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Slurry Mix Evaporator Batch Acceptability and Test Cases of the Product Composition Control System with Thorium as a Reportable Element

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EXECUTIVE SUMMARY

The Defense Waste Processing Facility (DWPF), which is operated by Savannah River Remediation, LLC (SRR), has recently begun processing Sludge Batch 6 (SB6) by combining it with Frit 418 at a nominal waste loading (WL) of 36%. A unique feature of the SB6/Frit 418 glass system, as compared to the previous glass systems processed in DWPF, is that thorium will be a reportable element for the resulting wasteform. Several activities were initiated based upon this unique aspect of SB6 including an investigation regarding the handling of thorium in the acceptability process at the Slurry Mix Evaporator (SME) hold-point for DWPF operations.

The conclusions provided in this report are that no changes need to be made to the SME acceptability process (i.e., no modifications to WSRC-TR-95-00364, Revision 5, are needed) and no changes need to be made to the Product Composition Control System (PCCS) itself (i.e. the spreadsheet utilized by Waste Solidification Engineering (WSE) for acceptability decisions does not require modification) in response to thorium becoming a reportable element for DWPF operations.

In addition, the inputs and results for the two test cases requested by WSE for use in confirming the successful activation of thorium as a reportable element for DWPF operations during the processing of SB6 are presented in this report.

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LIST OF ABBREVIATIONS

DWPF	Defense Waste Processing Facility
EPAR	Expected Property Acceptable Region
MAR	Measurement Acceptability Region
PAR	Property Acceptability Region
PCCS	Product Composition Control System
SB6	Sludge Batch 6
SME	Slurry Mix Evaporator
SRAT	Sludge Receipt and Adjustment Tank
SRNL	Savannah River National Laboratory
SRR	Savannah River Remediation
TC01	Test Case 1 (also TC01a and TC01b)
TC02	Test Case 2
TTR	Technical Task Request
TT&QA	Task Technical and Quality Assurance
T_L	Liquidus Temperature
WL	Waste Loading
WSE	Waste Solidification Engineering
wt%	weight percent
ΔG_p	An estimate of the free energy of hydration of a glass in kcal/mole derived from the composition of the glass.

1.0 Introduction

The Defense Waste Processing Facility (DWPF), which is operated by Savannah River Remediation, LLC (SRR), has recently begun processing Sludge Batch 6 (SB6) by combining it with Frit 418 at a nominal waste loading (WL) of 36%. A unique feature of the SB6/Frit 418 glass system, as compared to the previous glass systems processed in DWPF, is that thorium will be a reportable element (i.e., concentrations of elemental thorium in the final glass product greater than 0.5 weight percent (wt%)) for the resulting wasteform. Several activities were initiated based upon this unique aspect of SB6. One of these was an investigation into the impact of thorium on the models utilized in DWPF's Product Composition and Control System (PCCS). While the PCCS is described in more detail below, for now note that it is utilized by Waste Solidification Engineering (WSE) to evaluate the acceptability of each batch of material in the Slurry Mix Evaporator (SME) before this material is passed on to the melter. The evaluation employs models that predict properties associated with processability and product quality from the composition of vitrified samples of the SME material. The investigation of the impact of thorium on these models was conducted by Peeler and Edwards [1] and led to a recommendation that DWPF can process the SB6/Frit 418 glass system with ThO_2 concentrations up to 1.8 wt% in glass. Questions also arose regarding the handling of thorium in the SME batch acceptability process as documented by Brown, Postles, and Edwards [2]. Specifically, that document is the technical bases of PCCS, and while Peeler and Edwards confirmed the reliability of the models, there is a need to confirm that the current implementation of DWPF's PCCS appropriately handles thorium as a reportable element. Realization of this need led to a Technical Task Request (TTR) prepared by Bricker [3] that identified some specific SME-related activities that the Savannah River National Laboratory (SRNL) was requested to conduct. SRNL issued a Task Technical and Quality Assurance (TT&QA) plan [4] in response to the SRR request. The activities defined in the TT&QA plan that are addressed in this report are:

(1) Reviewing the current version of "SME Acceptability Determination for DWPF Process Control," WSRC-TR-95-00364, Revision 5, to assess if there is a need to update the technical basis for DWPF's PCCS to address the introduction of thorium as a reportable element and to complete this update, if needed, and

(2) Developing and documenting evaluations of PCCS test case scenarios that were provided to SRNL by WSE of SRR [5]. These test cases are to be utilized by WSE to confirm the successful implementation of the steps necessary to activate thorium as part of the input to PCCS.

WSE made an additional request to SRNL via electronic mail (see [4]). SRNL was requested to generate a white paper providing a statistical method for estimating thorium concentrations based on the established analysis of iron. This request has been rescinded by WSE via electronic mail (see Appendix C).

