Use of Uncertainty in Modeling DFLAW Treatment at Hanford – 17115

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ABSTRACT

Average or mean is understood by most; standard deviation (SD) is understood by few. Certainty is easy to model; uncertainty is not. The flowsheet simulation, described in this paper, placed uncertainties in the G2 model of the Hanford Tank Waste Treatment and Immobilization Plant's (WTP) Direct Feed Low-Activity Waste (DFLAW) process for performance and sensitivity evaluations. G2 is a dynamic material balance model that starts and proceeds with operating logic until all the feed is processed. Dynamic material balance is achieved by tracking the flows, storage, and change of all materials within the plant as time increments. Processing equipment and limitations of the flowsheet are modeled (e.g., equipment types, piping, volumes, flowrates, efficiencies, and physical and chemical environments that impact separations, phase equilibriums, and chemical reactions). Operating logic represents the rules and strategies of a running plant.

The G2 model simulated both certainty and uncertainty scenarios for comparison purposes. For the uncertainty scenarios, process decisions were made using presumed values to simulate various operational measurement errors and process variabilities. Presumed means that the known G2 values are adjusted to replicate measurement errors and variabilities. These include: 1) volume measurement, 2) sample analysis, 3) melter decontamination factor (DF), 4) glass former weighing, and 5) glass former composition variations. The errors were randomly generated in accordance with SD values of measurement devices, laboratory methods, and glass former composition ranges. The G2 model runs give insight on the DFLAW process' controllability and the expected range of glass properties.

INTRODUCTION

Coping with uncertainties can be a challenge. The DFLAW is the first treatment facility that will turn Hanford tank waste into glass on a production scale. Pumping, sampling, melter decontamination, glass former weighing, and variation of glass former compositions are among the uncertain factors that potentially impact the quantity and quality of glass made. This study presents the SD values of these operation parameters, based on WTP Project research and technology reports, and discusses the methods for incorporation in the G2 model [1]. Operating logic in the G2 model represent the rules and strategies of running the plant [2].

Producing Presumed Values

Every continuous, random variable *X* has an associated probability density function. The probability density function "records" the probabilities associated with *X* as areas under its graph. Figure 1 shows the probability curve that follows a normal distribution. Many or most large populations of characteristics or events in nature follow this distribution.

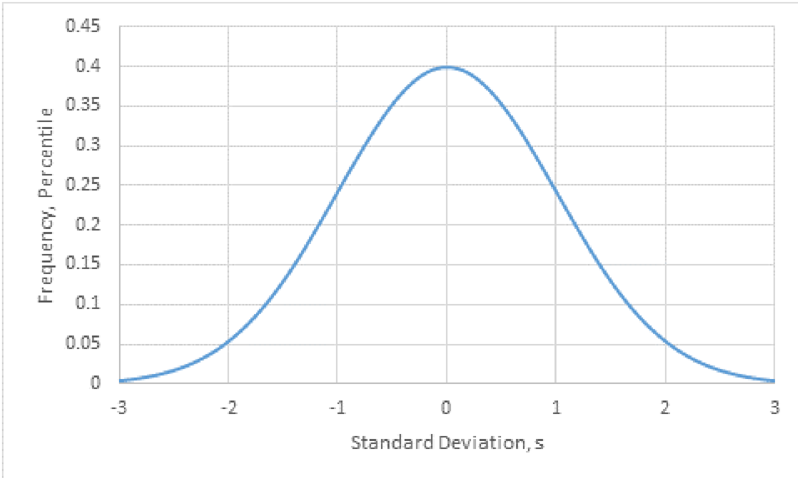

Fig. 1. Normal Probability Density Function.

