	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Selenium	78.96	0.0	mg/Liter	0.00E+00	Molar			0.00E+00
Silicon	28.0855	0.0	mg/Liter	0.00E+00	Molar			0.00E+00
Silver	107.8682	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Sodium	22.9898	108988.8	mg/Liter	4.74E+00	Molar		4.74E+00	

Tank AZ101 Supernate Composition								
Component	Molecular weight	**Concentration**	**Units**	**Concentration**	**Units**		Moles of plus	Moles of Minus
Strontium	87.62	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Sulfate	96.0576	17669.4	mg/Liter	1.84E-01	Molar			3.68E-01
Tellurium	127.6	0.0	mg/Liter	0.00E+00	Molar			0.00E+00
Titanium	47.88	0.0	mg/Liter	0.00E+00	Molar			0.00E+00
TIC	12.011	4618.7	mg/Liter	3.85E-01	Molar			
Vanadium	50.9415	0.0	mg/Liter	0.00E+00	Molar			0.00E+00
Zinc	65.38	0.0	mg/Liter	0.00E+00	Molar		0.00E+00	
Zirconium	91.22	3.1	mg/Liter	3.37E-05	Molar			6.73E-05
Totals							4.88	4.87

Table 45 Compound Calculations for Envelope B Simulant

							Formula Weight	Mass Needed	Mass of H2O
Compounds	Moles	Nitrate Moles	Contains [Na]	Moles of Na Needed	Wt % Carbon	Formula	grams	grams	grams
Aluminum trihydroxide	3.95E-01			3.95E-01		Al(OH)3	78	30.839	0.00E+00
Ammonium Nitrate	1.84E-02	1.84E-02				NH4NO3	80.04	1.470	
Barium Nitrate	0.00E+00	0.00E+00				Ba(NO3)2	261.35	0.000	
Boric Acid	0.00E+00			0.00E+00		H3BO3	61.83	0.000	
Cadmium Nitrate	0.00E+00	0.00E+00				Cd(NO3)2.4H2O	308.47	0.000	0.00E+00
Calcium Nitrate	0.00E+00	0.00E+00				Ca(NO3)2.4H2O	236.15	0.000	0.00E+00
Cesium Nitrate	2.81E-04	2.81E-04				CsNO3	194.91	0.055	
Sodium Chromate	1.40E-02		2.81E-02			Na2CrO4	161.97	2.274	
Copper Nitrate	0.00E+00	0.00E+00				Cu(NO3)2.2.5H2O	232.59	0.000	0.00E+00
Ethylenediaminetetraacetic acid	0.00E+00		0.00E+00	0.00E+00	32.3	Na2EDTA.2H2O	372.24	0.000	
Ferric Nitrate	0.00E+00	0.00E+00				Fe(NO3)3.9H2O	404	0.000	0.00E+00
Lanthanum Nitrate	0.00E+00	0.00E+00				La(NO3)3.6H2O	433.03	0.000	0.00E+00
Lead nitrate	0.00E+00	0.00E+00				Pb(NO3)2	331.2	0.000	

							Formula Weight	Mass Needed	Mass of H2O
Compounds	Moles	Nitrate Moles	Contains [Na]	Moles of Na Needed	Wt % Carbon	Formula	grams	grams	grams
Lithium Chloride	0.00E+00					LiCl	42.39	0.000	
Magnesium Nitrate	0.00E+00	0.00E+00				Mg(NO3)2.6H2O	256.41	0.000	0.00E+00
Manganous Chloride	0.00E+00					MnCl2.4H2O	197.9	0.000	0.00E+00
Potassium Molybdate	0.00E+00					K2MoO4	238.14	0.000	
Neodymium Nitrate	0.00E+00	0.00E+00				Nd(NO3)3.6H2O	438.35	0.000	0.00E+00
n-Hydroxyethylene diaminetriacetic acid	0.00E+00			0	43.2	HEDTA	278.26	0.000	
Nickel Nitrate	0.00E+00	0.00E+00				Ni(NO3)2.6H2O	290.81	0.000	0.00E+00
Potassium Nitrate	1.18E-01	1.18E-01				KNO3	101.1	11.956	
Sodium Perrhenate	0.00E+00		0.00E+00			NaReO4	273.19	0.000	
Rhodium Nitrate	0.00E+00	0.00E+00				Rh(NO3)3.2H2O	324.95	0.000	0.00E+00
Ruthenium Chloride	0.00E+00					RuCl3	207.43	0.000	
Selenium dioxide	0.00E+00			0.00E+00		SeO2	110.96	0.000	

							Formula Weight	Mass Needed	Mass of H2O
Compounds	Moles	Nitrate Moles	Contains [Na]	Moles of Na Needed	Wt % Carbon	Formula	grams	grams	grams
Sodium meta-silicate	0.00E+00		0.00E+00			Na2SiO3.9H2O	284.2	0.000	0.00E+00
Silver Nitrate	0.00E+00	0.00E+00				AgNO3	169.87	0.000	
Strontium Nitrate	0.00E+00	0.00E+00				Sr(NO3)2	211.63	0.000	
Tellurium Dioxide	0.00E+00			0.00E+00		TeO2	159.6	0.000	
Titanium Tetrachloride	0.00E+00					TiCl4	189.71	0.000	
Vanadium Pentoxide	0.00E+00			0.00E+00		V2O5	181.88	0.000	
Zinc Nitrate	0.00E+00	0.00E+00				Zn(NO3)2.6H2O	297.47	0.000	0
Zirconyl Nitrate	3.37E-05	6.73427E-05				ZrO(NO3)2.xH2O	249.23	0.008	0.000606085
Sodium Acetate	0.00E+00		0.00E+00		17.7	NaCH3COO.3H2O	136.08	0.000	0.00E+00
Sodium Bromide	0.00E+00		0.00E+00			NaBr	102.89	0.000	
Sodium Carbonate	3.85E-01		7.69E-01			Na2CO3	105.99	40.757	
Sodium Chloride	5.63E-03		5.63E-03			NaCl	58.44	0.329	
Sodium Fluoride	9.54E-02		9.54E-02			NaF	41.99	4.008	
Sodium Formate	0.00E+00		0.00E+00		17.7	HCOONa	68.01	0.000	
Glycolic Acid	0.00E+00			0.00E+00	31.6	HOCH2COOH, 70	76.05	0.000	0

							Formula Weight	Mass Needed	Mass of H2O
Compounds	Moles	Nitrate Moles	Contains [Na]	Moles of Na Needed	Wt % Carbon	Formula	grams	grams	grams
						wt%			
Sodium Nitrite	1.41E+00		1.41E+00			NaNO2	69	97.583	
Sodium Oxalate	0.00E+00		0.00E+00		17.9	Na2C2O4	134	0.000	
Sodium Phosphate	1.58E-02		4.75E-02			Na3PO4.12H2O	380.12	6.015	3.42E+00
Sodium Sulfate	1.84E-01		3.68E-01			Na2SO4	142.04	26.128	
Sodium Nitrate	1.08E+00	1.08E+00	1.08E+00			NaNO3	84.99	92.027	
Sodium Hydroxide	9.26E-01		9.26E-01			NaOH	40	37.052	
Totals		1.22E+00	4.74E+00					350.499	3.42E+00
Target		1.22E+00	4.74E+00						
		0.00E+00	3.83E-03						
Additional NaOH to match Na+	3.83E-03					NaOH	40	0.153	
Total NaOH	9.30E-01					NaOH	40	37.205	
Measured Density	1.2	grams/mL							

							Formula Weight	Mass Needed	Mass of H2O
Compounds	Moles	Nitrate Moles	Contains [Na]	Moles of Na Needed	Wt % Carbon	Formula	grams	grams	grams
Total Solution Mass	1200	grams/mL							
% Solids	2.92E+01								
Mass of Water	8.50E+02	grams							

Table 46 Best Basis Envelope B Recipe

Best Basis Inventory Envelope B Recipe

Volume of Feed	1000	mL

In a tared 1000 mL Volumetric Flask add

	grams	Actual Wt, grams
Water	200	

Transition Metals and Complexing agents

Compounds	Formula	Mass Needed	Actual Wt, grams
Ammonium Nitrate	NH4NO3	1.470	
Cesium Nitrate	CsNO3	0.055	
Potassium Nitrate	KNO3	11.956	
Zirconyl Nitrate	ZrO(NO3)2.xH2O	0.008	
Sodium Chloride	NaCl	0.329	
Sodium Fluoride	NaF	4.008	
Sodium Chromate	Na2CrO4	2.274	
Sodium Sulfate	Na2SO4	26.128	

In a separate container mix the following

Compounds	Formula	Mass Needed	Actual Wt, grams
Aluminum trihydroxide	Al(OH)3	30.839	
Sodium Hydroxide	NaOH	37.205	
Sodium Phosphate	Na3PO4.12H2O	6.015	

Add	grams	Actual Wt, grams
Water	300	

Mix thoroughly. Then add this solution to the volumetric flask.

Add	Formula	Mass Needed	Actual Wt, grams
Sodium Carbonate	Na2CO3	40.757	

Mix thoroughly.

Add	Formula	Mass Needed	Actual Wt, grams
Sodium Nitrate	NaNO3	92.027	
Sodium Nitrite	NaNO2	97.583	

Mix thoroughly.

Mix thoroughly and dilute to the mark.

Record Final Weight		grams

The final addition of water would be 349.50 grams based upon a density of 1.20 g/mL.