2.0 Background

While the SME acceptability process is fully described by Brown, Postles, and Edwards [2], an overview of its underlying philosophy is provided in this section. A decision on the acceptability of the waste glass product cannot be made at the melter or after it has been produced, since by then no further changes to the composition of the material are possible. Therefore, the acceptability decision is made on the upstream process, rather than on the downstream melt or glass product. That is, it is based on statistical process control rather than statistical quality control, and the acceptability decision is made at the SME. The SME is uniquely positioned in the process — it is both the first control point in the process wherein all necessary constituents are present and the last control point at which any change to these constituents can be effected. Thus, the control strategy involves monitoring the blended SME batch.

The monitoring of the SME is accomplished by sampling its contents. For each SME batch, a set of ($n \geq 4$) samples is taken to initiate an acceptability decision. Each of these samples is vitrified and the chemical compositions of the resulting n glasses are measured. The average of the measured chemical compositions for a minimum of 4 samples is determined, and this average composition serves as the basis for the acceptability decision for the SME batch.

However, the average chemical composition, while necessary, is not sufficient in and of itself, to complete the assessment of the performance of the SME contents against the constraints. Some of the constraints involve properties (either process or product quality) such as viscosity, liquidus temperature, and durability. These properties cannot be measured in situ, and thus, they must be predicted from models that relate these properties to glass composition. Not only must the model predictions satisfy their corresponding property constraints, but the constraints must also be appropriately met after the applicable modeling uncertainties are introduced into the acceptability decision.

For the constraints involving property-composition models and for most of the other constraints that directly involve composition, the uncertainties associated with the SME samples must also be accounted for as part of the acceptability decision. The uncertainties, labeled measurement uncertainties in this report, include those related to the collection of the slurry samples in the SME, the preparation of these samples for measurement, and the measurements themselves.

A glass composition representing the “average” content of a SME batch is deemed to be within the acceptable operating window for the DWPF if all of the applicable constraints are satisfied, at appropriate confidence levels, after all of the related property modeling and measurement uncertainties are accounted for. Conceptually, there is a layered approach to the acceptability decision. At the first step, the question is, does the average chemical composition representing the SME contents directly or through model predictions satisfy the constraints? If the answer is yes, the composition is said to be within the Expected Property Acceptable Region (EPAR). However, the EPAR does not account for uncertainties in the predicting models. If, after the property model uncertainties are accounted for (to be discussed later), the chemical composition still meets the constraints, then the composition is said to be within the Property Acceptable Region (PAR). Finally, if, after measurement uncertainties are accounted for (to be discussed later), the chemical composition still meets the constraints, then the composition is said to be within the Measurement Acceptable Region (MAR). A composition that is within the MAR for each of the applicable constraints is said to be within the acceptable operating window of the DWPF.

Some additional comments regarding the control strategy are warranted. As mentioned earlier, some of the constraints are directly related to composition and do not involve model predictions. For these constraints there would be fewer layers in the above description that would be applicable. Specifically, the PAR limits would be the same as the EPAR limits for such constraints since there is no property model uncertainty. In a similar fashion, if there is no need to apply property modeling or measurement uncertainties for a given constraint (which is true for a pair of constraints related to the reliability of the chemical composition measurement themselves), then the EPAR limit equals the PAR limit equals the MAR limit for that constraint. Finally, the

DWPF control strategy has evolved over the course of radioactive operations. Revisions to the strategy have introduced alternatives for satisfying some of the constraints as well as a new property-composition model for liquidus temperature and a constraint associated with the formation of a nepheline crystalline phase under certain heat treatments.

3.0 Discussion

The SME acceptability process, whose overview is described in the previous section, is implemented in DWPF's PCCS. In this section, the two topics of concern to this investigation that were outlined above regarding the introduction of thorium as a reportable element for DWPF are addressed. In Section 3.1, the current implementation of PCCS is investigated to confirm that if measurements for thorium are passed to that system they will be appropriately incorporated into the SME acceptability process, and in Section 3.2, the results, i.e., anticipated PCCS output, for two test cases described by Bricker and Ray [5] are presented. The second set of results provides WSE with a basis for validating the successful activation of thorium in the macros that link the measurements generated by the DWPF Laboratory to the inputs to PCCS. That is, in Section 3.2 values that represent the PCCS output for a given set of input values are given for the two test cases provided by Bricker and Ray [5].

3.1 <u>PCCS and Thorium</u>

To investigate how thorium is currently handled by PCCS, one may appeal to the most recent revision of the SME acceptability process as documented by Brown, Postles, and Edwards [2]. A review of that document clearly shows that ThO_2 is included in the list of oxides that is utilized to represent the composition of the vitrified SME material. That is, while thorium was not a reportable element for any of the previous glass systems processed at DWPF, there has been a "placeholder" for this element in PCCS since that system was created. For more details, the reader is referred to the discussion on the chemical composition measurements of SME samples in Appendix A of reference [2] and Tables A1-A3 in that appendix. ThO_2 is one of the oxides listed as a compositional component of the SME samples in the discussion of that appendix and in the tables indicated. Thus, when PCCS was created, a measured thorium concentration was anticipated as an input that would be needed (sooner or later) to represent the compositional information for SME samples. The processing of SB6 is the realization of that necessity.