The mathematical expression for the normal probability density function is given in Equation 1.

$$f(x) = \frac{1}{\sqrt{2\pi}}\, e^{-x^2} \qquad \text{(Eq. 1)}$$

There is another function, the cumulative distribution function, that records the same probabilities associated with *X*, but in a different way. The cumulative distribution function gives the accumulated probability up to *X*. Unfortunately, the e^{-x^2} function in Equation 1 does not have an elementary antiderivative. Therefore, numerical means must be used to evaluate its integrals involving the normal distribution. A Microsoft Excel[1] spreadsheet (Reference [3]) was used to derive the function and the curve in Figure 2.

[1] Microsoft Excel™ is a trademark of the Microsoft Corporation in the United States and/or other countries.

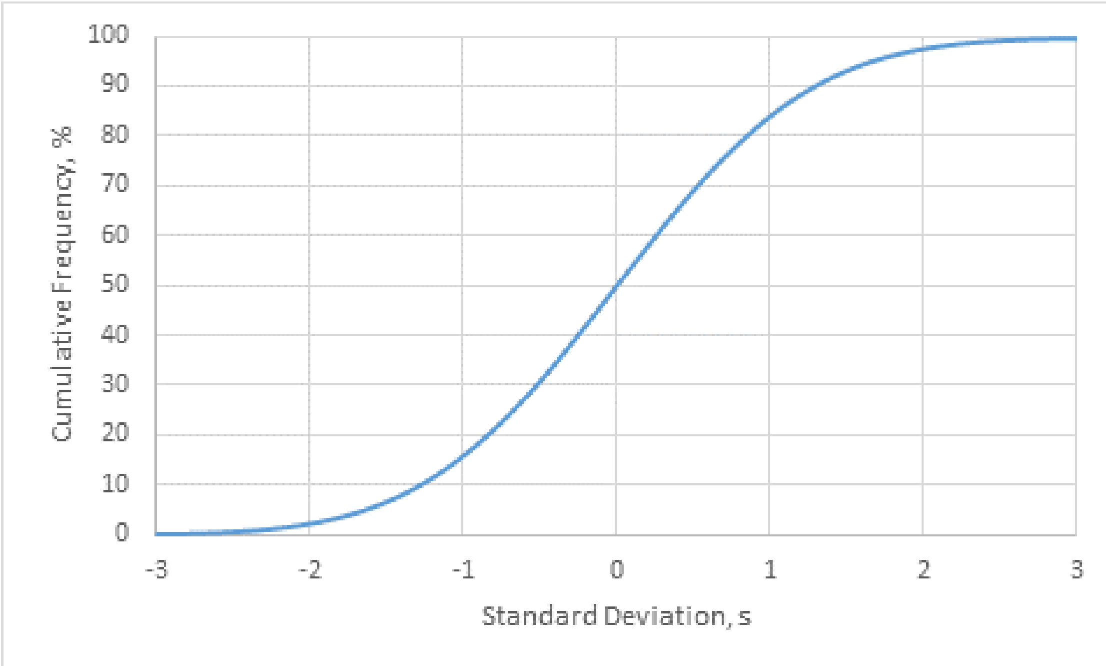

Fig. 2. Normal Cumulative Distribution Function.

Notice that the curve has *Cumulative Frequency, %* on the y-axis. However, to be useful for correlation with a random number generator in the G2 model, the axes were flipped in the spreadsheet—which produced Figure 3. Excel trendline functions were used to produce the best curve fit, as shown in the figure.

