

THE IMPACT OF THE PROPOSED ΔG_p LIMITS ON GLASS FORMULATION EFFORTS: Part I. Model-Based Assessments

D.K. Peeler
T.B. Edwards
A.S. Taylor

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Immobilization Technology Section
Savannah River National Laboratory
Aiken, SC 29808

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EXECUTIVE SUMMARY

The Savannah River National Laboratory (SRNL) has initiated studies to assess alternative durability options that may provide access to compositional regions of interest in support of the accelerated clean-up mission at the Defense Waste Processing Facility (DWPF) (Peeler and Edwards 2003a). One of the options being pursued is the redefinition of the durability model acceptability limits. In response, Edwards et al. (2003) identified and eliminated some of the conservative steps utilized in establishing the current limits without comprising the high confidence required for meeting the specification on the wasteform quality. The results led to a set of three new Property Acceptability Region (PAR) values for the preliminary glass dissolution estimator or free energy of hydration durability model (ΔG_p) (Jantzen et al. 1995) which have the potential to allow access to compositional regions of interest to improve melt rate or waste throughput.

Although these limits are available for implementation, there is currently no driving force to do so (i.e., the current Frit 418 – Sludge Batch 3 (SB3) system is liquidus temperature (T_L) limited). In this report, glass formulations were identified with the intent of generating incentive for applying the new durability limits for SB3. More specifically, higher alkali frit compositions were identified or developed to transition into and through the region of ΔG_p acceptability as defined by the current and proposed durability limits. All other property prediction criteria were satisfied.

An eight glass test matrix has been identified to meet these objectives. These glasses will be fabricated in the laboratory and their durability measured and compared to model predictions (and to the assessments by the index system). Although incentive for implementation of the proposed durability limits could be demonstrated through the measured durability response for these higher alkali systems, assessments of melt rate should also be performed to establish a clear motive or driver to implement a frit change. More specifically, a “significant” increase in melt rate may be required to provide the incentive for DWPF to implement the change rather than a “paper study” and/or durability assessment. The experimental results (both durability and melt rate) will be the focus of a subsequent report.

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LIST OF ACRONYMS

ADT	Alternative Durability Task
AGCR	Acceptable Glass Composition Region
CBU	Closure Business Unit
DWPF	Defense Waste Processing Facility
ΔG_p	preliminary glass dissolution estimator or free energy of hydration (in kcal/mol)
EA	Environmental Assessment
HLW	high level waste
MAR	Measurement Acceptability Region
PAR	Property Acceptability Region
PCCS	Product Composition Control System
PCS	Process and Control Services
PCT	Product Consistency Test
PHA	Precipitate Hydrolysis Aqueous
QA	quality assurance
SB	sludge batch
SME	Slurry Mix Evaporator
SRNL	Savannah River National Laboratory
T_L	liquidus temperature
TTR	technical task request
η	viscosity
WL	waste loading

1.0 INTRODUCTION

In support of accelerated mission goals, glass formulation efforts have been focused on melt rate and waste loading (WL) which ultimately dictate waste throughput for the Defense Waste Processing Facility (DWPF). With respect to melt rate, the general trend for improvement has been to enhance the total alkali concentration in the glass system by increasing the alkali concentration in the frit (Lambert et al. 2001), utilizing (or targeting) a less washed sludge, or using a combination of the two. Previous assessments have indicated that as higher alkali systems are pursued, a transition can occur in which predictions of durability begin limiting upper waste loadings rather than predictions of liquidus temperature (Peeler and Edwards 2002). Recent results have also suggested that the current durability model can lead to conservative decisions during the Slurry Mix Evaporator (SME) acceptability process (Peeler et al. 2001 and Cozzi et al. 2003). More specifically, the model has restricted access to glass compositional regions that could potentially enhance melt rate, waste loading, or waste throughput by classifying a specific glass composition as “unacceptable” whose experimentally determined durability (as defined by the Product Consistency Test (PCT)) is “acceptable” relative to the Environmental Assessment (EA) glass (WAPS 1996).

Part of the strategy used in establishing current SME acceptability criteria centered on the definition of an “acceptable” ΔG_p limit. This limit is currently used to classify a specific SME batch as acceptable (or unacceptable) from a product performance perspective (i.e., durability as measured by the PCT (ASTM 2002)). It is a model-based limit in that its value was developed through the application of models that relate the PCT response for boron, sodium, and lithium of a glass to the free energy of hydration (the ΔG_p) of the glass (Jantzen et al. 1995). The ΔG_p of a glass is determined from the chemical composition of the glass. For SME acceptability, the current Property Acceptability Region (PAR) ΔG_p limit is approximately -12.78 kcal/mol (as reported by Brown, Postles, and Edwards (2002)), and a predicted ΔG_p value (based on a measured SME analysis) less than this would result in the classification of the SME batch as “unacceptable” from a durability perspective.

As currently established, excessive conservatism is believed to be factored into this ΔG_p limit, which could potentially restrict the DWPF from accessing specific compositional regions that may be of interest. As previously noted, specific regions of interest include high-level waste (HLW) glasses at higher alkali concentrations. A recent example of the compositional restriction occurred during the development of Frit 320 for Sludge Batch 2 (SB2) (Peeler et al. 2001). Although Frit 304 (a higher alkali frit relative to Frit 320) demonstrated the highest melt rate for SB2, it was not recommended to DWPF for implementation due to ΔG_p predictions. The current model classified this glass (at 25% WL) as “unacceptable”, but experimental assessment indicated that the durability was acceptable (normalized boron release (NL [B]) was 1.09 g/L compared to 16.695 g/L associated with the EA glass (Jantzen et al. 1993)). The full extent of potential gains in melt rate for this sludge may not have been realized due to model predictions and the conservative limit for ΔG_p .

The Savannah River National Laboratory (SRNL) has initiated studies to assess alternative durability options that may provide access to compositional regions of interest in support of the accelerated clean-up mission at the DWPF. This effort is in response to a Technical Task Request (TTR) issued by DWPF (Occhipinti 2003). Four options are under study as potential replacements for or modifications to DWPF’s SME acceptability decision process. As described by Peeler and Edwards (2003a), the alternatives being considered are: (1) reassessing and/or redefining the current ΔG_p limit in the Product Composition Control System (PCCS), (2) utilizing

a non-parametric approach, (3) developing empirical models, and (4) defining an Acceptable Glass Composition Region (AGCR). The candidate options could have varying degrees of complexity in terms of their potential impact to PCCS modification and/or implementation and thus personnel in DWPF's Process and Control Services (PCS) were requested to perform an assessment of the possible advantages or disadvantages of each approach. In response to that request, Manz (2003) issued a supplementary report that indicated all four options appear to be technically feasible to incorporate into PCCS. The different options presented varying degrees of complexity for implementation. Based on that assessment, Manz (2003) suggested that the option associated with reestablishing the current ΔG_p limits option would have the least impact on PCCS given it is a one time change (i.e., it is not batch dependent) and essentially involves a rudimentary change to specific (but limited) values in the PCCS ΔG_p SME acceptability limits for boron, lithium and sodium.

Given the guidance by Manz (2003), Edwards et al. (2003) revisited the technical basis from which the current durability SME acceptability limits were established. The specific objective was to identify and eliminate some of the conservative steps utilized in establishing the current limits without comprising the high confidence required for meeting the specification on the wasteform quality. The results led to a set of three new values for ΔG_p : -14.1058, -13.8695, and -14.1991 kcal/mol for boron, lithium, and sodium, respectively. It should be noted that the more conservative limit (-13.8695 kcal/mol for lithium) is typically used to assess various compositions for acceptability.

Although these limits are available for implementation, there is currently no driving force to do so. More specifically, model-based predictions for the Frit 418 – SB3 system are liquidus temperature limited (followed closely by low viscosity). Predictions of durability are not an issue over the entire WL range of 25 – 60% for that system. However, the new durability limits could provide an opportunity to increase the total alkali content in the glass (either through the use of an alternative frit or by addition of trim chemicals) in an effort to increase melt rate and ultimately total waste throughput.¹

Objectives for this task are specified in Section 2.0. In Section 3.0, the nominal sludge composition used for these assessments is provided. Section 4.0 summarizes the glass selection strategy used to meet the stated objectives. In Section 5.0, the Measurement Acceptability Region (MAR) assessments are provided for various glass forming systems of interest. The discussions lead to the development of a test matrix which is presented in Section 6.0. A summary is provided in Section 7.0.

¹ Given SB3 has already been qualified and also contains Np, the ability to increase the alkali concentration in glass through sludge washing is no longer an option.

2.0 OBJECTIVE

The objective of this task is to investigate (and potentially generate) incentive for applying the proposed durability limits in PCCS from a glass formulation perspective. This task will assess compositional changes to the frit that could be made in an attempt to increase melt rate and/or waste loadings which together ultimately drive waste throughput issues for DWPF. The compositional changes will be specific to the SB3 system with Frit 418 serving as a baseline case from which alternatives will be assessed. The specific compositional adjustments to be made will include an assessment of higher alkali contents (given their known impact on melt rate) relative to Frit 418. Higher alkali containing frits will be developed and assessed that transition into and through the region of ΔG_p acceptability as defined by the current and proposed durability limits. Specifically, glasses will be defined that:

- (1) fail the MAR for the current durability limit (-12.78 kcal/mol) but pass the MAR for the proposed durability limit (-13.8 kcal/mol), and
- (2) fail the MAR for both the current and proposed durability limits while maintaining acceptable predictions for all other properties.

This work scope will be completed in a “phased” approach. The first phase (the focus of this report) will be a paper study assessment in which glass compositions meeting the stated objectives can be identified. The second phase will be an experimental assessment of the identified glasses in which measured durability responses will be compared to model predictions. The results of the experimental portion, Phase 2, will be documented in a subsequent report. In addition, assessments of melt rate should be performed on select glass forming systems to establish a clear motive or driver to implement a frit change. More specifically, a “significant” increase in melt rate may be required to provide the incentive for DWPF to implement the change. Assessments of melt rate will also be documented in a subsequent report.

It should be noted that although this study is focus on SB3, the incentive to implement the proposed durability limits may be advantageous to glass formulation efforts for future sludge batches. For example, access to higher alkali contents via the relaxed constraints may reduce liquidus temperatures for systems with relatively high concentrations of troublesome components (such as NiO, Cr₂O₃, and/or MnO).

The results of the current work will be the identification of alternative frits for SB3 that could be used to improve melt rate while still maintaining an acceptable product performance through the implementation of the proposed durability limits (see (1) above). Glasses will also be fabricated to “challenge” the proposed limits to identify additional conservatism within the use of the current durability approach (see (2) above). A positive result for this latter issue would provide incentive to continue the assessment of the other possible durability options as outlined by Peeler and Edwards (2003a).

This work has been prepared to address technical issues identified in a TTR (Occhipinti 2003) and in accordance with the Task Technical and Quality Assurance Plan (Peeler, Edwards, and Herman 2003). It is noted that this work is being performed under RW-0333P Quality Assurance (QA) requirements as specified in the TTR.

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3.0 SLUDGE COMPOSITION

Various SB3 compositional projections have been used recently to identify candidate frit compositions and to assess projected operating windows (Peeler and Edwards, 2003b). To support this task, the latest compositional projections from the Closure Business Unit (CBU) in March of 2004 will be used.² More specifically, the CBU provided three projected compositions based on various scenarios regarding SB3 given some uncertainties associated with the transfer volumes of Tank 40 and a secondary neptunium (Np) stream. These compositions were designated as: (1) baseline – Tank 51 + Tank 40 blended on 3/8/2004 + 70% of the Np solution in Tank 16, (2) Tank 40 current conditions + 4 of the 7 Np transfers, and (3) Tank 40 current conditions + 7 of the 7 Np transfers. The projected compositions are shown in Table 3-1. It is noted that the three compositional views are very similar with differences in the major oxides being less than 1.0% on a relative basis (i.e., Na₂O ranges from 20.773 wt% in the Tank 40 + 4 Np transfer case to 21.608 wt% in the baseline case). These minor differences have no significant impact on the sludge composition to be selected and used in this assessment. Since durability is the major focus of this report, the projected composition with the highest Na₂O concentration (the “baseline” case as defined by the CBU) was selected.