In establishing macros that were utilized to link the DWPF Laboratory measurements to the inputs to PCCS, WSE was able to simplify their systems by leaving as null entries the thorium measurements for the SME sample results. PCCS took these entries as zeros (i.e., indicating that there was no reportable thorium in that SME material) in the subsequent calculations supporting the acceptability decision for that SME batch. If positive values are entered into PCCS to represent the thorium concentrations in a set of SME samples, they will be appropriately handled in the subsequent calculations and will be correctly incorporated in the SME acceptability process. Thus, no changes need to be made to the SME acceptability process (i.e., reference [2] does not require a revision) and no changes need to be made to PCCS itself (i.e. the spreadsheet utilized by WSE for acceptability decisions does not require modification) in response to thorium becoming a reportable element for DWPF operations.

One other aspect of how thorium is handled in PCCS is worth mentioning as part of this discussion, and that is with regard to uncertainty, specifically compositional measurement uncertainty. Please note that the entries for measurement uncertainty for thorium as indicated in Tables B1 through B3 of Appendix B in reference [2] are all zero. This is a consequence of how uncertainties were originally determined: based upon DWPF Laboratory measurements of simulants analyzed as part of the qualification of DWPF for radioactive operations. Since thorium (a radioactive element) was not present during this testing, its uncertainty information was set to zero in PCCS as was the uncertainty information for uranium (another radioactive component) obviously not included in the DWPF simulant.

3.2 PCCS Test Cases

In this section, the results, i.e., anticipated PCCS output, for two test cases described by Bricker and Ray [5] are presented. These results provide WSE with a basis for validating the successful activation of thorium in the macros that link the measurements generated by the DWPF Laboratory to the inputs to PCCS. That is, in this section, values that represent the PCCS output for a given set of input values are given for the two test cases provided by Bricker and Ray [5]. Table 1 provides the two test cases from [5] that are to be addressed in this section.

Table 1. PCCS Test Cases for Verification of Thorium Activation.

Test Case (TC) Number	Description of Test Case
TC01	PCCS constraints (at a minimum, derived values) are equivalent for a specified composition (excluding thorium) before and after activation.
TC02	PCCS constraints (at a minimum, derived values) for B, Li, and Na leaching; and sum of oxides for a specified composition (including thorium) match results anticipated from models after activation.

The intent of test case TC01 is to show that activating thorium as a zero entry in the link between the measurements from the DWPF Laboratory and the inputs to PCCS introduces no changes to the output from the PCCS calculations without this zero entry. The intent of test case TC02 is to demonstrate that once a positive value for the concentration of thorium is entered into PCCS the constraints whose evaluations depend on thorium are appropriately modified. As indicated in the description of TC02, the only constraints that should be affected are the durability constraints (i.e., those associated with the predicted leaching of boron, lithium, and sodium) and the sum of oxides constraints. These are the only constraints that should change. This is seen by a review of the information in Table 6-12 and Table 8-3 of reference [2].

Table 6-12 of reference [2] shows that thorium does not influence the outcome of the predictions of the PCCS liquidus temperature (T_L) model, and thus, thorium does not affect the outcome of the T_L constraint. Table 8-3 in reference [2] provides the coefficients for the other PCCS constraints. That table is reproduced in this report as Table 2 and the row of coefficients associated with thorium is highlighted to clearly show those constraints that are affected by thorium. Those are the constraints with nonzero entries in the highlighted row; that is, the constraints associated with B, Li, and Na leaching (the durability model constraints) and the constraints associated with “Low Conserv” and “High Conserv” (the conservation of mass or sum of oxides constraints).

Each test case developed in this section consists of four values for each analyte of interest. These four values represent measurements of that analyte from four (hypothetical) samples – the minimum number allowable by PCCS.

Table 2. Constraint Vectors and PAR Limits (Offsets, β's) for All Constraints Except Liquidus Temperature