Appendix C Envelope C Simulant Spreadsheets

Table 47 Tank 241-AN-107 Supernate Composition

Tank An107 Supernate Composition											
										TOC	
Component	Molecular weight	**Concentration**	**Units**	**Concentration**	**Units**		Moles of plus	Moles of Minus	% Carbon	mg/Liter	
Acetate	59.04462	1100	mg/Liter	1.86E-02	M			1.86E-02	40.68	448	
Aluminum	26.98154	386	mg/Liter	1.43E-02	M			1.43E-02			
Ammonium	18.03846	22	mg/Liter	1.22E-03	M		1.22E-03				
Barium	137.33	7	mg/Liter	5.42E-05	M		1.08E-04				
Boron	10.81	35	mg/Liter	3.24E-03	M			9.71E-03			
Bromide	79.904	1150	mg/Liter	1.44E-02	M			1.44E-02			
Cadmium	112.41	64	mg/Liter	5.70E-04	M		1.14E-03				
Calcium	40.08	591	mg/Liter	1.47E-02	M		2.95E-02				
Carbonate	60.0092	83936	mg/Liter	1.40E+00	M			2.80E+00			
Cerium	140.12	53	mg/Liter	3.77E-04	M		1.13E-03				
Chloride	35.453	1830	mg/Liter	5.16E-02	M			5.16E-02			
Chromium	51.996	176	mg/Liter	3.38E-03	M			6.77E-03			

Tank An107 Supernate Composition											
										TOC	
Component	Molecular weight	**Concentration**	**Units**	**Concentration**	**Units**		Moles of plus	Moles of Minus	% Carbon	mg/Liter	
Copper	63.546	30	mg/Liter	4.74E-04	M		9.47E-04				
Ethylenediaminetetraacetic acid	288.20824	5620	mg/Liter	1.95E-02	M			7.80E-02	41.67	2342	
Fluoride	18.9984	133	mg/Liter	7.00E-03	M			7.00E-03			
Formate	45.01774	10400	mg/Liter	2.31E-01	M			2.31E-01	26.68	2775	
Glycolate	75.04206	18600	mg/Liter	2.48E-01	M			2.48E-01	32.01	5954	
Hydroxide	17.00734	340	mg/Liter	2.00E-02	M			2.00E-02			
Iron	55.847	1690	mg/Liter	3.03E-02	M		9.08E-02				
Lanthanum	138.9055	46	mg/Liter	3.28E-04	M		9.83E-04				
Lead	207.2	388	mg/Liter	1.87E-03	M		3.75E-03				
Magnesium	24.305	25	mg/Liter	1.03E-03	M		2.06E-03				
Manganese	54.938	563	mg/Liter	1.02E-02	M		2.05E-02				
Molybdenum	95.94	36	mg/Liter	3.73E-04	M			7.46E-04			
Neodymium	144.24	96	mg/Liter	6.65E-04	M		1.99E-03				
n-Hydroxyethylenedi	275.23618	2140	mg/Liter	7.78E-03	M			2.33E-02	43.64	934	

Tank An107 Supernate Composition											
										TOC	
Component	Molecular weight	**Concentration**	**Units**	**Concentration**	**Units**		Moles of plus	Moles of Minus	% Carbon	mg/Liter	
aminetriacetic acid											
Nickel	58.69	530	mg/Liter	9.03E-03	M		1.81E-02				
Nitrate	62.0049	230000	mg/Liter	3.71E+00	M			3.71E+00			
Nitrite	46.0055	61000	mg/Liter	1.33E+00	M			1.33E+00			
Oxalate	88.0196	826	mg/Liter	9.38E-03	M			1.88E-02	27.29	225	
Phosphate	94.97136	1110	mg/Liter	1.17E-02	M			3.51E-02			
Potassium	39.0983	1810	mg/Liter	4.63E-02	M		4.63E-02				
Selenium	78.96	1	mg/Liter	6.33E-06	M			1.27E-05			
Silicon	28.0855	#VALUE!	mg/Liter	#VALUE!	M			?????			
Silver	107.8682	14	mg/Liter	1.33E-04	M		1.33E-04				
Sodium	22.9898	195000	mg/Liter	8.48E+00	M		8.48E+00				
Sulfate	96.0576	8250	mg/Liter	8.59E-02	M			1.72E-01			
TIC	12.011	16800	mg/Liter	1.40E+00	M						
TOC		40400	mg/Liter	40.40	g/L						
Uranium		127	mg/Liter	1.27E+02	ug/mL						

Tank An107 Supernate Composition

Component	Molecular weight	**Concentration**	**Units**	**Concentration**	**Units**		Moles of plus	Moles of Minus	% Carbon	TOC mg/Liter	
Zinc	65.38	45	mg/Liter	6.93E-04	M			1.39E-03			
Zirconium	91.22	70	mg/Liter	7.67E-04	M		3.07E-03				
						Total	8.703675583	8.78E+00	Moles/Liter		
Additional Organics(based upon PNNL Report on FY1997 Results)											
Nitrilotriacetic Acid	188.11618	561	mg/Liter	2.98E-03	M			8.95E-03	Moles/Liter		
Citric Acid	189.09618	8495	mg/Liter	4.49E-02	M			1.35E-01	Moles/Liter		
Iminodiacetic Acid	131.08412	5947	mg/Liter	4.54E-02	M			9.07E-02	Moles/Liter		
Source	Agreement on Gluconate from Bill Wilmarth based upon Fe titration Test										
Sodium Gluconate	218.14	3927	mg/Liter	1.80E-02	M		1.80E-02	0.0			
						Total	8.72	9.04		12452	mg/Liter
						Short	0.31			27948	mg/Liter
Density (average)		1.4									

Table 48 Compound Calculations for AN-107 Simulant

Organic from 96 TOC	40.4									
							Formula Weight	Mass Needed	Mass of H2O	TOC
Compounds	Moles	Nitrate Moles		Moles of Na	Wt % Carbon	Formula	grams	grams	grams	Grams
Aluminum Nitrate	1.43E-02	4.29E-02		5.72E-02		Al(NO3)3.9H2O	375.13	5.37	2.32	
Ammonium Acetate	1.22E-03					NH4Ch3COO	77.08	0.09		
Barium Nitrate	5.42E-05	1.08E-04				Ba(NO3)2	261.35	0.01		
Boric acid	3.24E-03			9.71E-03		H3BO3	61.83	0.20		
Cadmium Nitrate	5.70E-04	1.14E-03				Cd(NO3)2.4H2O	308.47	0.18	0.04	
Calcium Nitrate	1.47E-02	2.95E-02				Ca(NO3)2.4H2O	236.15	3.48	1.06	
Cerium Nitrate	3.77E-04	1.13E-03				Ce(NO3)3.6H2O	434.23	0.16	0.04	
Cesium Nitrate	1.40E-04	1.40E-04				CsNO3	194.91	0.027		
Copper Nitrate	4.74E-04	9.47E-04				Cu(NO3)2.2.5H2O	232.59	0.11	0.00	
EDTA	1.95E-02			3.90E-02	32.3	Na2EDTA	372.24	7.26		2.34
Ferric Nitrate	3.03E-02	9.08E-02				Fe(NO3)3.9H2O	404	12.23	4.90	
HEDTA	7.78E-03			2.33E-02	43.2	HEDTA	278.26	2.16		0.93
Lanthanum Nitrate	3.28E-04	9.83E-04				La(NO3)3.6H2O	433.03	0.14	0.04	

Organic from 96 TOC	40.4									
							Formula Weight	Mass Needed	Mass of H2O	TOC
Compounds	Moles	Nitrate Moles		Moles of Na	Wt % Carbon	Formula	grams	grams	grams	Grams
Lead nitrate	1.87E-03	3.75E-03				Pb(NO3)2	331.2	0.62		
Magnesium Nitrate	1.03E-03	2.06E-03				Mg(NO3)2.6H2O	256.41	0.26	0.11	
Manganous Chloride	1.02E-02					MnCl2.4H2O	197.9	2.03	0.74	
Neodymium Nitrate	6.65E-04	1.99E-03				Nd(NO3)3.6H2O	438.35	0.29	0.07	
Nickel Nitrate	9.03E-03	1.81E-02				Ni(NO3)2.6H2O	290.81	2.63	0.98	
Potassium Nitrate	4.55E-02	4.55E-02				KNO3	101.1	4.60		
Silver Nitrate	1.33E-04	1.33E-04				AgNO3	169.87	0.023		
Strontium Nitrate	7.54E-05	1.51E-04				Sr(NO3)2	211.63	0.016		
Zinc Nitrate	6.93E-04	1.39E-03				Zn(NO3)2.6H2O	297.47	0.21	0.07	
Zirconyl Nitrate	7.67E-04	1.53E-03					249.23	0.19	0.01	
Glycolic Acid	2.48E-01			2.48E-01	31.6	HOCH2COOH, 70 wt%	76.05	26.93		5.95
Sodium Gluconate	1.80E-02			0.00E+00	33.0		218.14	3.93		1.30
Citric Acid	4.49E-02			1.35E-01	34.3		210.14	9.44	0.81	3.24
Nitrilotriacetic Acid	2.98E-03			8.95E-03	37.7		191.14	0.57		0.21
Iminodiacetic Acid	4.54E-02			9.07E-02	36.1		133.1	6.04		2.18

Organic from 96 TOC	40.4									
							Formula Weight	Mass Needed	Mass of H2O	TOC
Compounds	Moles	Nitrate Moles		Moles of Na	Wt % Carbon	Formula	grams	grams	grams	Grams
Total		2.42E-01		6.12E-01						16.16
		Sodium Moles								
Sodium Chloride	3.11E-02	3.11E-02				NaCl	58.44	1.82		
Sodium Fluoride	7.00E-03	7.00E-03				NaF	41.99	0.29		
Sodium Chromate	3.38E-03	6.77E-03				Na2CrO4	161.97	0.55		
Sodium Carbonate	1.40E+00	2.80E+00				Na2CO3	105.99	148.25		
Sodium Hydroxide	2.00E-02	2.00E-02				NaOH	40	0.80		
Sodium Nitrite	1.33E+00	1.33E+00				NaNO2	69	91.49		
Sodium Phosphate	1.17E-02	3.51E-02				Na3PO4.12H2O	380.12	4.44	2.52	
Potassium Molybdate	3.73E-04					K2MoO4	238.14	0.09		
Sodium Sulfate	8.59E-02	1.72E-01				Na2SO4	142.04	12.20		
Sodium formate	2.31E-01	2.31E-01			17.7	NaHCOO	68.01	15.71		2.77
Sodium Acetate	1.74E-02	1.74E-02			17.7	NaCH3COO.3H2O	136.08	2.37	0.94	0.42
Sodium Oxalate	9.38E-03	1.88E-02			17.9	Na2C2O4	134	1.26		0.23

Organic from 96 TOC	40.4									
							Formula Weight	Mass Needed	Mass of H2O	TOC
Compounds	Moles	Nitrate Moles		Moles of Na	Wt % Carbon	Formula	grams	grams	grams	Grams
Total		4.66E+00						Total	13.68	19.58
Sodium Nitrate	3.47E+00	3.47E+00				NaNO3	84.99	294.67		
Sodium Hydroxide	6.12E-01	6.12E-01				NaOH	40	24.46		
Total		8.77E+00								
						Gram of Solids		688.85		
		Grams								
Total Slurry Mass/Liter		1429								
		.								
Mass of Water to add		740.24								
Water		52.76	%							
TOC % 0f Actual		48.46								