Table 3-1. Projected Compositions for Three SB3 Cases.

(compositions provided by H.H. Elder on 3/15/04)

Oxide	Baseline	Tank 40 + 4 Np Transfers	Tank 40 + 7 Np Transfers
Al ₂ O ₃	15.022	14.946	14.870
BaO	0.145	0.156	0.156
CaO	2.854	2.966	2.952
Ce ₂ O ₃	0.234	0.258	0.258
Cr ₂ O ₃	0.234	0.248	0.248
CuO	0.088	0.100	0.100
Fe ₂ O ₃	32.082	33.083	32.897
K ₂ O	0.205	0.229	0.229
La ₂ O ₃	0.114	0.140	0.127
MgO	3.499	3.532	3.515
MnO	6.559	6.353	6.327
Na ₂ O	21.608	20.773	21.218
NiO	1.731	1.731	1.731
PbO	0.140	0.162	0.162
SiO ₂	3.038	2.909	2.888
ThO ₂	0.034	0.046	0.046
TiO ₂	0.033	0.033	0.017
U ₃ O ₈	10.082	10.094	10.047
ZnO	0.149	0.174	0.174
ZrO ₂	0.261	0.313	0.313
Total	98.113	98.246	98.275

² This effort was started prior to the introduction of SB3 into DWPF. Although a projected composition is being used to support this study, recent DWPF analyses indicate no significant differences in the oxide concentrations. The compositional projections were made available by H.H. Elder on March 15, 2004.

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4.0 GLASS SELECTION STRATEGY

To meet the stated task objectives (see Section 2.0), model-based assessments were performed to identify a series of glass compositions that would transition from “acceptable” to “unacceptable” as predicted by both the current and proposed durability limits. Initial assessments were performed with Frit 418 with supplemental frits being developed to challenge durability predictions with the primary focus being increased alkali content. In addition, Frit 202 was assessed in terms of the projected operating window and predicted properties given recent interest in the potential impact of viscosity on pour stream stability. Recent DWPF operations have been hampered by the need to clean the pour spout bellows due to the accumulation of glass. Theories have surfaced that relate the interval between required cleanings to the predicted viscosity of the glass. More specifically, a “soft” link has been made that suggests that as the viscosity of the glass decreases, the time between cleanings decreases (cleaning more frequently). Overall attainment is not only linked to melt rate (the primary driver for higher alkali systems) but also to down-time due to “maintenance” (canisters are not being filled during the bellows cleaning operation) among other factors. This sets up a potential need to balance “optimizing” melt rate (with higher alkali systems) and the overall attainment (with a higher viscosity system, assuming other physical changes such as the heated bellows are not effective). Therefore, model-based assessments were performed with Frit 202 (which should yield a higher predicted viscosity relative to Frit 418) and with other alternative (higher alkali) frits to improve melt rate. These model-based assessments will be supplemented by experimental assessments of durability and melt rate which will be documented in subsequent reports.

Figure 4-1 shows a conceptual view (not to scale) of the frit development efforts needed to meet the stated objectives of this study. Model based predictions indicate that the Frit 418 – SB3 system is T_L limited with durability not being an issue over the entire WL interval of 25 – 60% WL. Therefore, the Frit 418 – SB3 system is shown to the right of the current SME acceptability limit indicating it is acceptable from a durability prediction standpoint. The Frit 202 – SB3 system is expected to have even a more positive ΔG_p value (relative to the Frit 418 – SB3 system) given the lower total alkali content. It is anticipated that the MAR-based assessments for the Frit 202 – SB3 system will not be restricted by durability predictions but by T_L as is the Frit 418 system.

Point A represents a glass system in which the current ΔG_p limits are not met but the proposed limits would classify as acceptable. Point B represents a glass system which fails both the current and proposed limits. Note, the EA glass is also shown in this region. Again, the strategy is to increase the alkali content in Frit 418 to transition into and through the region of ΔG_p acceptability as defined by the current and proposed durability limits. Once the task objectives are satisfied on paper (based on model-predictions), glasses will be fabricated and their durability measured via the PCT (ASTM 2002). Measured durabilities will be compared to model predictions to provide additional data regarding the confidence of the proposed limits as well as the potential (or additional) conservatism of the ΔG_p model.

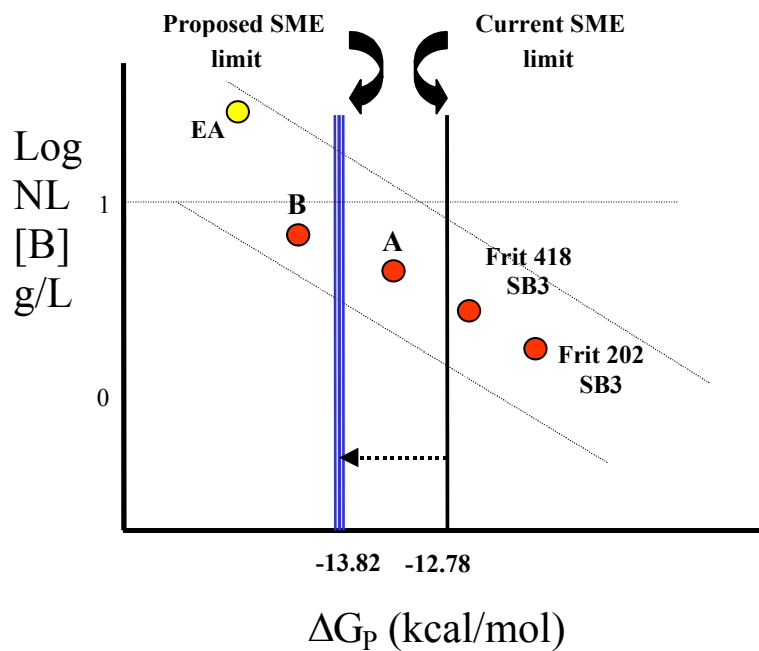


Figure 4-1. Conceptual View of log NL [B] (g/L) Versus ΔG_p .³

³ The vertical lines shown in Figure 4-1 represent the PAR limits associated with the current and proposed durability limits. The points representing the targeted glass compositions have been placed relative to these PAR limits based on assessments at the MAR for this conceptual view.

5.0 MAR ASSESSMENTS

The property predictions assessed in this study included the durability response in terms of ΔG_p using the current (Jantzen et al. (1995)) and proposed (Edwards et al. (2003)) limits, viscosity at 1150°C ($\eta_{1150^\circ\text{C}}$), T_L , and Al_2O_3 and alkali concentrations. Jantzen et al. (1995) and Brown et al. (2001) provide a more detailed discussion on the development of these models. To establish or project operational windows for sludge/frit scenarios of interest, the predicted properties must be assessed relative to established acceptance criteria. Acceptable predicted properties for this assessment are based on satisfying the more restrictive MAR limits. Brown, Postles, and Edwards (2002) provide a detailed discussion of how the MAR limits are utilized in PCCS.

Appendix A provides some of the key property predictions and glass compositional information for the systems of interest which ultimately were used for the PCCS MAR assessment. The last column of Table A1 in Appendix A provides a summary of the MAR assessment at each WL. The presence of a “-” indicates that the targeted glass composition is classified as processable based upon PCCS model predictions (i.e., all process and product performance predictions are acceptable at the MAR). The presence of “hvisc”, T_L , “Del Gp”, and/or “lvisc” indicate that predictions of high viscosity, liquidus temperature, durability, and/or low viscosity exceed their respective MAR limits.

Table 5-1 summarizes the MAR assessments for various frits when coupled with the SB3 baseline composition (see Table 3-1). In Table 5-1, the projected operating windows (expressed in terms of a WL interval) are provided along with the property (or properties) that limit access to higher WLs. For each system, projected operating windows are provided based on the use of the current and proposed durability limits. Appendix B provides details associated with each system assuming implementation of the proposed ΔG_p limits.⁴ The nominal frit compositions are shown in Table 5-2.

Since this task was initiated, DWPF has begun processing SB3 using Frit 418. Table 5-1 indicates that the projected operating window is relatively large (25 – 46% WL) using the nominal baseline SB3 composition and the current durability limits. At 47% WL, the system is both T_L and low viscosity limited. Implementation of the new durability limits does not change the projected operating window for the Frit 418-based system given it is T_L and low viscosity limited – providing no incentive to implement the proposed ΔG_p limits for SB3 with Frit 418.

Frit 202 was developed as a frit for “generic” coupled operations (sludge plus high alkali from precipitate hydrolysis aqueous (PHA)) (Jantzen 1988). Although “coupled” operations is not anticipated during processing of SB3, the fact that the sludge was “underwashed” to provide higher sodium concentrations makes Frit 202 an attractive alternative candidate for SB3. The projected operating window for the Frit 202-based system is 28 – 39% WL based on the use of the current durability limits. Predictions of viscosity exceeding the upper control limit restrict access to lower WLs (below 28%) – an indication that the viscosity of that system is higher as compared to the Frit 418 based system at each WL. Predictions of T_L limit access to WLs of 40% and greater. Although Frit 202 has a smaller window than the Frit 418-based system, the window still provides access to rather high WLs as compared to current DWPF processing (targeting ~34% WL). The assessment suggests that Frit 202 could be implemented in DWPF in an attempt to evaluate the impact of the higher viscosity glass system on pour stream stability. However, it

⁴ Appendix C summarizes the MAR assessments for the Frit 433 – SB3 system. Frit 433 was identified through the use of a “compositional grid” as discussed in a later section.

should be recognized that the more refractory frit (less total alkali) may result in a lower melt rate and, therefore, assessments of melt rate should be performed prior to implementation. Although melt rate may be lower, overall attainment may improve assuming down-time for bellows cleaning is minimized. As with the Frit 418-based system, there is no driver to implement the proposed durability limits with Frit 202 and SB3 (i.e., the system is not durability limited).

Table 5-1. MAR Results for Frit 202 and Frit 418 with the Nominal Baseline SB3 Composition.

	Projected Operating Window (using current ΔG_p limits)	Projected Operating Window (using proposed ΔG_p limits)
Frit 418	25 – 46 (T_L / low η)	25 – 46 (T_L / low η)
Frit 202	28 – 39 (T_L)	28 – 39 (T_L)
Frit 425	28 – 40 (ΔG_p)	28 – 41 (low η)
Frit 320	None	28 – 36 (ΔG_p /low η)
Frit 433	None	None

Table 5-2. Nominal Compositions of the Primary and Alternative Frits.

Oxide	Frit 202	Frit 418	Frit 425	Frit 320	Frit 433
B ₂ O ₃	8	8	8	8	8
Li ₂ O	7	8	8	8	5
Na ₂ O	6	8	10	12	15
SiO ₂	77	76	74	72	72
MgO	2	-	-	-	-
Total	100	100	100	100	100

To meet programmatic objectives, alternative frit compositions were needed that transition to and through the region of “acceptability” from a durability limit perspective (refer to Figure 4-1).⁵ Frit 418 and Frit 202 are classified as acceptable over a relatively large operating window and fail to challenge either durability limit approach.