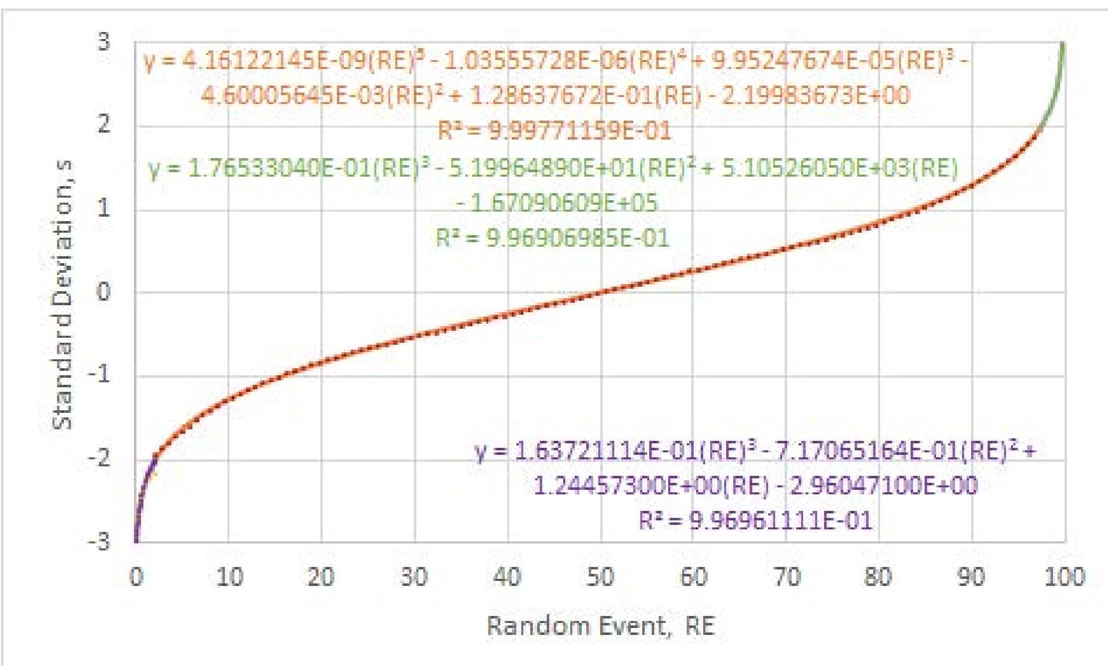

Fig. 3. Approximating Equations for the Number of Standard Deviations Versus Random Events.

A random number generator (between 0 and 100) can be used with this curve fit to incorporate uncertainty into the flowsheet. For example, if the random number generator picked the following random event numbers:

- 50.00, then the presumed sample value would be right at 0.00 SD.
- 2.61, then the presumed sample value would be at −2.00 SD.
- 97.49, then the presumed sample value would be at +2.00 SD.

Placing Uncertainty in Analytical Sample Values

The DOE is funding research and technology efforts to develop higher waste loading[2] for low-activity waste (LAW) glasses. Part of this effort is described in Reference [4]. That report tabulates the one-SD values for most of the elements that will be analyzed by plant operators. Table I in this study is an excerpt of Table A-2 from the cited report. Even though the values were derived with the concentrate receipt vessel (CRV) sampling in mind, the values were applied to all sampling in the G2 flowsheet. Figure 4 shows a simplified schematic of the DFLAW process, which is housed in three facilities. The WTP LAW Facility houses the vitrification equipment. The CRV vessel is in the LAW concentrate receipt process system's icon shown in Figure 4. The CRV vessel receives pretreated LAW from the low-activity waste pretreatment system (LAWPS) and recycles from the Effluent Management Facility (EMF). The recycles essentially consist of captured emissions from the vitrification process that have been removed by the WTP LAW offgas treatment system, sent to the EMF, and concentrated by the evaporator therein.

Table I gives analytical high values and analytical low values in percent relative standard deviation, which means the values tend to be higher or lower than the median value. The G2 flowsheet assumes that three samples are taken and then the results are averaged. Taking three samples greatly reduces the uncertainty.

The previous paragraph describes analytical variability of the sample, assuming that the sample is representative. Table I cites the representativeness of the samples varying by an SD of ±1.47%.

[2] Waste loading is the percentage of the glass mass comprised of Hanford tank waste. Mass is calculated as oxide(s). For example, sodium as Na_2O, calcium as CaO, and sulfur as SO_3.