Table 49 AN-107 Supernate Simulant Recipe

Final C Simulant Recipe

Volume of Feed	1000	mL

In a tared 1000 mL Volumetric Flask add

	grams	Actual Wt, grams
Water	200	

Transition Metals and Complexing agents

Compounds	Formula	Mass Needed	Actual Wt, grams
Calcium Nitrate	Ca(NO3)2.4H2O	3.48	
Cerium Nitrate	Ce(NO3)3.6H2O	0.16	
Cesium Nitrate	CsNO3	0.027	
Copper Nitrate	Cu(NO3)2.2.5H2O	0.11	
Ferric Nitrate	Fe(NO3)3.9H2O	12.23	
Lanthanum Nitrate	La(NO3)3.6H2O	0.14	
Lead nitrate	Pb(NO3)2	0.62	
Magnesium Nitrate	Mg(NO3)2.6H2O	0.26	

Manganous Chloride	MnCl2.4H2O	2.03	
Neodymium Nitrate	Nd(NO3)3.6H2O	0.29	
Nickel Nitrate	Ni(NO3)2.6H2O	2.63	
Potassium Nitrate	KNO3	4.60	
Strontium Nitrate	Sr(NO3)2	0.016	
Zinc Nitrate	Zn(NO3)2.6H2O	0.21	
Zirconyl Nitrate		0.19	
EDTA	Na2EDTA	7.26	
HEDTA	HEDTA	2.16	
Sodium Gluconate		3.93	
Glycolic Acid		26.93	
Citric Acid		9.44	
Nitrilotriacetic Acid		0.57	
Iminodiacetic Acid		6.04	
Boric acid	H3BO3	0.20	
Sodium Chloride	NaCl	1.82	
Sodium Fluoride	NaF	0.29	
Sodium Chromate	Na2CrO4	0.55	
Sodium Sulfate	Na2SO4	12.20	
Potassium Molybdate	K2MoO4	0.09	

In separate container mix the following

Add	Formula	Mass Needed	Actual Wt, grams
Sodium Hydroxide	NaOH	25.26	
Aluminum Nitrate	Al(NO3)3.9H2O	5.37	
Sodium Phosphate	Na3PO4.12H2O	4.44	
Sodium formate	NaHCOO	15.71	
Sodium Acetate	NaCH3COO.3H2O	2.37	
Sodium Oxalate	Na2C2O4	1.26	

Add	grams	Actual Wt, grams
Water	200	

Mix thoroughly. Then add this solution to the volumetric flask.

Add	Formula	Mass Needed	Actual Wt, grams
Sodium Carbonate	Na2CO3	148.25	

Mix thoroughly.

Mix	Formula	Mass Needed	Actual Wt, grams
Sodium Nitrate	NaNO3	297.29	

Sodium Nitrite	NaNO2	91.49	
Water		100	

Add and Mix thoroughly.

Mix thoroughly and dilute to the mark.

Record Final Weight		grams

The final addition of water would be 240.24 grams based upon a density of 1.429 g/mL.

Appendix D Envelope D Simulant Spreadsheets

Table 50 Solids Composition for Tank AZ-101 Core #1

Sample ID	101-AZ Core #1		Caustic leach assumed to remove 60% of Al
	Before		**After Caustic Leach**
Weight Fraction	0.094		0.086
Density	1.04		1.03
Solids Weight/ Liter	97.76		88.30

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
Ag	107.868	0.0475	0.494	0.005	0.505	AgO	123.868	0.580		0.559	0.642	5594
Al	26.9815	0.8020	8.3408	0.309	8.532	Al2O3	101.961	16.121		3.778	7.139	37782
As	74.9216	0.0380	0.3952	0.005	0.404	As2O3	197.841	0.534	<	0.448	0.591	4475
B	10.81	0.0020	0.0208	0.002	0.021	B2O3	69.6182	0.069		0.024	0.076	236
Ba	137.33	0.0153	0.15912	0.001	0.163	BaO	153.329	0.182		0.180	0.201	1802
Be	9.01218		0	0.000	0.000	BeO	25.0116	0.000	<DL	0.000	0.000	0
Ca	40.08	0.0620	0.6448	0.016	0.660	CaO	56.0794	0.923		0.730	1.022	7302

Sample ID	101-AZ Core #1		Caustic leach assumed to remove 60% of Al
	Before		**After Caustic Leach**
Weight Fraction	0.094		0.086
Density	1.04		1.03
Solids Weight/ Liter	97.76		88.30

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
Cd	112.41	0.1040	1.0816	0.010	1.106	CdO	128.409	1.264		1.225	1.399	12249
Ce	140.12	0.0335	0.3484	0.002	0.356	Ce2O3	328.238	0.417		0.395	0.462	3945
Co	58.9332	0.0205	0.2132	0.004	0.218	Co2O3	165.865	0.307		0.241	0.340	2414
Cr	51.996	0.0465	0.4836	0.009	0.495	Cr2O3	151.99	0.723		0.548	0.800	5477
Cu	63.546	0.0080	0.0832	0.001	0.085	CuO	79.5454	0.107		0.094	0.118	942
Dy	162.5	0.0015	0.0156	0.000	0.016	Dy2O3	372.998	0.018		0.018	0.020	177
Fe	55.847	2.3300	24.232	0.434	24.787	Fe2O3	159.692	35.439		27.441	39.234	274415
K	39.0983	0.0800	0.832	0.021	0.851	K2O	94.196	1.025		0.942	1.135	9422
La	138.906	0.0450	0.468	0.003	0.479	La2O3	325.809	0.561		0.530	0.622	5300
Li	6.941	0.0000	0	0.000	0.000	Li2O	29.8814	0.000	<	0.000	0.000	0

Sample ID	101-AZ Core #1		Caustic leach assumed to remove 60% of Al
	Before		**After Caustic Leach**
Weight Fraction	0.094		0.086
Density	1.04		1.03
Solids Weight/ Liter	97.76		88.30

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
Mg	24.305	0.0130	0.1352	0.006	0.138	MgO	40.3044	0.229		0.153	0.254	1531
Mn	54.938	0.1040	1.0816	0.020	1.106	MnO2	86.9368	1.751		1.225	1.938	12249
Mo	95.94	0.0020	0.0208	0.000	0.021	Mo2O3	239.878	0.027		0.024	0.029	236
Na	22.9898	0.9700	10.088	0.439	10.319	Na2O	61.979	13.910		11.424	15.399	114241
Nd	144.24	0.0440	0.4576	0.003	0.468	Nd2O3	336.478	0.546		0.518	0.604	5182
Ni	58.69	0.0800	0.832	0.014	0.851	NiO	74.6894	1.083		0.942	1.199	9422
P	30.9738	0.1030	1.0712	0.035	1.096	P2O5	141.945	2.511		1.213	2.780	12131
Pb	207.2	0.0725	0.754	0.004	0.771	PbO	223.199	0.831		0.854	0.920	8539
Re	186.207		0	0.000	0.000	?	420.412	0.000	<	0.000	0.000	0
Rh	102.906		0	0.000	0.000	Rh2O3	253.809	0.000	<	0.000	0.000	0

Sample ID	101-AZ Core #1		Caustic leach assumed to remove 60% of Al
	Before		**After Caustic Leach**
Weight Fraction	0.094		0.086
Density	1.04		1.03
Solids Weight/ Liter	97.76		88.30

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
Ru	101.07		0	0.000	0.000	Ru2O3	250.138	0.000	<	0.000	0.000	0
Sb	121.75		0	0.000	0.000	Sb2O5	323.497	0.000	<	0.000	0.000	0
Se	78.96		0	0.000	0.000	SeO2	110.959	0.000	<	0.000	0.000	0
Si	28.0855	0.1740	1.8096	0.064	1.851	SiO2	60.0843	3.960		2.049	4.384	20493
Sr	87.62	0.0105	0.1092	0.001	0.112	SrO	103.619	0.132		0.124	0.146	1237
Te	127.6		0	0.000	0.000	TeO2	159.599	0.000	<	0.000	0.000	0
Th	232.038	0.0185	0.1924	0.001	0.197	ThO2	264.037	0.224		0.218	0.248	2179
Ti	47.88	0.0040	0.0416	0.001	0.043	TiO2	79.8788	0.071		0.047	0.079	471
Tl	204.383		0	0.000	0.000	Tl2O3	456.764	0.000	<	0.000	0.000	0
U	238.029	0.2950	3.068	0.013	3.138	UO3	286.027	3.771		3.474	4.175	34744

Sample ID	101-AZ Core #1	Caustic leach assumed to remove 60% of Al	
	Before		**After Caustic Leach**
Weight Fraction	0.094		0.086
Density	1.04		1.03
Solids Weight/ Liter	97.76		88.30

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
V	50.9415		0	0.000	0.000	V2O3	149.881	0.000	<	0.000	0.000	0
Zn	65.38	0.0135	0.1404	0.002	0.144	ZnO	81.3794	0.179		0.159	0.198	1590
Zr	91.22	0.5060	5.2624	0.058	5.383	ZrO2	123.219	7.271		5.959	8.050	59594
NO2-	46.0055	0.4020	4.1808	0.091	4.277	NO2-	46.0055	4.277		4.735	4.735	47345
NO3-	62.0049	0.4120	4.2848	0.069	4.383	NO3-	62.0049	4.383		4.852	4.852	48523
F-	18.9984	0.0129	0.13416	0.007	0.137	F-	18.9984	0.137		0.152	0.152	1519
Cl-	35.453	0.0032	0.03328	0.001	0.034	Cl-	35.453	0.034		0.038	0.038	377
SO4-2	96.0576	0.1060	1.1024	0.011	1.128	SO4-2	96.0576	1.128		1.248	1.248	12484
PO4-3	78.972	0.0160	0.1664	0.002	0.170	PO4-3	78.972	0.170		0.188	0.188	1884
TIC	12.011	0.1300	1.352	0.113	1.383	TIC	12.011	1.383		1.531	1.531	15311

Sample ID	101-AZ Core #1		Caustic leach assumed to remove 60% of Al
	Before		**After Caustic Leach**
Weight Fraction	0.094		0.086
Density	1.04		1.03
Solids Weight/ Liter	97.76		88.30

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
CO3-2	60.0092	0.6495	6.755	0.113	6.910	CO3-2	60.0092	6.910		7.650	7.650	76495
Totals			79.53		81.36			94.76		65.54	94.2	