First, consider the use of Frit 425 (nominal composition shown in Table 5-2). Relative to Frit 418, Frit 425 has a 2% higher Na₂O concentration with the difference being accounted for by a 2% increase in SiO₂. The increased Na₂O concentration may potentially enhance melt rate given recent trends observed (Smith et al. 2003). Table 5-1 indicates a projected operating window of 28 – 40% WL given the current durability limits (see Appendix A for more details). At 41% WL, the system becomes durability limited with low viscosity also becoming a limiting factor at 42% WL. Given the system is durability limited, implementation of the proposed ΔG_p limits is expected to have some benefit – although in this case it is minimal. Application of the proposed

⁵ Although some glasses may fail the current SME acceptability criteria for durability, all other process properties will be satisfied.

limits results in a projected operating window of 28 – 41% WL for the Frit 425-based system. At 42% WL, the system is still low viscosity limited – that property prediction does not change with implementation of the proposed durability limits. The 1% increase in WL with the proposed limits is potentially not the incentive needed to either implement the limit change or transition to Frit 425. It is noted, however, that implementation of the proposed limits for the Frit 425 system results in predictions of durability being a non-issue over the entire 25 – 60% WL interval (see Appendix B for more details). Frit development efforts that could delay the onset of the low viscosity limitation in terms of WL could result in a larger operating window given implementation of the proposed durability limits – see discussion below.

Next, consider the use of Frit 320 with the baseline SB3 composition. Frit 320, a higher alkali frit relative to Frit 418, was developed and implemented (Peeler et al. 2001; Lambert et al. 2002) for SB2 to improve melt rate. Given the higher alkali content of both Frit 320 (as compared to Frit 418) and SB3 (as compared to SB2 due to washing), the combination of the two is a step in the right direction in terms of meeting programmatic objectives (i.e., challenging durability). The results of the projected operating windows with the current and proposed ΔG_p limits for the Frit 320-based systems are shown in Table 5-1 (property predictions for these two cases are shown in Appendix A and Appendix B, respectively). With the current ΔG_p limits, Frit 320 is prohibited from use over the entire WL range of interest (25 – 60%) due primarily to predictions of durability. Low viscosity is also a limiting constraint for WLs of 37% and higher. Implementation of the proposed ΔG_p limits results in an operating window of 28 – 36% WL with the system being low viscosity limited at 37% WL. Implementation of the proposed limits would allow Frit 320 to be used with SB3 up to WLs of 36% (based on the nominal SB3 composition used in this study). If melt rate (or waste throughput) is significantly increased (without having a negative impact on pour stream stability given the system is low viscosity limited), there may be incentive to implement the proposed durability limits and transition to Frit 320 for SB3. An assessment of the impact of WL on melt rate and waste throughput is recommended if Frit 320 is considered for use.

The use of Frit 425 could provide a melt rate advantage over Frit 418 given its higher alkali content. However, given the trends observed by Smith et al. (2003), the reduction in upper WL may ultimately reduce waste throughput given melt rate decreases with WL. In addition, there is very little (if any) driving force to implement the proposed durability limits given predictions of low viscosity. Use of Frit 320 does provide some incentive for implementation of the proposed limits. It transitions into the “acceptable” composition region based on the proposed limits but predictions of low viscosity limit the upper WL to a point less than desirable (36% or less).

The last programmatic objective was to develop or identify a frit that challenged both existing and proposed durability limits while maintaining all other properties as acceptable. Keeping with the simple strategy of adding Na_2O to Frit 418 (with the difference being made up by an increase in SiO_2 content), additional alkali increases to Frit 320 would continue to challenge durability predictions. However, as Na_2O contents increase in this system, viscosity predictions decrease. With the Frit 320 – SB3 system being low viscosity limited at 37% WL, any significant increase in alkali (in an attempt to produce a significant increase in melt rate given the less conservative durability limits) would only reduce the upper WL that could be achieved based on low viscosity – a direction DWPF does not wish to take. Instead of a “trial-and-error” approach and given the predicted properties are equation based, the mathematical “grid-approach” (developed by Peeler and Edwards 2003c) was used to identify a frit that could potentially increase the total alkali content and allow access to relatively high WLs (upper 30’s to lower 40’s at a minimum) while challenging both the current and new durability limits.

To do this, a grid was defined based on minimum and maximum oxide ranges for potential frit components (see Table 5-3). To support the development of the compositional grid, incremental steps for each frit oxide were established at 1.0 wt%. This resulted in 4 Al_2O_3 values, 5 B_2O_3 , 5 Li_2O , 8 Na_2O , and 3 ZrO_2 values. It should be noted that the SiO_2 values were allowed to float to provide a sum of oxides of 100%. This approach led to $4 \times 5 \times 5 \times 8 \times 3 = 2,400$ frits in the grid.

Table 5-3. Minimum and Maximum Values for Candidate Frit Oxides.

Oxide	Minimum	Maximum	Increment
Al_2O_3	0	3	1
B_2O_3	8	12	1
Li_2O	4	8	1
Na_2O	8	15	1
SiO_2	60	80	1
ZrO_2	0	2	1

The 2,400 frits were then combined with the nominal SB3 composition at each WL over a range from 30 – 45%. Given 16 individual WLs were used for each of the 2,400 frits, a total of 38,400 glass compositions were developed. To provide guidance on possible frits that would challenge the proposed ΔG_p limits but would maintain all other properties as acceptable, a plot of ΔG_p versus viscosity was produced (see Figure 5-1). These two parameters were selected as a guide given the desire to increased alkali content and the relation between durability and viscosity – in general, as alkali increases, both viscosity and durability decrease. The plot was utilized to identify a set of glasses that challenged the proposed durability limits but maintained acceptable viscosities. Anticipating a ΔG_p MAR value of approximately -13.4 kcal/mol (derived by reducing the -13.82 kcal/mol PAR criteria proposed by Edwards et al. (2003) by a rough estimate of the measurement uncertainty), those glasses with ΔG_p values less than approximately -13.25 kcal/mol with the highest viscosities were selected. This process resulted in 260 glasses being identified. MAR assessments were performed on all 260 glasses over the WL interval of 25 – 60% of which 161 glasses were found to meet all of the programmatic criteria (i.e., failed the PCT MAR based on the proposed limits but maintained all other properties as acceptable). From this list of 161 glasses, one of the “grid frits” was found to allow WLs up to 37% WL (although frits with potentially higher WL may have been possible given the gross nature in which the 260 glasses were selected). This frit was compositionally identified, labeled as Frit 433 (see Table 5-2 for its nominal composition), and used to make a more formal MAR assessment over the entire WL interval from 25 – 60% WL. Appendix C summarizes the MAR based assessments for the Frit 433 – SB3 system. The basis for developing and selecting this frit was to increase the total alkali content, allow access to relatively high WLs (upper 30’s to lower 40’s at a minimum) while challenging both the current and new durability limits. Glasses within this system failed the durability MAR (based on the proposed constraints) over the entire WL range of 25 – 60%. Ignoring durability predictions, the projected operating window would range from 28 – 41% WL with the system being low viscosity limited at 42% WL. Although an upper WL in the low 40’s was achieved, it is interesting to note that with the implementation of the proposed durability limits, predictions of low viscosity become the limiting property for these higher alkali containing frits. In addition, it is noted that the total alkali content of Frit 433 is 20% which is identical to Frit 320 – the difference being the partitioning between Li_2O and Na_2O concentrations. It will be interesting to note any significant differences between these two systems in terms of their response to the PCT or melt rate assessments.

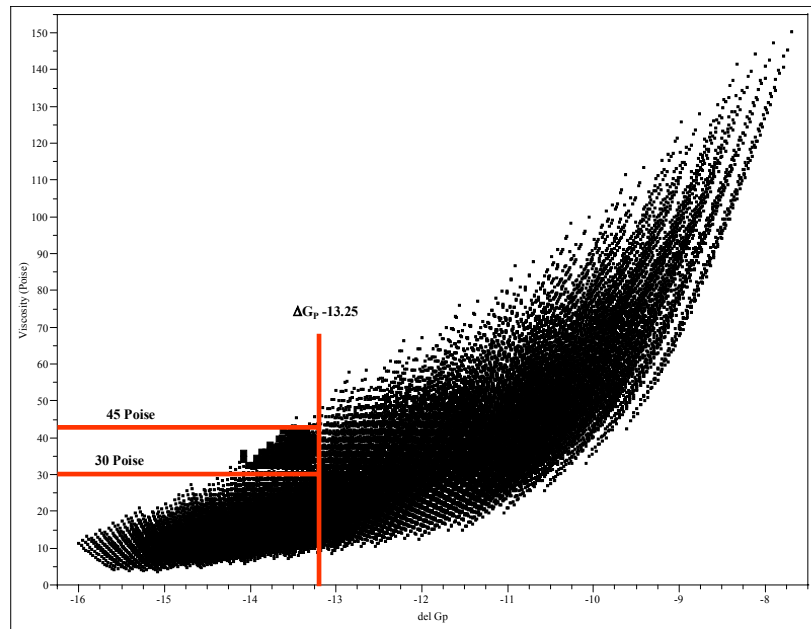


Figure 5-1. Viscosity versus Durability Relationship for Grid-Based Frits.

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6.0 TARGET GLASS COMPOSITIONS

Based on the MAR assessments performed in Section 5.0, glasses can be selected to investigate the incentive of implementing the proposed durability limits in PCCS from a glass formulation perspective. More specifically, glass compositions based on specific frits and targeting specific WLs can be selected to challenge the current ΔG_p limits, the proposed ΔG_p limits, or both. Experimental assessments of durability for these glasses will either confirm the proposed durability limits or possibly identify additional conservatism (Peeler and Edwards (2003a) providing incentive to continue the assessments of the other possible durability options).

In this section, a series of glasses is identified for experimental assessments of durability and/or melt rate. For each frit-based system, two glasses will be selected to meet one of the stated programmatic objectives. Based on a review of the information presented in Section 5.0, Appendix A, Appendix B, and Appendix C, WLs of 35% and 40% were selected to meet the stated objectives. A more detailed analysis of each glass system at 35% and 40% WL and how the selection process fills in the technical gaps is provided below. Table 6-1 summarizes the targeted compositions of the Alternative Durability Task (ADT) glasses. The reader is also referred to Figure 6-1 which provides a conceptual view of the relation between the targeted glass composition (dependent upon frit, sludge, and WL) and programmatic objectives (i.e., the targeted glasses transition into and through the compositional regions of acceptability based on the various durability limits).

6.1 Frit 202 – SB3

Based on the MAR assessments (refer to Section 5.0), the Frit 202 – SB3 system is not durability limited over the entire WL interval of 25 – 60% (regardless of the durability limits used). Based on model predictions, fabricating glasses that target 35% and 40% WL will not provide any insight into “challenging” the current or proposed limits. However, these glasses will provide a basis for the PCT response in case Frit 202 is used in DWPF with SB3 to adjust viscosity (to potentially minimize pour stream instability and increase overall attainment). It is noted that the 35% WL Frit 202 – SB3 glass (ADT-1) is classified as acceptable but the 40% WL glass (ADT-2) fails the T_L MAR.

6.2 Frit 425 – SB3

The Frit 425 – SB3 system becomes durability limited at 41% WL with the current durability limits (projected operating window is 28 – 40% WL). Experimental assessment of durability for Frit 425-based glasses targeting 35 (ADT-3) and 40% (ADT-4) WL also will not provide any insight with respect to challenging the current limits (given ADT-4 is classified as acceptable with the current limits). However, ADT-4 does push the envelope in terms of the upper WL that could be targeted in that system (i.e., at 41% WL predictions of durability are unacceptable).

6.3 Frit 320 – SB3

There is no projected operating window for this system with the use of the current durability limits. Given implementation of the proposed limits, the projected operating window is 28 – 36% WL. Therefore, fabricating Frit 320-based glasses at 35 (ADT-5) and 40% (ADT-6) WL will challenge the use of the current limits at both WLs. In addition, ADT-5 (35% WL) will confirm the use of the proposed limits while ADT-6 (40% WL) could provide insight into additional conservatism. This series of glasses transitions through the compositional region defined by the

current durability limits and into (and ultimately through) an expanded compositional region which is classified as acceptable based on the proposed durability limits.

6.4 Frit 433 – SB3

ADT-7 (35% WL) and ADT-8 (40% WL) will challenge both the current and proposed limits. Both Frit 433-based glasses are predicted to be unacceptable with respect to durability based on model predictions.

