TOWARDS PREDICTIVE CONTROL OF FERROALLOY FURNACES: COMBINING THERMOCHEMISTRY, INVENTORY MODELLING AND SYSTEMS ENGINEERING

J.J. Eksteen[1], S. J. Frank[2] and M.A.Reuter[3]

[1]Department of Process Engineering, University of Stellenbosch, Private Bag X1, Matieland, 7602, South Africa.
E-mail: jeksteen@sun.ac.za
[2]Crusader Systems (Pty) Ltd P.O. Box 98040, Waterkloof Heights, 0065, South Africa. E-mail sjfrank@crusader.co.za
[3]Department of Applied Earth sciences, Delft University of Technology, Mijnbouwstraat 120, 2628 RX Delft,
The Netherlands. E-mail: M.A.Reuter@citg.tudelft.nl

ABSTRACT

Ferroalloy furnaces are well known to be extremely difficult to control from a metallurgical perspective. Mostly metallurgical control is still reactive in nature, causing a significant amount of reworking and product blending to achieve a proper product specification. Despite numerous efforts towards the model based control of primary smelting operations, actual metallurgical feedforward control seems to remain elusive. One of the key reasons in the failure to model these metallurgical reactors well, is that fundamentally orientated pyrometallurgists, statisticians, data miners and control engineers very often have diverging ideas how to model these systems. Furthermore, metallurgists have often come to rely on their ability to develop empirical regression models of furnace behaviour, as they have lost their faith in the ability of thermochemical and metallurgical engineering fundamentals to accurately predict the outcomes from furnaces. This paper shows how good thermochemical modelling can be combined with proper technological and systems analysis, as well as a proper inventory model, to predict the alloy and slag chemistry with good accuracy one tap into the future, at a time horizon of typically around 4 to 6 hours. For this modelling approach, a number of tools will be used, such as data reconciliation, thermodynamic modelling using FactSage®, inventory and heel estimation, neural networks and statistical data exploration. Furthermore, systems identification theory will be combined with the approaches given above to develop a truly dynamic predictive model. This paper seeks to demonstrate the need for a hybrid approach, which incorporates plant data and readily accessible thermodynamic data to develop a proper dynamic model.

1. INTRODUCTION

Metallurgical process control is still a major challenge in the metallurgical process industry. Primary bath smelting operations are characterised by multiphase reactions and complex chemistry, as well as ill-defined kinetic-, momentum, heat and mass transfer phenomena. The processes in burden-type furnaces are even more complex.

Ideally, metallurgical control for bath type furnaces would eventually seek to achieve a few important goals:

- Control of the predicted assay of the bulk slag / alloy / dust.
- Control of the expected yields of bulk slag / alloy / dust.
- Control of the rheology of the product phases to ensure tapability, with minimum metal entrainment (For example, alloy produced is normally seen as alloy tapped - not what is available in the furnace).
- Minimisation of the specific energy input while still maintaining yields and product specifications
- Control to minimise environmental impact.
- Control for cost minimisation or income maximisation

It is important to realise that not all of the above could be control objective functions at the same time. One of the above-mentioned aspects becomes the main control objective while the other are specified as constraints.

Proceedings: Tenth International Ferroalloys Congress;
INFACON X: '*Transformation through Technology*'
ISBN: 0-9584663-5-1

1 – 4 February 2004
Cape Town, South Africa
Produced by: Document Transformation Technologies

Some advanced modelling techniques such as computational fluid dynamic (CFD) modelling have been used to aid in process characterisation. However, while CFD modelling has aided many metallurgists in analysing waste heat reboilers, ladle processing and casting operations, the nature of the primary smelting operations remains too ill-characterised to develop reliable phenomenological models where the parameters are known with a high degree of certainty. The long time to converge (if they converge at all) still limits CFD to off-line model development. A pure thermodynamic approach also fails. A detailed thermodynamic simulation may aid in predicting the type and amounts of stable phases, and the deportment of elements in phases. This may give a general idea of the equilibrium state, but this ideal equilibrium state is never perfectly achieved. Thermodynamic simulation is therefore seen, as for CFD, as an off-line tool for process development and design, not as a tool for on-line process control. Moreover, when thermodynamic analyses are done on raw data from primary smelting operations, the plant outcomes are often poorly correlated with the thermodynamic predictions. On the other hand, data miners and control engineers very often take a totally empirical or black-box approach which very often leads to short term process accuracy, but long term instability. This is also the reason why one finds so few working dynamic (empirical) process models, despite the claim of accuracy. This is due to the fact that very often these models are non-linear (non-linear parameters estimation is bound to run into convergence and instability problems) and they are based on a certain time frame of historic data. However, very often changes are made in the fundamental operating characteristics of the process, due to the plant changing to another raw material supplier, modifications to the feed pre-treatment system etc., which fundamentally shift the normal operating position into a region outside the boundaries of the original data set used for parameters estimation.