Oxide	B Leaching	Li Leaching	Na Leaching	High Viscosity	Low Viscosity	Homogeneity	Al_2O_3	Low Conserv	High Conserv	Low Frit	High Frit	TiO_2	NaCl	NaF	Cr_2O_3	Na_2SO_4	Cu	R_2O	. Neph
Al_2O_3	37.680	37.680	37.680	-2	2	575.8565	101.961	101.961	-101.9612	0	0	0	0	0	0	0	0	0	-63.2159
B_2O_3	-10.430	-10.430	-10.430	1	-1	111.6360	0	69.620	-69.6202	69.6202	-69.6202	0	0	0	0	0	0	0	0
BaO	-23.180	-23.180	-23.180	0	0	0	0	153.339	-153.3394	0	0	0	0	0	0	0	0	0	0
HCOO	0.000	0.000	0.000	0	0	0	0	0.000	0.0000	0	0	0	0	0	0	0	0	0	0
CaO	-13.790	-13.790	-13.790	0	0	316.7253	0	56.079	-56.0794	0	0	0	0	0	0	0	0	0	0
Ce_2O_3	-44.990	-44.990	-44.990	0	0	1853.8236	0	328.238	-328.2382	0	0	0	0	0	0	0	0	0	0
NaCl	0.000	0.000	0.000	0	0	0	0	0.000	0.0000	0	0	0	-58.4428	0	0	0	0	0	0
Cr_2O_3	11.950	11.950	11.950	0	0	0	0	151.990	-151.9902	0	0	0	0	0	-151.9902	0	0	0	0
Cs_2O	-80.380	-80.380	-80.380	2	-2	451.8814	0	281.809	-281.8094	281.8094	-281.8094	0	0	0	0	0	0	-281.8094	0
CuO	-4.955	-4.955	-4.955	0	0	0	0	75.544	-75.5439	0	0	0	0	0	0	0	-63.5383	0	0
NaF	0.000	0.000	0.0000	0	0	0	0	0.000	0.0000	0	0	0	0	-41.9882	0	0	0	0	0
Fe_2O_3	14.560	14.560	14.560	2	-2	901.9096	0	159.692	-159.6922	0	0	0	0	0	0	0	0	0	0
K_2O	-76.410	-76.410	-76.410	2	-2	151.0552	0	94.203	-94.2034	94.2034	-94.2034	0	0	0	0	0	0	-94.2034	0
La_2O_3	-48.590	-48.590	-48.590	0	0	1840.1560	0	325.818	-325.8182	0	0	0	0	0	0	0	0	0	0
Li_2O	-24.040	-24.040	-24.040	2	-2	47.9084	0	29.877	-29.8774	29.8774	-29.8774	0	0	0	0	0	0	-29.8774	0
MgO	-6.570	-6.570	-6.570	0	0	0	0	40.311	-40.3114	0	0	0	0	0	0	0	0	0	0
MnO	-24.440	-24.440	-24.440	0	0	0	0	70.937	-70.9374	0	0	0	0	0	0	0	0	0	0
MoO_3	16.460	16.460	16.460	0	0	812.9341	0	143.938	-143.9382	0	0	0	0	0	0	0	0	0	0
NO_2	0.000	0.000	0.000	0	0	0	0	0.000	0.0000	0	0	0	0	0	0	0	0	0	0
NO_3	0.000	0.000	0.000	0	0	0	0	0.000	0.0000	0	0	0	0	0	0	0	0	0	0
Na_2O	-53.090	-53.090	-53.090	2	-2	99.3833	0	61.979	-61.9790	61.9790	-61.9790	0	0	0	0	0	0	-61.9790	-38.4270
Na_2SO_4	0.000	0.000	0.000	0	0	0	0	0.000	0.0000	0	0	0	0	0	0	-142.0412	0	0	0
Nd_2O_3	-37.790	-37.790	-37.790	0	0	1900.3616	0	336.478	-336.4782	0	0	0	0	0	0	0	0	0	0
NiO	0.370	0.370	0.370	0	0	0	0	74.709	-74.7094	0	0	0	0	0	0	0	0	0	0
P_2O_5	-26.550	-26.550	-26.55	0	0	0	0	141.945	-141.9446	0	0	0	0	0	0	0	0	0	0
PbO	21.050	21.050	21.050	0	0	0	0	223.189	-223.1894	0	0	0	0	0	0	0	0	0	0
SiO_2	4.050	4.050	4.050	-0.78734	1.19412	96.3460	0	60.085	-60.0848	60.0848	-60.0848	0	0	0	0	0	0	0	22.8322
ThO_2	19.230	19.230	19.230	0	0	0	0	264.037	-264.0368	0	0	0	0	0	0	0	0	0	0
TiO_2	16.270	16.270	16.270	0	0	0	0	79.899	-79.8988	0	0	-79.8988	0	0	0	0	0	0	0
U_3O_8	-23.770	-23.770	-23.770	0	0	0	0	842.085	-842.0852	0	0	0	0	0	0	0	0	0	0
Y_2O_3	-12.910	-12.910	-12.910	0	0	1275.3196	0	225.808	-225.8082	0	0	0	0	0	0	0	0	0	0
ZnO	0.920	0.920	0.920	0	0	0	0	81.369	-81.3694	0	0	0	0	0	0	0	0	0	0
ZrO_2	17.490	17.490	17.490	0	0	0	0	123.219	-123.2188	0	0	0	0	0	0	0	0	0	0
PAR	-14.1058	-13.8695	-14.1991	0	0	210.9203	3.0	95.000	-105	70	-85	-2	-1	-1	-0.3	-0.59	-0.5	-19.3	0

3.2.1 *Test Case TC01*

The intent of test case TC01 is to show that activating thorium as a zero entry in the link between the measurements from the DWPF Laboratory and the inputs to PCCS introduces no changes to the output from the PCCS calculations without this zero entry. Thus, for this test case, the PCCS output is provided for a set values representing SME sample measurements without thorium values. This same set of PCCS output is then generated for the same set of SME sample measurements modified to have zero entries for thorium content.

Table A1 in Appendix A provides the measurements that are to be entered into PCCS to represent the SME samples before thorium entry is activated. This set of measurements is identified as TC01a. Table A2 in Appendix A provides the same set of measurements with zeros entered for the thorium content of these SME samples. These values are to be entered into PCCS after thorium has been activated in the link between the DWPF Laboratory information and PCCS. This set of measurements is identified as TC01b.