**Table 6-1. Target Compositions of the Alternative Durability Task (ADT) Glasses.
(wt%, oxide calcine basis)**

Glass ID	ADT-1	ADT-2	ADT-3	ADT-4	ADT-5	ADT-6	ADT-7	ADT-8
	Frit 202	Frit 202	Frit 425	Frit 425	Frit 320	Frit 320	Frit 433	Frit 433
WL	35%	40%	35%	40%	35%	40%	35%	40%
Oxide	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%
Al ₂ O ₃	5.359	6.124	5.359	6.124	5.359	6.124	5.359	6.124
B ₂ O ₃	5.200	4.800	5.200	4.800	5.200	4.800	5.200	4.800
BaO	0.052	0.059	0.052	0.059	0.052	0.059	0.052	0.059
CaO	1.018	1.164	1.018	1.164	1.018	1.164	1.018	1.164
Ce ₂ O ₃	0.084	0.096	0.084	0.096	0.084	0.096	0.084	0.096
Cr ₂ O ₃	0.083	0.095	0.083	0.095	0.083	0.095	0.083	0.095
CuO	0.031	0.036	0.031	0.036	0.031	0.036	0.031	0.036
Fe ₂ O ₃	11.445	13.080	11.445	13.080	11.445	13.080	11.445	13.080
K ₂ O	0.073	0.084	0.073	0.084	0.073	0.084	0.073	0.084
La ₂ O ₃	0.041	0.047	0.041	0.047	0.041	0.047	0.041	0.047
Li ₂ O	4.550	4.200	5.200	4.800	5.200	4.800	3.250	3.000
MgO	2.548	2.626	1.248	1.426	1.248	1.426	1.248	1.426
MnO	2.340	2.674	2.340	2.674	2.340	2.674	2.340	2.674
Na ₂ O	11.608	12.410	14.208	14.810	15.508	16.010	17.458	17.810
NiO	0.617	0.706	0.617	0.706	0.617	0.706	0.617	0.706
PbO	0.050	0.057	0.050	0.057	0.050	0.057	0.050	0.057
SiO ₂	51.134	47.439	49.184	45.639	47.884	44.439	47.884	44.439
ThO ₂	0.012	0.014	0.012	0.014	0.012	0.014	0.012	0.014
TiO ₂	0.012	0.014	0.012	0.014	0.012	0.014	0.012	0.014
U ₃ O ₈	3.597	4.110	3.597	4.110	3.597	4.110	3.597	4.110
ZnO	0.053	0.061	0.053	0.061	0.053	0.061	0.053	0.061
ZrO ₂	0.093	0.107	0.093	0.107	0.093	0.107	0.093	0.107
Total	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

Figure 6-1 is a conceptual view of the ADT glasses on a log NL [B] (g/L) versus ΔG_p plot which provides a perspective of how each glass relates to the stated programmatic objectives – glass compositions that transition to and through the region of “acceptability” from a durability perspective. Glass compositions resulting from Frit 425, Frit 320, and Frit 433 (at 35 and 40% WL) will provide an opportunity to assess and challenge the proposed durability limits. The

results could provide continued incentive (assuming durable glasses result for most if not all glasses tested) to pursue implementation of the proposed limits or alternative options to control durability. Assessment of the Frit 202 glasses will provide a basis for the use of this frit with SB3 in case a higher viscosity system is pursued.

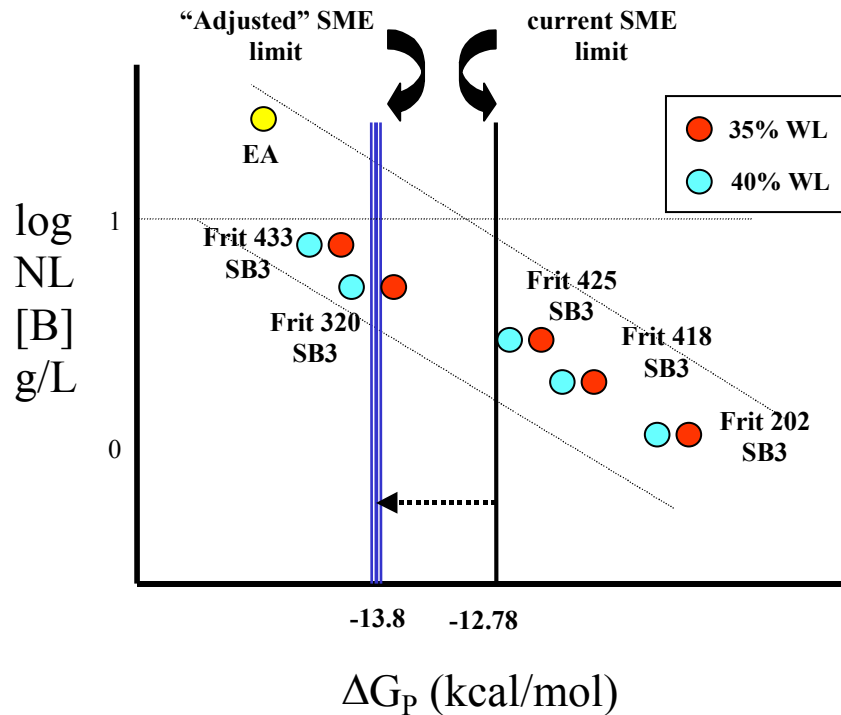


Figure 6-1. Conceptual View of the ADT Glasses within the ΔG_p versus $\log NL [B]$ Diagram.⁶

6.5 Application of the Index System

Although perhaps premature, the index system developed by Brewer et al. (2003) was applied to the targeted ADT compositions (listed in Table 6-1). The index system was developed to account for the fact that single component constraints (either individually or when used in series) were not adequate to describe the cumulative effects, whether positive or negative, of several components simultaneously. In general, the index system consists of two separate indices, the “Good” index (those oxides that enhance durability) and the “bad” index (those oxides that deteriorate durability). The “bad” index is subtracted from the “good” index, and if the remainder is greater than -0.24 the glass is classified as acceptable. The term “acceptable” (in reference to a PCT response) was defined as a glass whose $\log NL [B]$ (g/L) is less than 1.0 (or $NL [B] < 10$ g/L). This is consistent with the limit used by Edwards and Brown (1998) to set the $\Sigma alkali$ and Al_2O_3 criteria for relaxing the homogeneity constraint from the MAR to the PAR for Tank 42. This definition is also considered to be conservative relative to the EA glass as reported by Jantzen et

⁶ The Frit 418 – SB3 glasses shown in Figure 6-1 are not specific ADT glasses. SB2/3-4 and SB2/3-7 from Lorier et al. (2003) will be used to represent these two glasses.

al. (1993) with uncertainties considered as well as conservative relative to the requirements as specified in the WAPS. It should be noted that a direct comparison between the ability of the ΔG_p model and the index system to classify glasses as “acceptable” or “unacceptable” is not a 1-to-1 comparison. That is, the index system utilizes an “acceptance” limit of 10 g/L or less while the ΔG_p values used for acceptability translate into approximately 2.5 and 4.0 g/L for the current and proposed limits, respectively, per the following equation.

$$\log_{10}\{NL[B \text{ (g/L)}]\} = -1.901 - 0.181\Delta G_p$$

Therefore, there is a higher probability that a composition would be deemed acceptable by the index system as compared to the use of the new durability limits – especially for those systems which challenge durability.

The results of the index system assessment are summarized in Table 6-2. All “ADT” glasses are classified as “acceptable” based on this system and the 10 g/L limit. Assuming the experimental assessments of the ADT glasses are “positive” and any issues associated with implementation are resolved, the index system could allow access to compositional regions not attainable through the ΔG_p model even with the less conservative, durability limits proposed by Edwards et al. (2003).

Table 6-2. Results of Index System Assessment.

Glass ID	Index Classification
ADT-1	Acceptable
ADT-2	Acceptable
ADT-3	Acceptable
ADT-4	Acceptable
ADT-5	Acceptable
ADT-6	Acceptable
ADT-7	Acceptable
ADT-8	Acceptable

7.0 SUMMARY

In support of accelerated mission goals, glass formulation efforts have been focused on melt rate and WL which ultimately dictate waste throughput for the DWPF. With respect to melt rate, the general trend for improvement has been to enhance the total alkali concentration in the glass system by increasing the alkali concentration in the frit (Lambert et al. 2001), utilizing (or targeting) a less washed sludge, or using a combination of the two. Previous assessments have indicated that as higher alkali systems are pursued, a transition can occur in which predictions of durability begin limiting upper waste loadings rather than predictions of liquidus temperature (Peeler and Edwards 2002). Recent results have also suggested that the current durability model can lead to conservative decisions during the SME acceptability process (Peeler et al. 2001 and Cozzi et al. 2003). More specifically, the model has restricted access to glass compositional regions that could potentially enhance melt rate, waste loading, or waste throughput by classifying a specific glass composition as “unacceptable” whose experimentally determined durability (as defined by the PCT) is “acceptable” relative to the EA glass (WAPS 1996).

SRNL has initiated studies to assess alternative durability options that may provide access to compositional regions of interest in support of the accelerated clean-up mission at the DWPF. One of the options being pursued is the redefinition of the durability model acceptable limits. In response, Edwards et al. (2003) identified and eliminated some of the conservative steps utilized in establishing the current limits without comprising the high confidence required for meeting the specification on the wasteform quality. The results led to a set of three new PAR values for ΔG_p which has the potential to allow access to compositional regions of interest to improve melt rate or waste throughput.

Although these limits are available for implementation, there is currently no driving force to do so (i.e., the current Frit 418 – SB3 system is T_L limited). The objectives of this task were to investigate (and generate) the incentive of applying the new durability limits in PCCS from a glass formulation perspective. Higher alkali frit compositions were identified or developed to transition into and through the region of acceptability as defined by the current and proposed durability limits. Specifically, glasses were defined that:

- (1) fail the MAR for the current durability limit (-12.78 kcal/mol) but pass the MAR for the proposed durability limit (-13.8 kcal/mol), and
- (2) fail the MAR for both the current and proposed durability limits while maintaining acceptable predictions for all other properties.

An eight glass test matrix has been identified to meet these objectives. The “ADT” glasses will be fabricated in the laboratory and their PCTs measured and compared to model predictions (and to the assessments by the index system). These glasses will be batched and melted under oxidizing conditions that target the projected compositions. Durability (as measured by the PCT) will be measured on each glass in triplicate using standard procedures. The measured response will then be compared to model based predictions to assess the applicability and/or potential conservatism of the various limits or durability approaches.

Although incentive for implementation of the proposed durability limits could be demonstrated through this study in terms of the measured durability response for higher alkali systems, assessments of melt rate will also be performed to establish a clear motive or driver to implement a frit change. More specifically, a “significant” increase in melt rate may be required to provide the incentive for DWPF to implement the change rather than a “paper study” incentive or PCT assessment. The experimental results (both PCT and melt rate) will be the focus of subsequent reports.