Ideally, one would therefore seek for a modelling approach or algorithm that would be able to:

- Capture the fundamental trend characteristics of the process through a fundamental submodel.
- Limit nonlinearities of non-linear parameter estimation to the pre-derived (or off-line derived) fundamental models. Once the non-linear parameters are derived they should preferably remain fixed. This model therefore becomes a non-linear transformation of the input parameters.
- Characterise the distributed nature of the materials entering and leaving the reactor using statistical techniques, both in space and time. This also has to be done for the non-material operating variables as far as it is practical.
- Pretreat the data to close the material balances over an extended time horizon in a way that is statistically acceptable (i.e. a way that takes into account the statistical nature of the data). In other words the data should be reconciled within its statistical variance.
- Use the pretreated data set, in conjunction with the non-linear transformation model, to develop a dynamic process model which is linear in the parameters (although the variables themselves may be non-linearly transformed).
- Recursively estimate the linear parameters. The re-estimation instant should be triggered by non-conformance to a statistical condition.
- Incorporate the dynamic process model into a standard model predictive control architecture.

It is apparent that multiple levels of knowledge would be required which are not typical of any single engineering curriculum. Moreover, it would be preferable that all these knowledge types reside within one person due to the interactions of the knowledge categories. Although the requirements above superficially appear as a linear series, deeper analysis will show that the categories interact at various levels. The requirements presented above will be discussed below. The paper will show that fundamental equilibrium modelling, process dynamics and systems modelling and process data characterisation all have their own part to play in the development of an overall model, which may then be implemented into model predictive control. Leaving out either the fundamental model, or the dynamic model component, or the data characterisation, will lead to process models which are either inaccurate, or overly complex, or unable to deal with fundamental shifts in process conditions.

2. THERMODYNAMIC MODELLING OF REDUCTIVE CHROMITE BATH SMELTING AND THE “INTELLIGENT MAPPING” THEREOF

This paragraph will focus on a specific type of fundamental submodel for chromite bath smelting operations, namely a representative thermodynamic submodel, which will become a component of the overall dynamic process model. While thermodynamic modelling remains a powerful prediction tool, it should be kept in

mind that thermodynamic equilibrium cannot predict the process dynamics, which are inherent to all metallurgical processes. Bath type furnaces are intensive smelting operations, i.e. very small processing volumes are used to achieve very high mass and heat transfer rates and rapid kinetics. Production engineers often assume that these reactors would closely approach an equilibrium state, derived from the feeds to the process (in contrast to post-analysis based on slag-metal equilibrium where the actual feed is not taken into account).

One approach, to predict equilibrium based on the reactor feeds, would be to use one of a number of commercially available thermodynamic software packages (MTData ® [1] by NPL in the UK, FactSage ® [2] by CRCT in Montreal, Canada , MPE ® [3] by the CSIRO in Australia, Thermo-Calc ®, [4], by Thermo-Calc, Sweden) to perform the equilibrium predictions based on a Gibbs Free Energy minimisation algorithm which is used in conjunction with pure component properties and non-ideal solution properties. For the purposes of the work done at the University of Stellenbosch and the Delft University of Technology, FactSage ® will be used as a typical example. All the above mentioned software packages are powerful in their ability to calculate non-ideal thermochemical equilibrium and their databases are frequently updated with the most recent, critically assessed, solution parameter sets. The basis of the thermodynamic calculations is the Solgasmix ® Gibbs Free Energy (GFE) minimiser [5]. The software uses the modified quasichemical model for short-range ordering [6], [7], [8] to model molten slags and mattes. Sublattice models [9] are used for the solid solutions, and polynomial expansions or the unified interaction parameters formalism are used to model alloy melts. Although these software packages are ideal for design and process development, neither the software, nor the format of the results lend it to direct on-line prediction.

A way to overcome this challenge, is to use an alternative mapping function which maps process inputs to predicted equilibrium outputs, as predetermined by, say, FactSage ®. A convenient and powerful way to perform this mapping is through the use of non-parametric models such as standard feedforward back propagation neural networks [10]. It has been shown that these networks can represent the complex equilibrium thermodynamics to a near-perfect accuracy [11]. For example, in the case of high carbon ferrochrome (HCFeCr) production from chromite, fluxes and anthracite in an open arc furnace, one needs to perform up to 50000 simulations, using an input table constructed using the principle of 3^n factorial design to cover the complete input space with as few as possible simulations. The range of the input space is determined by the range of plant data with a 20% increase in the maximum range. In this specific case, a multi layer perceptron neural network has been trained with 8 inputs (Temperature, and the ratios of Fe, Mg, Al, Ca, Si, O and C to Cr elements in feed), 40 hidden nodes, over 45000 training exemplars, and tested on over 13000 test cases. Prediction accuracy of the quantity and chemistry of every phase were obtained with an R^2 above 95%. The thermodynamics of the furnace can therefore be reliably predicted within the boundaries of the trained data generated by FactSage. As FactSage predicts the amount of each phase (for example the lime, periclase, spinels, mullite, pyroxene, and corundum solid solutions, molten slag and molten alloy and alloy carbide precipitates), the data has to be reworked to relate it to the form industry normally would measure it. For instance, where oxidic solid solutions precipitate, the actual slag analysis will reflect the overall analysis of the combined molten and entrained solid components. On the other hand, FactSage will predict the composition of the liquid and solid phases separately. The overall composition has therefore to be reconstituted from the FactSage predictions. Similarly one has to recalculate the actual alloy phase from the liquid alloy and the alloy solid solution and intermetallic precipitates. Therefore, as industrial slags and alloys are analysed based on bulk material chemistry, the assay of a specific element, say carbon in the alloy has to be recalculated from the carbon in the liquid alloy and the carbon as distributed amongst all the solid (carbide) phases.

