The WTP Immobilized LAW Formulation Algorithm: Recent Efforts Toward Software Development – 17342

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ABSTRACT

The immobilized low-activity waste (ILAW) product from WTP must meet certain requirements and processing constraints. The strategy for controlling ILAW product composition uses the ILAW formulation algorithm. This algorithm is approved by the DOE Office of River Protection (ORP) for use in calculating melter feed recipes that will produce acceptable ILAW product during Low-Activity Waste (LAW) Facility commissioning. The calculations performed by the algorithm have been demonstrated using a sophisticated spreadsheet, but this spreadsheet is not expected to support continuous operation. Efforts are underway to develop software that will support glass formulation during operation. Recent work toward software development includes an examination of assumptions made in the algorithm about expected LAW Facility operation, and spreadsheet calculations to formulate glass for potential LAW compositions under the direct feed LAW (DFLAW) strategy that ORP has adopted.

The documentation of the ILAW algorithm is the planned basis for software development. However, some assumptions made in the current algorithm’s mass balance logic do not match the matured design and expected operation of the LAW Facility. A self-assessment effort evaluated the validity of these assumptions by reviewing design documents, in order to identify opportunities to align the algorithm’s mass balance logic with the matured design and ensure that the developed software supports continuous LAW Facility operation. Several improvement opportunities were identified and are discussed. The results of ILAW algorithm calculations to formulate glass for eighteen challenging LAW compositions indicate that the current WTP baseline LAW glass models are sufficiently robust to accommodate DFLAW.

INTRODUCTION

The immobilized low-activity waste (ILAW) product that will be produced from the Hanford Tank Waste Treatment and Immobilization Plant (WTP) must be processable in joule-heated, ceramic lined melters, and meet requirements stipulated by the WTP Contract for composition, waste loading, and properties of the glass wasteform [1]. The ILAW Product Compliance Plan (PCP) [2], a WTP Contract deliverable [3], documents the strategy for controlling the composition of the ILAW product to meet the requirements and constraints, which involves the use of the ILAW formulation algorithm [4]. This algorithm has been approved by the US Department of Energy (DOE) Office of River Protection (ORP) for use in calculating melter feed recipes, in order to produce acceptable ILAW during the commissioning phase of Low-Activity Waste (LAW) Facility operations [3, 5]. The calculations performed by the LAW algorithm have been demonstrated using a sophisticated spreadsheet and documented in the ILAW algorithm report [4]. The spreadsheet demonstration is not expected to support continuous operation of the LAW Facility; therefore, efforts are underway to develop software that will be used for glass formulation calculations during operations.

This paper begins with a brief description of the ILAW algorithm and the product requirements and constraints it uses to formulate acceptable ILAW product, to provide a foundation from which to discuss recent work that has been performed toward the development of glass formulation software for WTP. Since the ILAW algorithm report [4] is planned to be the basis for software development, a self-assessment was conducted recently to ensure that software developers responsible for implementing the ILAW algorithm into software have the most current and accurate information on how the LAW Facility is designed and planned to operate [6]. The methods, results, and follow-up actions of this effort are summarized in this paper.

In addition to the self-assessment, the spreadsheet demonstration of the ILAW algorithm has been used to evaluate potentially challenging waste compositions that may be realized under the Direct Feed LAW (DFLAW) strategy that has been adopted by ORP for early commissioning of the LAW Facility [7]. According to this strategy, LAW that has been pretreated to remove suspended solids by ultrafiltration and cesium by ion exchange will be fed directly to one of two concentrate receipt vessels (CRV) in the LAW Facility [8]. One aspect of this strategy that was initially considered problematic is recycling the LAW Effluent Management Facility (EMF) evaporator bottoms directly to the CRVs, because the recycle stream is expected to contain significant concentrations of sulfate and halides, which can limit the achievable waste loading in the glass wasteform. The calculation approach and results are presented and discussed.

