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THE DWPF PRODUCT COMPOSITION CONTROL SYSTEM AT SAVANNAH RIVER : STATISTICAL PROCESS CONTROL ALGORITHM (U)

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INTRODUCTION

The DWPF Process batch-blends aqueous radwaste (PHA) with solid radwaste (Sludge) in a waste receipt vessel (the SRAT). The resulting SRAT-Batch is transferred to the next process vessel (the SME) and there blended with ground glass (Frit) to produce a batch of feed slurry. The SME-Batch is passed to a subsequent hold tank (the MFT) which feeds a Melter continuously. The Melter produces a molten glass wasteform which is poured into stainless steel canisters for cooling and, ultimately, shipment to and storage in a geologic Repository.

The Repository will require that the glass wasteform be resistant to leaching by any underground water that might contact it. In addition, there are processing constraints on Viscosity and Liquidus Temperature of the melt:

Processibility	Acceptability
Liquidus Temperature ≤ 1050°C 20 ≤ Melt Viscosity ≤ 100 poise	Leach Rate ≤ 1 $gm/m^2/day$

THE PCCS STATISTICAL PROCESS CONTROL (SPC) ALGORITHM

What Is It?

The Product Composition Control System (PCCS) is the system intended to ensure that the *melt will be Processible* and that the *glass wasteform will be Acceptable.* Within the PCCS, the SPC Algorithm is the device which *guides control of the DWPF process.*

Why Is It?

The SPC Algorithm is needed to control the *multivariate* DWPF process *in the face of uncertainties (variances and covariances)* which arise from this process and its supply, sampling, modeling, and measurement systems.

What Does It Do?

The SPC Algorithm

- *derives a Target-Blend* (mass fractions *p* pf PHA, *s* of Sludge, and *f* of Frit) which will combine with current SRAT and SME Heels to produce a SME-Batch with desirably high waste-loading,

- *monitors a pending SME-Batch* composition for Melt Processibility and Product Acceptability prior to clearing it for transfer to the Melter Feed Tank,

- and *derives a Remediation-Blend* of trim chemicals to correct an Unacceptable SME-Batch

in such a way that *the resulting melt will likely process into good product.* The essentials of the DWPF Process and the PCCS are illustrated in Figure 1. However, for simplicity we limit the discussion here to *monitoring*.

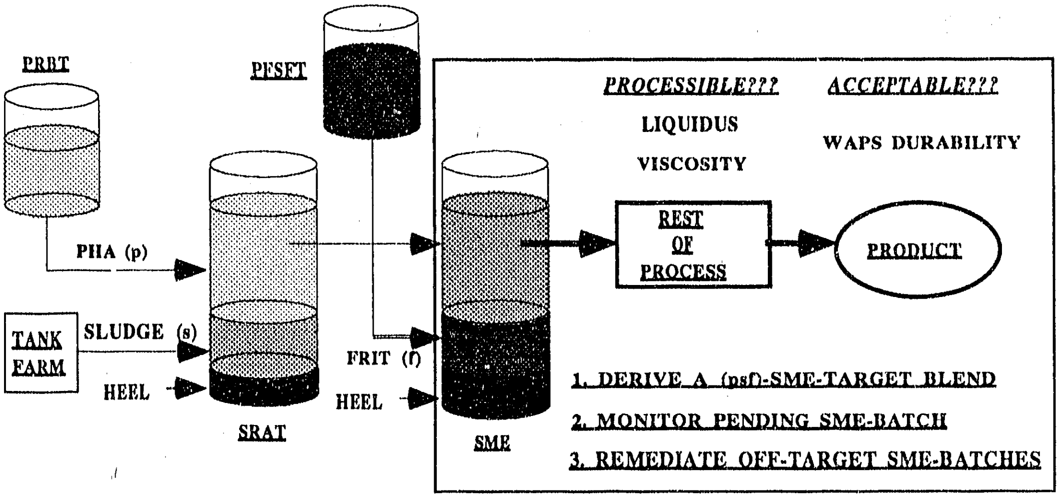

Figure 1 Product Composition Control System

To monitor the SME-Batch composition, the PCCS SPC algorithm takes into account:

- uncertainties inherent in slurry *sampling*, sample *preparation* and *measurement*;

- uncertainty in *prediction of properties* from slurry composition;

- the *simultaneous* variation of the individual constituent concentrations;

- mass-balance process information to *augment the measurement data*;

- and the *Waste Acceptance criteria* (WAPS).