From a control perspective the actual composition of the separate solid phases is not so important. However, it is important to calculate the fraction of the reconstituted slag that is solids, as it significantly influences the furnace behaviour through influencing the melt rheology, and therefore such phenomena such as metal entrainment in slag, slag foaming, and melt phase tapability and mixing. For the purpose of viscosity estimation one would require the composition and temperature of the liquid-only slag component of the slag / alloy, and the total fraction of solids associated with the bulk phase. For this purpose, the correlations of Urbain [12], [13]or Riboud [14] may be used to calculate the viscosity of the liquid-only slag phase, while the Einstein-Roscoe [15] equation may be used to estimate the observed bulk viscosity, once the relative amounts of liquid and total solids are known. A-priori knowledge of the viscosity, even within an order of

magnitude would allow production staff to gauge if they could expect problems with tapping, foaming or significant entrainment.

It was shown in this section that thermodynamics has an important role to play to predict the overall trends to be expected in furnace data, as well some direct production aspects which are for instance influenced by melt viscosity. It was also shown that the data requires reworking before it could be used for neural network training. The neural network becomes an "artificial intelligent" predictor of the thermodynamics in a way that is readily accessible to the production staff, i.e. the data is presented in the same way it is measured in industry. It should be stressed that only the thermodynamic equilibrium predictions are modelled using a neural network, not the plant data. The neural network also does this in a way which presents the outcomes in directly useful form for process interpretation. A way must now be found to make plant data accessible for modelling (both as input to the thermodynamic models, as well as the system models discussed later in this paper), and to determine the limits of model prediction accuracy.

3. CHARACTERISING THE RAW DATA – DISTRIBUTIONS AND VARIANCE

Why do even very complex models (thermochemical models, fundamental dynamic models and CFD) fail to accurately predict the measured outcomes of processes? Due to economic and logistic constraints, the melts from furnaces are seldom sampled more than once per tap. It is therefore assumed by production staff that the sample is representative of the bulk melt, which implies that the alloy or slag has to be well mixed. While it is often assumed that melts of bath type furnaces are well mixed, some recent research points to the contrary [16]. The impact of the well mixedness of the reactor product phases has a significant impact on the representativeness of the final assay, the reliability of the data associated with each melt sample, and how the assay data will subsequently be treated. The results for Si in ferrochrome alloys and CrO in chromite smelting slags have been reported by the authors [17]. In this paper, sulphur is investigated as it has such a significant influence on the metallurgy and the subsequent material properties of stainless steels produced from ferrochrome. Especially when there is a direct transfer of hot material from the ferrochrome producer to the stainless steel producer, the effects of an uncertain sulphur assays become problematic, as no product blending (which involves rework) takes place to smooth out assay discrepancies. To characterise the homogeneity / mixedness of the melt, sampling campaigns were run over two different periods, involving more than 10 taps each. Each tap was analysed based on 6 equispaced samples throughout the duration of the tap, once the flow of the melt through the launder to the ladle was fully developed, i.e. flowing rapidly. The average sulphur assay of each tap was calculated and the % relative deviation from the tap average was calculated for each sample throughout the tap. When the distribution is represented as a frequency histogram (Figure 1), it becomes apparent that the melt is far from well mixed.

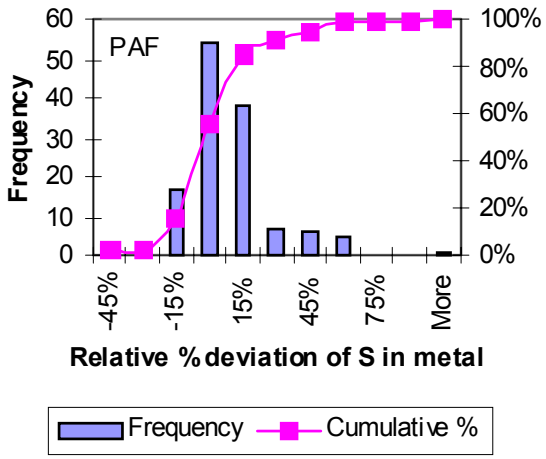

Figure 1. Histogram of the % relative deviation of the Sulphur assay in HCFeCr alloys.

It was shown [17] that for certain elements, such as silicon, the deviation is much more severe. It is apparent from the figures above that the deviation is much more than could be ascribed to analytical instrument imprecision (typically less than 2% relative). It also shows that elements such as Si and S are most definitely not well mixed. Each element in the alloy and the slag should therefore be monitored in a similar way, as the mixedness of a specific element is not necessarily related to the mixedness of another element. It was found that most transition metals show small standard deviations in the alloy melt, which means they can be modelled more reliably than S and Si.

For the case of sulphur presented above, the absolute mean relative deviation has been found to be about 25%. If a 95% confidence interval is used, the standard error is twice the standard deviation, which would imply a relative sample error of ±50% which gives the upper and lower limits within which a sample assay may be readjusted using data reconciliation techniques as discussed in the following paragraph. It is also apparent that, no matter how complicated a process model is developed, the model predictions cannot be expected to perform better than the inherent error level associated with the variable to be predicted. In the case of sulphur given above, with the model predicting the mean and the measurements allowed to vary with a relative standard deviation of 25% around the mean, the model can never achieve an R^2 greater than 0.55 (multiple runs with over 100 data points). If two different models both perform better, it cannot be stated with any certainty that the one model is inherently more accurate than another. The simplest model of the two would then be the best choice.