TABLE I. Vessel Analytical, Mixing, and Sampling Percent Relative Standard Deviation per Immobilized Low-Activity Waste Algorithm

Element	MRQ mg/L	Analytical High %RSD	Analytical Low %RSD	CRV mix/samp %RSD
Ac	NA	NA	NA	NA
Ag	0.2	20	5	1.47%
Al	18	5	5	1.47%
Am	NA	NA	NA	NA
As	2.8	25	10	1.47%
B	0.4	25	10	1.47%
Ba	0.4	15	5	1.47%
Be	0.03	25	5	1.47%
Bi	0.9	15	10	1.47%
Ca	2	15	5	1.47%
Cd	0.06	10	5	1.47%
Ce	2	25	10	1.47%
Cl	19	10	10	1.47%
Cm	NA	NA	NA	NA
Co	0.1	25	10	1.47%

Note: MRQ = minimum reportable quantity; %RSD = percent relative standard deviation; NA = not applicable

Analytical Sample Locations

The G2 flowsheet model's sampling were performed at LAWPS staging vessels and EMF recycle/return vessels and not the CRV itself, which is in line with the WTP Project's present sampling strategy[3]. The G2 model made decisions on transfers between systems shown in Figure 4, which were based only on measured analytical sample results and measured tank volumes (with the uncertainties incorporated).

Placing Uncertainty in Tank Level-Volume Measurement

According to studies in Reference [5], the one-SD in height that can be measured by radar in vessels is 0.394 inches (rounded up to 0.4 inches). Based on this, the one-SD values for the concerned vessels are given in Table II.

TABLE II. Standard Deviation per Volume Measured in a Vessel

Vessel	ID, ft.	RSD_{TL}, gal	$RSD_{TL,}$ liter
CRV-00001/00002	14	38.38	145.3
MFPV-00001/00003[4]	11	23.70	89.71

Note: ID = inner diameter; RSD = relative standard deviation

[3] *Sampling the CRV itself will require a costly around-the-clock laboratory staff and possible sampling delays awaiting sampling results.*
[4] *The MFPVs are fed by the CRV. The MFPV also receive the glass former chemicals, per the glass recipe, which are fed to glass melters.*

