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Intelligent Software Sensors and Process Prediction for Glass Container Forming Processes based on Multivariate Statistical Process Control Techniques

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***Abstract*— Glass container forming processes have attracted more attention over the past years due to the problem of lacking process information and correlation for key variables within the processes. In this paper an approach to develop process modeling and intelligent software sensing is presented for application based on multivariate statistical process control methods. The intelligent software sensors are able to provide real time estimation of key variables, and Partial Least Squares (PLS) techniques have allowed for forward prediction of final product quality variables. An application of software sensors used for container forming blank temperature is presented along with PLS being applied to predict the wall and base dimensions of glass container products. Initial results show that these methods are very promising in providing a significant improvement within this area which is usually unmonitored and is susceptible to long time delays between forming and quality inspection.**

Keywords- Glass Container Forming; Batch Control, Software Sensors; Condition Monitoring; MSPC, PLS, PCA

I. INTRODUCTION

The Glass container manufacturing industry is a huge global sector of package manufacturing which produces products for various industrial sectors such as cosmetics, pharmaceutical and the food and beverage industry. Glass containers are produced by the melting of raw materials mainly sand, soda ash and limestone in a gas or electric fired furnace at temperatures above 1200 °C. The glass once molten is then distributed away from the furnace along channels known as fore-hearths which are at set controlled temperatures to the relevant glass forming machines, where upon arrival the molten glass is allowed to drain through an orifice. The molten glass is then cut as it leaves the orifice at a precise set rate to allow for enough molten material for the particular product being formed. This 'cut' molten glass is then delivered to the glass forming machine, typically in double or triple cavities.

At this stage high capacity, high volume production machinery is used to mould the molten glass into the various batches of containers that one manufacturing facility may produce. It is this part of the Glass Container Forming Processes which have been a difficult challenge to engineers. Difficulties with the harsh nature of the environment and obtaining accurate information relating to its process make it extremely challenging. The lack of on-line sensing for process variables has been a serious obstruction and has left the process to somewhat a 'black art' over the years. Now with higher expectations and demands from customers this process has never been as important to monitor and refine. At present almost all control methods and policies applied are based on off line information for the process operators and supervision, this compromises quality as the delays between product formation and inspection is so large that abnormalities can go undetected for a while. It is also relatively unknown at this stage as to the actual limits and constraints that exist on the variables within this part of the process or as to the actual combined contribution that each of these variables actually has upon the final product being made.

Multivariate Statistical process control methods based upon linear projection have attracted interest and have been are proven method for producing empirical models for Industrial processes. Principle Component Analysis (PCA) and Partial Least Squares (PLS) techniques have been applied to many practical regression problems to estimate quality related variables. Zhang and Lennox [1] applied these techniques to batch fed fermentation processes with the focus on the adoption and application of PLS and PCA techniques for sensor failure detection and prediction. Other promising results were achieved within batch fermentation processes with various publications made [2][3][4][5], applications have also been deployed within the steel industries and used for advanced monitoring of plant functions to determine the relationship between process variables and production quality [6].

The applications of the above-mentioned PLS and PCA techniques have proved successful in providing soft-sensing techniques and linear regression model prediction for process variables.

This paper aims to develop software sensors and also linear regression model prediction of glass container forming quality related variables using PLS techniques. Also the paper will demonstrate the ability of PCA to provide abnormal condition detection and isolation within glass container forming processes.