Once the data has been statistically characterised and limits have been determined as to the best possible performance of model predictions compared to measurements, one may use the statistical properties of the data (such as its variance) to process the data for further model development. This data processing, is the essence of the following section.

4. RECONCILING THE DATA – A LOW PASS FILTERING TECHNIQUE

Once the standard deviations are known, the data could be reconciled to obtain mass balance closure. The material balances could be reconciled within the shortest timeframe within which the quantities of all streams and inventories could be determined with reasonable accuracy. Two factors normally make it difficult to reduce the time-horizon to less than a day – the flue dust composition is not analysed often, and the fluctuating melt inventory and unknown furnace freeze lining contribute to tap-to-tap uncertainty. If these two aspects are addressed to obtain a good estimate of the freeze line on the furnace wall and of the dust analysis, the time horizon may be reduced.

If the variances have been characterised, the data may be reconciled using a standard non-linear programming technique, such as the generalised reduced gradient method. In principle the problem is a quadratic optimisation problem with linear mass balance constraints. In general, a measurement vector for every stream ($\boldsymbol{x}_m$), which contains all the assays of all the components, may be written as:

$$x_m = x_{adjusted} + e \tag{1}$$

where $x_{adjusted}$ is the vector of the adjusted (reconciled) values of the variables, x_m, the vector of unbiased random measurement errors normally distributed with a zero mean and covariance matrix V.

The reconciliation problem can therefore be stated as a constrained least squares estimation problem where the weighted sum of adjustments is to be minimised to constraints:

$$\min_{x_{adjusted}} \left(x_m - x_{adjusted}\right)^T V^{-1} \left(x_m - x_{adjusted}\right) \tag{2}$$

subject to

$$f\left(x_{adjusted}\right) = 0 \tag{3}$$

which is the steady state mass balance for an element over the reconciliation period,

where $V \in \Re^{n_x \times n_x}$ is the covariance matrix of the measured variables x_m. In the discussed case the linear constraints arise from the linear mass balance equations for the different elements of the system, and the overall material balance. Additional constraints arise due to stoichiometric relationships, which constrain the maximum and minimum carbon to oxygen ratio in the gas stream and the minimum and maximum amount of oxygen that may be associated with the elements in the slag and dust. When the data may be biased, the systematic bias may be estimated as a parameter, where the objective function is reformulated as follows:

$$\min J(x) = \min \sum_{i=1}^{k} \frac{\left(\bar{x}_i - \left(x_m - \hat{b}_i\right)\right)^2}{V_i} \tag{4}$$

subject to the mass balance and stoichiometric constraints, as well as upper and lower bounds on the adjusted variables and biases:

$$\begin{aligned} & f\left(\bar{x}_i\right) = 0 \\ & \bar{x}_{lower,i} \le \bar{x}_i \le \bar{x}_{upper,i} \qquad \forall i \\ & \hat{b}_{lower,i} \le \hat{b}_i \le \hat{b}_{upper,i} \qquad \forall i \end{aligned} \tag{5}$$

In the case where both total flows as well as compositions are to be adjusted, equation (4) becomes:

$$\min\left\{J\left(x,Q\right)\right\} = \min\left\{\sum_{j=1}^{n} \frac{\left(\bar{Q}_j - \left(Q_m - \hat{b}_j\right)\right)^2}{V_j} + \sum_{j=1}^{n}\sum_{i=1}^{k} \frac{\left(\bar{x}_{ij} - \left(x_{m,j} - \hat{b}_{ij}\right)\right)^2}{V_{ij}}\right\} \tag{6}$$

subject to the same constraints as (4) with the additional total stream mass balance constraint:

$$\sum_{j=1}^{n} \bar{Q}_j = 0 \tag{7}$$

where b_i or b_{ij} is the bias associated with a measurement of component i in stream j, and Q_j is the reconciled stream mass flow rate of stream j. The optimisation can be done off-line using a nonlinear programming software package (for instance using the advanced solver in Excel) or it can be done as part of the larger algorithm when the optimisation is done using a dynamic link library (DLL) to other subroutines used in the overall furnace model development.

Eksteen and Reuter [17] have shown how data reconciliation can significantly reduce the noise component associated with carbon assays, the data reconciliation process therefore serving as an advanced type of low-pass filter for the data. Once reconciled, the data has added value, as it now conform to natural mass conservation laws, and could be analysed with process engineering principles based on the conservation of mass and energy. It was also shown that where there is significant bias in the data reconciliation adjustments, the adjustments may lend themselves to dynamic predictability [16].

