[AMN05] Inferential control of fatty acid fractionation column

Lim Wan Piang[1] and Arshad Ahmad[2]

[1,2] Laboratory of Process Control, Faculty of Chemical and Natural Resources Engineering, University Teknologi Malaysia, 81310 Skudai, Johor, Malaysia.

Introduction

Nowadays, chemical production is moving towards full capacity operation with high profitability while aiming to achieve zero accidents and zero emissions. Process control and monitoring is amongst the important factors that will help to accomplish these targets. Successful implementation of process control in operating plant requires relevant control strategies with reliable on-line measurement. However, difficulties in on-line measurement for some product qualities still exist due to large time delay, low sampling rate, high cost and unavailability of soft sensors. Recently, inferential control has been considered as a good strategy to deal with the limitations.

The study of inferential control has started since 1970s. This concept utilised the measurable secondary measurements, such as temperature and pressure, to capture the behaviour of the primary measurements, such as product quality. Its application in distillation columns is common, where the product compositions are always inferred using the readily measured intermediate tray temperatures of the column. One of the examples is control of the bottom product quality of an industrial debutaniser (Joseph and Brosilow, 1978). The feed flow rate and the tray temperatures were chosen as the secondary variables and results showed that the performance was much improved compare to the steady state control. Tham *et al.* (1991) also evaluated the application of inferential control on a high purity distillation column. The predicted top product compositions using feed flow rate, reflux flow rate and tray temperatures were very close to the composition analyser response. Recently, Amirthalingam *et al.* (2000) proposed a two-step procedure for building an inferential control model, which used both historical operation data and plant test data. This model was implemented to a multi-component distillation column. Tray temperatures were chosen to feed into the multirate Kalman filter in order to estimate the product compositions.

Various estimation approaches for the construction of process estimator have been widely studied by researchers. Available techniques can be categorised into fundamental and empirical approaches. Fundamental approach is theory based where the estimation model is built using first principle equations of the entire system consisting of mass and energy balances, thermodynamics and reaction kinetics. Although it is the direct approach, its application has not been widely explored due to financial and time constraints. The limitations of fundamental models had motivated researchers to utilise the historical input and output data for the development of empirical models. Recently, application of partial least square regression (PLS) in developing composition estimator has been gaining popularity. The use of PLS model in chemical process estimation was started in the early 1990s (Mejdell and Skogestad, 1991). The proposed estimators that were based on steady-state data and multiple temperature measurements had performed well in various conditions such as multi-component mixtures, pressure variations, and non-linearity. Budman *et al.* (1992) and Kano *et al.* (2000) had also examined the application of the PLS model in the same field.

In this paper, an on-line estimation model, which was established using Partial Least Squares (PLS) regression in the previous work (Lim and Ahmad, 2003) is applied. The model is designed to predict the overhead product composition of a fatty acid fractionation column. Several refinements are introduced to enhance the robustness and accuracy. It is further implemented in inferential control of the product composition. Its performance is evaluated against various process uncertainties.

Materials and Methods

Case Study

In this section, brief description of the selected process is illustrated. The light-cut column is one of the columns in the fatty acid fractionation plant. Separation of fatty acids ranging from C_{10} to C_{18} is carried out in this column. The feedstock of the column is the bottom product from the pre-cut column. Distillate product consists of around 98% C_{12} fatty acid. The bottom products that are mainly C_{14} to C_{18} are then fed to the next column for further processing. Further details on the process description and physical properties of the column can be referred in the work of Lim and Ahmad (2003).

Overview of PLS Model

The identification model was built using Partial Least Squares regression proposed by Geladi and Kowalski (1986). It is known to be a superior linear identification model in dealing with a large set of correlated data. The structure of PLS model is briefly discussed in this section.

It consists of two outer relations and an inner relation. The outer relations are the matrices of independent and dependent variables, which can be represented by **X** and **Y**, respectively. The input **X** is projected into the latent space by the input-loading factor, **P** to obtain the input scores, **T**. Similarly, the output scores, **U** is obtained by projecting the output **Y** into latent space through the output-loading factor, **Q**. These relations are in matrix form and are written in Equation (1) and (2).

Outer relations: $$\mathbf{X} = \mathbf{TP}^{\mathbf{T}} + \mathbf{E}_f \quad (1)$$
$$\mathbf{Y} = \mathbf{UQ}^{\mathbf{T}} + \mathbf{F}_f \quad (2)$$

The matrices $\mathbf{E}_f$ and $\mathbf{F}_f$ are residuals of **X** and **Y**, respectively. **X** and **Y** are linked by a linear regression called inner relation to capture the relationships between the inputs and output latent scores. The notation of the inner relation is written in Equation (3).