Table 51 Solids Composition for Tank AZ-101 Core #2

Sample ID	101-AZ Core #2		Caustic leach assumed to remove 60% of Al
			After Caustic Leach
Weight Fraction	0.186		0.178
Density	1.14		1.13
Solids Weight/ Liter	212.04		201.16

Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**After Caustic Leach Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
Ag	107.8682	0.0174	0.1984	0.002	0.094	AgO	123.8676	0.107		0.099	0.113	986
Al	26.98154	0.8420	9.5988	0.356	4.527	Al2O3	101.96128	8.553		1.909	3.606	19087
As	74.9216	0.0240	0.2736	0.004	0.129	As2O3	197.8414	0.170	<	0.136	0.180	1360
B	10.81	0.0200	0.2280	0.021	0.108	B2O3	69.6182	0.346	<	0.113	0.365	1133
Ba	137.33	0.0435	0.4959	0.004	0.234	BaO	153.3294	0.261		0.247	0.275	2465
Be	9.01218	0.0041	0.0467	0.005	0.022	BeO	25.01158	0.031		0.023	0.064	232

Sample ID	101-AZ Core #2		Caustic leach assumed to remove 60% of Al
			After Caustic Leach
Weight Fraction	0.186		0.178
Density	1.14		1.13
Solids Weight/ Liter	212.04		201.16

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
Ca	40.08	0.1890	2.1546	0.054	1.016	CaO	56.0794	1.422		1.071	1.499	10711
Cd	112.41	0.5110	5.8254	0.052	2.747	CdO	128.4094	3.138		2.896	3.308	28959
Ce	140.12	0.0460	0.5244	0.004	0.247	Ce2O3	328.2382	0.290	<	0.261	0.305	2607
Co	58.9332	0.0590	0.6726	0.011	0.317	Co2O3	165.8646	0.446	<	0.334	0.471	3344
Cr	51.996	0.0184	0.2098	0.004	0.099	Cr2O3	151.9902	0.145		0.104	0.152	1043
Cu	63.546	0.0193	0.2200	0.003	0.104	CuO	79.5454	0.130		0.109	0.137	1094
Dy	162.5	0.0028	0.0319	0.000	0.015	Dy2O3	372.9982	0.017	<	0.016	0.018	159
Fe	55.847	5.6200	64.0680	1.147	30.215	Fe2O3	159.6922	43.199		31.850	45.536	318496
K	39.0983	0.1000	1.1400	0.029	0.538	K2O	94.196	0.648	<	0.567	0.683	5667

Sample ID	101-AZ Core #2		Caustic leach assumed to remove 60% of Al
			After Caustic Leach
Weight Fraction	0.186		0.178
Density	1.14		1.13
Solids Weight/ Liter	212.04		201.16

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
La	138.9055	0.2720	3.1008	0.022	1.462	La2O3	325.8092	1.715		1.541	1.808	15415
Li	6.941	0.0031	0.0353	0.005	0.017	Li2O	29.8814	0.036	<	0.018	0.038	176
Mg	24.305	0.0319	0.3637	0.015	0.172	MgO	40.3044	0.284		0.181	0.300	1808
Mn	54.938	0.0853	0.9724	0.018	0.459	MnO2	86.9368	0.726		0.483	0.765	4834
Mo	95.94	0.0021	0.0239	0.000	0.011	Mo2O3	239.8782	0.014	<	0.012	0.015	119
Na	22.9898	1.3700	15.6180	0.679	7.366	Na2O	61.979	9.929		7.764	10.466	77640
Nd	144.24	0.1690	1.9266	0.013	0.909	Nd2O3	336.4782	1.060		0.958	1.117	9578
Ni	58.69	0.4040	4.6056	0.078	2.172	NiO	74.6894	2.764		2.290	2.914	22895
P	30.9738	0.1900	2.1660	0.070	1.022	P2O5	141.9446	2.341	<	1.077	2.467	10768

Sample ID	101-AZ Core #2		Caustic leach assumed to remove 60% of Al
			After Caustic Leach
Weight Fraction	0.186		0.178
Density	1.14		1.13
Solids Weight/ Liter	212.04		201.16

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
Pb	207.2	0.0224	0.2554	0.001	0.120	PbO	223.1994	0.130		0.127	0.137	1269
Re	186.207	0.0043	0.0490	0.000	0.023	Re2O3?	420.4122	0.026	<	0.024	0.055	244
Rh	102.9055	0.0270	0.3078	0.003	0.145	Rh2O3	253.8092	0.179	<	0.153	0.189	1530
Ru	101.07	0.0451	0.5141	0.005	0.242	Ru2O3	250.1382	0.300		0.256	0.316	2556
Sb	121.75	0.0790	0.9006	0.007	0.425	Sb2O5	323.497	0.564	<	0.448	0.595	4477
Se	78.96	0.0260	0.2964	0.004	0.140	SeO2	110.9588	0.196	<	0.147	0.207	1473
Si	28.0855	0.2240	2.5536	0.091	1.204	SiO2	60.0843	2.576		1.269	2.716	12694
Sr	87.62	0.0314	0.3580	0.004	0.169	SrO	103.6194	0.200		0.178	0.210	1779
Te	127.6	0.0170	0.1938	0.002	0.091	TeO2	159.5988	0.114	<	0.096	0.121	963

Sample ID	101-AZ Core #2		Caustic leach assumed to remove 60% of Al
			After Caustic Leach
Weight Fraction	0.186		0.178
Density	1.14		1.13
Solids Weight/ Liter	212.04		201.16

Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**After Caustic Leach Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
Th	232.0381	0.0330	0.3762	0.002	0.177	ThO2	264.0369	0.202	<	0.187	0.213	1870
Ti	47.88	0.0038	0.0433	0.001	0.020	TiO2	79.8788	0.034		0.022	0.036	215
Tl	204.383	0.4200	4.7880	0.023	2.258	Tl2O3	456.7642	2.523	<	2.380	2.660	23802
U	238.0289	0.4050	4.6170	0.019	2.177	UO3	286.0271	2.616		2.295	2.758	22952
V	50.9415	0.0024	0.0274	0.001	0.013	V2O3	149.8812	0.019	<	0.014	0.020	136
Zn	65.38	0.0112	0.1277	0.002	0.060	ZnO	81.3794	0.075		0.063	0.079	635
Zr	91.22	2.1300	24.2820	0.266	11.452	ZrO2	123.2188	15.469		12.071	16.305	120711
NO2-	46.0055	0.6100	6.9540	0.151	3.280	NO2-	46.0055	3.280		3.457	3.457	34570
NO3-	62.0049	0.3100	3.5340	0.057	1.667	NO3-	62.0049	1.667		1.757	1.757	17568

Sample ID	101-AZ Core #2		Caustic leach assumed to remove 60% of Al
			After Caustic Leach
Weight Fraction	0.186		0.178
Density	1.14		1.13
Solids Weight/ Liter	212.04		201.16

										After Caustic Leach		
Element or Anion	**Mole Wt**	**wt %**	**g/L**	**Moles/L**	**Wt % of Solids**	**Oxide**	**Mole Wt**	**Oxide wt %of Solids**	**<?**	**Wt % of Solids**	**Oxide wt %of Solids**	**microg/g solids**
F-	18.9984	0.0260	0.2964	0.016	0.140	F-	18.9984	0.140		0.147	0.147	1473
Cl-	35.453	0.0040	0.0456	0.001	0.022	Cl-	35.453	0.022		0.023	0.023	227
SO4-2	96.0576	0.1500	1.7100	0.018	0.806	SO4-2	96.0576	0.806		0.850	0.850	8501
PO4-3	78.972	0.0310	0.3534	0.004	0.167	PO4-3	78.972	0.167		0.176	0.176	1757
TIC	12.011	0.0760	0.8664	0.072	0.409	TIC	12.011	0.409		0.431	0.431	4307
CO3-2	60.0092	0.3797	4.3287	0.072	2.041	CO3-2	60.0092	2.041		2.152	2.152	21519
Totals			171.41		80.84			103.00		73.79	103.22	

Table 52 Tank AZ-101 Blend Solids Composition

Tank	AZ-101	AZ-101	Blend	Blend	Blend	
Volume, Gallons	35000	35000	35000			
Volume, Liters	132489	132489	132489			
Weight Fraction	0.094	0.186	0.142			
Density	1.040	1.140	1.090			
Solids Weight/ Liter	97.760	212.040	154.900			
Element or Anion	**grams/Liter**	**grams/Liter**	**grams/Liter**	**grams/gram solids**	**microgram/gram**	**<?**
Ag	0.494	0.198	0.346	2.23E-03	2235	
Al	8.341	9.599	8.970	5.79E-02	57907	
As	0.395	0.274	0.334	2.16E-03	2159	<
B	0.021	0.228	0.124	8.03E-04	803	
Ba	0.159	0.496	0.328	2.11E-03	2114	
Be	0.000	0.047	0.023	1.51E-04	151	<

Tank	AZ-101	AZ-101	Blend	Blend	Blend	
Volume, Gallons	35000	35000	35000			
Volume, Liters	132489	132489	132489			
Weight Fraction	0.094	0.186	0.142			
Density	1.040	1.140	1.090			
Solids Weight/ Liter	97.760	212.040	154.900			
Element or Anion	**grams/Liter**	**grams/Liter**	**grams/Liter**	**grams/gram solids**	**microgram/gram**	**<?**
Ca	0.645	2.155	1.400	9.04E-03	9036	
Cd	1.082	5.825	3.454	2.23E-02	22295	
Ce	0.348	0.524	0.436	2.82E-03	2817	
Co	0.213	0.673	0.443	2.86E-03	2859	<
Cr	0.484	0.210	0.347	2.24E-03	2238	
Cu	0.083	0.220	0.152	9.79E-04	979	
Dy	0.016	0.032	0.024	1.53E-04	153	<
Fe	24.232	64.068	44.150	2.85E-01	285023	

Tank	AZ-101	AZ-101	Blend	Blend	Blend	
Volume, Gallons	35000	35000	35000			
Volume, Liters	132489	132489	132489			
Weight Fraction	0.094	0.186	0.142			
Density	1.040	1.140	1.090			
Solids Weight/ Liter	97.760	212.040	154.900			
Element or Anion	**grams/Liter**	**grams/Liter**	**grams/Liter**	**grams/gram solids**	**microgram/gram**	**<?**
K	0.832	1.140	0.986	6.37E-03	6365	<
La	0.468	3.101	1.784	1.15E-02	11520	
Li	0.000	0.035	0.018	1.14E-04	114	
Mg	0.135	0.364	0.249	1.61E-03	1610	
Mn	1.082	0.972	1.027	6.63E-03	6630	
Mo	0.021	0.024	0.022	1.44E-04	144	
Na	10.088	15.618	12.853	8.30E-02	82976	
Nd	0.458	1.927	1.192	7.70E-03	7696	