For both PCCS entries TC01a and TC01b, the PCCS output should be identical. The output that should be generated by PCCS for each of these two sets of SME sample measurements is provided in Table B1 of Appendix B. Specifically, the lines of output labeled as TC01 in this table should be used for comparisons between the output for TC01a and TC01b.

3.2.2 *Test Case TC02*

The intent of test case TC02 is to demonstrate that once a positive value for the concentration of thorium is entered into PCCS the constraints whose evaluations depend on thorium are appropriately modified. As indicated in the discussion above, the constraints involved are those associated with B, Li, and Na leaching (the durability model constraints) and the constraints associated with “Low Conserv” and “High Conserv” (the conservation of mass or sum of oxides constraints). To keep these comparisons simple yet comprehensive, the sample measurements for this test case will be the same as those for TC01 with the exception of the sample values for the thorium concentrations. The values for thorium will be selected so as to lead to an average of 1 weight percent elemental thorium for TC02. This is indicated in Table A3 of Appendix A.

Since the only change between the sample measurements of TC01 and those of TC02 is the thorium concentrations and since thorium activation leads to changes only in the constraints associated with B, Li, and Na leaching (the durability model constraints) and the constraints associated with “Low Conserv” and “High Conserv” (the conservation of mass or sum of oxides constraints), the PCCS output for TC02 should be identical to the output for TC01 for all of the other constraints. The PCCS output for TC02 is provided in Table B1 of Appendix B. Specifically, the lines of output labeled as TC02 in this table should be used to validate the PCCS output for TC02.

Please note that the derived values for ΔG_p increase slightly as one goes from TC01 to TC02 (i.e., the values go from -10.4607 to -10.3779 kcal/mole). This is a reflection of the positive coefficient for ThO_2 in the durability models as seen in Table 2. Also, please note that the derived value for sum of oxides increases from TC01 to TC02 (i.e., 97.3507 wt% to 98.4886 wt%). The difference is 1.1379, the gravimetric factor for ThO_2.

4.0 Conclusions and Recommendations

The effort documented in this report indicates that no changes need to be made to the SME acceptability process (i.e., no modifications to [2] are needed) and no changes need to be made to the PCCS itself (i.e. the spreadsheet utilized by WSE for acceptability decisions does not require modification) in response to thorium becoming a reportable element for DWPF operations.

The inputs and results for the two test cases requested by WSE for use in confirming the successful activation of thorium as a reportable element for DWPF operations during the processing of SB6 are presented in this report. Appendix A provides the inputs for the two test cases, and Appendix B provides the results that should be generated by PCCS for each of these test cases. The arrangement of the output information in Appendix B is not identical to that provided in PCCS but all of the information critical for complete and successful comparisons is provided in that appendix.

While offering an independent path for confirming the successful activation of thorium as a reportable element for DWPF's processing of SB6, this approach does introduce the possibility for some round off errors, so care should be taken in comparing the test case results presented here to those generated by the modified link between the DWPF Laboratory information and PCCS. It is believed, however, that for most of the results provided in this report the values should be reproducible to five significant digits, when available, or to within 1%.

5.0 References

[1] Peeler, DK and TB Edwards, "Impact of Thorium on PCCS Predictions within the Frit 418 –Sludge Batch 6 System," SRNL-L3100-2010-00099, May 2010.

[2] Brown, KG, RL Postles, and TB Edwards, "SME Acceptability Determination for DWPF Process Control," WSRC-TR-95-00364, Revision 5, September 2006.

[3] Bricker, JM, Technical Task Request: SME Acceptability and PCCS Test Cases – Activation/Confirmation of Thorium," HLW-DWPF-TTR-2010-00015, Revision 0, May 2010.

[4] Edwards, TB, "Task Technical and Quality Assurance Plan: Slurry Mix Evaporator Batch Acceptability and Test Cases for the Product Composition Control System with Thorium as a Reportable Element," SRNL-RP-2010-01022, June 2010.

[5] Bricker, JM and JW Ray, "Proposed Test Cases for Activating Thorium in the Input Links to the Product Composition Control System (PCCS)," SRR-WSE-2010-00193, September 2010.