Inner relation: $$\mathbf{U} = \mathbf{TB} \quad (3)$$

The determinations of scores and loadings factors are carried out sequentially from the first factor to the f_{th} factor. Scores and loading vectors for each factor is calculated from the previous residual matrices as shown in Equation (4) and (5), where initially $\mathbf{E}_0 = \mathbf{X}$ and $\mathbf{F}_0 = \mathbf{Y}$.

For **X**: $$\mathbf{E}_f = \mathbf{E}_{f\text{-}1} - \mathbf{T}_f\,\mathbf{P}_f^{\mathbf{T}} \quad (4)$$

For **Y**: $$\mathbf{F}_f = \mathbf{F}_{f\text{-}1} - \mathbf{U}_f\,\mathbf{Q}_f^{\mathbf{T}} \quad (5)$$

Calculation of the inner and outer relations is performed until the last factor, f or when residual matrices are below certain threshold.

Non-linear PLS

In the ordinary PLS, the transformed input and output variables are related using a simple linear regression. This representation is found to be insufficient for the fatty acids fractionation column in this study due to the highly non-linear behaviour between primary and secondary variables. Regarding to this limitation, various non-linear functions are possible to replace the linear regression in order to enhance its ability in capturing non-linear system (Wold *et al.*, 1989).

In this study, a neural network is chosen as the substitution. The non-linear PLS model is constructed based on the NNPLS model proposed by Qin and McAvoy (1992). The inner model is made up of a SISO feedforward network. The notation of the inner model is represented by Equation (6):

Inner relation: $$\mathbf{U}_f = \mathcal{N}(\mathbf{t}_f) + \mathbf{r}_f \quad (6)$$

where $\mathcal{N}(\bullet)$ stands for the non-linear relation represented by a feedforward network and $\mathbf{r}_f$ is the residual of the network. Here, the input and output scores served as the training data to obtain corresponding network weights. The procedure of determining the scores and loading factors is carried out sequentially from the first factor to the fth factor.

Smoothing Filter

Process disturbances and measurement noise are common uncertainties in real industry. In order to produce a more reliable estimation model in dynamic process, a smoothing filter is added. The filter helps to refine the predicted output and to eliminate outliers. It utilises the previous predicted results at time, t_f to serve as bias values to correct the estimated data based on a weight value. The weight of the bias values, β was ranging from 0 to 1. Both bias and estimated values can be added based on Equation 7.

$$\hat{y}_t^c = \beta\hat{y}_t + (1-\beta)\hat{y}_{t_f}^c \quad (7)$$

Here, $\hat{y}_t^c$ is the filtered output, $\hat{y}_t$ is the predicted value at current time, and $\hat{y}_{t_f}^c$ is the previous corrected predicted value at time t_f. Various weight values are tested and a final value of 0.7 is used.

Results and Discussion

On-line Estimation

All variables are scaled around mean and unit variances before on-line estimation of product composition. The enhanced model was tested against three sets of data with different process uncertainties. The output data of data set A, B and C show moderate, mild and severe fluctuation, respectively. The mean-squared error (MSE) of prediction using the enhanced and ordinary PLS models are summarised in Table1. The enhanced PLS model performs better than the conventional model where lower MSE are noted in all cases. The model is able to capture the movement of the output value ranging from 0.7 to 1.0 as illustrated in Figure 1 where solid line indicates the actual output and dotted line indicates the estimated output.

TABLE 1 The performance of models in on-line estimation

Data ($MSE \times 10^{-4}$)	**Ordinary PLS**	**Enhanced PLS**
Data A	1.5573	0.4894
Data B	0.1333	0.0748
Data C	30.802	15.406