LAW VITRIFICATION PROCESS OVERVIEW

Fig. 1 is a simplified process flow diagram of the LAW vitrification process. The LAW feed is received in one of two CRVs in the LAW vitrification facility, and is transferred in batches from the CRVs to the melter feed preparation vessels (MFPV), where GFCs are added and the melter feed is blended. LAW 6, a sample of the blended melter feed, is taken for process verification. The blended melter feed is then transferred in batches to the melter feed vessels (MFV), which continuously provide melter feed to the melters. The melt is poured into containers where it cools and solidifies into glass, which is the ILAW product.

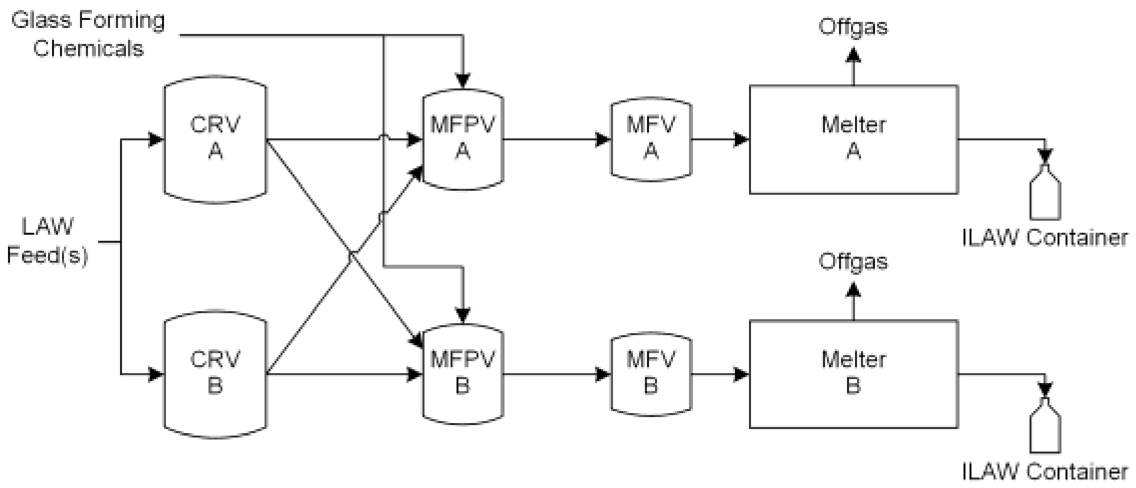

Fig. 1. Simplified Flow Diagram of the LAW Vitrification Process.

A BRIEF DESCRIPTION OF THE ILAW FORMULATION ALGORITHM

Glass Formulation Models, Rules and Constraints

The ILAW algorithm is composed of the following:

- The baseline WTP glass models for predicting properties based on glass composition [9]:
    - Normalized release of boron measured by the Product Consistency Test (PCT)
    - Normalized release of sodium measured by PCT
    - Alteration depth measured by the Vapor Hydration Test (VHT) at 200°C
    - Melt viscosity as a function of glass pool temperature
    - Melt electrical conductivity as a function of glass pool temperature
    - Statistical information for each model used to calculate prediction uncertainties
- Mathematical "rules" used in glass formulation calculations to determine the waste loading that can be achieved based on waste composition:
    - Na_2O-SO_3-K_2O rules [10]
    - Cl-F-SO_3 rules [11]
    - Cr_2O_3-K_2O-P_2O_5 rules [11]
- Constraints on glass composition and properties to ensure the ILAW product is acceptable and processable, and to ensure validity of model predictions of glass properties, which include:
    - Upper limits on normalized PCT release of boron and sodium
    - An upper limit on alteration depth measured by VHT
    - Upper limits on radionuclide activities in accordance WTP Contract requirements
    - Minimum loadings of waste Na_2O stipulated for discrete LAW envelopes
    - Ranges of acceptable melt properties (i.e., melt viscosity and electrical conductivity)

    - Model validity constraints on glass composition and glass properties to ensure validity of glass model predictions
- Mass balance logic to support continuous operation of the LAW Facility, which includes Monte Carlo simulations to propagate uncertainties in glass composition

Overview of Mass Balance Logic

The current ILAW algorithm performs the following steps in its mass balance logic:

1. In the first step, waste composition and radionuclide activity data from the Analytical Laboratory (Lab) is evaluated and converted. An initial target glass composition is estimated based on the converted data. A final target glass composition and radionuclide activities that account for the composition of available glass forming chemicals (GFC) are calculated. A target volume of waste to transfer from the CRV to the MFPV is calculated, as stipulated by the target glass composition. The final target glass composition and its properties are checked against constraints, and adjustments are made to the target glass composition and target waste transfer volume, if necessary. The final target glass composition and waste transfer volume are reported to operations staff as guidance to perform a waste transfer.
2. Based on the measured waste volume transferred from the CRV to the MFPV, the target GFC masses and dilution water volume are adjusted accordingly. These target quantities are reported to operations staff as guidance to prepare a batch of GFCs to blend with the waste in the MFPV.
3. Based on the measured waste transfer volume, measured GFC masses, and measured dilution water volume, the final composition and properties of the melter feed batch is calculated.
4. The melter feed batch results from Step 3 are assessed against algorithm constraints to ensure that the MFPV batch will yield an acceptable ILAW product. If constraints are satisfied, the melter feed batch is sampled and transferred to the MFV. If constraints are not satisfied, qualified staff will be prompted to intervene and determine alternatives.
5. If the final glass composition and properties satisfy the constraints, transfer of the melter feed batch is authorized, and calculations are performed to support ILAW production documentation and reporting.

SELF-ASSESSMENT METHODOLOGY FOR EXAMINING ILAW ALGORITHM ASSUMPTIONS

The self-assessment had two major aspects. First, the information related to the glass property-compositions models and glass formulation rules in the ILAW algorithm report was compared with source documents [9, 10, 11]. Verification and validation of the models and their associated constraints was part of the quality assurance program of the subcontractor who established them. While the validity of the glass-property composition models was not in question, verification of correct transcription of the information related to the models and to glass formulation rules from source documents was performed. After a thorough review, the information related to the glass models and most of the glass formulation rules was found to be consistent. There was an inconsistency identified in one of the Na_2O-SO_3-K_2O rules: the ILAW algorithm report lists a maximum sulfate limit of 0.77 wt%; however, Muller et al. proposes a maximum of 0.70 wt% [10]. Upon further investigation and correspondence with the authors of the ILAW algorithm report, it was determined that 0.70 wt% sulfate should be used [12]. A preliminary assessment of the impact of this change indicated no change in the glass formulation results documented in the ILAW algorithm report. The mathematical equations for the Na_2O-SO_3-K_2O rules are listed and visualized in Fig. 2.

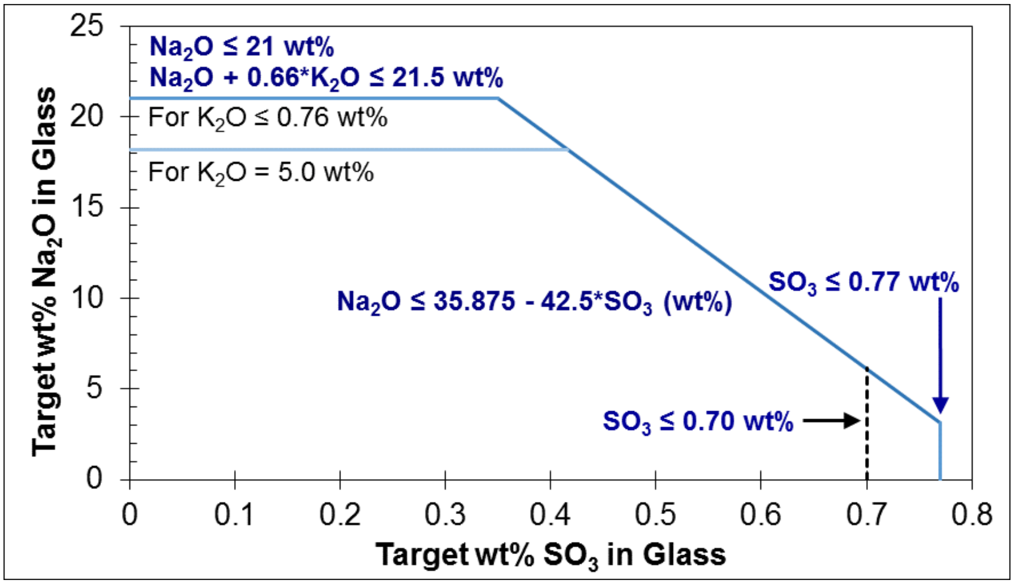

Fig. 2. Na_2O-SO_3-K_2O rules.