5. THE ROLE OF THE MELT RESIDUAL AFTER TAPPING

It was shown by Eksteen and Reuter [17] that significant amounts of alloy or slag may be left in the furnace after tapping. These melt residuals (heel) automatically becomes part of the feed to the next tap. The larger the heel relative to the feed, the more the influence of the heel. The quantity of the remaining heel has therefore to be estimated and calculated. Estimation of the heel is done based on the amounts of alloy and slag produced, the physical design of the furnace, and the amount tapped from the furnace. The calculation therefore incorporates the mass balance, design and operational aspects. In the case of the ferrochrome furnace studied, Figures 2 and 3 show the small percentage of the slag and alloy inventories that are tapped (nearly always < 50%). The graphs clearly point out the significant buffer that remains within the furnace, significantly increasing the furnace time constant and stabilisation time. This seriously impedes the furnace controllability that can be achieved with short term feed changes (for example a feed change from one tap to

the next) - any feed recipe change therefore has to be maintained throughout several taps. It also indicates that the alloy and slag heels are the largest contributors on a mass basis to the metallurgical outcomes of subsequent taps. It also shows clearly that any thermochemical equilibrium predictions made cannot only rely on the reported feed composition and masses from the feed bins. Therefore pure thermochemical equilibrium simulators can never predict the performance of this type of furnace.

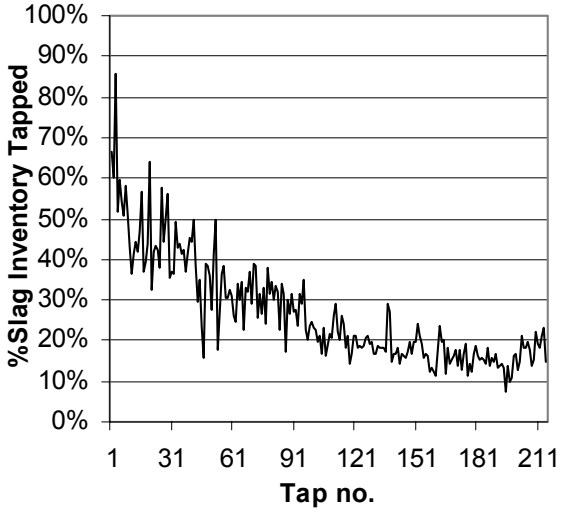

Figure 2. Percentage of available slag tapped.

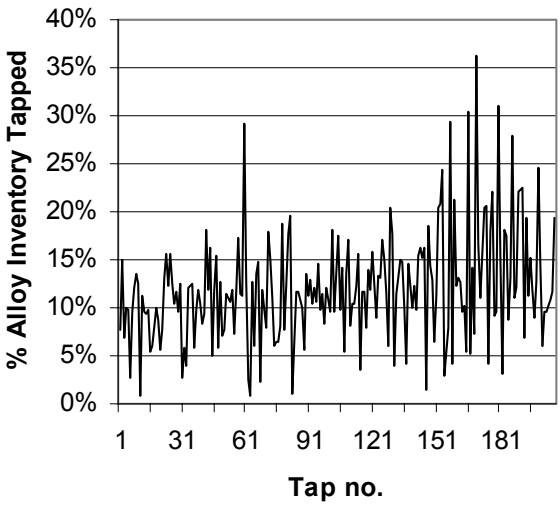

Figure 3. Percentage of available alloy tapped.

6. FROM RECONCILED DATA AND FUNDAMENTALS TO SYSTEM MODELS

It should now be clear that, while thermodynamics can give a good prediction of phase and chemical equilibria, it remains a predictor of equilibrium at infinite time, which assumes homogeneous compositions (within a phase) of the interacting phases. As infinite time is never achieved, nor are the phases internally homogeneous, some method is required to perform true dynamic prediction. The data reconciliation described above is not dynamic, it is only a way to process the data in a scientifically accountable way. The true dynamics in the reconciled data still has to be modelled, incorporating chemical equilibrium predictions in some way.

Once the data has been reconciled within its natural variance and the system thermodynamics have been simulated and used to train a representative neural network, a systems model could be developed. As mentioned earlier, such a model should capture the dynamics and should have all parameters estimated in a linear relationship to each other. A standard way of achieving this in the digital control engineering field is through transfer function models, such as models of the ARX or ARMAX structures [18]. Transfer function models normally relate a measured output $y(k)$, (or $\Delta y(k)$, in the case of integrated models) with the model variables types shown in Table 1.

Table 1. Model Variable Types.

Variable	Variable type	Model type
$y(k\text{-}1),\ldots, y(k\text{-}n)$	Its own history	Autoregressive (AR)
$e(k\text{-}1), \ldots, e(k\text{-}n)$	Past model errors, $e(k\text{-}1)= \hat{y}(k\text{-}1)- y(k\text{-}1)$, where $\hat{y}(k\text{-}1)$ is the model estimate of $y(k\text{-}1)$.	Moving average (MA)
$u(k\text{-}d\text{-}1),\ldots, u(k\text{-}d\text{-}n)$	External forcing function, or exogenous variables with delay d.	Exogenous (X)
$\Delta y(k\text{-}1),\ldots, \Delta y(k\text{-}n)$	Integrated noise structure where $\Delta y(k\text{-}1) = y(k\text{-}1) - y(k\text{-}2)$	Integrated (I)

These elements can be combined to form ARMA, ARIMA, ARX, ARMAX, ARIMAX, MAX type models. If the relationships between the variables are non-linear, the model types are prefixed with a capital N, for example NARMAX would imply non-linear autoregressive moving average model with exogenous variable inputs. The model order refers to the number of historic variables used for the AR, MA, and X components. A mixed order results when all the model components do not have the same order. A typical autoregressive moving average model with exogenous inputs takes on the general form:

$$y(k)+a_1y(k-1)+\ldots+a_ny(k-n)=b_0+b_1u(k-d)+\ldots+b_mu(k-d-m)+e(k)+c_1e(k-1)+\ldots c_re(k-r) \quad (8)$$