II. Statistical Modelling and Soft-sensing using Multivariate Statistical Process Control Techniques

A. *Principle Component Analysis*

Principle Component analysis (PCA) is a multivariate statistical method for identifying patterns within data sets by highlighting similarities and differences within the data presented. PCA attempts to find combinations of factors or variables that describe trends within the data, after data assembly PCA mathematically it is a method of writing a matrix of X variables of rank R as the sum of R matrices of rank 1 initially assuming the data are mean cantered [7].

$$X = M1 + M2 + ... + M3 + ... + Mr \tag{1}$$

Each matrix with *m* rows and *n* columns, and each variable being a column and each sample a row

PCA decomposes the matrix X as the sum of *r* t_i and p_i pairs where *r* is the rank of the matrix X

$$X = t_1 pT_1 + t_2 pT_2 + ... + t_k pT_k + ... + t_r pT_r \tag{2}$$

The t_i, p_i pairs are ordered by the amount of variance captured. The t_i vectors are known as scores and contain information on how the samples relate to each other. The p_i vectors are known as loadings and contain information on how the variables relate to each other. Mathematically, PCA relies upon an eigenvector decomposition of the covariance or correlation matrix of the process variables. For a given data matrix X with m rows and n columns, the covariance matrix of X is

$$\mathrm{cov(X)} = \frac{X^T X}{m-1} \tag{3}$$

provided that the columns of X have been "mean-cantered" by subtracting off the original mean of each column.

In the PCA decomposition, the p_i vectors are eigenvectors of the covariance matrix;

$$\mathrm{cov(X)} p_i = \lambda_i p_i \tag{4}$$

where λ_i is the eigenvalue associated with the eigenvector p_i. The score vector t_i is the linear combination of the original X variables defined by p_i.

Another way to look at this is that the t_i are the projections of X onto the pi. The t_i, p_i pairs are arranged in descending order according to the associated λ_i. The λ_i are a measure of the amount of variance described by the t_i, p_i pair. The first pair captures the largest amount of information in the decomposition and each subsequent pair captures the greatest possible amount of variance remaining after subtracting $t_i p_i$ from X.

B. *Partial Least Squares*

PLS is a system identification tool that is capable of identifying the relationships between input (X) and output (Y) variables. The advantage that this approach offers over more traditional identification techniques, such as ordinary least squares, is that it is able to extract robust models even in applications involving large numbers of highly correlated and noisy process variable measurements.

The approach works by selecting factors of cause variables in a sequence that successively maximizes the explained covariance between the cause and effect variables. Given a matrix of cause data, **X**, and effect data, **Y**, a factor of the cause data, $\mathbf{t}_k$, and effect data, $\mathbf{u}_k$, is evaluated, such that:

$$X = \sum_{k=1}^{np<nx} t_k p_k^T + E \tag{5}$$

and

$$Y = \sum_{k=1}^{np<nx} u_k q_k^T + F \tag{6}$$

where **E** and **F** are residual matrices, *np* is the number of inner components that are used in the model and *nx* is the number of causal variables. $\mathbf{p}_k$ and $\mathbf{q}_k$ are referred to as loading vectors.

These equations are referred to as the *outer relationships*. The vectors $\mathbf{t}_k$ are mutually orthogonal. These vectors and $\mathbf{u}_k$ are selected so as to maximise the covariance between each pair, ($\mathbf{t}_k$, $\mathbf{u}_k$). Linear regression is performed between the $\mathbf{t}_k$ and the $\mathbf{u}_k$ vectors to produce the inner relationship, such that:

$$u_k = b_k t_k + \varepsilon_k \tag{7}$$

where b_k is a regression coefficient, and ε_k refers to the prediction error. The PLS method provides the potential for a regularised model through selecting an appropriate number of latent variables, $\mathbf{u}_k$ in the model (*np*). The number of latent variables is typically generated through the use of cross validation.

III. Advanced Monitoring Techniques using PCA

A. *PCA Arrangement*

PCA does not attempt to resolve any relationship between input and output data but it identifies patterns within data, as the glass container forming process is constant, by analysing the data present at one condition would give a suitable set of data to train a PCA model for identification of process changes. The data was constructed into a Matrix (X), where each column was a variable and each row a sample of the variables at a specific point in time.

$$X = \begin{bmatrix} & & \\ x_{11} & x_{21} \cdots & x_{n1} \\ x_{12} & x_{22} \cdots & x_{n2} \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ x_{1(86)} & x_{2(86)} \cdots & x_{n(86)} \end{bmatrix}$$

B. *Implementation Of Advanced Monitoring Using PCA*

A PCA Model was generated which consisted of 4 principle components which described 95% of the entire variation within the data sets , this model was then used to test against known faulty conditions which occurred within the glass container forming process.