It also will take into account *process and input feed variations*, as they become known during operation.

CHARACTERIZING THE PROCESS PRIOR TO MAKING PRODUCT

The process is characterized prior to making product *by relating glass and melt Properties to feed slurry Composition.* The composition is expressed through a hybrid combination of elements denoted ξ. Each property has its own unique ξ. Both glass chemistry theory and empirical least-squares fitting show that *straight-line regressions* relate the glass property (Leach Rate) and the process melt properties (Viscosity and Liquidus Temperature) to the ξ's. Thus, to characterize the process *prior to making and inspecting either the melt or product*, these properties are *predicted* from measured feed slurry composition using straight-line regressions in ξ. Back-solving any such regression line to get the ξ-value corresponding to its property limit transforms the constraint on that property into an equivalent constraint on its ξ. This constraint on ξ, in turn, becomes a constraint on the concentrations of the individual constituent oxides (the "x's"). For example,

the Liquidus regression is: $T_L = 803.8698 + 2276.8724\xi_t$

and its ξ is: $\xi_t = \dfrac{134[Fe_2O_3]}{156[SiO_2] - 360[Al_2O_3]}$.

Its property limit is: $T_L \leq 1050°C$

which transforms to: $\xi_t \leq \left[\underline{0.108} = \dfrac{1050 - 803.8698}{2276.8724}\right]$.

Graphically, this is illustrated in Figure 2.

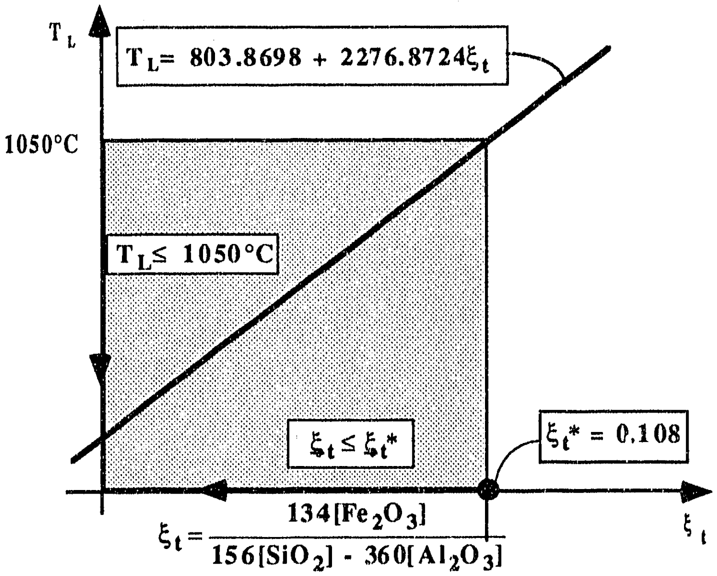

Figure 2 Liquidus Correlation

Thus, $T_L \leq 1050°C$ becomes: $134[Fe_2O_3] \leq 0.108\left(156[SiO_2] - 360[Al_2O_3]\right)$

or: $$\left(134[Fe_2O_3] - 16.848[SiO_2] + 38.88[Al_2O_3]\right) \leq 0$$

or: $$[\underline{x}_t]\,[\underline{\alpha}_t]' \leq 0$$

where: $[\underline{x}_t] = ([Fe_2O_3],[SiO_2],[Al_2O_3])$ and $[\underline{\alpha}_t] = [134, -16.848, 38.88]$.