The second major aspect of the self-assessment was to determine the alignment of the ILAW algorithm's mass balance logic with design basis documents for the LAW Facility. Design basis documents for the LAW facility were reviewed for information relevant to glass formulation to evaluate the alignment [1, 2, 13-17]. In addition, a prior independent, informal review of the ILAW algorithm report was leveraged to determine gaps that should be addressed in development of the software that will be used to support glass formulation during operation [18]. Based on the review of design documents related to the LAW Facility and of the observations made in the prior informal review, the mass balance logic of the ILAW algorithm does not fully match the matured design of the LAW Facility. Opportunities for improvement identified include the following:

- Using limits in the ILAW algorithm for working volumes of vessels in the vitrification process that are practical and consistent with conduct of operations
- The calculation approach for radionuclide inventory
- The calculation approach for reporting ILAW composition and properties on a lot basis
- How the ILAW algorithm accounts for heel compositions of previous MFPV batches

To capture the findings of the self-assessment and identify additional gaps in the ILAW algorithm mass balance logic, a gap analysis is currently underway.

EVALUATION OF WASTE COMPOSITIONS UNDER DIRECT FEED LAW (DFLAW) STRATEGY

Purpose

While the ILAW algorithm is the only DOE-approved algorithm available for use in calculating recipes of ILAW product that can meet WTP Contract requirements and constraints for processing, it had not been used to perform glass formulation calculations using waste compositions that may be realized under the DFLAW strategy recently adopted by ORP. One important feature of the ILAW algorithm is that it accounts for uncertainties associated with the following: the predictions of glass and melt properties using the glass models; chemical analysis of waste samples; mixing and sampling of vessels; and the composition of glass forming chemicals. The DFLAW strategy has been modeled using the Dynamic (G2) Model. While G2 uses the same glass property-composition models as the ILAW algorithm, it does not account for the uncertainties like the ILAW algorithm can. The purpose of the spreadsheet calculations was to evaluate the feasibility of using the ILAW algorithm, with existing model validity regions and uncertainties, to formulate ILAW product recipes to immobilize waste feed compositions that may be realized under the DFLAW strategy [7].

Assumptions

This study evaluated the feasibility of producing compliant glasses from waste feed compositions under the DFLAW strategy in which feed produced from the LAW Pretreatment System is blended with EMF evaporator bottoms in the CRVs of the LAW vitrification process. The current ILAW algorithm logic assumes the CRVs are sampled in order to determine the composition of the waste feed. To simulate DFLAW operation using the logic of the current algorithm, CRV compositions were derived from simulated chemical composition data for one CRV in a recent G2 model run [19]. Waste compositions were derived from only one CRV, because the LAW vitrification process has duplicate melter trains and no significant differences were observed between the chemical compositions of the contents of each CRV over time. The referenced model run simulated 85% and 100% recycle of EMF evaporator bottoms into the CRV for three different setpoints for the specific gravity of the recycle stream. The CRV compositions were evaluated using established sampling and analytical uncertainties, as if the CRV is sampled three times and each sample is analyzed once. This is the baseline strategy described in the ILAW PCP that is approved by ORP [2, 3], and demonstrated using the ILAW algorithm [3]. The CRV compositions of interest for this study were those possessing high concentrations of sulfate and halides, due to the concern presented by significant concentrations of sulfate and halides expected in the recycle stream from the EMF. Other components that may limit achievable waste loading are potassium, chromium, and phosphorus; however, these were present in sufficiently low concentrations such that they were not anticipated to limit achievable waste loadings. Therefore, the waste compositions of interest for glass formulation calculations in this study were selected for high halide, high sulfate, and low sulfate concentrations.