This modelling approach is slightly adapted to include the equilibrium prediction from the thermochemical model (the neural network equivalent of FactSage ® equilibrium predictions). The equilibrium prediction (a non-linear transformation of the input variables) may be viewed as an exogenous variable, but it should be kept in mind that it is in itself a function of multiple variables. This approach, named the Equilibrium-ARMAX approach in previous publications [17], [19], [20] changes (8) above to the form in equation (9)

$$\hat{y}(t)=a_0\cdot\underset{Equilibrium}{\tilde{y}_{Thermochemical}}(t)+\sum_{i=1}^{m}a_i\cdot y(t-i)+\sum_{i=1}^{n}\sum_{j=1}^{r}b_{ij}\cdot u_j(t-i-d)+\sum_{i=1}^{p}c_i\cdot e(t-i) \quad (9)$$

The order (m, n, and r in the above equation) and the coefficients can be estimated from the reconciled data, as has been previously indicated by the authors and co-workers [17], [19]. The parameter estimation could be done through a simple least squares technique. As the parameters are linear, their estimation could be done directly using matrix techniques, without any iterations.

Figure 4 shows the time series of the Equilibrium-Armax prediction, the equilibrium prediction only and reconciled measured data for carbon in HCFeCr alloy. It is apparent that the Equilibrium-ARMAX model follows the reconciled data time series very closely, without any delay or lag. It is also apparent that, although the pure-equilibrium model (without the ARMAX component) corresponds to the reconciled data sometimes, it is in general poorly modelled based on chemical equilibrium only. The system is therefore not at chemical equilibrium. Despite its poor correlation to the reconciled data, equilibrium cannot be ignored either. It has been shown [17] that the Equilibrium-ARMAX performs significantly better than the Equilibrium model only, or the ARMAX model only. The Equilibrium and ARMAX components contribute in a synergistic manner toward an improved overall model.

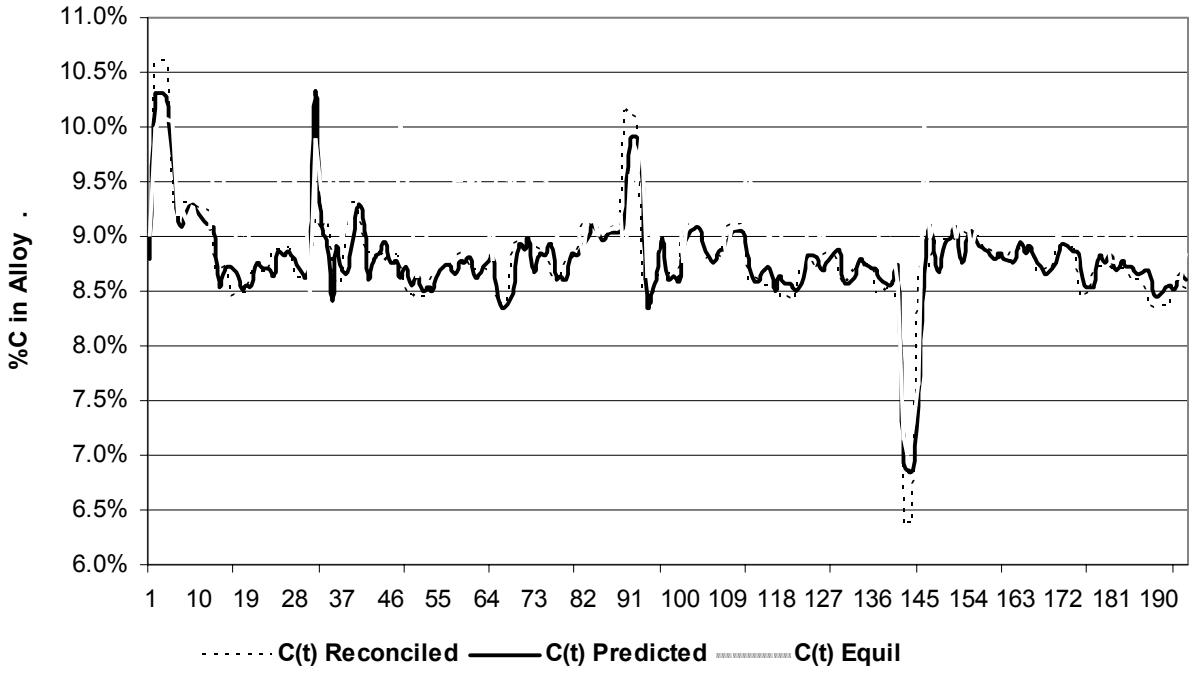

Figure 4. Time series of carbon in HCFeCr alloy.

Finally, it should be stated that process dynamics is not equivalent to kinetics. Process dynamics is strongly dependent on the reactor geometry, the residual amounts of material in the reactor, mixedness of the process melts and the operating practice. Kinetics on the other hand, refer to mass-laws for chemical reaction or mass transfer control which, for metallurgical smelting operations, are normally first order processes. A system may therefore have higher order dynamics despite having first order kinetics.