The inequality thus formed determines a region in measured composition space ($\underline{x}$-Space), all points of which give predicted values of T_L that are Acceptable (ie, ≤ 1050°C). Denote this region the *Expected Property Acceptable Region (EPAR).* Figure 3 illustrates the EPAR for Liquidus (using only 2-dimensions for clarity).

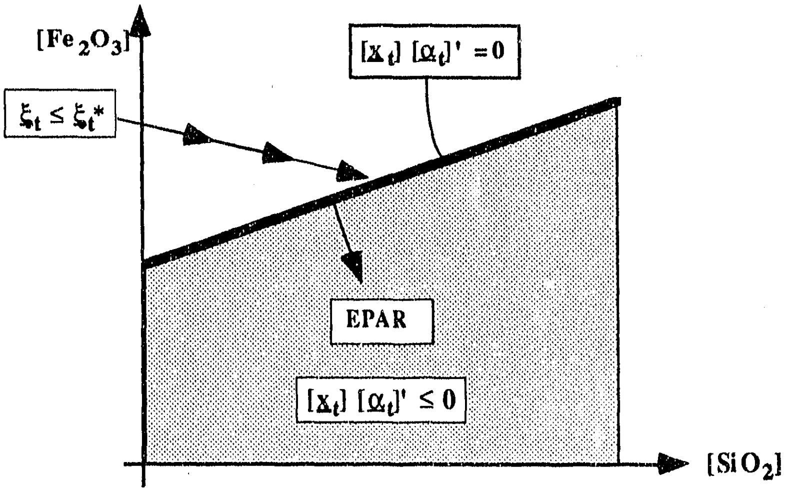

Figure 3 Liquidus EPAR in 2 Dimensions

ACCOUNTING FOR PREDICTION UNCERTAINTY

To monitor an already blended SME-Batch, the algorithm first accounts for the (random) uncertainty of prediction through use of *Scheffé simultaneous confidence bands*[1] around the straight-line regressions:

Scheffe-type Bands: $$\text{Model Value} \pm s_r\sqrt{q\,F(q,n-q)}\sqrt{\xi_0(X'X)^{-1}\xi_0'}$$

These bands utilize the estimate of the random error standard deviation (s_r), the design of the parent data $(X'X)^{-1}$, and the F-statistic to provide at any $\xi = \xi_0$ confidence limits on the model value which hold simultaneously for all ξ. They are appropriate for *repeated* use of the line.

Back-solving the appropriate (upper and/or lower) *confidence band* for a new ξ-limit ξ^* corresponding to the acceptable property limit produces other inequalities like those which generated the EPAR. These new inequalities are *constraint hyperplanes* in $\underline{x}$-Space which accommodate the random uncertainty in the predictions. Call them Constraint Uncertainty Planes and denote them as $\underline{x}$-*CUP's*. These new inequalities generate the *Property Acceptable Region (PAR),* the locus of all compositions which give acceptable property predictions even *allowing for* *the random uncertainty of prediction.* The PAR is interior to (and thus everywhere more conservative than) the EPAR. See Figure 4 for illustration for Liquidus. (There are corresponding but different cases for Viscosity and Durability.)