Tank	AZ-101	AZ-101	Blend	Blend	Blend	
Volume, Gallons	35000	35000	35000			
Volume, Liters	132489	132489	132489			
Weight Fraction	0.094	0.186	0.142			
Density	1.040	1.140	1.090			
Solids Weight/ Liter	97.760	212.040	154.900			
Element or Anion	**grams/Liter**	**grams/Liter**	**grams/Liter**	**grams/gram solids**	**microgram/gram**	**<?**
Ni	0.832	4.606	2.719	1.76E-02	17552	
P	1.071	2.166	1.619	1.04E-02	10449	<
Pb	0.754	0.255	0.505	3.26E-03	3258	<
Re	0.000	0.049	0.025	1.58E-04	158	<
Rh	0.000	0.308	0.154	9.94E-04	994	<
Ru	0.000	0.514	0.257	1.66E-03	1660	
Sb	0.000	0.901	0.450	2.91E-03	2907	<
Se	0.000	0.296	0.148	9.57E-04	957	<

Tank	AZ-101	AZ-101	Blend	Blend	Blend	
Volume, Gallons	35000	35000	35000			
Volume, Liters	132489	132489	132489			
Weight Fraction	0.094	0.186	0.142			
Density	1.040	1.140	1.090			
Solids Weight/ Liter	97.760	212.040	154.900			
Element or Anion	**grams/Liter**	**grams/Liter**	**grams/Liter**	**grams/gram solids**	**microgram/gram**	**<?**
Si	1.810	2.554	2.182	1.41E-02	14084	
Sr	0.109	0.358	0.234	1.51E-03	1508	
Te	0.000	0.194	0.097	6.26E-04	626	<
Th	0.192	0.376	0.284	1.84E-03	1835	<
Ti	0.042	0.043	0.042	2.74E-04	274	
Tl	0.000	4.788	2.394	1.55E-02	15455	<
U	3.068	4.617	3.843	2.48E-02	24806	<
V	0.000	0.027	0.014	8.83E-05	88	<

Tank	AZ-101	AZ-101	Blend	Blend	Blend	
Volume, Gallons	35000	35000	35000			
Volume, Liters	132489	132489	132489			
Weight Fraction	0.094	0.186	0.142			
Density	1.040	1.140	1.090			
Solids Weight/ Liter	97.760	212.040	154.900			
Element or Anion	**grams/Liter**	**grams/Liter**	**grams/Liter**	**grams/gram solids**	**microgram/gram**	**<?**
Zn	0.140	0.128	0.134	8.65E-04	865	
Zr	5.262	24.282	14.772	9.54E-02	95366	
NO2-	4.181	6.954	5.567	3.59E-02	35942	
NO3-	4.285	3.534	3.909	2.52E-02	25238	
F-	0.134	0.296	0.215	1.39E-03	1390	
Cl-	0.033	0.046	0.039	2.55E-04	255	<
SO4-2	1.102	1.710	1.406	9.08E-03	9078	<
PO4-3	0.166	0.353	0.260	1.68E-03	1678	<

Tank	AZ-101	AZ-101	Blend	Blend	Blend	
Volume, Gallons	35000	35000	35000			
Volume, Liters	132489	132489	132489			
Weight Fraction	0.094	0.186	0.142			
Density	1.040	1.140	1.090			
Solids Weight/ Liter	97.760	212.040	154.900			
Element or Anion	**grams/Liter**	**grams/Liter**	**grams/Liter**	**grams/gram solids**	**microgram/gram**	**<?**
TIC	1.352	0.866	1.109	7.16E-03	7161	
CO3-2	6.755	4.329	5.542	3.58E-02	35776	

Table 53 Compound Calculations for AZ-101 Simulated Sludge

									OH- required	Na	
Element or Anion	**Mole Wt**	**grams/Liter**	**moles/Liter**	**Source**	**Formula**	**Mole Wt**	**moles/Liter**	**grams/Liter**	**moles/Liter**	**Moles/Liter**	
Ag	107.8682	0.346	3.21E-03	Silver Nitrate	AgNO3	169.88	3.21E-03	0.545	3.21E-03		
Al	26.98154	8.970	3.32E-01	Aluminum Oxide	Al2O3	101.96	1.66E-01	16.948			
As	74.9216	0.334	4.46E-03								<
B	10.81	0.124	1.15E-02	Boric Acid	H3BO3	61.83	1.15E-02	0.712	3.45E-02		<
Ba	137.33	0.328	2.38E-03	Barium Nitrate	Ba(NO3)2	261.35	2.38E-03	0.623	4.77E-03		
Be	9.01218	0.023	2.59E-03								
Ca	40.08	1.400	3.49E-02	Calcium Nitrate	Ca(NO3)2.4H2O	236.15	3.49E-02	8.247	6.98E-02		
Cd	112.41	3.454	3.07E-02	Cadmium Nitrate	Cd(NO3)2.4H2O	308.47	3.07E-02	9.477	6.14E-02		
Ce	140.12	0.436	3.11E-03	Cerium Nitrate	Ce(NO3)3.6H2O	434.23	3.11E-03	1.352	9.34E-03		
Co	58.9332	0.443	7.52E-03	Cobalt nitrate	Co(NO3)2.6H2O	291.03	7.52E-03	2.187	1.50E-02		
Cr	51.996	0.347	6.67E-03	Chromium Nitrate	Cr(NO3)3.9H2O	400.14	6.67E-03	2.668			
Cu	63.546	0.152	2.39E-03	Copper Nitrate	Cu(NO3)2.3H2O	241.6	2.39E-03	0.576	4.77E-03		
Dy	162.5	0.024	1.46E-04	Dysprosium Nitrate	Dy(NO3)3.5H2O	438.59	1.46E-04	0.064	4.39E-04		

									OH- required	Na	
Element or Anion	**Mole Wt**	**grams/Liter**	**moles/Liter**	**Source**	**Formula**	**Mole Wt**	**moles/Liter**	**grams/Liter**	**moles/Liter**	**Moles/Liter**	
Fe	55.847	44.150	7.91E-01	Ferric Nitrate	Fe(NO3)3.9H2O	404	7.91E-01	319.383	2.37E+00		
K	39.0983	0.986	2.48E-02	Potassium Nitrate	KNO3	101.11	2.48E-02	2.503			
La	138.9055	1.784	1.28E-02	Lanthanum Nitrate	La(NO3)3.6H2O	433.01	1.28E-02	5.563	3.85E-02		
Li	6.941	0.018	2.55E-03								<
Mg	24.305	0.249	1.03E-02	Magnesium Nitrate	Mg(NO3)2.6H2O	256.41	1.03E-02	2.631	2.05E-02		
Mn	54.938	1.027	1.87E-02	Manganese dioxide							
Mo	95.94	0.022	2.33E-04	Potassium Molybdate	K2MoO4	238.14	2.33E-04	0.056			
Na	22.9898	12.853	5.59E-01	Sodium hydroxide	NaOH	40	5.59E-01	22.363			
Nd	144.24	1.192	8.26E-03	Neodymium nitrate	Nd(NO3)3.6H2O	438.34	8.26E-03	3.623	2.48E-02		
Ni	58.69	2.719	4.63E-02	Nickel Nitrate	Ni(NO3)2.6H2O	290.81	4.63E-02	13.472	9.26E-02		
P	30.9738	1.619	5.23E-02								
Pb	207.2	0.505	2.44E-03	Lead Nitrate	Pb(NO3)2	331.2	2.44E-03	0.807	4.87E-03		
Re	186.207	0.025	1.32E-04	Sodium perrhenate	NaReO4	273.19	1.32E-04	0.036		1.32E-04	<
Rh	102.9055	0.154	1.50E-03	Rhodium Nitrate	Rh(NO3)3 Soln, 4.933wt% Rh			3.120	4.49E-03		<
Ru	101.07	0.257	2.54E-03	Ruthenium Trichloride	RuCl3 41.74wt% Ru			0.616	7.63E-03		<

									OH- required	Na	
Element or Anion	**Mole Wt**	**grams/Liter**	**moles/Liter**	**Source**	**Formula**	**Mole Wt**	**moles/Liter**	**grams/Liter**	**moles/Liter**	**Moles/Liter**	
Sb	121.75	0.450	3.70E-03								<
Se	78.96	0.148	1.88E-03	Selenium dioxide	SeO2	110.96	1.88E-03	0.208			<
Si	28.0855	2.182	7.77E-02	Silica	SiO2	60.0843	7.77E-02	4.667			
Sr	87.62	0.234	2.67E-03	Strontium nitrate	Sr(NO3)2	211.63	2.67E-03	0.564	5.33E-03		
Te	127.6	0.097	7.59E-04								<
Th	232.0381	0.284	1.23E-03								<
Ti	47.88	0.042	8.87E-04	Titanium dioxide	TiO2	79.9	8.87E-04	0.071			
Tl	204.383	2.394	1.17E-02								<
U	238.0289	3.843	1.61E-02								
V	50.9415	0.014	2.69E-04								<
Zn	65.38	0.134	2.05E-03	Zinc Nitrate	Zn(NO3)2.6H2O	297.47	2.05E-03	0.610	4.10E-03		
Zr	91.22	14.772	1.62E-01	Zirconyl Nitrate	ZrO(NO3)2.xH2O x~6	339.322	1.62E-01	54.950	6.48E-01		
NO2-	46.0055	5.567	1.21E-01		NaNO2	69	1.21E-01	8.350		1.21E-01	
NO3-	62.0049	2.909	4.69E-02		NaNO3	84.99	4.69E-02	3.988		4.69E-02	
F-	18.9984	0.215	1.13E-02		NaF	41.99	1.13E-02	0.476		1.13E-02	