7. FROM PREDICTION TO PREDICTIVE CONTROL

Once a reliable predictive control model has been developed, one may incorporate the process model into a model predictive control architecture. Model predictive control (MPC) is a generalised approach to multiple input multiple output (MIMO) control, where the process model is used to predict future outputs over a time period longer than the longest measurement time delay. Model predictive control is defined as a control scheme in which the controller repeatedly determines or optimises the manipulated variable profile, that optimises an open loop performance on a time interval extending from the current time plus a prediction horizon. Feedback is incorporated by using process measurements, as soon as they become available, to update the optimisation problem for the next time step. The receding horizon technique is introduced as a natural computationally feasible feedback law. The method has proven to have desirable stability properties for non-linear systems. As a consequence of its structure (Figure 5), a MPC is a feedforward controller for known process changes and a feedback controller for unknown process changes [21]. Thus, MPC can reject measured disturbances more rapidly than conventional controllers, by anticipating their impact on the process.

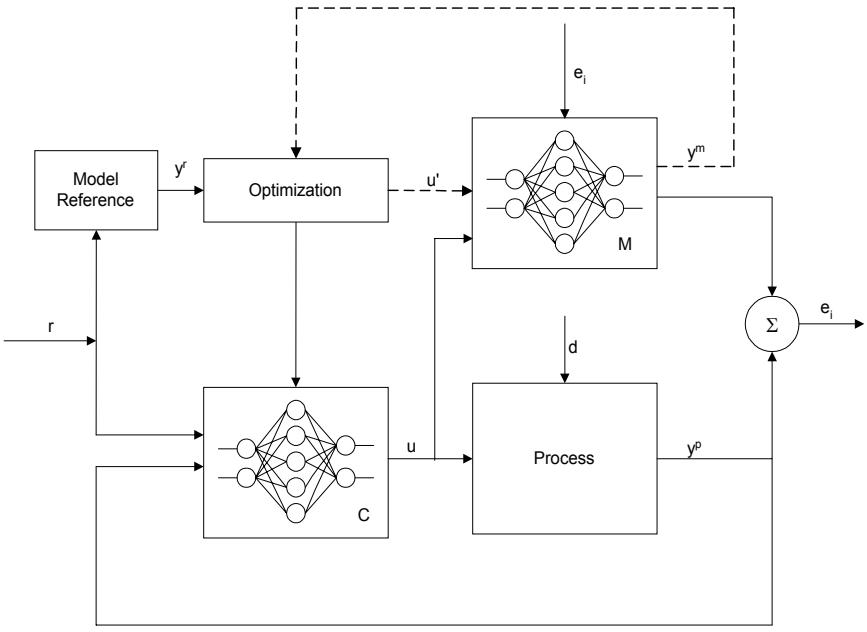

Figure 5. Model predictive control structure using neural networks [21].

Setpoint changes are achieved efficiently through their ability to predict an optimal sequence of manipulated input values to be implemented. The feedback element of MPC compensates for the effects of unmeasured disturbances on the process outputs and deviations between model outputs and those measured (process / model mismatch). The prediction horizon allows the MPC controller to take control action at the current time in response to forecast error, even though the error at current time is zero. Also the MPC may be given information about future constraints and future inputs such as planned setpoint changes of forecasts of loads or disturbances.

Implementing MPC with a neural network approach, involves utilising a neural network to provide predictions of future plant response over the specified horizon. The predictions supplied to the neural network are passed to a numerical optimisation routine (quadratic programming, genetic algorithms), which attempts to minimise a specified performance criterion in the calculation of a suitable control signal.

The control signal may be chosen so as to minimise a quadratic performance criterion, e.g.:

$$J = \sum_{j=N_1}^{N_2} \left[y^r(t+j) - y^m(t+j) \right]^2 + \sum_{j=1}^{N_2} \lambda_j \cdot \left[u'(t+j-1) - u'(t+j-2) \right]^2 \tag{10}$$

subject to the constraints of the dynamic model. The constants N_1 and N_2 define the horizons over which the tracking error and control increments are considered. The values of λ are the control weights. The remaining parameters are illustrated in Figure 5.

Another alternative is to train a further neural network to mimic the action of the optimisation routine. The controller network is consequently trained to produce the same control output for a given plant output [21].

The multi-step strategy of MPC has proven performance in controlling processes in unstable operating regimes. However, the MPC approach remains sensitive to modelling errors in these unstable regions. A disadvantage of the MPC approach lies in that the execution of the optimisation algorithm is computationally intensive, especially where linearization of non-linear systems is not applicable. Also, the solution of the optimisation problem - therefore the controller behaviour - depends on a number of tuning parameters, such as weighting coefficients in the objective function, the convergence criterion, and the scaling of variables [22].

8. CONCLUSIONS

This paper reviewed the philosophy to develop dynamic predictive control models which incorporate thermodynamic submodels. The equilibrium outcomes from thermodynamic models can be conveniently represented through an artificial intelligent mapping system such as a neural network. However, it has been shown that reprocessing of the equilibrium data is required to present it in a format that is useful for process monitoring and control. Bulk material properties have to be recalculated from the distribution within the constituent phases.