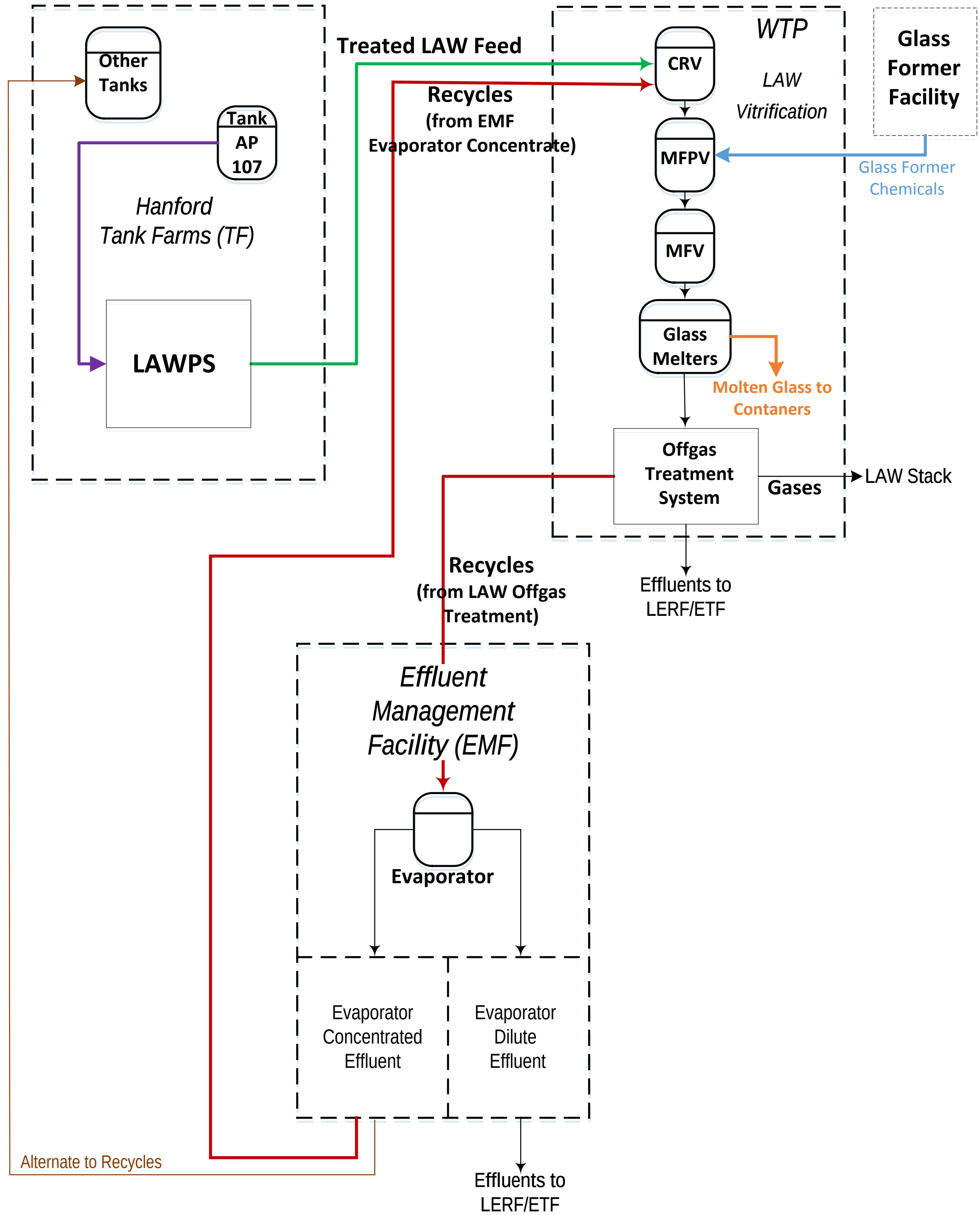

Fig. 4. Simplified Schematic of the DFLAW Treatment System.

Determining Glass Formers for DFLAW Glass

Glass former amounts were added to the melter feed preparation vessels (MFPV) as determined with a LAW glass chemistry known as the LAW Glass Shell, version 2.0 routine using presumed data [6]. The glass routine is consistent with Reference [4].

Melter Off-Gas Uncertainty

What the melter releases to the offgas system and then recycles through EMF can vary considerably from batch to batch. The Vitreous State Laboratory discovered this through various melter runs it performed and reported in Reference [7]. Table A-3 of Reference [5] presents a compilation of the various reports and expresses the variability with results from a PERT (Program Evaluation and Review Technique) simulation program. The same results are shown in Table III. The uncertainty curve for this distribution is not a typical bell shape, but a lopsided triangle, used with asymmetrical DF values.

TABLE III. Melter DF in Ln(DF) (only a portion of table shown)

Component	ln(DF), Min	ln(DF), Median	ln(DF), Max	Notes[a]	ν_b, Nominal[b]
Ac2O3	2.9601	6.8772	11.1239	Non-volatile	0.99721
Ag2O	1.8563	4.1940	6.4944	Semi-volatile	0.97803
Al2O3	5.0764	7.0814	8.8901	Non-volatile from data	0.99888
Am2O3	1.8563	4.1940	6.4944	Semi-volatile	0.97803
As2O5	0.0945	1.5296	4.2370	Volatile	0.77121
B2O3	3.7080	4.5886	5.8519	Semi-volatile from data	0.98968
BaO	2.9601	6.8772	11.1239	Non-volatile	0.99721
BeO	2.9601	6.8772	11.1239	Non-volatile	0.99721
Bi2O3	1.8563	4.1940	6.4944	Semi-volatile	0.97803
CaO	5.2311	7.0825	8.6034	Non-volatile from data	0.99892
CdO	2.9601	6.8772	11.1239	Non-volatile	0.99721
Ce2O3	2.9601	6.8772	11.1239	Non-volatile	0.99721
Cl	0.0979	0.7583	1.9095	Volatile from data	0.54407
Cm2O3	2.9601	6.8772	11.1239	Non-volatile	0.99721
CoO	2.9601	6.8772	11.1239	Non-volatile	0.99721
Cr2O3	1.8563	3.0681	5.3033	Semi-volatile from data	0.95261