Appendix A
Test Case Inputs

Table A1 Inputs for Test Case TC01a

Case ID	Average TC01a	Sample 1 TC01a-S1	Sample 2 TC01a-S2	Sample 3 TC01a-S3	Sample 4 TC01a-S4
Solids	42.6025	42.2400	43.0400	42.3200	42.8100
Calcined Solids	36.1275	35.8000	36.4400	35.7400	36.5300
Spec. Gravity	1.38925	1.3730	1.4250	1.3650	1.3940
Al (wt%)	4.62050	4.6300	4.6390	4.6450	4.5680
B (wt%)	1.53600	1.5170	1.5440	1.5510	1.5320
Ba (wt%)					
Ca (wt%)	0.36475	0.3520	0.3870	0.3690	0.3510
Ce (wt%)					
Cr (wt%)	0.02125	0.0210	0.0190	0.0220	0.0230
Cs (wt%)					
Cu (wt%)	0.01250	0.0100	0.0120	0.0150	0.0130
Fe (wt%)	5.96800	5.9850	5.9730	6.0200	5.8940
K (wt%)	0.05975	-0.0380	0.0750	-0.0980	0.3000
La (wt%)					
Li (wt%)	2.34900	2.3420	2.3400	2.3810	2.3330
Mg (wt%)	0.20025	0.2040	0.1930	0.2040	0.2000
Mn (wt%)	1.73975	1.8130	1.7990	1.6710	1.6760
Mo (wt%)					
Na (wt%)	10.36825	10.5670	10.3200	10.2870	10.2990
Nd (wt%)					
Ni (wt%)	0.68950	0.7010	0.6550	0.7060	0.6960
Pb (wt%)					
Si (wt%)	23.32900	23.5320	23.3570	23.4320	22.9950
Th (wt%)					
Ti (wt%)	0.03775	0.1330	0.0070	0.0070	0.0040
U (wt%)	1.53900	1.5850	1.5580	1.5050	1.5080
Y (wt%)					
Zn (wt%)					
Zr (wt%)	0.09475	0.0980	0.0930	0.0950	0.0930
Cl (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
F (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
HCOO (ppm)	35246.0000	35657.0000	33443.0000	35054.0000	36830.0000
NO2 (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
NO3 (ppm)	14179.0000	14039.0000	13640.0000	13808.0000	15229.0000
PO4 (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
SO4 (ppm)	1024.7500	1051.0000	992.0000	1054.0000	1002.0000
TOC (ppm)	3655.0000	14620.0000	0.0000	0.0000	0.0000

Table A2. Inputs for Test Case TC01b

Case ID	Average TC01b	Sample 1 TC01b-S1	Sample 2 TC01b-S2	Sample 3 TC01b-S3	Sample 4 TC01b-S4
Solids	42.6025	42.2400	43.0400	42.3200	42.8100
Calcined Solids	36.1275	35.8000	36.4400	35.7400	36.5300
Spec. Gravity	1.38925	1.3730	1.4250	1.3650	1.3940
Al (wt%)	4.62050	4.6300	4.6390	4.6450	4.5680
B (wt%)	1.53600	1.5170	1.5440	1.5510	1.5320
Ba (wt%)					
Ca (wt%)	0.36475	0.3520	0.3870	0.3690	0.3510
Ce (wt%)					
Cr (wt%)	0.02125	0.0210	0.0190	0.0220	0.0230
Cs (wt%)					
Cu (wt%)	0.01250	0.0100	0.0120	0.0150	0.0130
Fe (wt%)	5.96800	5.9850	5.9730	6.0200	5.8940
K (wt%)	0.05975	-0.0380	0.0750	-0.0980	0.3000
La (wt%)					
Li (wt%)	2.34900	2.3420	2.3400	2.3810	2.3330
Mg (wt%)	0.20025	0.2040	0.1930	0.2040	0.2000
Mn (wt%)	1.73975	1.8130	1.7990	1.6710	1.6760
Mo (wt%)					
Na (wt%)	10.36825	10.5670	10.3200	10.2870	10.2990
Nd (wt%)					
Ni (wt%)	0.68950	0.7010	0.6550	0.7060	0.6960
Pb (wt%)					
Si (wt%)	23.32900	23.5320	23.3570	23.4320	22.9950
Th (wt%)	0	0	0	0	0
Ti (wt%)	0.03775	0.1330	0.0070	0.0070	0.0040
U (wt%)	1.53900	1.5850	1.5580	1.5050	1.5080
Y (wt%)					
Zn (wt%)					
Zr (wt%)	0.09475	0.0980	0.0930	0.0950	0.0930
Cl (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
F (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
HCOO (ppm)	35246.0000	35657.0000	33443.0000	35054.0000	36830.0000
NO2 (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
NO3 (ppm)	14179.0000	14039.0000	13640.0000	13808.0000	15229.0000
PO4 (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
SO4 (ppm)	1024.7500	1051.0000	992.0000	1054.0000	1002.0000
TOC (ppm)	3655.0000	14620.0000	0.0000	0.0000	0.0000