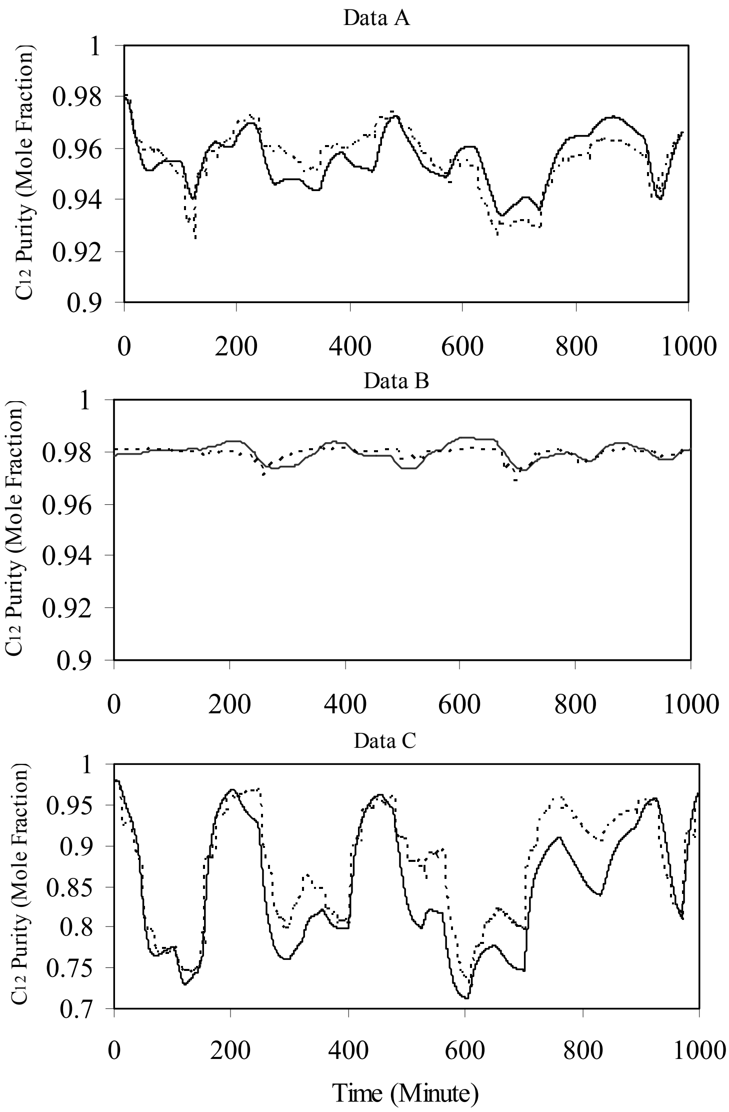


FIGURE 1 On-line estimation using enhanced PLS model

Inferential Control of Product Composition

The inferential estimation model constructed in the previous section is now tested for composition control of the fractionation column. A PID controller is selected to control the overhead product composition by manipulating the reflux flow rate. The general structure of inferential control scheme is depicted in Figure 2.

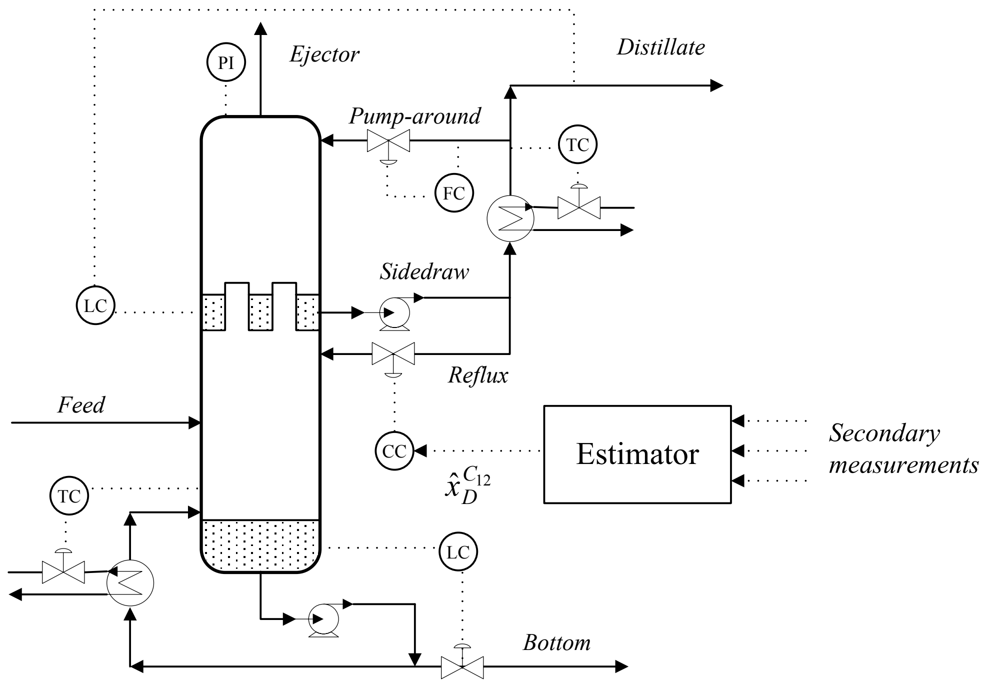
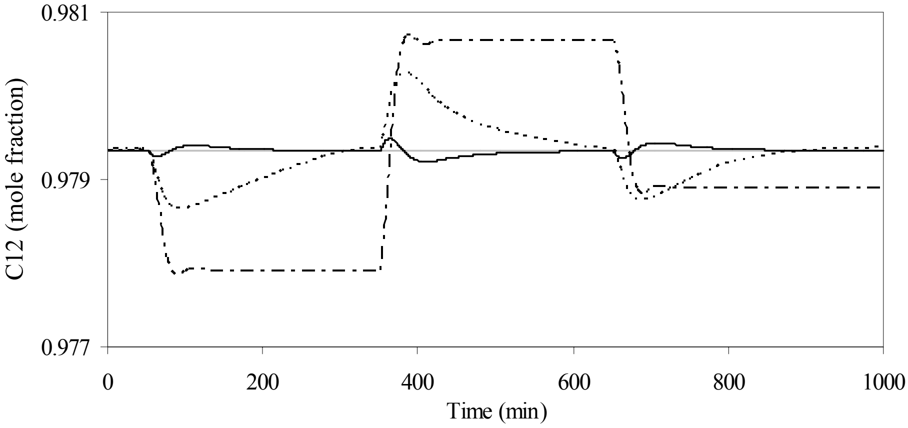