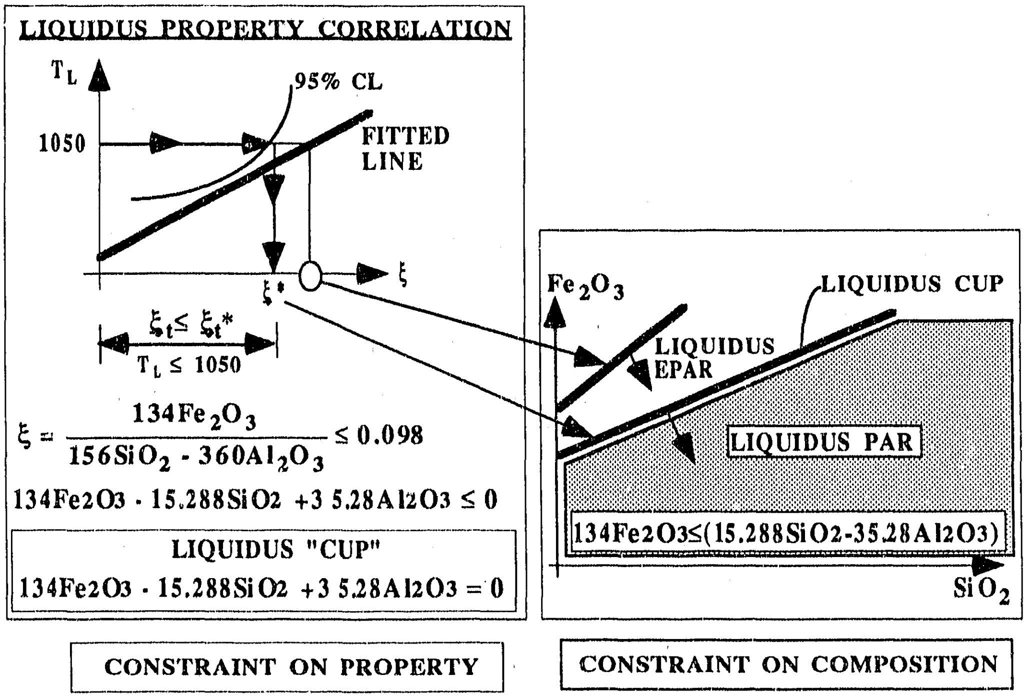

Figure 4 Liquidus Property Acceptability

There is a separate PAR for each property. The confluence of all 4 such PAR's forms the *overall PAR*. (Actually, only 3 determine the overall PAR since only one of the Lo Viscosity and Hi Viscosity constraint pair will apply to a particular case.) *Any point located within the overall PAR represents a SME-Batch measured composition which will give predicted properties that meet all the stated limits, even allowing for predictive uncertainty.* The PAR is illustrated in Figure 5.

ACCOUNTING FOR SAMPLING & MEASUREMENT UNCERTAINTY

The PAR accommodates the random uncertainty inherent in property prediction arising from uncertainty only in the properties themselves. But, in operation, the composition of the feed slurry will not be measured to the same accuracy and precision as that of the standard glasses on which the predicting relations are based. Thus, *there will be appreciable errors in ξ.* It remains to deal with this component of uncertainty *from the sampling and measurement systems which produce the composition measurement.*

A current SME-Batch composition measurement $\underline{x}^m$ is a 1xq row-vector of measurements on *several constituent oxides simultaneously* :

$$\underline{x}^m = ([Fe_2O_3] , [SiO_2] , \ldots, [MgO]) = [x_1 , x_2 , \ldots, x_q].$$

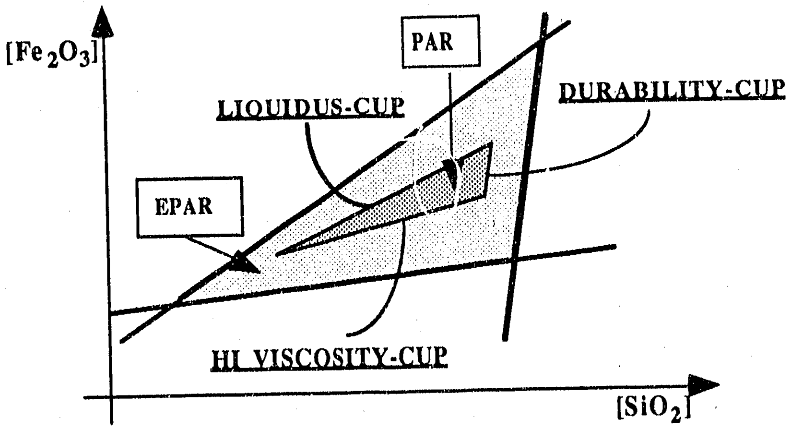

Figure 5 The DWPF Property Acceptable Region (PAR)