Element or Anion	Mole Wt	grams/Liter	moles/Liter	Source	Formula	Mole Wt	moles/Liter	grams/Liter	OH- required moles/Liter	Na Moles/Liter	
Cl-	35.453	0.039	1.11E-03		NaCl	58.44	1.11E-03	0.065		1.11E-03	
SO4-2	96.0576	1.406	1.46E-02		Na2SO4	142.04	1.46E-02	2.079		2.93E-02	
PO4-3	78.972	4.127	5.23E-02		Na3PO4.12H2O	380.12	5.23E-02	19.864		1.57E-01	
TIC	12.011	1.109	9.23E-02								
CO3-2	60.0092	5.542	9.23E-02		Na2CO3	105.99	9.23E-02	9.788		1.85E-01	
								Totals	3.43E+00	5.51E-01	
								Total-CO3		3.67E-01	

Manganese Dioxide Calculations

	Moles/Liter
Mn needed	1.87E-02

Stoichiometry 3Mn(NO3)2 + 2KMnO4 + 2H2O = 2KNO3 + 5MnO2 + 4HNO3

Mole Wt	grams/Liter

									OH- required	Na	
Element or Anion	**Mole Wt**	**grams/Liter**	**moles/Liter**	**Source**	**Formula**	**Mole Wt**	**moles/Liter**	**grams/Liter**	**moles/Liter**	**Moles/Liter**	
Mn(NO3)2	1.12E-02	178.95	2.01	50 wt% Mn(NO3)2	50 wt% Mn(NO3)2	178.95	1.12E-02	4.014			
KMnO4	7.48E-03	158.03	1.18	Potassium Permanganate	KMnO4	158.03	7.48E-03	1.182			

Table 54 Final Simulated Sludge Recipe for Envelope D Waste

Simulated Sludge Recipe AZ-101

Volume of Feed 1000 mL

	grams	Actual Wt, grams
Water	500	

Manganese Dioxide Production

Add to the kettle:

Compounds	Formula	Mass Needed	Actual Wt, grams
Potassium Permanganate	KMnO4	1.18	

Compound should completely dissolve.

Add to the kettle:

Compounds	Formula	Mass Needed	Actual Wt, grams
Manganous Nitrate Solution	50 Wt % solution	4.01	

Mix thoroughly. Will produce fine black solids, which will remain suspended while being agitated.

Add to the kettle the following compounds with mixing to insure complete solution:

Transition Metals and Complexing agents

Compounds	Formula	Mass Needed	Actual Wt, grams
Ferric Nitrate	Fe(NO3)3.9H2O	319.383	
Nickel Nitrate	Ni(NO3)2.6H2O	13.472	
Zirconyl nitrate	ZrO(NO3)2.xH2O x~6	54.950	
Cerium nitrate	Ce(NO3)3.6H2O	1.352	
Lanthanum nitrate	La(NO3)3.6H2O	5.563	
Neodymium Nitrate	Nd(NO3)3.6H2O	3.623	
Barium Nitrate	Ba(NO3)2	0.623	
Calcium Nitrate	Ca(NO3)2.4H2O	8.247	
Cadmium Nitrate	Cd(NO3)2.4H2O	9.477	
Chromium Nitrate	Cr(NO3)3.9H2O	2.668	
Cobalt Nitrate	Co(NO3)2.6H2O	2.187	
Copper Nitrate	Cu(NO3)2.3H2O	0.576	
Dysprosium Nitrate	Dy(NO3)3.5H2O	0.064	
Magnesium Nitrate	Mg(NO3)2.6H2O	2.631	
Lead Nitrate	Pb(NO3)2	0.807	
Rhodium Nitrate	Rh(NO3)3 Soln, 4.933wt% Rh	3.120	

Ruthenium Trichloride	RuCl3 41.74wt% Ru	0.616	
Strontium Nitrate	Sr(NO3)2	0.564	
Zinc Nitrate	Zn(NO3)2.6H2O	0.610	
Silver Nitrate	AgNO3	0.545	

Mix thoroughly to completely dissolve everything except the fine black solids of MnO2.

Standardize a pH electrode with pH 4, 7 and 10 buffers.

Place the pH electrode in the precipitation vessel with the metal nitrates and measure the pH.

pH	

With the nitrate solution agitating, slowly add 8 molar NaOH,

200	grams of NaOH plus	600	grams of Water	(Info only)

, until the pH reaches 10.

pH	

Continue mixing for 1 Hour and then recheck pH.

pH	

Next add 400 milliliters of a 0.6 molar sodium carbonate solution

Thoroughly mix the slurry to insure good mixing.

pH	

Allow the slurry to settle overnight or over a weekend.

Decant the supernate .

Wash the settled solids with a 0.01 M NaOH and 0.01 M $NaNO_2$ Solution

until the supernate is l**ess than 1000 mg/L Nitrate.**

Washing can be accomplished by multiple dilutions with gravity settling or by continuous crossflow filtration.

Concentrate the washed solids until the final volume desired is obtained.

	Goal, mL	Actual, mL
Final Volume	1000	

Final Insoluble Compounds Addition

Compounds	Formula	Mass Needed	Actual Wt, grams	Required Particle Size
Titanium dioxide	TiO2	0.071		< 5 microns
Silica	SiO2	4.67		< 5 microns
Aluminum Oxide	Al2O3	16.95		< 5 microns

Mix thoroughly for 30 minutes.

Final Soluble Compound Addition

Salts

Compounds	Formula	Mass Needed	Actual Wt, grams
Sodium Perrhenate	NaReO4	0.036	
Potassium Nitrate	KNO3	2.503	
Potassium Molybdate	K2MoO4	0.056	
Boric Acid	H3BO3	0.712	
Sodium Chloride	NaCl	0.065	
Sodium Fluoride	NaF	0.476	
Sodium Sulfate	Na2SO4	2.079	
Sodium Phosphate	Na3PO4.12H2O	19.864	
Sodium Nitrate	NaNO3	3.988	
Sodium Nitrite	NaNO2	8.350	

Mix the slurry for an hour to completely dissolve the added salts.

Appendix E Envelope A Entrained Solids Simulant Spreadsheet

Table 55 AN-105 Entrained Solids

Component	grams/100 grams Sample	Mole Wt	Moles	Compound	Moles	Mole Wt	Wt	Wt % of sample	Wt % simulant
TOC	0.065	12.011	5.41E-03	Oxalate	2.71E-03	88.024	0.238	41.79	
Al	0.025	26.98	9.27E-04	Al2O3	4.63E-04	101.96	0.047	8.29	9.2
Ca	0.008	40.08	2.00E-04	CaOxalate	2.00E-04	128.1	0.026	4.49	5.0
Cr	0.103	58.93	1.75E-03	Cr2O3	8.74E-04	152.02	0.133	23.31	26.0
Fe	0.004	55.85	7.16E-05	Fe2O3	3.58E-05	159.7	0.006	1.00	1.1
Mn	0.001	54.94	1.82E-05	MnO2	1.82E-05	86.94	0.002	0.28	0.3
Na	0.092	22.99	4.00E-03	NaOxalate	2.00E-03	134	0.268	47.04	52.4
Ni	0.002	58.69	3.41E-05	NiO	3.41E-05	74.71	0.003	0.45	0.5
Si	0.013	28.09	4.63E-04	SiO2	4.63E-04	60.09	0.028	4.88	5.4
Solids	0.57					Total	0.511	89.7	100.0
						% of Solids	89.7		
				%Oxalate used					
				81.32					

Recipe	grams/100 grams of
Al2O3	9.2
CaOxalate	5.0
Cr2O3	26.0
Fe2O3	1.1
MnO2	0.3
NaOxalate	52.4
NiO	0.5
SiO2	5.4

Appendix F Envelope C Entrained Solids Simulant Spreadsheet

Table 56 First Wash of AN-107 Solids

								Assume Dilution Factor is 8.8		
First Wash				Initial AN-107	Initial AN-107	Dilution Factor	Status	Diluted Conc.		Due to Dissolution
Component	mg/Liter	MW	Molar	mg/Liter	Molar			Molar	mg/Liter	mg/Liter
Aluminum	1140	26.98154	4.23E-02	386	1.43E-02	0.3	Dissolving	1.63E-03	43.9	**1096.1**
Calcium	70	40.08	1.75E-03	591	1.47E-02	8.4	dilution	1.68E-03	67.2	XXXXX
Cadmium	7.3	112.41	6.49E-05	64	5.69E-04	8.8	dilution	6.47E-05	7.3	XXXXX
Chromium	59.8	51.996	1.15E-03	176	3.38E-03	2.9	Dissolving	3.85E-04	20.0	**39.8**
Copper	3.8	58.9332	6.45E-05	30	5.09E-04	7.9	dilution	5.78E-05	3.4	XXXXX
Iron	3.1	55.847	5.55E-05	1690	3.03E-02	545.2	Sol. Limited	3.44E-03	192.0	XXXXX
Potassium	183	39.0983	4.68E-03	1810	4.63E-02	9.9	Dilution	5.26E-03	205.7	XXXXX
Manganese	1	54.938	1.82E-05	563	1.02E-02	563.0	Sol. Limited	1.16E-03	64.0	XXXXX
Sodium	32900	22.98977	1.43E+00	195000	8.48E+00	5.9	Dissolving	9.64E-01	22159.1	**10740.9**

								Assume Dilution Factor is 8.8		
First Wash				Initial AN-107	Initial AN-107	Dilution Factor	Status	Diluted Conc.		Due to Dissolution
Nickel	58.6	58.69	9.98E-04	530	9.03E-03	9.0	Dilution	1.03E-03	60.2	XXXXX
Phosphorus	73.9	30.97376	2.39E-03							XXXXX
Lead	46	207.2	2.22E-04	388	1.87E-03	8.4	Dilution	2.13E-04	44.1	XXXXX
Silicon	17.3	28.0855	6.16E-04							**17.3**
Zinc	2.4	65.38	3.67E-05	45	6.88E-04	18.8	SolLimited	7.82E-05	5.1	XXXXX
TOC	7550	12.011	6.29E-01	40400	3.36E+00	5.4	Dissolving	3.82E-01	4590.9	**2959.1**
TIC	3070	12.011	2.56E-01	16800	1.40E+00	5.5	Dissolving	1.59E-01	1909.1	**1160.9**
Chloride	230	35.453	6.49E-03	1830	5.16E-02	8.0	Dilution	5.87E-03	208.0	XXXXX
Fluoride	1050	18.998	5.53E-02	133	7.00E-03	0.1	Dissolving	7.96E-04	15.1	**1034.9**
Nitrate	26150	62.0049	4.22E-01	230000	3.71E+00	8.8	Dilution	4.22E-01	26136.4	XXXXX
Sulfate	1530	96.0576	1.59E-02	8250	8.59E-02	5.4	Dissolving	9.76E-03	937.5	**592.5**
Phosphate	1240	94.97136	1.31E-02	1110	1.17E-02	0.9	Dissolving	1.33E-03	126.1	**1113.9**