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APPENDIX A

OPERATING WINDOWS WITH CURRENT ΔG_p LIMITS

Table A.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Current Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁷ wt%	R ₂ O MAR	MAR Status
Frit 202/SB2-3 Baseline	25	-12.3950	-8.8458	852.59	1003.59	108.68	3.83	15.31	18.64	hvisc
Frit 202/SB2-3 Baseline	26	-12.3950	-8.9153	866.20	1005.43	104.59	3.98	15.40	18.64	hvisc
Frit 202/SB2-3 Baseline	27	-12.3950	-8.9849	879.44	1007.14	100.56	4.13	15.49	18.64	hvisc
Frit 202/SB2-3 Baseline	28	-12.3950	-9.0545	892.33	1008.74	96.58	4.29	15.59	18.64	-
Frit 202/SB2-3 Baseline	29	-12.3950	-9.1241	904.86	1010.21	92.66	4.44	15.68	18.64	-
Frit 202/SB2-3 Baseline	30	-12.3950	-9.1937	917.07	1011.56	88.81	4.59	15.77	18.64	-
Frit 202/SB2-3 Baseline	31	-12.3950	-9.2633	928.97	1012.78	85.01	4.75	15.86	18.64	-
Frit 202/SB2-3 Baseline	32	-12.3950	-9.3329	940.56	1013.87	81.27	4.90	15.95	18.64	-
Frit 202/SB2-3 Baseline	33	-12.3950	-9.4024	951.86	1014.82	77.61	5.05	16.05	18.64	-
Frit 202/SB2-3 Baseline	34	-12.3950	-9.4720	962.88	1015.63	74.01	5.21	16.14	18.64	-
Frit 202/SB2-3 Baseline	35	-12.3950	-9.5416	973.63	1016.30	70.48	5.36	16.23	18.64	-
Frit 202/SB2-3 Baseline	36	-12.3950	-9.6112	984.13	1016.83	67.02	5.51	16.32	18.64	-
Frit 202/SB2-3 Baseline	37	-12.3950	-9.6808	994.38	1017.22	63.64	5.66	16.42	18.64	-
Frit 202/SB2-3 Baseline	38	-12.3950	-9.7504	1004.39	1017.49	60.33	5.82	16.51	18.64	-
Frit 202/SB2-3 Baseline	39	-12.3950	-9.8200	1014.16	1017.64	57.10	5.97	16.60	18.64	-
Frit 202/SB2-3 Baseline	40	-12.3950	-9.8895	1023.72	1017.67	53.95	6.12	16.69	18.64	TL
Frit 202/SB2-3 Baseline	41	-12.3950	-9.9591	1033.06	1017.62	50.89	6.28	16.79	18.64	TL
Frit 202/SB2-3 Baseline	42	-12.3950	-10.0287	1042.19	1017.39	47.90	6.43	16.88	18.64	TL
Frit 202/SB2-3 Baseline	43	-12.3950	-10.0983	1051.12	1016.88	45.01	6.58	16.97	18.64	TL
Frit 202/SB2-3 Baseline	44	-12.3950	-10.1679	1059.86	1016.32	42.20	6.74	17.06	18.64	TL
Frit 202/SB2-3 Baseline	45	-12.3950	-10.2375	1068.41	1015.72	39.48	6.89	17.15	18.64	TL
Frit 202/SB2-3 Baseline	46	-12.3950	-10.3071	1076.78	1015.08	36.85	7.04	17.25	18.64	TL
Frit 202/SB2-3 Baseline	47	-12.3950	-10.3766	1084.97	1014.42	34.31	7.20	17.34	18.64	TL
Frit 202/SB2-3 Baseline	48	-12.3950	-10.4462	1093.00	1013.73	31.87	7.35	17.43	18.64	TL
Frit 202/SB2-3 Baseline	49	-12.3950	-10.5158	1100.86	1013.02	29.52	7.50	17.52	18.64	TL
Frit 202/SB2-3 Baseline	50	-12.3950	-10.5854	1108.56	1012.30	27.27	7.66	17.62	18.64	TL
Frit 202/SB2-3 Baseline	51	-12.3950	-10.6550	1116.10	1011.57	25.12	7.81	17.71	18.64	TL
Frit 202/SB2-3 Baseline	52	-12.3950	-10.7246	1123.50	1010.82	23.06	7.96	17.80	18.64	TL lvisc
Frit 202/SB2-3 Baseline	53	-12.3950	-10.7941	1130.75	1010.07	21.10	8.11	17.89	18.63	TL lvisc

⁷ R₂O represents the sum of alkali where R = Na, Li, K, and Cs.

Table A.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Current Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁷ wt%	R ₂ O MAR	MAR Status
Frit 202/SB2-3 Baseline	54	-12.3950	-10.8637	1137.86	1009.31	19.24	8.27	17.99	18.63	TL lvisc
Frit 202/SB2-3 Baseline	55	-12.3950	-10.9333	1144.83	1008.55	17.47	8.42	18.08	18.63	TL lvisc
Frit 202/SB2-3 Baseline	56	-12.3950	-11.0029	1151.67	1007.78	15.81	8.57	18.17	18.62	TL lvisc
Frit 202/SB2-3 Baseline	57	-12.3950	-11.0725	1158.38	1007.02	14.24	8.73	18.26	18.62	TL lvisc
Frit 202/SB2-3 Baseline	58	-12.3950	-11.1421	1164.97	1006.25	12.77	8.88	18.35	18.61	TL lvisc
Frit 202/SB2-3 Baseline	59	-12.3928	-11.2117	1171.43	1005.48	11.40	9.03	18.45	18.61	TL lvisc
Frit 202/SB2-3 Baseline	60	-12.3890	-11.2812	1177.77	1004.72	10.12	9.19	18.54	18.61	TL lvisc
Frit 320/SB2-3 Baseline	25	-12.3520	-13.3121	709.67	990.70	41.90	3.83	20.56	18.55	Del Gp R2O
Frit 320/SB2-3 Baseline	26	-12.3506	-13.3222	724.78	993.00	40.25	3.98	20.58	18.55	Del Gp R2O
Frit 320/SB2-3 Baseline	27	-12.3491	-13.3322	739.57	995.19	38.62	4.13	20.60	18.55	Del Gp R2O
Frit 320/SB2-3 Baseline	28	-12.3477	-13.3422	754.04	997.26	37.02	4.29	20.63	18.55	Del Gp
Frit 320/SB2-3 Baseline	29	-12.3462	-13.3523	768.22	999.24	35.44	4.44	20.65	18.54	Del Gp
Frit 320/SB2-3 Baseline	30	-12.3447	-13.3623	782.11	1001.13	33.90	4.59	20.67	18.54	Del Gp
Frit 320/SB2-3 Baseline	31	-12.3433	-13.3723	795.72	1002.93	32.38	4.75	20.69	18.54	Del Gp
Frit 320/SB2-3 Baseline	32	-12.3418	-13.3824	809.06	1004.65	30.89	4.90	20.71	18.54	Del Gp
Frit 320/SB2-3 Baseline	33	-12.3403	-13.3924	822.15	1006.30	29.43	5.05	20.74	18.54	Del Gp
Frit 320/SB2-3 Baseline	34	-12.3388	-13.4024	834.99	1007.88	28.00	5.21	20.76	18.54	Del Gp
Frit 320/SB2-3 Baseline	35	-12.3373	-13.4125	847.60	1009.39	26.60	5.36	20.78	18.54	Del Gp
Frit 320/SB2-3 Baseline	36	-12.3359	-13.4225	859.97	1010.83	25.23	5.51	20.80	18.54	Del Gp
Frit 320/SB2-3 Baseline	37	-12.3344	-13.4325	872.11	1012.20	23.90	5.66	20.83	18.53	Del Gp lvisc
Frit 320/SB2-3 Baseline	38	-12.3329	-13.4426	884.04	1013.49	22.60	5.82	20.85	18.53	Del Gp lvisc
Frit 320/SB2-3 Baseline	39	-12.3314	-13.4526	895.76	1014.40	21.34	5.97	20.87	18.53	Del Gp lvisc
Frit 320/SB2-3 Baseline	40	-12.3299	-13.4626	907.28	1015.16	20.10	6.12	20.89	18.53	Del Gp lvisc
Frit 320/SB2-3 Baseline	41	-12.3284	-13.4727	918.59	1015.86	18.91	6.28	20.92	18.53	Del Gp lvisc
Frit 320/SB2-3 Baseline	42	-12.3269	-13.4827	929.72	1016.50	17.75	6.43	20.94	18.53	Del Gp lvisc
Frit 320/SB2-3 Baseline	43	-12.3254	-13.4927	940.66	1017.06	16.63	6.58	20.96	18.53	Del Gp lvisc
Frit 320/SB2-3 Baseline	44	-12.3239	-13.5028	951.41	1017.54	15.54	6.74	20.98	18.52	Del Gp lvisc
Frit 320/SB2-3 Baseline	45	-12.3224	-13.5128	961.99	1017.92	14.50	6.89	21.00	18.52	Del Gp lvisc
Frit 320/SB2-3 Baseline	46	-12.3209	-13.5228	972.40	1018.21	13.49	7.04	21.03	18.52	Del Gp lvisc
Frit 320/SB2-3 Baseline	47	-12.3194	-13.5329	982.64	1018.38	12.52	7.20	21.05	18.52	Del Gp lvisc
Frit 320/SB2-3 Baseline	48	-12.3179	-13.5429	992.71	1018.45	11.59	7.35	21.07	18.52	Del Gp lvisc
Frit 320/SB2-3 Baseline	49	-12.3164	-13.5529	1002.63	1018.42	10.70	7.50	21.09	18.52	Del Gp lvisc

Table A.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Current Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁷ wt%	R ₂ O MAR	MAR Status	
Frit 320/SB2-3 Baseline	50	-12.3149	-13.5630	1012.39	1018.27	9.84	7.66	21.12	18.52	Del Gp	lvisc
Frit 320/SB2-3 Baseline	51	-12.3133	-13.5730	1022.01	1018.03	9.03	7.81	21.14	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	52	-12.3118	-13.5830	1031.47	1017.70	8.26	7.96	21.16	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	53	-12.3103	-13.5931	1040.79	1017.29	7.53	8.11	21.18	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	54	-12.3088	-13.6031	1049.97	1016.81	6.83	8.27	21.21	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	55	-12.3073	-13.6131	1059.01	1016.27	6.18	8.42	21.23	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	56	-12.3057	-13.6232	1067.92	1015.67	5.57	8.57	21.25	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	57	-12.3042	-13.6332	1076.69	1015.02	4.99	8.73	21.27	18.50	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	58	-12.3027	-13.6432	1085.34	1014.34	4.46	8.88	21.29	18.50	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	59	-12.3012	-13.6533	1093.87	1013.62	3.96	9.03	21.32	18.50	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	60	-12.2996	-13.6633	1102.27	1012.87	3.50	9.19	21.34	18.50	Del Gp TL	lvisc
Frit 418/SB2-3 Baseline	25	-12.3950	-10.5402	756.73	994.42	72.89	3.83	17.56	18.64	-	
Frit 418/SB2-3 Baseline	26	-12.3950	-10.5872	771.86	996.70	70.14	3.98	17.62	18.64	-	
Frit 418/SB2-3 Baseline	27	-12.3950	-10.6342	786.61	998.85	67.42	4.13	17.68	18.64	-	
Frit 418/SB2-3 Baseline	28	-12.3950	-10.6812	801.00	1000.88	64.74	4.29	17.75	18.64	-	
Frit 418/SB2-3 Baseline	29	-12.3950	-10.7282	815.04	1002.81	62.10	4.44	17.81	18.64	-	
Frit 418/SB2-3 Baseline	30	-12.3950	-10.7751	828.76	1004.64	59.50	4.59	17.87	18.64	-	
Frit 418/SB2-3 Baseline	31	-12.3950	-10.8221	842.16	1006.37	56.94	4.75	17.93	18.64	-	
Frit 418/SB2-3 Baseline	32	-12.3950	-10.8691	855.25	1008.02	54.43	4.90	17.99	18.64	-	
Frit 418/SB2-3 Baseline	33	-12.3950	-10.9161	868.06	1009.56	51.96	5.05	18.06	18.64	-	
Frit 418/SB2-3 Baseline	34	-12.3950	-10.9631	880.58	1011.02	49.53	5.21	18.12	18.64	-	
Frit 418/SB2-3 Baseline	35	-12.3950	-11.0101	892.83	1012.39	47.16	5.36	18.18	18.64	-	
Frit 418/SB2-3 Baseline	36	-12.3950	-11.0571	904.82	1013.66	44.83	5.51	18.24	18.63	-	
Frit 418/SB2-3 Baseline	37	-12.3950	-11.1041	916.56	1014.83	42.56	5.66	18.31	18.63	-	
Frit 418/SB2-3 Baseline	38	-12.3950	-11.1511	928.06	1015.89	40.34	5.82	18.37	18.63	-	
Frit 418/SB2-3 Baseline	39	-12.3950	-11.1981	939.32	1016.85	38.17	5.97	18.43	18.62	-	
Frit 418/SB2-3 Baseline	40	-12.3950	-11.2451	950.35	1017.55	36.05	6.12	18.49	18.62	-	
Frit 418/SB2-3 Baseline	41	-12.3950	-11.2921	961.17	1017.92	33.99	6.28	18.56	18.62	-	
Frit 418/SB2-3 Baseline	42	-12.3950	-11.3391	971.77	1018.19	31.99	6.43	18.62	18.62	-	
Frit 418/SB2-3 Baseline	43	-12.3950	-11.3861	982.16	1018.34	30.05	6.58	18.68	18.61	-	
Frit 418/SB2-3 Baseline	44	-12.3950	-11.4330	992.36	1018.39	28.16	6.74	18.74	18.61	-	
Frit 418/SB2-3 Baseline	45	-12.3950	-11.4800	1002.36	1018.33	26.34	6.89	18.80	18.61	-	