To describe its uncertainty thus necessitates use of *multivariate* statistical techniques.† If the concentrations of the individual constituents can be assumed multivariate Gaussian, then traditional methods of multivariate normal theory apply. Assuming the process to be q-variate Gaussian centered at $\underline{x}^m$, the uncertainty around this measurement due to "usual and customary" noise is described by *Hotelling's* T^2. Hotelling's T^2 is the multivariate analog[2] of the square of "Student's t":

$$T^2 = [\underline{x} - \underline{x}^m]\, S_M^{-1} [\underline{x} - \underline{x}^m]'.$$

S_M is the covariance matrix based on an historic sample of several such measurements (but not including $\underline{x}^m$). S_M consists of the variances within and covariances between the "q" individual constituents:

$$S_M = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1q} \\ s_{12} & s_{22} & \cdots & s_{2q} \\ & & & \\ s_{1q} & s_{2q} & \cdots & s_{qq} \end{bmatrix}$$

where the s_{ij} are the sample variances (i=j) and covariances (i≠j):

$$s_{ij} = \frac{1}{n-1}\sum\left(x_{ik} - \underline{x}_i\right)\left(x_{jk} - \underline{x}_j\right)$$

---

† A more simplistic alternative, that of applying several sets of univariate control limits independently, is theoretically and pragmatically counterproductive since it causes the false-reject rate to sky-rocket. If there are q=10 constituents to be controlled, and if 95% control limits are applied independently on each, from probability considerations alone some 40% of the candidate feed batches will be rejected even though they are good feed material.

$$\underline{x}_j = \frac{1}{n}\sum x_{jk} \qquad k = 1,2,\ldots,n.$$

The locus of all points $\underline{x}$ such that $T^2 \leq T_c^2$ is a q-dimensional ellipsoid which represents the uncertainty envelope around the measurement $\underline{x}^m$. This ellipsoid is denoted the *Measurement & Sampling uncertainty Ellipsoid (MSE).* The aspect ratios and tilts of the MSE are determined by S_M^{-1}, the inverse of the covariance matrix S_M. The size (ie, probability volume) of the MSE is determined by the number and allocation of samples and measurements, and by the critical value T_c^2 of Hotelling's T^2 corresponding to whatever confidence level is chosen. If "r" replicate measurements are averaged to get $\underline{x}^m$, the covariance matrix becomes $\underline{S}_M = r^{-1}S_M$; and thus the expression above corresponds to the case of a single measurement, r=1. T^2 is distributed as:

$$T^2 \sim \left[\frac{(n+1)}{n}\right]\left[\frac{q(n-1)}{n-q}\right]F(q,\ n\text{-}q)$$

where F(q, n-q) is the variance-ratio statistic with "q" numerator and "n-q" denominator degrees of freedom.[3] Thus, the "radius" T_c of the MSE can be set according to the probability level appropriate for the test. See Figure 6 for continued illustration of the Liquidus case.

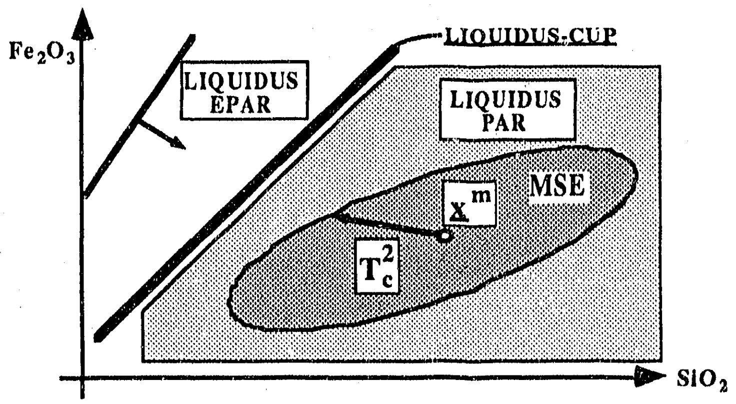

Figure 6 Measurement and Sampling Uncertainty Ellipsoid

MONITORING A SME-BATCH

With the property modeling uncertainty accommodated by the CUP and the composition measurement uncertainties accommodated by the MSE, it remains to *determine whether the MSE is everywhere inside the PAR and distinct from the CUP*. If it is, not only is the composition measurement itself Acceptable, but it is also far enough away from the CUP to be *statistically distinguishable* from it. The algorithm now *decides* whether $\underline{x}^m$ meets both these criteria; if so, the SME-Batch is judged to be *Property and Measurement Acceptable* for that property. To decide this, it determines whether or not the point on the CUP "nearest" the MSE is geometrically distinct from it. Denote that nearest point $\underline{x}^+$, and denote its T^2-value by T_+^2:

$$T_+^2 = [\underline{x}^+ - \underline{x}^m]\, S_M^{-1}\, [\underline{x}^+ - \underline{x}^m]' = \min_x \left\{ [\underline{x}^+ - \underline{x}^m]\, S_M^{-1}\, [\underline{x}^+ - \underline{x}^m]' \right\}.$$

To determine T_+^2, do a Lagrangian minimization of T^2 subject to the auxiliary condition that $\underline{x}$ be on an $\underline{x}$-CUP. This means that $\underline{x}\,\underline{a}' + \varepsilon = 0$ where $\varepsilon = 0$ for Liquidus and Viscosity, $\varepsilon = 5.67$ for Durability, and the $\underline{a}$ are known constants deriving from the back-solution of the confidence bands around the property model. Thus:

Minimize T^2 subject to the constraint: $\phi = \underline{x}\,\underline{a}' + \varepsilon = 0.$

Construct the Lagrangian: $F = T^2 + \lambda\,\phi$

Solve for the $\underline{x}$ which minimizes F, which by Lagrange is also the $\underline{x}$ which minimizes T^2. Find the partial derivatives:

$$\frac{\partial F}{\partial \underline{x}} = \frac{\partial T^2}{\partial \underline{x}} + \lambda \frac{\partial \phi}{\partial \underline{x}} = 2 S_M^{-1} [\underline{x} - \underline{x}^m]' + \lambda\,\underline{a}'$$

$$\frac{\partial F}{\partial \lambda} = \underline{x}\,\underline{a}' + \varepsilon$$

Set the partials to zero and solve for x+: $2 S_M S_M^{-1} [\underline{x}^+ - \underline{x}^m]' + S_M \lambda\,\underline{a}' = 0$

$$[\underline{x}^+]' = [\underline{x}^m]' - \left(\frac{\lambda}{2}\right) S_M\,\underline{a}'$$

$$\underline{x}^+\underline{a}' + \varepsilon = 0 \rightarrow \underline{x}^m\underline{a}' - \left(\frac{\lambda}{2}\right) \underline{a}\, S_M\,\underline{a}' + \varepsilon = 0$$

$$\frac{\lambda}{2} = \frac{\underline{x}^m\underline{a}' + \varepsilon}{\underline{a}\, S_M\,\underline{a}'}$$

The solution is: $\underline{x}^+ = \underline{x}^m - \left[\dfrac{\underline{x}^m\underline{a}' + \varepsilon}{\underline{a}\, S_M\,\underline{a}'}\right] \underline{a}\, S_M .$

This solution gives the minimum, since there can be no maximum. The minimum T^2 corresponding to this is:

$$_{\min}T^2 = T_+^2 = \frac{(\underline{x}^m\underline{a}' + \varepsilon)^2}{\underline{a}\, S_M\,\underline{a}'} .$$

Thus, the test devolves to: $\dfrac{(\underline{x}^m\underline{a}' + \varepsilon)^2}{\underline{a}\, S_M\,\underline{a}'} : T_c^2 .$

for the case of a single measurement (r=1). For the average of r >1 replicates:

$$\left(T_+^2\right)_r = r\,T_+^2$$

and the test becomes: $$r\,\frac{(\underline{x}^m\underline{a}' + \varepsilon)^2}{\underline{a}\,S_M\,\underline{a}'} : T_c^2 \qquad r = 2,3,\ldots$$

If $T_+^2 > T_c^2$, then $\underline{x}^+$ is outside of, and thus does not touch, the MSE. If this is true for $\underline{x}^+$, it being "nearest" the measurement, then it must be true for *all points on the* $\underline{x}$*-CUP*. If this is true for all 4 $\underline{x}^+$, then $\underline{x}^m$ is statistically distinct from all CUP's, and $\underline{x}^m$ differs from $\underline{x}^+$ by more than sampling and measurement noise, and is judged to be statistically distinct from it. See Figure 7 for continuation of the Liquidus illustration.