It was shown that the distributive nature of the melts being produced by the reactor directly influences the subsequent model development. Not only does variance due to spatial distributions influence the maximum accuracy of model prediction, but it can (and should) be used constructively to weigh data during variance based data reconciliation.

Finally it was shown that a dynamic systems model may be developed through a judicious combination of AR, MA, X and Equilibrium components. This dynamic model may then be incorporated into a model predictive control architecture, should automatic control be required. Alternatively, it may be used to suggest the best operating conditions through an operator guidance system, or more simply, the model is simple enough to be used in Excel on a manager's desk.

9. REFERENCES

[1] Davies, R.H., Dinsdale, A.T., Gisby, J.A., Robinson, J.A., Martin, S.M., "MTData – Thermodynamic and Phase Equilibrium Software from the National Physical Laboratory", Calphad, 26(2), pp.229-271, 2002.

[2] Bale, C.W., Chartrand, P., Degterov, S.A., Eriksson, G., Hack, K., Ben Mahfoud, R., Melançon, J., Pelton, A.D., Petersen, S, "FactSage Thermochemical Software and Databases", Calphad, 26(2), pp. 189-228, 2002.

[3] Zhang, L., Jahanshahi, S., Sun, S., Chen, C., Bourke, B., Wright, S., Somerville, M., "CSIRO's Multiphase Reaction Models and Their Application", Journal of Metals, 54(11), pp.51- 56, 2002.

[4] Andersson, J.-O., Helander, T., Höglund, Shi, P., Sundman, B., "Thermo-Calc and DICTRA: Computational Tools for Materials Science", Calphad, 26(2), pp. 273-312, 2002.

[5] Eriksson, G., Chemica Scripta, 8, pp. 100-103, 1975.

[6] Blander, M., Pelton, A.D., Geochimica et Cosmochimica Acta, 51, pp. 85-95, 1987.

[7] Pelton, A.D., Blander M., Proceedings of the AIME Symposium on Molten Salts and Slags, AIME, Warrendale, PA, pp. 281—294, 1984.

[8] Pelton, A.D., Blander M., “Thermodynamic Analysis of Ordered Liquid Solutions using the Quasichemical Approach – Application to Silicate Slags”, Metallurgical and Materials Transactions B, 17B, 805-815, 1997.
[9] Pelton, A.D., “Solution Models”, in Advanced Physical Chemistry for Process Metallurgy, Eds., N. Sano, W-K. Lu, P.V. Riboud, M. Maeda, Academic Press, San Diego, pp. 87-117, 1997.
[10] Reuter, M.A., Van der Walt, T.J., and Van Deventer, J.S.J., “Modelling of Metal-slag Equilibrium Processes Using Neural Nets”, Metallurgical and Materials Transactions B, 23B, pp. 643 – 650, 1992.
[11] Georgalli, G.A., Eksteen, J.J., Anderson, D.K., “Prediction of the dynamic behaviour of iron and sulphur during nickel-copper matte conversion using semi-empirical models”, Proceedings of the 10th IFAC Symposium on Automation in Mining, Mineral and Metal Processing, September 4-6, Tokyo, pp. 241-246, 2001.
[12] Urbain, G., Steel Research, 58, pp. 111-116, 1987.
[13] Urbain, G., Boiret, M., Iron and Steelmaking, 17, pp. 255-260, 1990.
[14] Riboud, P.V., Roux, Y., Lucas, D., Gaye, H., Fachber. Hüttenprax., Metallweiterverarb., 19, 859-869, 1987.
[15] Roscoe, R., Brittish Journal of Applid Physics, 3, pp. 267-269, 1952.
[16] Eksteen, J.J., Frank, S.J., Reuter, M.A., “Dynamic structures in variance based data reconciliation adjustments for a chromite smelting furnace”, Minerals Engineering, Vol. 15, No. 11, pp. 931-943, 2002.
[17] Eksteen, J.J. and Reuter, M.A., “A generic approach to the development of semi-empirical predictive models for bath type furnaces”, Proceedings of the XXII International Mineral Processing Congress, 28 Sep. - 3 Oct., Cape Town, South Africa, Accepted for publication, 2003.
[18] Kanjilal, P.P., “Adaptive Prediction and Predictive Control”, IEE Control Engineering Series 52, London, Peter Peregrinus Ltd., 1995.
[19] Eksteen, J.J., Georgalli, G.A. and Reuter, M.A, “Online Prediction of the Actual Melt Chemistry in an Ausmelt Converter Using a Thermodynamic- System Identification Hybrid Modelling Technique”, Third International Sulphide Smelting Symposium, TMS, pp. 457-468, 2002.
[20] Georgalli, G.A. Eksteen, J.J. and Reuter, M.A., “An Integrated Thermochemical-Systems Approach to the Prediction of Matte Composition Dynamics in an Ausmelt Nickel-Copper Matte Converter”, Minerals Engineering, 15(11), pp. 909-917, 2002.
[21] Hunt, K.J., Sbarbaro, D., Zbikowski, R., Gawthrop, P.J., “Neural Networks for Control Systems - A Survey”. Automatica, 28(6): p. 1083-1112, 1992.
[22] Psichogios, D.C. and L.H. Ungar, “Direct and Indirect Model Based Control Using Artificial Neural Networks”, Industrial and Engineering Chemistry Research, 30, p. 2564-2573, 1991.