Table 57 Second Wash of Solids from Tank AN-107

								Assume Dilution Factor is		25
Second Wash				First Wash	First Wash	Dilution Factor	Status	Diluted Conc.		Due to Dissolution
Component	mg/Liter	MW	Molar	mg/Liter	Molar			Molar	mg/Liter	mg/Liter
Aluminum	83.4	26.98154	3.09E-03	1140	4.23E-02	13.7	Dissolving	1.69E-03	45.6	**37.8**
Calcium	1.3	40.08	3.24E-05	70	1.75E-03	53.8	Sol. Limited	6.99E-05	2.8	XXXXX
Cadmium	0.3	112.41	2.67E-06	7.3	6.49E-05	24.3	Dilution	2.60E-06	0.3	XXXXX
Chromium	17.1	51.996	3.29E-04	59.8	1.15E-03	3.5	Dissolving	4.60E-05	2.4	**14.7**
Copper	0.3	58.9332	5.09E-06	3.8	6.45E-05	12.7	Dissolving	2.58E-06	0.2	0.1
Iron	0.6	55.847	1.07E-05	3.1	5.55E-05	5.2	Dissolving	2.22E-06	0.1	0.5
Potassium		39.0983	0.00E+00	183	4.68E-03	XXXXXX		XXXXXX	XXXXXX	XXXXX
Manganese	0.15	54.938	2.73E-06	1	1.82E-05	6.7	Dissolving	7.28E-07	0.0	XXXXX
Sodium	1500	22.98977	6.52E-02	32900	1.43E+00	21.9	Dilution	5.72E-02	1316.0	XXXXX
Nickel	2.1	58.69	3.58E-05	58.6	9.98E-04	27.9	Dilution	3.99E-05	2.3	XXXXX

								Assume Dilution Factor is		25
Second Wash				First Wash	First Wash	Dilution Factor	Status	Diluted Conc.		Due to Dissolution
Phosphorus	3	30.97376	9.69E-05	73.9	2.39E-03	24.6	Dilution	9.54E-05	3.0	XXXXX
Lead	1.9	207.2	9.17E-06	46	2.22E-04	24.2	Dilution	8.88E-06	1.8	XXXXX
Silicon	24.9	28.0855	8.87E-04	17.3	6.16E-04	0.7	Dissolving	2.46E-05	0.7	**24.2**
Zinc	0.3	65.38	4.59E-06	2.4	3.67E-05	8.0	Dissolving	1.47E-06	0.1	0.2
TOC	244	12.011	2.03E-02	7550	6.29E-01	30.9	Dilution	2.51E-02	302.0	XXXXX
TIC	286	12.011	2.38E-02	3070	2.56E-01	10.7	Dissolving	1.02E-02	122.8	**163.2**
Chloride	12	35.453	3.38E-04	230	6.49E-03	19.2	Dissolving	2.59E-04	9.2	2.8
Fluoride	75	18.998	3.95E-03	1050	5.53E-02	14.0	Dissolving	2.21E-03	42.0	**33.0**
Nitrate	960	62.0049	1.55E-02	26150	4.22E-01	27.2	Dilution	1.69E-02	1046.0	XXXXX
Sulfate	65	96.0576	6.77E-04	1530	1.59E-02	23.5	Dilution	6.37E-04	61.2	XXXXX
Phosphate	55	94.97136	5.79E-04	1240	1.31E-02	22.5	Dilution	5.22E-04	49.6	XXXXX

Table 58 Third Wash of Solids From tank AN-107

								Assume Dilution Factor is	16	
Third Wash				Second Wash	First Wash	Dilution Factor	Status	Diluted Conc.		Due to Dissolution
Component	mg/Liter	MW	Molar	mg/Liter	Molar			Molar	mg/Liter	mg/Liter
Aluminum	44.6	26.98154	1.65E-03	83.4	3.09E-03	1.9	Dissolving	1.93E-04	5.2	**39.4**
Calcium		40.08	XXXXX	1.3	3.24E-05	XXXXX	<DL	2.03E-06	0.1	XXXXX
Cadmium		112.41	XXXXX	0.3	2.67E-06	XXXXX	<DL	1.67E-07	0.0	XXXXX
Chromium	10.2	51.996	1.96E-04	17.1	3.29E-04	1.7	Dissolving	2.06E-05	1.1	**9.1**
Copper	0.1	58.9332	1.70E-06	0.3	5.09E-06	3.0	Dissolving	3.18E-07	0.0	0.1
Iron	4.9	55.847	8.77E-05	0.6	1.07E-05	0.1	Dissolving	6.71E-07	0.0	4.9
Potassium		39.0983	XXXXX	0	0.00E+00	XXXXX	<DL	XXXXX	XXXXX	XXXXX
Manganese	0.8	54.938	1.46E-05	0.15	2.73E-06	0.2	Dissolving	1.71E-07	0.0	XXXXX
Sodium	354	22.98977	1.54E-02	1500	6.52E-02	4.2	Dilution	4.08E-03	93.8	XXXXX
Nickel	0.2	58.69	3.41E-06	2.1	3.58E-05	10.5	Dil+Wash	2.24E-06	0.1	XXXXX

								Assume Dilution Factor is		16
Third Wash				Second Wash	First Wash	Dilution Factor	Status	Diluted Conc.		Due to Dissolution
Component	mg/Liter	MW	Molar	mg/Liter	Molar			Molar	mg/Liter	mg/Liter
Phosphorus	2.8	30.97376	9.04E-05	3	9.69E-05	1.1	Dilution	6.05E-06	0.2	XXXXX
Lead		207.2	XXXXX	1.9	9.17E-06	XXXXX	<DL	5.73E-07	0.1	XXXXX
Silicon	23.9	28.0855	8.51E-04	24.9	8.87E-04	1.0	Dissolving	5.54E-05	1.6	**22.3**
Zinc		65.38	XXXXX	0.3	4.59E-06	XXXXX	<DL	2.87E-07	0.0	XXXXX
TOC		12.011	XXXXX	244	2.03E-02	XXXXX	<DL	1.27E-03	15.3	XXXXX
TIC	127	12.011	1.06E-02	286	2.38E-02	2.3	Dissolving	1.49E-03	17.9	**109.1**
Chloride	2	35.453	5.64E-05	12	3.38E-04	6.0	Dilution	2.12E-05	0.8	1.3
Fluoride	23	18.998	1.21E-03	75	3.95E-03	3.3	Dissolving	2.47E-04	4.7	**18.3**
Nitrate	58	62.0049	9.35E-04	960	1.55E-02	16.6	Dilution	9.68E-04	60.0	XXXXX
Sulfate	5	96.0576	5.21E-05	65	6.77E-04	13.0	Dilution	4.23E-05	4.1	XXXXX
Phosphate	3	94.97136	3.16E-05	55	5.79E-04	18.3	Dilution	3.62E-05	3.4	XXXXX

Sodium Wash		22.98977		230	0.01

Table 59 Fourth Wash of Solids from Tank AN-107

								Assume Dilution Factor is	8.3	
Fourth Wash				Third Wash	Third Wash	Dilution Factor	Status	Diluted Conc.		Due to Dissolution
Component	mg/Liter	MW	Molar	mg/Liter	Molar			Molar	mg/Liter	mg/Liter
Aluminum	28.2	26.98154	1.05E-03	44.6	1.65E-03	1.6	Dissolving	1.99E-04	5.4	**22.8**
Calcium	0.6	40.08	1.50E-05		XXXXXXXX	XXXXXXXX	<DL	XXXXXX	XXXXXX	XXXXXXXX
Cadmium		112.41	XXXXXX		XXXXXXXX	XXXXXXXX	<DL	XXXXXX	XXXXXX	XXXXXXXX
Chromium	5.9	51.996	1.13E-04	10.2	1.96E-04	1.7	Dissolving	2.36E-05	1.2	**4.7**
Copper		58.9332	0.00E+00	0.1	1.70E-06	XXXXXXXX	<DL	2.04E-07	0.0	0.0
Iron	9	55.847	1.61E-04	4.9	8.77E-05	0.5	Dissolving	1.06E-05	0.6	**8.4**
Potassium		39.0983	XXXXXX		XXXXXXXX	XXXXXXXX	<DL	XXXXXX	XXXXXX	XXXXXXXX
Manganese	1.6	54.938	2.91E-05	0.8	1.46E-05	0.5	Dissolving	1.75E-06	0.1	**1.5**
Sodium	243	22.98977	1.06E-02	354	1.54E-02	1.5	Dil+Wash	1.86E-03	42.7	XXXXXXXX
Nickel		58.69	0.00E+00	0.2	3.41E-06	XXXXXXXX	<DL	4.11E-07	0.0	XXXXXXXX

								Assume Dilution Factor is	8.3	
Fourth Wash				Third Wash	Third Wash	Dilution Factor	Status	Diluted Conc.		Due to Dissolution
Component	mg/Liter	MW	Molar	mg/Liter	Molar			Molar	mg/Liter	mg/Liter
Phosphorus	1.7	30.97376	5.49E-05	2.8	9.04E-05	1.6	Dilution	1.09E-05	0.3	1.4
Lead	0.4	207.2	1.93E-06		XXXXXXXX	XXXXXXXX	<DL	XXXXXX	XXXXXX	XXXXXXXX
Silicon	16.6	28.0855	5.91E-04	23.9	8.51E-04	1.4	Dissolving	1.03E-04	2.9	**13.7**
Zinc	0.1	65.38	1.53E-06		XXXXXXXX	XXXXXXXX	<DL	XXXXXX	XXXXXX	XXXXXXXX
TOC		12.011	XXXXXX		XXXXXXXX	XXXXXXXX	<DL	XXXXXX	XXXXXX	XXXXXXXX
TIC	110	12.011	9.16E-03	127	1.06E-02	1.2	Dissolving	1.27E-03	15.3	**94.7**
Chloride	3	35.453	8.46E-05	2	5.64E-05	0.7	Dissolving	6.80E-06	0.2	2.8
Fluoride	12	18.998	6.32E-04	23	1.21E-03	1.9	Dissolving	1.46E-04	2.8	**9.2**
Nitrate	7	62.0049	1.13E-04	58	9.35E-04	8.3	Dilution	1.13E-04	7.0	XXXXXXXX
Sulfate	3	96.0576	3.12E-05	5	5.21E-05	1.7	Dissolving	6.27E-06	0.6	**2.4**
Phosphate	3	94.97136	3.16E-05	3	3.16E-05	1.0	Dissolving	3.81E-06	0.4	**2.6**