DFLAW Glass Former Uncertainty

Glass Former Chemical Weighing Uncertainty

Equation 2 is from Appendix E of Reference [4]. Appendix E is titled *Uncertainties for GFC Mass Measurements*. The equation calculates the expected precision (as an SD value) for weighing each glass former chemical (GFC).

$$s_{weight}^{WH} = \sqrt{3\left(\frac{2}{3}SPC_{CE}{}^{2} + SPC_{NR}{}^{2}\right)} \qquad \text{(Eq. 2)}$$

Where:

s_{weight}^{WH} = SD for weigh hopper weight measurement (kg)

SPC_{CE} = Specification for combined error, as given in the data sheet for each load cell, which includes linearity and hysteresis errors (kg)
SPC_{NR} = Specification for non-repeatability, as given in the data sheet for each load cell (kg)
3 = Three load cells

There are two different types of weighing stations; their use depends on the amount of GFC normally used. The SD is different for each.

<u>Standard Deviation for Achieving Weighing Target</u>
This error relates to timing and control of weighing. For example, how quickly the equipment can stop placing GFC in the weighing station when the scale shows the target amount is reached. The error's estimate is assumed to be usually within 1 kg. This number will be better known after process startup and operations.

<u>Multiple Weighings of Glass Former Chemical</u>
Most GFCs require several weighings in order to supply the amount needed for the MFPV batch. Each weighing will require a newly calculated event with its SD.

<u>Supplied Glass Former Chemical Uncertainty</u>
The composition of oxides in GFCs are considered to vary within each new GFC truckload. The distribution of variance in the GFC is envisioned as being lopsided, with more being to either the left or right side of the distribution. Refer to Appendix G of Reference [4] for more details on GFC values. The G2 model changed the oxide composition of GFCs in the silo when a new GFC truck delivery arrives.

RESULTS

The WTP Project still needs to perform model runs with the glass former uncertainties. Even so, the results may be surprising because of the wide range of variables and uncertainties; therefore, it is expected to have large differences with the certainties incorporated. Table IV lists the key differences for the DFLAW runs thus far. The uncertainties included in the "With" scenario are analyte concentrations, sample volume, and tank volume. The "With Offgas DFs" scenario also includes impacts from melter decontamination factors (DFs) fluctuations, which (in turn) cause fluctuations in the process offgas, then recycle streams, and then finally glass production.

TABLE IV. Mission Key Results

Uncertainty	Containers Made	Treatment Duration, years
Without (Baseline)	14,789	7.65
With	15,155	7.80
With Offgas DFs included	15,230	7.78

In addition, the sodium waste loading in the LAW glass made is good. Figure 5 shows that, while modeling uncertainty, there are some fluctuations in the process, but they are mild. Individual MFPV batches may have slightly higher or slightly lower waste loadings, but the process stays in check.