Evaluation Results

For the waste compositions with relatively high halide and sulfate concentrations, glass compositions formulated using the current ILAW algorithm met the WTP Contract requirements and processing constraints listed. The waste loading for these wastes was limited by halide concentration. For waste compositions with low sulfate concentrations, initial glass formulations possessed predicted electrical conductivity values (including uncertainties) exceeding the upper limit of 0.7 S/cm. It was also observed that predicted alteration depths (including uncertainty) exceeded the upper limit of 453 μm; however, this was not consistently observed between multiple Monte Carlo simulations. Glass formulations were adjusted by decreasing the waste loading by between 0.33 and 0.37 wt% in order to decrease the electrical conductivity below the upper limit. After adjustment, values for alteration depth including uncertainty did not exceed the corresponding upper limit.

The maximum waste loadings (after applying melter retention) projected for each recycle case by the ILAW algorithm and by G2 are listed in TABLE I. Fig. 3 provides a visual comparison of waste loadings projected for waste compositions derived from the G2 scenario assuming 85% recycle and evaporator bottoms with a specific gravity of 1.2. The dotted lines represent the minimum waste Na_2O loadings for Envelopes A (14 wt%), B (3 wt%), and C (10 wt%) waste designations. Envelope C is limited to complexed tank wastes from Hanford tanks AN-102 and AN-107 in accordance with the WTP Contract. These lines are for illustrative purposes only, because the envelope assigned to DFLAW operation according to the WTP Contract is Envelope E, which has not been assigned a minimum loading for waste Na_2O at the time the calculations were performed.

TABLE I. Target Glass Waste Loadings Projected by ILAW Algorithm and G2.

Composition Characteristic	DFLAW Recycle Case	Max waste Na_2O loading (wt%)		Max overall waste loading (wt%)	
		ILAW algorithm	G2	ILAW algorithm	G2
High Halides	85%	13.83%	13.53%	16.08%	16.00%
	100%	13.21%	11.92%	15.49%	14.22%
Low Sulfate	85%	20.55%	20.96%	23.23%	23.94%
	100%	20.53%	20.95%	23.28%	24.03%
High Sulfate	85%	9.62%	8.79%	11.42%	10.63%
	100%	8.87%	7.85%	10.71%	9.64%

One fundamental difference between G2 and the ILAW algorithm is that the ILAW algorithm accounts for process mixing, sampling, analytical, and mass balance uncertainty to ensure (at a 90% confidence level) that the glass product does not fail any glass performance constraints. Providing a statistical confidence statement for glass performance is a commitment in the ILAW PCP approved by DOE [1]. While this is the case, the results suggest that the ILAW algorithm and G2 project waste loading estimates are within ~1 wt% of each other.