Figure 1 shows the impact of the erroneous data upon the first two principle components. It depicts the new loaded data to exist well outside that of known good limits, this breach alone could be used to detect process abnormality. There are other components of further interest when performing Principle Component Analysis these are that of the Q residuals and Hoitelling T2 charts. The Q residuals give an indication of the measure of difference 'or residual' between a sample of data and its projection onto the components retained in the original model and the Hoi telling T2 contributions describe how much variation is within each sample to that retained within the model. Figure 2 shows this information.

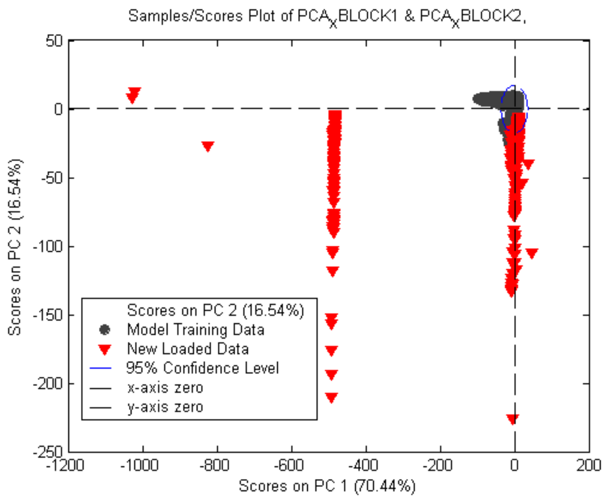

Figure 1 First two PC's loaded against Model Data

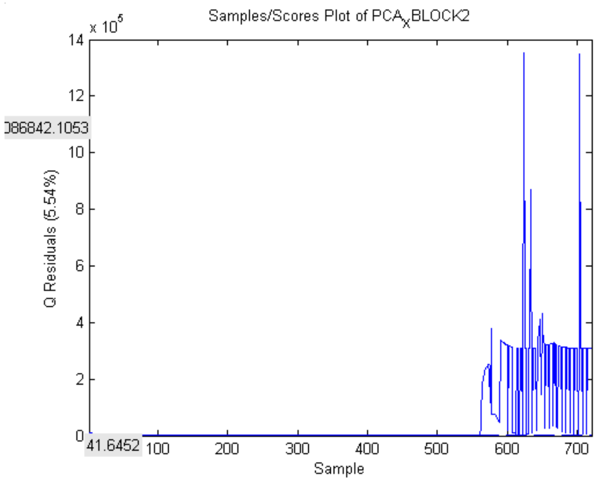

Figure 2 Q residual chart of new loaded PCA data

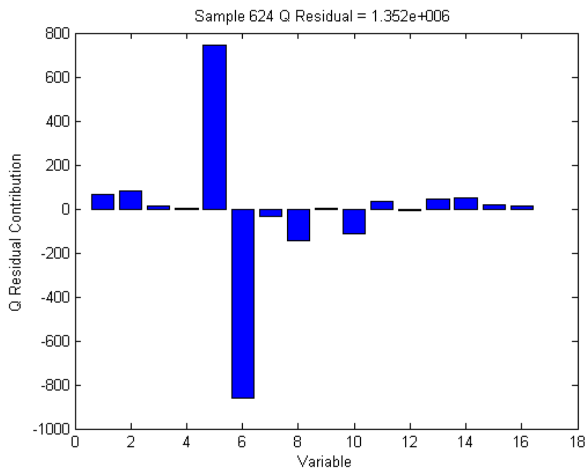

Figure 3 Q Residual Contributions at point of detection

From Figure 2, it can be seen that at around sample 570 a difference between the data in the model and the data now loaded is detected, this difference becomes even worse, at around sample 624 where the Q residual value goes extremely large. What we are actually experiencing here is an indication that something is wrong, to what we deem normal operating conditions for blank temperatures. Further investigation into the data at sample 624 shows that variables 5 and 6 are the main cause of this anomaly.