Table A3. Inputs for Test Case TC02

Case ID	Average TC02	Sample 1 TC02-S1	Sample 2 TC02-S2	Sample 3 TC02-S3	Sample 4 TC02-S4
Solids	42.6025	42.2400	43.0400	42.3200	42.8100
Calcined Solids	36.1275	35.8000	36.4400	35.7400	36.5300
Spec. Gravity	1.38925	1.3730	1.4250	1.3650	1.3940
Al (wt%)	4.62050	4.6300	4.6390	4.6450	4.5680
B (wt%)	1.53600	1.5170	1.5440	1.5510	1.5320
Ba (wt%)					
Ca (wt%)	0.36475	0.3520	0.3870	0.3690	0.3510
Ce (wt%)					
Cr (wt%)	0.02125	0.0210	0.0190	0.0220	0.0230
Cs (wt%)					
Cu (wt%)	0.01250	0.0100	0.0120	0.0150	0.0130
Fe (wt%)	5.96800	5.9850	5.9730	6.0200	5.8940
K (wt%)	0.05975	-0.0380	0.0750	-0.0980	0.3000
La (wt%)					
Li (wt%)	2.34900	2.3420	2.3400	2.3810	2.3330
Mg (wt%)	0.20025	0.2040	0.1930	0.2040	0.2000
Mn (wt%)	1.73975	1.8130	1.7990	1.6710	1.6760
Mo (wt%)					
Na (wt%)	10.36825	10.5670	10.3200	10.2870	10.2990
Nd (wt%)					
Ni (wt%)	0.68950	0.7010	0.6550	0.7060	0.6960
Pb (wt%)					
Si (wt%)	23.32900	23.5320	23.3570	23.4320	22.9950
Th (wt%)	1.00000	0.9000	1.0000	1.1000	1.0000
Ti (wt%)	0.03775	0.1330	0.0070	0.0070	0.0040
U (wt%)	1.53900	1.5850	1.5580	1.5050	1.5080
Y (wt%)					
Zn (wt%)					
Zr (wt%)	0.09475	0.0980	0.0930	0.0950	0.0930
Cl (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
F (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
HCOO (ppm)	35246.0000	35657.0000	33443.0000	35054.0000	36830.0000
NO2 (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
NO3 (ppm)	14179.0000	14039.0000	13640.0000	13808.0000	15229.0000
PO4 (ppm)	536.5000	550.0000	525.0000	532.0000	539.0000
SO4 (ppm)	1024.7500	1051.0000	992.0000	1054.0000	1002.0000
TOC (ppm)	3655.0000	14620.0000	0.0000	0.0000	0.0000

Appendix B
Test Case Results

Table B1. Results for Test Cases

Test	ΔG_p PAR Value (kcal/mole)		
Case ID	Boron	Lithium	Sodium
TC01	-14.1058	-13.8695	-14.1991
TC02	-14.1058	-13.8695	-14.1991

Test	ΔG_p MAR Value (kcal/mole)			ΔG_p Derived Value (kcal/mole)		
Case ID	Boron	Lithium	Sodium	Boron	Lithium	Sodium
TC01	-13.7200	-13.4837	-13.8133	-10.4607	-10.4607	-10.4607
TC02	-13.7200	-13.4837	-13.8133	-10.3779	-10.3779	-10.3779

Test	ΔG_p MAR Difference (kcal/mole)			Constraints Met	Property Values (g/L)		
Case ID	Boron	Lithium	Sodium		Boron	Lithium	Sodium
TC01	3.2592	3.0229	3.3525	Yes	0.986	0.977	0.972
TC02	3.3421	3.1058	3.4354	Yes	0.953	0.950	0.941

	Liquidus	High	Low	Homogeneity			Low	High
Test	Temp (T_L)	Viscosity	Viscosity	PAR	Sum of Oxides PAR		Frit	Frit
Case ID	PAR Value	PAR Value	PAR Value	Value	Low	High	PAR Value	PAR Value
TC01	1032.4	0	0	210.9203	95	-105	70	-85
TC02	1032.4	0	0	210.9203	95	-105	70	-85
Units	^oC	unitless	unitless	wt%	wt%	wt%	wt%	wt%

	Liquidus	High	Low	Homogeneity			Low	High
Test	Temp (T_L)	Viscosity	Viscosity	MAR	Sum of Oxides MAR		Frit	Frit
Case ID	MAR Value	MAR Value	MAR Value	Value	Low	High	MAR Value	MAR Value
TC01	1008.908	0.01187	0.025807	219.5137	95	-105	73.1656	-81.8344
TC02	1008.908	0.01187	0.025807	219.5137	95	-105	73.1656	-81.8344
Units	^oC	unitless	unitless	wt%	wt%	wt%	wt%	wt%

	Liquidus	High	Low		Sum of Oxides		Low	High
Test	Temp (T_L)	Viscosity	Viscosity	Homogeneity	Derived Value		Frit	Frit
Case ID	Derived Value	Derived Value	Derived Value	Derived Value	Low	High	Derived Value	Derived Value
TC01	853.428	0.1437	0.1942	218.9730	97.3507	-97.3507	73.9590	-73.9590
TC02	853.428	0.1437	0.1942	218.9730	98.4886	-98.4886	73.9590	-73.9590
Units	^oC	unitless	unitless	wt%	wt%	wt%	wt%	wt%

	Liquidus	High	Low		Sum of Oxides		Low	High
Test	Temp (T_L)	Viscosity	Viscosity	Homogeneity	MAR Diff		Frit	Frit
Case ID	MAR Diff	MAR Diff	MAR Diff	MAR Diff	Low	High	MAR Diff	MAR Diff
TC01	155.48	0.1319	0.1683	-0.5407	2.3507	7.6493	0.7934	7.8753
TC02	155.48	0.1319	0.1683	-0.5407	3.4886	6.5114	0.7934	7.8753
Units	^oC	unitless	unitless	wt%	wt%	wt%	wt%	wt%