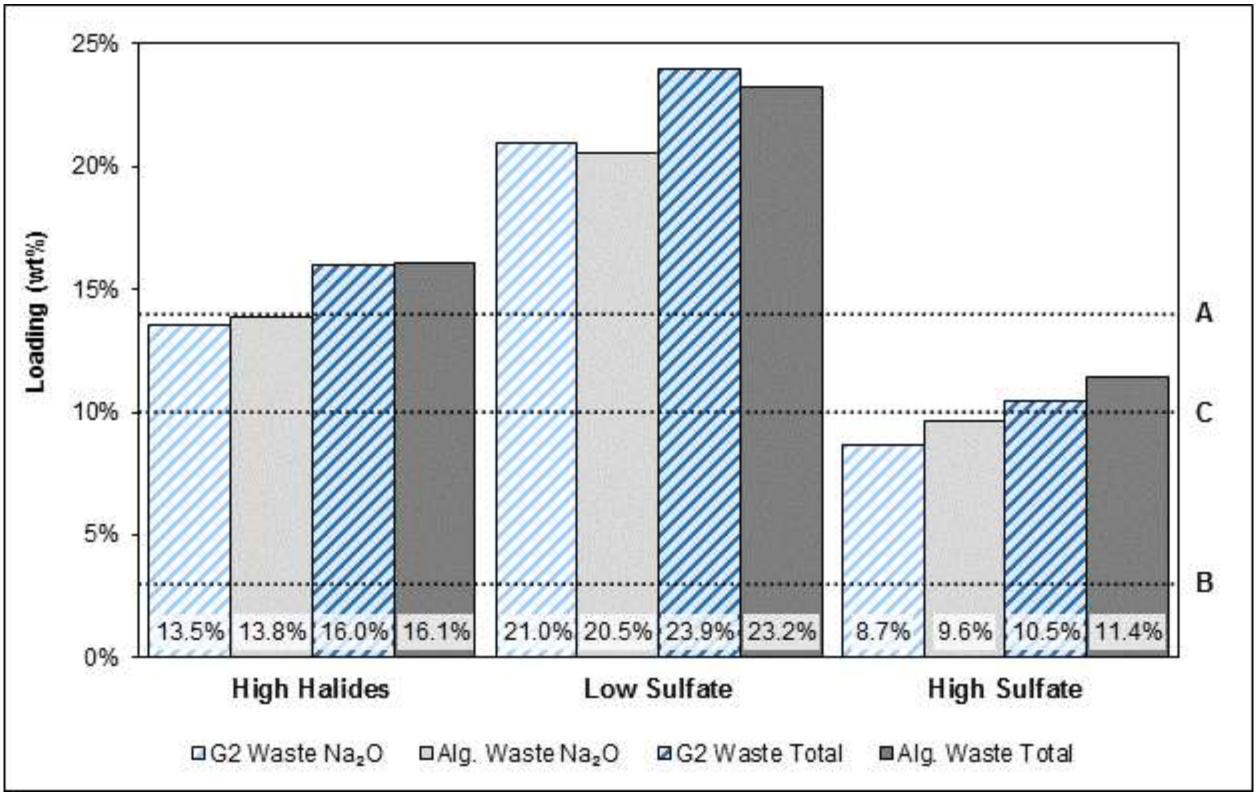

Fig. 3. Waste loadings calculated by ILAW algorithm and by G2.

CONCLUSION

Based upon the results of the self-assessment, the information associated with the glass property-composition models in the ILAW algorithm Report [3] was verified to be accurate and consistent with source documents. The information related to most of the glass formulation rules was found to be consistent with source documents. To be consistent with the work of Muller et al. [10], the algorithm authors have recommended that the maximum sulfate limit in glass be changed from 0.77 wt% to 0.70 wt%, which is not expected to significantly impact glass formulation.

An initial evaluation of eighteen challenging waste feed compositions that may be realized under DFLAW indicates that the baseline WTP glass models are sufficiently robust to accommodate the operation strategy of returning EMF evaporator bottoms directly to the CRVs in the LAW facility. This was considered problematic particularly because of the recycle of halides and sulfates, but the waste loadings projected by the ILAW algorithm are comparable to that predicted by G2. Other potentially limiting species (i.e., potassium, chromium, and phosphorus) did not limit the waste loading of glass formulations for the CRV compositions tested in the evaluation.

While the baseline WTP glass models and glass formulation rules are well-established and can accommodate the DFLAW strategy of EMF recycle, the self-assessment effort determined that the mass balance methodology needs to be modified to be consistent with the matured design and expected operation of the LAW Facility. A gap analysis of the ILAW algorithm logic to identify what the limitations of the current algorithm are and the gaps that need to be addressed in the software that will be developed for glass formulation and manufacture is currently in progress.

ACRONYMS

CRV	Concentrate receipt vessel
DFLAW	Direct-feed low-activity waste
DOE	US Department of Energy
EMF	Effluent Management Facility
G2	Dynamic (G2) Model
GFC	Glass forming chemical
ILAW	Immobilized low-activity waste
LAW	Low-activity waste
MFPV	Melter feed preparation vessel
ORP	Office of River Protection
PCP	Product compliance plan
PCT	Product consistency test
VHT	Vapor hydration test
WTP	Hanford Tank Waste Treatment and Immobilization Plant

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