Looking at the data at this point indicates a sensor failure on IS station 3, variables 5 and 6. The above shows promising results that PCA techniques can be used for identifying process abnormalities.

IV. Construction of Intelligent Software Sensors

A. *PLS Model Development*

The first stage in the development of a suitable PLS Model is to obtain relevant training and model testing data. In this application Data was collected from two main process areas, the actual process variables themselves and the final product quality data measured and recorded by the operatives themselves.

There was also a further problem introduced within this process as there is huge transport lag between the process data recorded and the quality data obtained from the operatives, here an empirical approach was undertaken in order to calculate the desired transport lag and construct the data matrix for analysis to begin.

Finally a PLS Model was generated which contained 3 latent variables was developed using this data.

In this model the following measurements were used as input variables (X) 50 Psi I-S Station operating Air , 35 Psi I-S Station Operating Air , Plunger Cooling I-S Station Air and IS Station Blank Temperatures , with Output Variables (Y) of container wall thickness measurements and container base thickness Measurements.

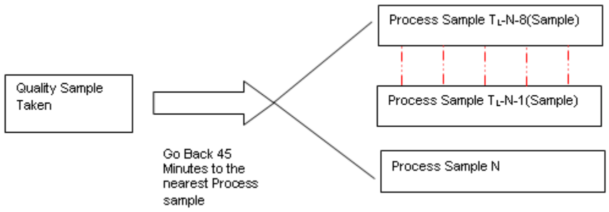

Figure 4 PLS Model Data Construction

The input Variables were constructed into the input variable matrix X and the output variables into the column vectors.

$$X = \begin{bmatrix} x_{11} & x_{21}\cdots & x_{n1} \\ x_{12} & x_{22}\cdots & x_{n2} \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ x_{1(86)} & x_{2(86)}\cdots & x_{n(86)} \end{bmatrix}, \quad Y_1 = \begin{bmatrix} y_1 \\ y_{12} \\ \cdots\cdots \\ \cdots\cdots \\ y_{1(86)} \end{bmatrix} Y_2 = \begin{bmatrix} y_2 \\ y_{22} \\ \cdots\cdots \\ \cdots\cdots \\ y_{2(86)} \end{bmatrix}$$

These data matrices were then split into two, half utilised for model training data and the remaining half utilised for model verification.

B. *Implementation of Software Sensors*

Based on the PLS model generated, a software sensing approach was investigated as due to the harsh nature of the environment it was common to experience sensor failures, so with the ability to predict these variables we would be at an advantage if required to adopt such soft sensing techniques for further applied control loops around this process. A 'software sensor' was developed to estimate a container forming IS station Blank temperature. The accuracy of this software sensor is illustrated in Figure 5, although there is some modelling error present this model development is a big step forward and as a basis to providing feasibility towards such applications. The figure gives good evidence that PLS based model prediction is feasible for 'soft sensing' applications on glass container forming processes.