Table A.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Current Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁷ wt%	R ₂ O MAR	MAR Status
Frit 418/SB2-3 Baseline	46	-12.3950	-11.5270	1012.17	1018.16	24.58	7.04	18.87	18.60	-
Frit 418/SB2-3 Baseline	47	-12.3948	-11.5740	1021.80	1017.91	22.88	7.20	18.93	18.60	TL lvisc
Frit 418/SB2-3 Baseline	48	-12.3919	-11.6210	1031.26	1017.56	21.24	7.35	18.99	18.60	TL lvisc
Frit 418/SB2-3 Baseline	49	-12.3890	-11.6680	1040.54	1017.14	19.67	7.50	19.05	18.60	TL lvisc
Frit 418/SB2-3 Baseline	50	-12.3860	-11.7150	1049.65	1016.66	18.16	7.66	19.12	18.59	TL lvisc
Frit 418/SB2-3 Baseline	51	-12.3831	-11.7620	1058.60	1016.11	16.72	7.81	19.18	18.59	TL lvisc
Frit 418/SB2-3 Baseline	52	-12.3801	-11.8090	1067.40	1015.52	15.34	7.96	19.24	18.59	TL lvisc
Frit 418/SB2-3 Baseline	53	-12.3772	-11.8560	1076.04	1014.88	14.03	8.11	19.30	18.58	TL lvisc
Frit 418/SB2-3 Baseline	54	-12.3743	-11.9030	1084.53	1014.21	12.79	8.27	19.37	18.58	TL lvisc
Frit 418/SB2-3 Baseline	55	-12.3713	-11.9500	1092.87	1013.51	11.61	8.42	19.43	18.58	TL lvisc
Frit 418/SB2-3 Baseline	56	-12.3684	-11.9970	1101.07	1012.79	10.50	8.57	19.49	18.57	TL lvisc
Frit 418/SB2-3 Baseline	57	-12.3654	-12.0440	1109.14	1012.04	9.46	8.73	19.55	18.57	TL lvisc
Frit 418/SB2-3 Baseline	58	-12.3625	-12.0909	1117.06	1011.28	8.48	8.88	19.61	18.57	TL lvisc
Frit 418/SB2-3 Baseline	59	-12.3595	-12.1379	1124.86	1010.50	7.56	9.03	19.68	18.57	TL lvisc
Frit 418/SB2-3 Baseline	60	-12.3565	-12.1849	1132.53	1009.70	6.71	9.19	19.74	18.56	TL lvisc
Frit 425/SB2-3 Baseline	25	-12.3950	-11.9262	732.33	992.50	55.67	3.83	19.06	18.61	R2O
Frit 425/SB2-3 Baseline	26	-12.3950	-11.9547	747.47	994.80	53.52	3.98	19.10	18.61	R2O
Frit 425/SB2-3 Baseline	27	-12.3950	-11.9832	762.26	996.97	51.41	4.13	19.14	18.60	R2O
Frit 425/SB2-3 Baseline	28	-12.3950	-12.0117	776.71	999.03	49.32	4.29	19.19	18.60	-
Frit 425/SB2-3 Baseline	29	-12.3950	-12.0402	790.84	1000.99	47.27	4.44	19.23	18.60	-
Frit 425/SB2-3 Baseline	30	-12.3945	-12.0687	804.66	1002.85	45.25	4.59	19.27	18.60	-
Frit 425/SB2-3 Baseline	31	-12.3924	-12.0972	818.18	1004.63	43.26	4.75	19.31	18.60	-
Frit 425/SB2-3 Baseline	32	-12.3902	-12.1258	831.43	1006.32	41.31	4.90	19.35	18.59	-
Frit 425/SB2-3 Baseline	33	-12.3880	-12.1543	844.39	1007.93	39.40	5.05	19.40	18.59	-
Frit 425/SB2-3 Baseline	34	-12.3858	-12.1828	857.10	1009.46	37.52	5.21	19.44	18.59	-
Frit 425/SB2-3 Baseline	35	-12.3836	-12.2113	869.54	1010.92	35.69	5.36	19.48	18.59	-
Frit 425/SB2-3 Baseline	36	-12.3814	-12.2398	881.74	1012.29	33.89	5.51	19.52	18.58	-
Frit 425/SB2-3 Baseline	37	-12.3792	-12.2683	893.71	1013.58	32.14	5.66	19.57	18.58	-
Frit 425/SB2-3 Baseline	38	-12.3770	-12.2968	905.44	1014.78	30.42	5.82	19.61	18.58	-
Frit 425/SB2-3 Baseline	39	-12.3748	-12.3253	916.95	1015.84	28.76	5.97	19.65	18.58	-
Frit 425/SB2-3 Baseline	40	-12.3726	-12.3539	928.25	1016.48	27.13	6.12	19.69	18.58	-
Frit 425/SB2-3 Baseline	41	-12.3704	-12.3824	939.33	1017.05	25.55	6.28	19.74	18.57	Del Gp

Table A.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Current Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁷ wt%	R ₂ O MAR	MAR Status	
Frit 425/SB2-3 Baseline	42	-12.3682	-12.4109	950.22	1017.53	24.01	6.43	19.78	18.57	Del Gp	lvisc
Frit 425/SB2-3 Baseline	43	-12.3660	-12.4394	960.90	1017.91	22.53	6.58	19.82	18.57	Del Gp	lvisc
Frit 425/SB2-3 Baseline	44	-12.3638	-12.4679	971.40	1018.19	21.09	6.74	19.86	18.57	Del Gp	lvisc
Frit 425/SB2-3 Baseline	45	-12.3616	-12.4964	981.71	1018.37	19.69	6.89	19.90	18.56	Del Gp	lvisc
Frit 425/SB2-3 Baseline	46	-12.3594	-12.5249	991.84	1018.43	18.35	7.04	19.95	18.56	Del Gp	lvisc
Frit 425/SB2-3 Baseline	47	-12.3571	-12.5535	1001.79	1018.39	17.06	7.20	19.99	18.56	Del Gp	lvisc
Frit 425/SB2-3 Baseline	48	-12.3549	-12.5820	1011.57	1018.25	15.81	7.35	20.03	18.56	Del Gp	lvisc
Frit 425/SB2-3 Baseline	49	-12.3527	-12.6105	1021.19	1018.00	14.62	7.50	20.07	18.56	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	50	-12.3505	-12.6390	1030.64	1017.67	13.48	7.66	20.12	18.55	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	51	-12.3482	-12.6675	1039.94	1017.26	12.39	7.81	20.16	18.55	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	52	-12.3460	-12.6960	1049.09	1016.79	11.35	7.96	20.20	18.55	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	53	-12.3438	-12.7245	1058.08	1016.25	10.36	8.11	20.24	18.55	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	54	-12.3416	-12.7530	1066.93	1015.66	9.43	8.27	20.29	18.54	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	55	-12.3393	-12.7816	1075.64	1015.02	8.54	8.42	20.33	18.54	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	56	-12.3371	-12.8101	1084.21	1014.34	7.71	8.57	20.37	18.54	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	57	-12.3348	-12.8386	1092.65	1013.64	6.93	8.73	20.41	18.54	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	58	-12.3326	-12.8671	1100.95	1012.90	6.20	8.88	20.45	18.54	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	59	-12.3304	-12.8956	1109.12	1012.14	5.52	9.03	20.50	18.53	Del Gp TL	lvisc
Frit 425/SB2-3 Baseline	60	-12.3281	-12.9241	1117.17	1011.37	4.88	9.19	20.54	18.53	Del Gp TL	lvisc

APPENDIX B

OPERATING WINDOWS WITH PROPOSED DURABILITY LIMITS

Table B.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Proposed Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁸ wt%	R ₂ O MAR	MAR Status
Frit 202/SB2-3 Baseline	25	-13.4837	-8.8458	852.59	1003.59	108.68	3.83	15.31	18.64	hvisc
Frit 202/SB2-3 Baseline	26	-13.4837	-8.9153	866.20	1005.43	104.59	3.98	15.40	18.64	hvisc
Frit 202/SB2-3 Baseline	27	-13.4837	-8.9849	879.44	1007.14	100.56	4.13	15.49	18.64	hvisc
Frit 202/SB2-3 Baseline	28	-13.4837	-9.0545	892.33	1008.74	96.58	4.29	15.59	18.64	-
Frit 202/SB2-3 Baseline	29	-13.4837	-9.1241	904.86	1010.21	92.66	4.44	15.68	18.64	-
Frit 202/SB2-3 Baseline	30	-13.4837	-9.1937	917.07	1011.56	88.81	4.59	15.77	18.64	-
Frit 202/SB2-3 Baseline	31	-13.4837	-9.2633	928.97	1012.78	85.01	4.75	15.86	18.64	-
Frit 202/SB2-3 Baseline	32	-13.4837	-9.3329	940.56	1013.87	81.27	4.90	15.95	18.64	-
Frit 202/SB2-3 Baseline	33	-13.4837	-9.4024	951.86	1014.82	77.61	5.05	16.05	18.64	-
Frit 202/SB2-3 Baseline	34	-13.4837	-9.4720	962.88	1015.63	74.01	5.21	16.14	18.64	-
Frit 202/SB2-3 Baseline	35	-13.4837	-9.5416	973.63	1016.30	70.48	5.36	16.23	18.64	-
Frit 202/SB2-3 Baseline	36	-13.4837	-9.6112	984.13	1016.83	67.02	5.51	16.32	18.64	-
Frit 202/SB2-3 Baseline	37	-13.4837	-9.6808	994.38	1017.22	63.64	5.66	16.42	18.64	-
Frit 202/SB2-3 Baseline	38	-13.4837	-9.7504	1004.39	1017.49	60.33	5.82	16.51	18.64	-
Frit 202/SB2-3 Baseline	39	-13.4837	-9.8200	1014.16	1017.64	57.10	5.97	16.60	18.64	-
Frit 202/SB2-3 Baseline	40	-13.4837	-9.8895	1023.72	1017.67	53.95	6.12	16.69	18.64	TL
Frit 202/SB2-3 Baseline	41	-13.4837	-9.9591	1033.06	1017.62	50.89	6.28	16.79	18.64	TL
Frit 202/SB2-3 Baseline	42	-13.4837	-10.0287	1042.19	1017.39	47.90	6.43	16.88	18.64	TL
Frit 202/SB2-3 Baseline	43	-13.4837	-10.0983	1051.12	1016.88	45.01	6.58	16.97	18.64	TL
Frit 202/SB2-3 Baseline	44	-13.4837	-10.1679	1059.86	1016.32	42.20	6.74	17.06	18.64	TL
Frit 202/SB2-3 Baseline	45	-13.4837	-10.2375	1068.41	1015.72	39.48	6.89	17.15	18.64	TL
Frit 202/SB2-3 Baseline	46	-13.4837	-10.3071	1076.78	1015.08	36.85	7.04	17.25	18.64	TL
Frit 202/SB2-3 Baseline	47	-13.4837	-10.3766	1084.97	1014.42	34.31	7.20	17.34	18.64	TL
Frit 202/SB2-3 Baseline	48	-13.4837	-10.4462	1093.00	1013.73	31.87	7.35	17.43	18.64	TL
Frit 202/SB2-3 Baseline	49	-13.4837	-10.5158	1100.86	1013.02	29.52	7.50	17.52	18.64	TL
Frit 202/SB2-3 Baseline	50	-13.4837	-10.5854	1108.56	1012.30	27.27	7.66	17.62	18.64	TL
Frit 202/SB2-3 Baseline	51	-13.4837	-10.6550	1116.10	1011.57	25.12	7.81	17.71	18.64	TL
Frit 202/SB2-3 Baseline	52	-13.4837	-10.7246	1123.50	1010.82	23.06	7.96	17.80	18.64	TL lvisc
Frit 202/SB2-3 Baseline	53	-13.4837	-10.7941	1130.75	1010.07	21.10	8.11	17.89	18.63	TL lvisc

⁸ R₂O represents the sum of alkali where R = Na, Li, K, and Cs.