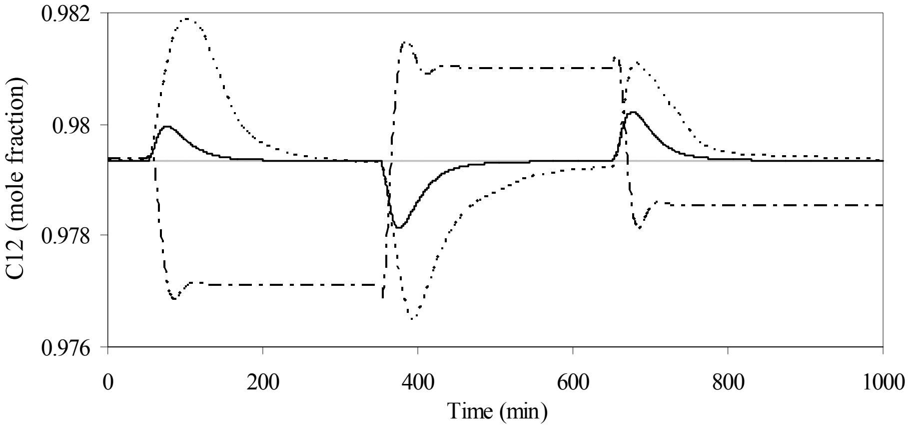
FIGURE 2 Configuration of inferential control

Disturbances are introduced to the feed stream of the light-cut column in order to evaluate the performance of inferential control. Two cases are investigated, which are fluctuation in feed flow rate and feed composition. Step changes are initiated at time 50, 350 and 650 minutes for both cases as shown in Figure 3. The total simulation time is 1000 minutes. ±5% changes of the composition of C_{12} fatty acid in the feed stream are introduced while the feed flow rate remained constant. On the other hand, maximum perturbation for feed flow rate is ±150 kg/hr with consistent feed composition.

The close-loop responses of the overhead product composition are plotted in Figure 3. Here, the solid line indicates the close-loop response of inferential control and the dotted line is the close-loop response of stage temperature control. Based on the results, the product composition is deviated from the desired value using stage temperature control. Conversely, the implementation of inferential control has successfully returned the overhead composition to the desired set point when disturbances are imposed to the feed stream. The performance is much better comparing with the responses using stage temperature control.



a) Close-loop response of product composition with fluctuation in feed flow rate



b) Close-loop response of product composition with fluctuation in feed composition

FIGURE 3 Close-loop response of product composition

Conclusion

In this paper, a PLS-based estimation model is constructed to estimate the product composition of a fatty acid fractionation column. The model is able to produce considerable results after some refinements. Inferential control of the product composition using the PLS-based estimator is implemented. The control scheme works adequately in rejecting process uncertainties and it is also more efficient comparing to the common indirect strategy using temperature control. As the conclusion, the proposed technique is a viable method for composition control in process industry.

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