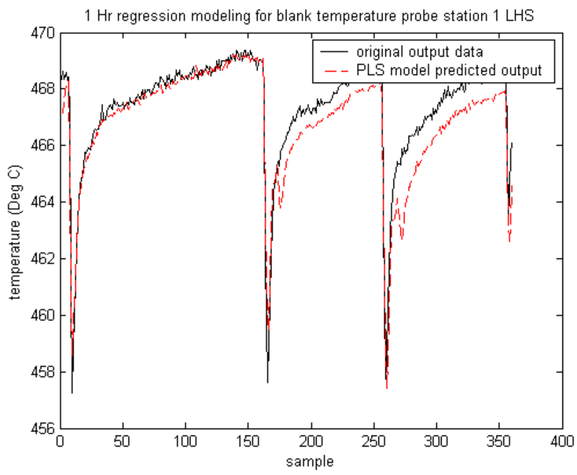

Figure 5 PLS Blank Temperature Prediction

V. Model Prediction of Glass Container Wall and Base Thickness

A. *PLS Model Development*

Using the data Matrices X, Y1 and Y2 previously constructed it is also possible to utilise the obtained process data to predict product quality variables.

B. *Implementation of Linear regression Modellling using PLS fitting*

In the previous section it was demonstrated that PLS techniques can be used for software sensing techniques within glass container forming processes, in this section it will be shown that the same techniques are able to be applied to predict two important glass container quality variables - container wall thickness and base thickness. Based upon the PLS model generated, real data measured for container base thickness and wall thickness are compared with what are predicted using the container forming process input variables, this is of great benefit as the ability to predict such variables would remove the transport times involved before any feedback is generated on glass container variables.

The PLS Model generated is found to be very good in this application and has the ability to predict the container wall thickness, the model generated actually does so to within 0.5mm. Further tests gave similar promising results with the ability to predict container base thickness as shown in Figures 6 and 7. Comparing with the real data collected from production (solid green line), PLS Model is found to predict these product quality variables and shows promising evidence that these techniques and methods are applicable to glass container forming processes.

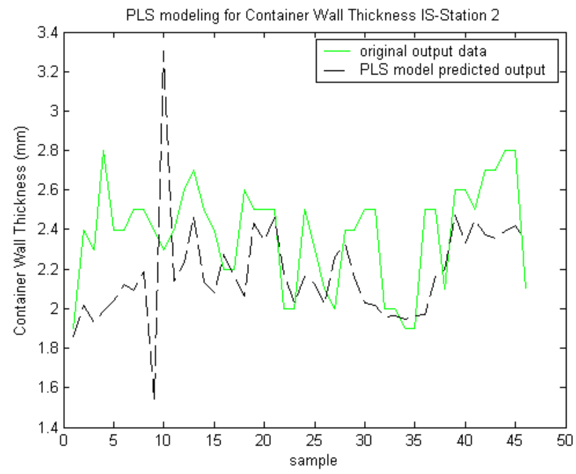

Figure 6 PLS Model Wall Thickness Prediction

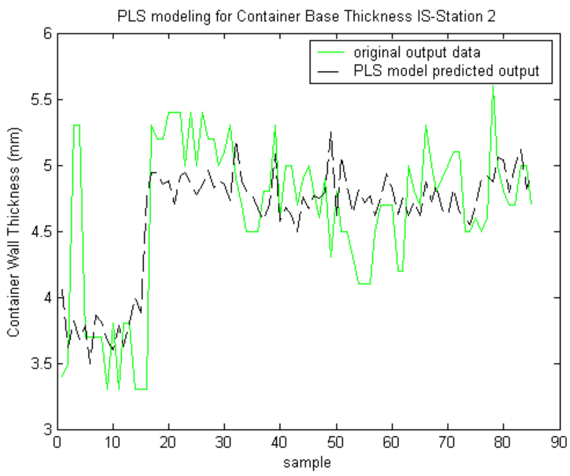

Figure 7 PLS Model Base Thickness Prediction

VI. CONCLUSIONS

In this paper, statistical models of a glass manufacturing IS machine processes have been produced. Comparisons between the real-world data and that produced from the developed models were produced and gave promising results towards the application of such techniques. Intelligent software sensors were also developed and discussed. All the initial results show that these methods are very promising in providing a significant improvement within this area which is usually unmonitored and is susceptible to long time delays between forming and quality inspection.

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