Table B.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Proposed Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁸ wt%	R ₂ O MAR	MAR Status	
Frit 202/SB2-3 Baseline	54	-13.4837	-10.8637	1137.86	1009.31	19.24	8.27	17.99	18.63	TL	lvisc
Frit 202/SB2-3 Baseline	55	-13.4837	-10.9333	1144.83	1008.55	17.47	8.42	18.08	18.63	TL	lvisc
Frit 202/SB2-3 Baseline	56	-13.4837	-11.0029	1151.67	1007.78	15.81	8.57	18.17	18.62	TL	lvisc
Frit 202/SB2-3 Baseline	57	-13.4837	-11.0725	1158.38	1007.02	14.24	8.73	18.26	18.62	TL	lvisc
Frit 202/SB2-3 Baseline	58	-13.4837	-11.1421	1164.97	1006.25	12.77	8.88	18.35	18.61	TL	lvisc
Frit 202/SB2-3 Baseline	59	-13.4815	-11.2117	1171.43	1005.48	11.40	9.03	18.45	18.61	TL	lvisc
Frit 202/SB2-3 Baseline	60	-13.4777	-11.2812	1177.77	1004.72	10.12	9.19	18.54	18.61	TL	lvisc
Frit 320/SB2-3 Baseline	25	-13.4407	-13.3121	709.67	990.70	41.90	3.83	20.56	18.55	R2O	
Frit 320/SB2-3 Baseline	26	-13.4393	-13.3222	724.78	993.00	40.25	3.98	20.58	18.55	R2O	
Frit 320/SB2-3 Baseline	27	-13.4378	-13.3322	739.57	995.19	38.62	4.13	20.60	18.55	R2O	
Frit 320/SB2-3 Baseline	28	-13.4364	-13.3422	754.04	997.26	37.02	4.29	20.63	18.55	-	
Frit 320/SB2-3 Baseline	29	-13.4349	-13.3523	768.22	999.24	35.44	4.44	20.65	18.54	-	
Frit 320/SB2-3 Baseline	30	-13.4334	-13.3623	782.11	1001.13	33.90	4.59	20.67	18.54	-	
Frit 320/SB2-3 Baseline	31	-13.4320	-13.3723	795.72	1002.93	32.38	4.75	20.69	18.54	-	
Frit 320/SB2-3 Baseline	32	-13.4305	-13.3824	809.06	1004.65	30.89	4.90	20.71	18.54	-	
Frit 320/SB2-3 Baseline	33	-13.4290	-13.3924	822.15	1006.30	29.43	5.05	20.74	18.54	-	
Frit 320/SB2-3 Baseline	34	-13.4275	-13.4024	834.99	1007.88	28.00	5.21	20.76	18.54	-	
Frit 320/SB2-3 Baseline	35	-13.4260	-13.4125	847.60	1009.39	26.60	5.36	20.78	18.54	-	
Frit 320/SB2-3 Baseline	36	-13.4246	-13.4225	859.97	1010.83	25.23	5.51	20.80	18.54	-	
Frit 320/SB2-3 Baseline	37	-13.4231	-13.4325	872.11	1012.20	23.90	5.66	20.83	18.53	Del Gp	lvisc
Frit 320/SB2-3 Baseline	38	-13.4216	-13.4426	884.04	1013.49	22.60	5.82	20.85	18.53	Del Gp	lvisc
Frit 320/SB2-3 Baseline	39	-13.4201	-13.4526	895.76	1014.40	21.34	5.97	20.87	18.53	Del Gp	lvisc
Frit 320/SB2-3 Baseline	40	-13.4186	-13.4626	907.28	1015.16	20.10	6.12	20.89	18.53	Del Gp	lvisc
Frit 320/SB2-3 Baseline	41	-13.4171	-13.4727	918.59	1015.86	18.91	6.28	20.92	18.53	Del Gp	lvisc
Frit 320/SB2-3 Baseline	42	-13.4156	-13.4827	929.72	1016.50	17.75	6.43	20.94	18.53	Del Gp	lvisc
Frit 320/SB2-3 Baseline	43	-13.4141	-13.4927	940.66	1017.06	16.63	6.58	20.96	18.53	Del Gp	lvisc
Frit 320/SB2-3 Baseline	44	-13.4126	-13.5028	951.41	1017.54	15.54	6.74	20.98	18.52	Del Gp	lvisc
Frit 320/SB2-3 Baseline	45	-13.4111	-13.5128	961.99	1017.92	14.50	6.89	21.00	18.52	Del Gp	lvisc
Frit 320/SB2-3 Baseline	46	-13.4096	-13.5228	972.40	1018.21	13.49	7.04	21.03	18.52	Del Gp	lvisc
Frit 320/SB2-3 Baseline	47	-13.4081	-13.5329	982.64	1018.38	12.52	7.20	21.05	18.52	Del Gp	lvisc
Frit 320/SB2-3 Baseline	48	-13.4066	-13.5429	992.71	1018.45	11.59	7.35	21.07	18.52	Del Gp	lvisc
Frit 320/SB2-3 Baseline	49	-13.4051	-13.5529	1002.63	1018.42	10.70	7.50	21.09	18.52	Del Gp	lvisc

Table B.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Proposed Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁸ wt%	R ₂ O MAR	MAR Status	
Frit 320/SB2-3 Baseline	50	-13.4036	-13.5630	1012.39	1018.27	9.84	7.66	21.12	18.52	Del Gp	lvisc
Frit 320/SB2-3 Baseline	51	-13.4020	-13.5730	1022.01	1018.03	9.03	7.81	21.14	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	52	-13.4005	-13.5830	1031.47	1017.70	8.26	7.96	21.16	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	53	-13.3990	-13.5931	1040.79	1017.29	7.53	8.11	21.18	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	54	-13.3975	-13.6031	1049.97	1016.81	6.83	8.27	21.21	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	55	-13.3960	-13.6131	1059.01	1016.27	6.18	8.42	21.23	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	56	-13.3944	-13.6232	1067.92	1015.67	5.57	8.57	21.25	18.51	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	57	-13.3929	-13.6332	1076.69	1015.02	4.99	8.73	21.27	18.50	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	58	-13.3914	-13.6432	1085.34	1014.34	4.46	8.88	21.29	18.50	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	59	-13.3899	-13.6533	1093.87	1013.62	3.96	9.03	21.32	18.50	Del Gp TL	lvisc
Frit 320/SB2-3 Baseline	60	-13.3883	-13.6633	1102.27	1012.87	3.50	9.19	21.34	18.50	Del Gp TL	lvisc
Frit 418/SB2-3 Baseline	25	-13.4837	-10.5402	756.73	994.42	72.89	3.83	17.56	18.64	-	
Frit 418/SB2-3 Baseline	26	-13.4837	-10.5872	771.86	996.70	70.14	3.98	17.62	18.64	-	
Frit 418/SB2-3 Baseline	27	-13.4837	-10.6342	786.61	998.85	67.42	4.13	17.68	18.64	-	
Frit 418/SB2-3 Baseline	28	-13.4837	-10.6812	801.00	1000.88	64.74	4.29	17.75	18.64	-	
Frit 418/SB2-3 Baseline	29	-13.4837	-10.7282	815.04	1002.81	62.10	4.44	17.81	18.64	-	
Frit 418/SB2-3 Baseline	30	-13.4837	-10.7751	828.76	1004.64	59.50	4.59	17.87	18.64	-	
Frit 418/SB2-3 Baseline	31	-13.4837	-10.8221	842.16	1006.37	56.94	4.75	17.93	18.64	-	
Frit 418/SB2-3 Baseline	32	-13.4837	-10.8691	855.25	1008.02	54.43	4.90	17.99	18.64	-	
Frit 418/SB2-3 Baseline	33	-13.4837	-10.9161	868.06	1009.56	51.96	5.05	18.06	18.64	-	
Frit 418/SB2-3 Baseline	34	-13.4837	-10.9631	880.58	1011.02	49.53	5.21	18.12	18.64	-	
Frit 418/SB2-3 Baseline	35	-13.4837	-11.0101	892.83	1012.39	47.16	5.36	18.18	18.64	-	
Frit 418/SB2-3 Baseline	36	-13.4837	-11.0571	904.82	1013.66	44.83	5.51	18.24	18.63	-	
Frit 418/SB2-3 Baseline	37	-13.4837	-11.1041	916.56	1014.83	42.56	5.66	18.31	18.63	-	
Frit 418/SB2-3 Baseline	38	-13.4837	-11.1511	928.06	1015.89	40.34	5.82	18.37	18.63	-	
Frit 418/SB2-3 Baseline	39	-13.4837	-11.1981	939.32	1016.85	38.17	5.97	18.43	18.62	-	
Frit 418/SB2-3 Baseline	40	-13.4837	-11.2451	950.35	1017.55	36.05	6.12	18.49	18.62	-	
Frit 418/SB2-3 Baseline	41	-13.4837	-11.2921	961.17	1017.92	33.99	6.28	18.56	18.62	-	
Frit 418/SB2-3 Baseline	42	-13.4837	-11.3391	971.77	1018.19	31.99	6.43	18.62	18.62	-	
Frit 418/SB2-3 Baseline	43	-13.4837	-11.3861	982.16	1018.34	30.05	6.58	18.68	18.61	-	
Frit 418/SB2-3 Baseline	44	-13.4837	-11.4330	992.36	1018.39	28.16	6.74	18.74	18.61	-	
Frit 418/SB2-3 Baseline	45	-13.4837	-11.4800	1002.36	1018.33	26.34	6.89	18.80	18.61	-	