Property Values

	Liquidus	High	Low		Sum of Oxides		Low	High
Test	Temp (T_L)	Viscosity	Viscosity	Homogeneity	Values		Frit	Frit
Case ID	Prediction	Pred Value	Pred Value	Value	Low	High	Value	Value
TC01	853.428	53.704	53.704	218.973	97.3507	97.3507	73.959	73.959
TC02	853.428	53.704	53.704	218.973	98.4886	98.4886	73.959	73.959
Units	^oC	Poise	Poise	wt%	wt%	wt%	wt%	wt%

Table B1. Results for Test Cases *(continued)*

MAR Values

	Al_2O_3	Al_2O_3[a]	Al_2O_3[b]	TiO_2	NaCl	NaF	Cr_2O_3	Na_2SO_4	Cu	R_2O	
Test	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	Units
Case ID	3	4	4.43	-2	-1	-1	-0.3	-0.59	-0.5	-19.3	PAR Value
TC01	3.3831	4.3831	4.8131	-1.9835	-1	-1	-0.2730	-0.59	-0.4875	-18.5999	
TC02	3.3831	4.3831	4.8131	-1.9835	-1	-1	-0.2730	-0.59	-0.4875	-18.5999	

Derived Values

Test	Al_2O_3	Al_2O_3	Al_2O_3	TiO_2	NaCl	NaF	Cr_2O_3	Na_2SO_4	Cu	R_2O	
Case ID	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	Units
TC01	8.7304	8.7304	8.7304	-0.0630	-0.2448	-0.3282	-0.0311	-0.4195	-0.0125	-19.1055	
TC02	8.7304	8.7304	8.7304	-0.0630	-0.2448	-0.3282	-0.0311	-0.4195	-0.0125	-19.1055	

MAR Differences

Test	Al_2O_3	Al_2O_3	Al_2O_3	TiO_2	NaCl	NaF	Cr_2O_3	Na_2SO_4	Cu	R_2O
Case ID	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%
TC01	5.3473	4.3473	3.9173	1.9205	0.7552	0.6718	0.2420	0.1705	0.4750	-0.5056
TC02	5.3473	4.3473	3.9173	1.9205	0.7552	0.6718	0.2420	0.1705	0.4750	-0.5056

Property Values

Test	Al_2O_3	Al_2O_3	Al_2O_3	TiO_2	NaCl	NaF	Cr_2O_3	Na_2SO_4	Cu	(R_2O)
Case ID	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%
TC01	8.7304	8.7304	8.7304	0.0630	0.2448	0.3282	0.0311	0.4195	0.0125	19.1055
TC02	8.7304	8.7304	8.7304	0.0630	0.2448	0.3282	0.0311	0.4195	0.0125	19.1055

Nepheline Constraint

Test Case ID	PAR	MAR	Derived Value	MAR Difference	Nepheline Value
TC01	0	0.67776	4.8867	4.2089	0.687
TC02	0	0.67776	4.8867	4.2089	0.687
Units	unitless	unitless	unitless	unitless	unitless

[a] This constraint on Al_2O_3 is not an explicit PCCS output; the constraint is used as an alternate to the homogeneity MAR evaluation.
[b] This constraint on Al_2O_3 is not an explicit PCCS output; the constraint is used as an alternate to the low frit MAR evaluation.

Appendix C
E-Mail Modifying Scope of Work for this Task

Email for Tommy Edwards

Deletion Request: HLW-DWPF-TTR-2010-00015, "SME Acceptability and PCCS Test Cases - Activation/Confirmation of Thorium"

Jonathan Bricker to: Tommy Edwards, Connie Herman, John Occhipinti, Terri Fellinger, Aaron Staub, Herbert Elder, Jeff Ray   10/06/2010 01:56 PM

History: This message has been replied to.

Tommy,

Per our discussion earlier this week, please delete the prior additional request to

"...generate a white paper providing a statistical method for estimating thorium concentrations based on the established analysis of iron..."

from the scope of work captured in HLW-DWPF-TTR-2010-00015. I suppose it can also be removed from the Test Case Report (SRNL-STI-2010-00557). I apologize for any confusion this may have caused. This was certainly a bit of a "knee-jerk" reaction on our part.

Thanks,
Jonathan Bricker
DWPF-Engineering
8.7164

Distribution:

Name:	Location:
Sharon Marra	773-A
Connie Herman	999-W
Allan Barnes	999-W
Patricia Lee	703-41A
Gene Shine	703-41A
Michael Stone	999-W
David Peeler	999-W
Tommy Edwards	999-W
Amanda Billings	999-W
Kevin Fox	999-W
Fabienne Johnson	999-W
Charles Crawford	773-42A
John Occhipinti	704-S
Jonathan Bricker	704-27S
John Iaukea	704-30S
Aaron Staub	704-27S
Jeff Ray	704-S
Robert Hinds	704-S
Terri Fellinger	704-26S
Amanda Shafer	704-27S
Mason Clark	704-27S
Helen Pittman	704-27S
Hank Elder	704-24S
Bill Holtzscheiter	704-15S
Pat Vaughan	773-41A