Sodium Wash		22.98977		230	0.01	

Table 60 Summary of Washes for Tank AN-107 Solids

	Wash 1	Wash 2	Wash 3	Wash 4
Factor (Volume)	18.837	17.824	18.054	18.325
	Dissolved	Dissolved	Dissolved	Dissolved
Component	microgm/mL	microgm/mL	microgm/mL	microgm/mL
Aluminum	1096.1	37.8	39.4	22.8
Calcium	XXXXXX	XXXXXX	XXXXXX	XXXXXXX
Cadmium	XXXXXX	XXXXXX	XXXXXX	XXXXXXX
Chromium	39.8	14.7	9.1	4.7
Copper	XXXXXX	0.1	0.1	0.0
Iron	XXXXXX	0.5	4.9	8.4
Potassium	XXXXXX	XXXXXX	XXXXXX	XXXXXXX
Manganese	XXXXXX	XXXXXX	XXXXXX	1.5
Sodium	10740.9	XXXXXX	XXXXXX	XXXXXXX
Nickel	XXXXXX	XXXXXX	XXXXXX	XXXXXXX
Phosphorus	XXXXXX	XXXXXX	XXXXXX	1.4
Lead	XXXXXX	XXXXXX	XXXXXX	XXXXXXX
Silicon	17.3	24.2	22.3	13.7
Zinc	XXXXXX	0.2	XXXXXX	XXXXXXX
TOC	2959.1	XXXXXX	XXXXXX	XXXXXXX
TIC	1160.9	163.2	109.1	94.7
Chloride	XXXXXX	2.8	1.3	2.8
Fluoride	1034.9	33.0	18.3	9.2

	Wash 1	Wash 2	Wash 3	Wash 4
Factor (Volume)	18.837	17.824	18.054	18.325
	Dissolved	Dissolved	Dissolved	Dissolved
Component	microgm/mL	microgm/mL	microgm/mL	microgm/mL
Nitrate	XXXXXX	XXXXXX	XXXXXX	XXXXXXX
Sulfate	592.5	XXXXXX	XXXXXX	2.4
Phosphate	1113.9	XXXXXX	XXXXXX	2.6

Table 61 Solids Calculation for Unwashed Entrained Solids in Tank AN-107

Total in Wash					Solids	Total							Mass	Simulant	After Wash
Component	microgm	microgm	microgm	microgm	microgm	microgm	MW	Moles	Moles +	Moles -	Form	MW	grams	wt %	
Aluminum	20647.9	673.7	711.1	418.3	2254	24705.1	26.98154	9.16E-04			Al2O3	101.96	0.042654	4.711761	32.06132
Calcium	XXXX	XXXX	XXXX	XXXX	256	256	40.08	6.39E-06	1.28E-05		Ca3(PO4)2	310.1827	0.00066	0.072951	0.496396
Cadmium	XXXX	XXXX	XXXX	XXXX			112.41	0.00E+00							
Chromium	749.7	262.2	164.9	85.6	1119	2381.3	51.996	4.58E-05		9.16E-05	Cr2O3	152.02	0.003481	0.384539	2.616608
Copper	XXXX	2.6	1.5	-0.2	11	14.9	58.9332	2.53E-07							
Iron	XXXX	8.5	87.8	154.1	30096	30346.4	55.847	5.43E-04			Fe2O3	159.69	0.043387	4.792659	32.61179
Potassium	XXXX	XXXX	XXXX	XXXX			39.0983	0.00E+00							
Manganese	XXXX	XXXX	XXXX	27.6	17721	17748.6	54.938	3.23E-04			MnO2	86.94	0.028087	3.102641	21.11201
Sodium	202326.5	XXXX	XXXX	XXXX	3079	205405.5	22.98977	8.93E-03	8.93E-03						
Nickel	XXXX	XXXX	XXXX	XXXX	87	87	58.69	1.48E-06	2.96E-06						

Total in Wash					Solids	Total							Mass	Simulant	After Wash
Component	microgm	microgm	microgm	microgm	microgm	microgm	MW	Moles	Moles +	Moles -	Form	MW	grams	wt %	
Phosphorus	XXXX	XXXX	XXXX	25.0	192	217.0	30.97376	7.00E-06							
Lead	XXXX	XXXX	XXXX	XXXX	2010	2010	207.2	9.70E-06							
Silicon	325.9	431.5	403.4	251.4	805	2217.2	28.0855	7.89E-05		1.58E-04	Na2O.Al2O3.(SiO2)2.5H2O	374.1852	0.01477	1.631542	11.10188
Zinc	XXXX	3.6	XXXX	XXXX	150	153.6	65.38	2.35E-06							
TOC	55740.4	XXXX	XXXX	XXXX		55740.4	12.011	4.64E-03		4.64E-03	Na2C2O4	134	0.310932	34.34689	
TIC	21868.0	2908.9	1970.1	1735.4		28482.4	12.011	2.37E-03		4.74E-03	Na2CO3.H2O	124	0.294049	32.48188	
Chloride	XXXX	49.9	22.6	50.6		123.0	35.453	3.47E-06		3.47E-06					
Fluoride	19494.2	588.2	330.6	169.1		20582.1	18.998	1.08E-03		1.08E-03	NaF	41.99	0.045491		
Nitrate	XXXX	XXXX	XXXX	XXXX			62.0049	0.00E+00							
Sulfate	11160.9	XXXX	XXXX	43.9		11204.9	96.0576	1.17E-04		2.33E-04	Na2SO4.10H2O	322.2	0.037584	4.151662	
Phosphate	20981.8	XXXX	XXXX	48.4		21030.2	94.97136	2.21E-04		4.43E-04	Na3PO4.12H2O	380.13	0.084175	9.298324	
Others															
Magnesium					113	113	24.305	4.65E-06							

Total in Wash					Solids	Total							Mass	Simulant	After Wash
Component	microgm	microgm	microgm	microgm	microgm	microgm	MW	Moles	Moles +	Moles -	Form	MW	grams	wt %	
Barium					167	167	137.33	1.22E-06							
Lanthanum					228	228	138.9055	1.64E-06							
Zirconium					282	282	91.22	3.09E-06							
					total	423495.5		Total	8.95E-03	1.14E-02	With Soluble Salts	Total	0.90527		
											Without Soluble Salts	Total	0.133039		

Table 62 Recipe for Unwashed Entrained Solids from Tank AN-107

Wet First Wash Solids	**1.8**	**grams**
Washed Solids	**0.106**	**grams/Liter**

					Minus
	Sample Solids		**Mass**	**Simulant**	**Sol Salts**

Component	Moles	Form	Formula Wt	Grams	Wt %	Wt %
Aluminum	9.16E-04	Al2O3	101.96	0.0467	5.13	34.06
Calcium	6.39E-06	Ca3(PO4)2	310.18	0.00066	0.07	0.48
Chromium	4.58E-05	Cr2O3	152.02	0.0035	0.38	2.54
Iron	5.43E-04	Fe2O3	159.69	0.0434	4.77	31.65
Manganese	3.23E-04	MnO2	86.94	0.0281	3.09	20.49
Sodium	8.93E-03					
Silicon	7.89E-05	Na2O.Al2O3.(SiO2)2.5H2O	374.19	0.0148	1.62	10.78
TOC as Carbon	4.64E-03	Na2C2O4	134.00	0.3109	34.19	
TIC (Carbonate)	2.37E-03	Na2CO3.H2O	124.00	0.2940	32.34	
Fluoride	1.08E-03	NaF	41.99	0.0455	5.00	
Sulfate	1.17E-04	Na2SO4.10H2O	322.20	0.0376	4.13	
Phosphate	2.21E-04	Na3PO4.12H2O	380.13	0.0842	9.26	
		Including Soluble Salts	Total	0.9093	100.00	
		Without Soluble Salts	Total	0.1371		100.00

Recipe	CAS #	Formula	grams/100 grams of solids
Aluminum Oxide	1344-28-1	Al2O3	5.1

Calcium Phosphate, tribasic	12167-74-7	Ca3(PO4)2	0.1
Chromic Oxide	1308-38-9	Cr2O3	0.4
Ferric Oxide	1309-37-1	Fe2O3	4.8
Manganese Dioxide	1313-13-9	MnO2	3.1
Sodium Aluminosilicate		Na2O.Al2O3.(SiO2)2.5H2O	1.6
Sodium Oxalate	62-76-0	Na2C2O4	34.2
Sodium Carbonate Monohydrate	5968-11-6	Na2CO3.H2O	32.3
Sodium Fluoride	7681-49-4	NaF	5.0
Sodium Sulfate Decahydrate	7727-73-3	Na2SO4.10H2O	4.1
Sodium Phosphate Dodecahydrate	10101-89-0	Na3PO4.12H2O	9.3
		Total	100.0

Appendix G Analytical Methods

Analyte	Analysis Method*
Ag	ICP-AES
Al	ICP-AES
B	ICP-AES
Ba	ICP-AES
Ca	ICP-AES
Ce	ICP-AES
Cr	ICP-AES
Cs	ICP-AES, AA
Cu	ICP-AES
Fe	ICP-AES
K	ICP-AES, AA
La	ICP-AES
Mg	ICP-AES
Mn	ICP-AES
Mo	ICP-AES
Na	ICP-AES, AA
Nd	ICP-AES
Ni	ICP-AES
P	ICP-AES
Pb	ICP-AES
Sr	ICP-AES
Zn	ICP-AES
Zr	ICP-AES
Chloride	IC
Fluoride	IC
Formate	IC, HPLC
Nitrate	IC
Nitrite	IC
Oxalate	IC
Phosphate	IC
Sulfate	IC
TIC/TOC	CO_2 measurement
EDTA	HPLC
HEDTA	HPLC
Glycolate	HPLC
Citrate	HPLC
Acetate	HPLC
Iminodiacetic Acid	GCMS
Hydroxide	Titration
Carbonate	Titration

Analysis Methods:

ICP-AES	Inductively Coupled Plasma – Atomic Emission Spectrophotometer
AA	Atomic Absorption Spectrophotometer
IC	Ion Chromatography
HPLC	High Performance Liquid Chromatography

GCMS	Derivatization Gas Chromatography-Mass Spectrometry
CO_2 measurement	Wet Persulfate Oxidation

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