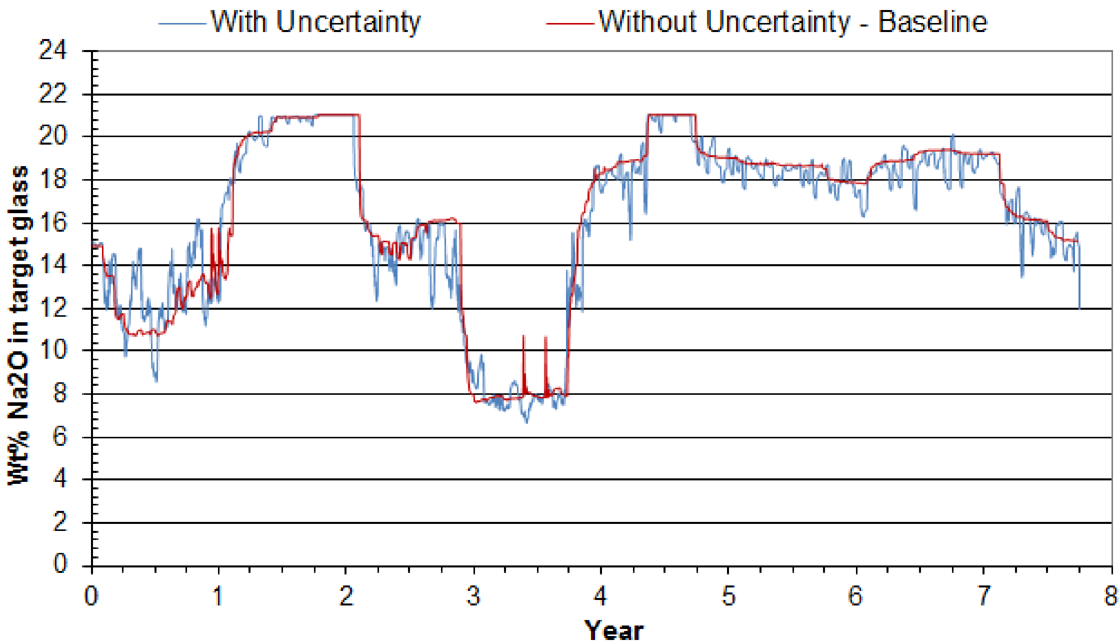

Figure 5. Sodium Waste Loading (Na_2O) in Low-Activity Waste Glass.

With good waste loading shown from the uncertainty modeled, the glass is also still good. Figure 6 shows that modeling uncertainty places some fluctuations in the glass properties, but they are mild. The glass viscosity and electrical conductivity of the glass are always within or close to normal ranges. Some of the uncertainty batches drop a little below the Baseline curve; however, this is manageable. This can be dampened by the mass of glass in the melter. There are about three days' worth of glass in the melter. Almost all batches for the product consistency test, which is important for disposal, are within the limit (2.0 g/m^2). Those batches that are not within that limit are only slightly outside the range, but they are offset by the next batch(es) that are below the limit. Also, some batches are outside the vapor of hydration limit (50 g/m^2·per day) for both the certain and uncertain scenarios. This is because the vapor of hydration property model has a sodium concentration term that is squared—i.e., $(Na_2O)^2$—and it is very sensitive to high-sodium concentrations. Reducing the sodium concentration to around 19.5 wt% would eliminate the problem in both scenarios.