Table B.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Proposed Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁸ wt%	R ₂ O MAR	MAR Status
Frit 418/SB2-3 Baseline	46	-13.4837	-11.5270	1012.17	1018.16	24.58	7.04	18.87	18.60	-
Frit 418/SB2-3 Baseline	47	-13.4835	-11.5740	1021.80	1017.91	22.88	7.20	18.93	18.60	TL lvisc
Frit 418/SB2-3 Baseline	48	-13.4806	-11.6210	1031.26	1017.56	21.24	7.35	18.99	18.60	TL lvisc
Frit 418/SB2-3 Baseline	49	-13.4777	-11.6680	1040.54	1017.14	19.67	7.50	19.05	18.60	TL lvisc
Frit 418/SB2-3 Baseline	50	-13.4747	-11.7150	1049.65	1016.66	18.16	7.66	19.12	18.59	TL lvisc
Frit 418/SB2-3 Baseline	51	-13.4718	-11.7620	1058.60	1016.11	16.72	7.81	19.18	18.59	TL lvisc
Frit 418/SB2-3 Baseline	52	-13.4688	-11.8090	1067.40	1015.52	15.34	7.96	19.24	18.59	TL lvisc
Frit 418/SB2-3 Baseline	53	-13.4659	-11.8560	1076.04	1014.88	14.03	8.11	19.30	18.58	TL lvisc
Frit 418/SB2-3 Baseline	54	-13.4630	-11.9030	1084.53	1014.21	12.79	8.27	19.37	18.58	TL lvisc
Frit 418/SB2-3 Baseline	55	-13.4600	-11.9500	1092.87	1013.51	11.61	8.42	19.43	18.58	TL lvisc
Frit 418/SB2-3 Baseline	56	-13.4571	-11.9970	1101.07	1012.79	10.50	8.57	19.49	18.57	TL lvisc
Frit 418/SB2-3 Baseline	57	-13.4541	-12.0440	1109.14	1012.04	9.46	8.73	19.55	18.57	TL lvisc
Frit 418/SB2-3 Baseline	58	-13.4512	-12.0909	1117.06	1011.28	8.48	8.88	19.61	18.57	TL lvisc
Frit 418/SB2-3 Baseline	59	-13.4482	-12.1379	1124.86	1010.50	7.56	9.03	19.68	18.57	TL lvisc
Frit 418/SB2-3 Baseline	60	-13.4452	-12.1849	1132.53	1009.70	6.71	9.19	19.74	18.56	TL lvisc
Frit 425/SB2-3 Baseline	25	-13.4837	-11.9262	732.33	992.50	55.67	3.83	19.06	18.61	R2O
Frit 425/SB2-3 Baseline	26	-13.4837	-11.9547	747.47	994.80	53.52	3.98	19.10	18.61	R2O
Frit 425/SB2-3 Baseline	27	-13.4837	-11.9832	762.26	996.97	51.41	4.13	19.14	18.60	R2O
Frit 425/SB2-3 Baseline	28	-13.4837	-12.0117	776.71	999.03	49.32	4.29	19.19	18.60	-
Frit 425/SB2-3 Baseline	29	-13.4837	-12.0402	790.84	1000.99	47.27	4.44	19.23	18.60	-
Frit 425/SB2-3 Baseline	30	-13.4832	-12.0687	804.66	1002.85	45.25	4.59	19.27	18.60	-
Frit 425/SB2-3 Baseline	31	-13.4811	-12.0972	818.18	1004.63	43.26	4.75	19.31	18.60	-
Frit 425/SB2-3 Baseline	32	-13.4789	-12.1258	831.43	1006.32	41.31	4.90	19.35	18.59	-
Frit 425/SB2-3 Baseline	33	-13.4767	-12.1543	844.39	1007.93	39.40	5.05	19.40	18.59	-
Frit 425/SB2-3 Baseline	34	-13.4745	-12.1828	857.10	1009.46	37.52	5.21	19.44	18.59	-
Frit 425/SB2-3 Baseline	35	-13.4723	-12.2113	869.54	1010.92	35.69	5.36	19.48	18.59	-
Frit 425/SB2-3 Baseline	36	-13.4701	-12.2398	881.74	1012.29	33.89	5.51	19.52	18.58	-
Frit 425/SB2-3 Baseline	37	-13.4679	-12.2683	893.71	1013.58	32.14	5.66	19.57	18.58	-
Frit 425/SB2-3 Baseline	38	-13.4657	-12.2968	905.44	1014.78	30.42	5.82	19.61	18.58	-
Frit 425/SB2-3 Baseline	39	-13.4635	-12.3253	916.95	1015.84	28.76	5.97	19.65	18.58	-
Frit 425/SB2-3 Baseline	40	-13.4613	-12.3539	928.25	1016.48	27.13	6.12	19.69	18.58	-
Frit 425/SB2-3 Baseline	41	-13.4591	-12.3824	939.33	1017.05	25.55	6.28	19.74	18.57	-

Table B.1 Projected Operating Windows and Predicted Properties for Various SB3 Systems Using Proposed Durability Limits.

Category	WL (%)	Li Del Gp MAR (kcal/mol)	B Del Gp Value (kcal/mol)	T _L Pred (°C)	T _L MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁸ wt%	R ₂ O MAR	MAR Status
Frit 425/SB2-3 Baseline	42	-13.4569	-12.4109	950.22	1017.53	24.01	6.43	19.78	18.57	lvisc
Frit 425/SB2-3 Baseline	43	-13.4547	-12.4394	960.90	1017.91	22.53	6.58	19.82	18.57	lvisc
Frit 425/SB2-3 Baseline	44	-13.4525	-12.4679	971.40	1018.19	21.09	6.74	19.86	18.57	lvisc
Frit 425/SB2-3 Baseline	45	-13.4503	-12.4964	981.71	1018.37	19.69	6.89	19.90	18.56	lvisc
Frit 425/SB2-3 Baseline	46	-13.4481	-12.5249	991.84	1018.43	18.35	7.04	19.95	18.56	lvisc
Frit 425/SB2-3 Baseline	47	-13.4458	-12.5535	1001.79	1018.39	17.06	7.20	19.99	18.56	lvisc
Frit 425/SB2-3 Baseline	48	-13.4436	-12.5820	1011.57	1018.25	15.81	7.35	20.03	18.56	lvisc
Frit 425/SB2-3 Baseline	49	-13.4414	-12.6105	1021.19	1018.00	14.62	7.50	20.07	18.56	TL lvisc
Frit 425/SB2-3 Baseline	50	-13.4392	-12.6390	1030.64	1017.67	13.48	7.66	20.12	18.55	TL lvisc
Frit 425/SB2-3 Baseline	51	-13.4369	-12.6675	1039.94	1017.26	12.39	7.81	20.16	18.55	TL lvisc
Frit 425/SB2-3 Baseline	52	-13.4347	-12.6960	1049.09	1016.79	11.35	7.96	20.20	18.55	TL lvisc
Frit 425/SB2-3 Baseline	53	-13.4325	-12.7245	1058.08	1016.25	10.36	8.11	20.24	18.55	TL lvisc
Frit 425/SB2-3 Baseline	54	-13.4303	-12.7530	1066.93	1015.66	9.43	8.27	20.29	18.54	TL lvisc
Frit 425/SB2-3 Baseline	55	-13.4280	-12.7816	1075.64	1015.02	8.54	8.42	20.33	18.54	TL lvisc
Frit 425/SB2-3 Baseline	56	-13.4258	-12.8101	1084.21	1014.34	7.71	8.57	20.37	18.54	TL lvisc
Frit 425/SB2-3 Baseline	57	-13.4235	-12.8386	1092.65	1013.64	6.93	8.73	20.41	18.54	TL lvisc
Frit 425/SB2-3 Baseline	58	-13.4213	-12.8671	1100.95	1012.90	6.20	8.88	20.45	18.54	TL lvisc
Frit 425/SB2-3 Baseline	59	-13.4191	-12.8956	1109.12	1012.14	5.52	9.03	20.50	18.53	TL lvisc
Frit 425/SB2-3 Baseline	60	-13.4168	-12.9241	1117.17	1011.37	4.88	9.19	20.54	18.53	TL lvisc

APPENDIX C

MAR ASSESSMENT FOR FRIT 433

Table C.1. MAR Assessment for Frit 433 – SB3.

WL (%)	B Del Gp MAR (kcal/mol)	Li Del Gp MAR (kcal/mol)	T _L Pred (°C)	TL MAR (°C)	Visc Pred (Poise)	Al ₂ O ₃ wt%	R ₂ O ⁹ wt%	R ₂ O MAR	MAR Status
25	-13.6564	-13.4201	710.96	990.26	56.69	3.83	20.56	18.54	Del Gp R2O
26	-13.6552	-13.4189	726.00	992.57	54.44	3.98	20.58	18.53	Del Gp R2O
27	-13.6540	-13.4177	740.71	994.77	52.23	4.13	20.60	18.53	Del Gp R2O
28	-13.6528	-13.4165	755.11	996.86	50.05	4.29	20.63	18.53	Del Gp
29	-13.6516	-13.4153	769.21	998.85	47.91	4.44	20.65	18.53	Del Gp
30	-13.6504	-13.4141	783.03	1000.75	45.81	4.59	20.67	18.53	Del Gp
31	-13.6493	-13.4130	796.56	1002.58	43.74	4.75	20.69	18.53	Del Gp
32	-13.6481	-13.4118	809.84	1004.33	41.72	4.90	20.71	18.53	Del Gp
33	-13.6469	-13.4106	822.85	1006.01	39.74	5.05	20.74	18.53	Del Gp
34	-13.6457	-13.4094	835.62	1007.62	37.79	5.21	20.76	18.52	Del Gp
35	-13.6445	-13.4082	848.16	1009.16	35.90	5.36	20.78	18.52	Del Gp
36	-13.6433	-13.4070	860.46	1010.64	34.04	5.51	20.80	18.52	Del Gp
37	-13.6421	-13.4058	872.54	1012.05	32.23	5.66	20.83	18.52	Del Gp
38	-13.6409	-13.4046	884.40	1013.32	30.47	5.82	20.85	18.52	Del Gp
39	-13.6396	-13.4033	896.06	1014.18	28.75	5.97	20.87	18.52	Del Gp
40	-13.6384	-13.4021	907.51	1015.01	27.09	6.12	20.89	18.52	Del Gp
41	-13.6372	-13.4009	918.77	1015.78	25.47	6.28	20.92	18.51	Del Gp
42	-13.6360	-13.3997	929.83	1016.49	23.90	6.43	20.94	18.51	Del Gp lvisc
43	-13.6348	-13.3985	940.71	1017.13	22.38	6.58	20.96	18.51	Del Gp lvisc
44	-13.6336	-13.3973	951.41	1017.69	20.91	6.74	20.98	18.51	Del Gp lvisc
45	-13.6323	-13.3960	961.94	1018.16	19.49	6.89	21.00	18.51	Del Gp lvisc
46	-13.6311	-13.3948	972.30	1018.54	18.13	7.04	21.03	18.51	Del Gp lvisc
47	-13.6299	-13.3936	982.49	1018.80	16.82	7.20	21.05	18.51	Del Gp lvisc
48	-13.6287	-13.3924	992.52	1018.95	15.56	7.35	21.07	18.51	Del Gp lvisc
49	-13.6274	-13.3911	1002.39	1018.98	14.36	7.50	21.09	18.50	Del Gp lvisc
50	-13.6262	-13.3899	1012.11	1018.90	13.21	7.66	21.12	18.50	Del Gp lvisc
51	-13.6250	-13.3887	1021.68	1018.71	12.11	7.81	21.14	18.50	Del Gp TL lvisc

⁹ R₂O represents the sum of alkali where R = Na, Li, K, and Cs.

Table C.1. MAR Assessment for Frit 433 – SB3.

52	-13.6237	-13.3874	1031.10	1018.42	11.07	7.96	21.16	18.50	Del Gp	TL	lvise
53	-13.6225	-13.3862	1040.39	1018.04	10.08	8.11	21.18	18.50	Del Gp	TL	lvise
54	-13.6212	-13.3849	1049.53	1017.58	9.15	8.27	21.21	18.50	Del Gp	TL	lvise
55	-13.6200	-13.3837	1058.54	1017.05	8.27	8.42	21.23	18.50	Del Gp	TL	lvise
56	-13.6187	-13.3824	1067.42	1016.46	7.45	8.57	21.25	18.50	Del Gp	TL	lvise
57	-13.6175	-13.3812	1076.17	1015.82	6.67	8.73	21.27	18.49	Del Gp	TL	lvise
58	-13.6162	-13.3799	1084.79	1015.13	5.95	8.88	21.29	18.49	Del Gp	TL	lvise
59	-13.6150	-13.3787	1093.29	1014.40	5.28	9.03	21.32	18.49	Del Gp	TL	lvise
60	-13.6137	-13.3774	1101.67	1013.65	4.66	9.19	21.34	18.49	Del Gp	TL	lvise