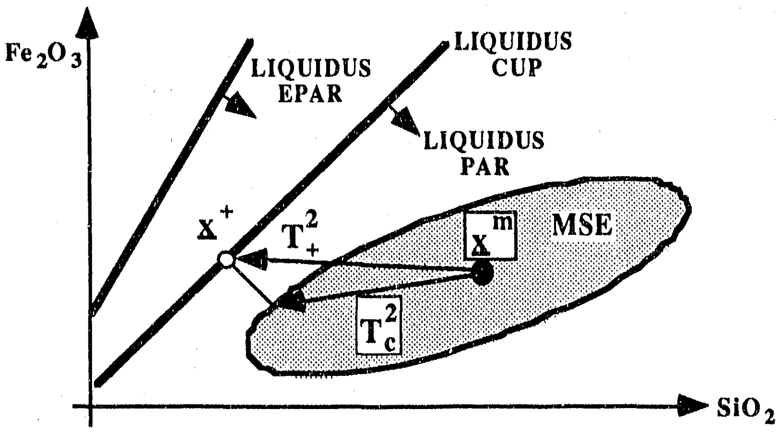

Figure 7 Property and Measurement Acceptability

If $T_+^2 > T_c^2$ for *all properties*, the SME-Batch is judged to be *overall Property and Measurement Acceptable.* It is then cleared for transfer to the MFT.

INCORPORATING OTHER PROCESS INFORMATION

In order to improve the precision of the measurements, the algorithm augments the measurement information available for process control by incorporating other relevant process information into the measurement system through use of a *Kalman Filter*[4] *mass-transfer state model.* The KF mass-transfer state model gives a *state projection* for the SME composition after receipt of the SRAT transfer but prior to the control lab measurement:

[State Projection for Mass in SME Now] =

[Mass out of SRAT+Mass into SME]/2 + [SME Heel]

The Kalman-filtered state estimate is the following combination of this state-model projection and the relevant lab measurement:

[SME State Estimate] =

[State Projection] + K[Lab Measurement - State Projection]

where the "Kalman Gain" K varies over (0,1) to favor the State Projection or the Lab Measurement as its current notion about the uncertainties in each dictates.

ADVANTAGES OF THE ALGORITHM

By correctly accommodating the multivariate uncertainty of the composition measurement system, and by incorporating the uncertainty of property prediction, it *correctly maintains the false-alarm rate* (proportion of good SME-Batches wrongly judged to need remediation) at a reasonable level.

By incorporating mass transfer measurements into the composition measurement system, it *increases the useful information* and thus relieves some of the stress on the composition measurements. The built-in redundancy of the mass transfer measurements with the composition measurements also provides a means of *detecting aberrations ("outliers")* in either.

By devising a Target Blend to give acceptable properties, it *smooths out batchwise differences in feed composition* to give an "on-aim" type of control scheme on properties rather than a "within-limits" type of control on composition. In so doing, it has the effect of constructing a Property "Macro-Batch" out of possibly variable input feed material.

Its quantification of process control enables DWPF *to take quantitative credit for the control efforts upstream of the MFT*; thereby relegating the MFT sample measurements to a "confirmatory" rather than a "determining" role. This translates into fewer MFT samples and less MFT measurements for equal confidence.

Expressed another way: without such an algorithm, the pre-MFT prior model is a "total ignorance" prior; namely, that the feed slurry arrives at the MFT *at random*. In that case, all the load of Waste Qualification falls on the MFT samples and measurements.

ACKNOWLEDGEMENTS

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