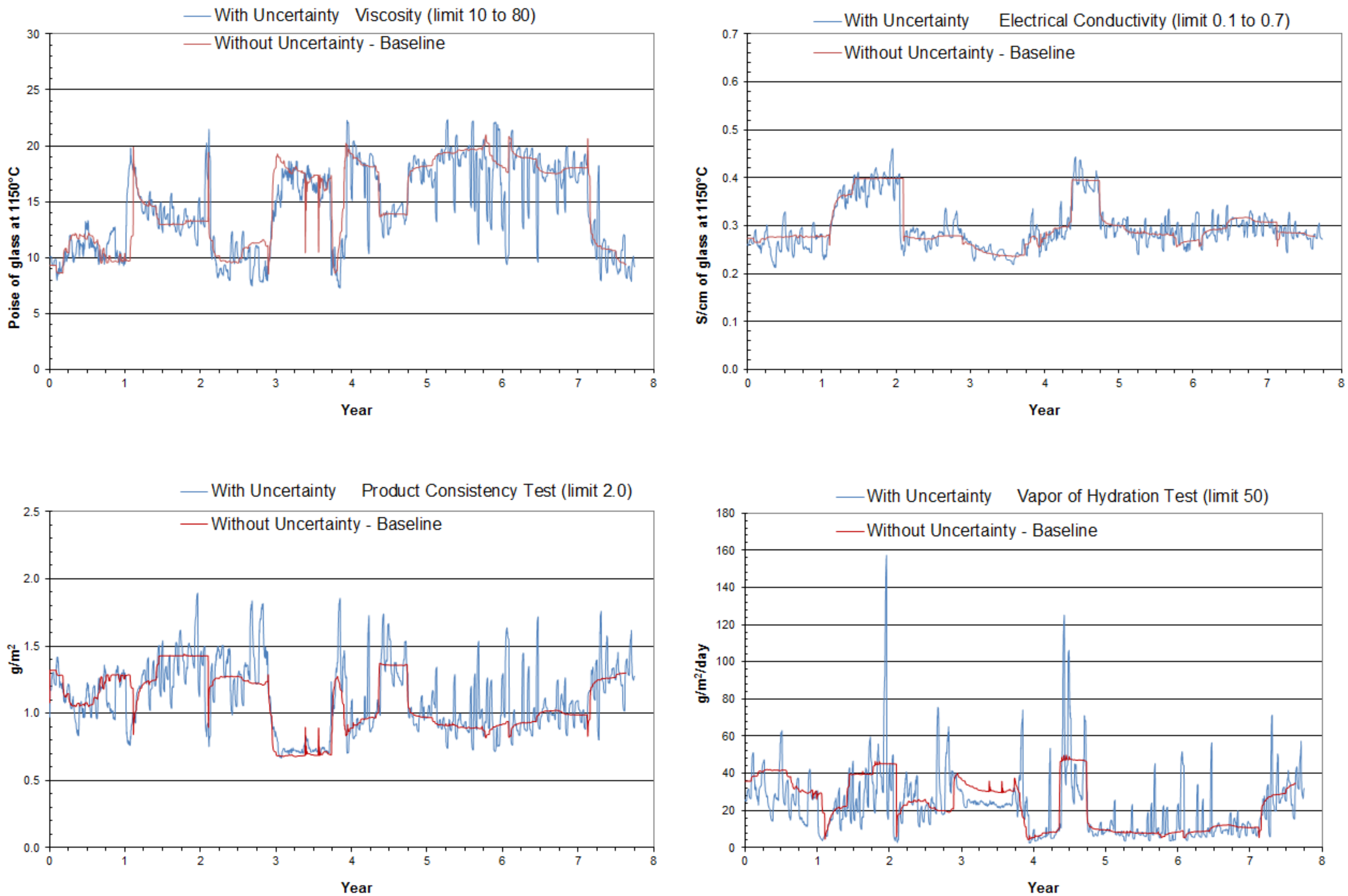

Fig. 6. Glass Properties of the Immobilized Low-Activity Waste Glass Made.

CONCLUSION

Without a sophisticated flowsheet model, process engineers and statisticians calculate the collective impacts of a large system by adding the extreme values of individual uncertainties. The G2 model runs for the DFLAW process show that this combined effect rarely happens and the properties of the actual glass normally hover around the mean values. The results show that uncertainty does affect the process; however, the effects are not as serious as initially thought. The process can be operated when taking measurement and analytical results at face value and making process decisions accordingly. Uncertainty does produce frequent up-and-down spikes in the process, which results in changes to the batches feeding the melters. However, the properties of the glass generally remain within acceptable limits. A few batches may spike outside the acceptable range, but that spike can be mitigated by the large inventory of glass in the melter itself that can dampen sudden change.

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ACKNOWLEDGEMENTS

This work is performed in support of the US Department of Energy, under DOE Contract DE-AC27-01RV14136.