Proceedings of the 11th
KACC, October 1996

ESTIMATION OF PRODUCT COMPOSITIONS FOR MULTICOMPONENT DISTILLATION COLUMNS

°Joonho Shin*, Moonyong Lee**, and Sunwon Park *

* Dept. of Chem. Eng., KAIST, Taejon 305-701, Korea
Tel : +82-42-869-3960; Fax : +82-42-869-3910; E-mail : swpark@convex.kaist.ac.kr

** School of Chem. Eng. & Tech., Yeungnam Univ., Kyongsan 712-749, Korea
Tel : +82-53-810-2512; Fax : +82-53-814-8790; E-mail : mynlee@ynucc.yeungnam.ac.kr

Abstract

In distillation column control, secondary measurements such as temperatures and flows are widely used in order to infer product composition. This paper addresses the design of static estimators using the secondary measurements for estimating the product compositions of the multicomponent distillation columns. Based on the unified framework for the estimator problems, the relationships among several typical static estimators are discussed including the effect of the measured inputs. Design guidelines for the composition estimator using PLS regression are also presented. The estimator based on the guidelines is robust to sensor noise and has a good predictive power.

Keywords

Composition estimator, PLS(Partial-Least-Squares) regression.

INTRODUCTION

Product quality measurement is one of the major difficulties associated with the composition control of distillation columns. Although on-line analyzers such as Gas Chromatography(GC) have the advantage of directly measuring the product quality, the composition control by the analyzers has not been preferred yet because of large measurement delays, high investment/maintenance costs and low reliability. Instead, temperature control using a single tray temperature is perhaps the most popular means of controlling product composition. However, it also has many limitations due to low sensitivity, non-key component effect, disturbance effect, and dynamic lags. For these reasons, many workers (Weber and Brosilow, 1972; Joseph and Brosilow, 1978; Kresta, Marlin and MacGregor, 1994; Mejdell and Skogestad, 1991; Piovoso and Kosanovich, 1994) have studied the inferential models using multiple secondary measurements. The design issues for the composition estimator using secondary measurements are : (1) the selection of the estimator type; (2) the determination of the number of factors if PCR or PLS regression is used; (3) the selection of the secondary measurements to be used; (4) the selection of the most effective variable transformation and scaling. In this paper, we will present the design guidelines by addressing the issues mentioned above.

ESTIMATOR PROBLEM

Assume that a process behaves linearly within the operation range. Then the process can be described by the linear form as

$$\theta = \mathbf{F_u u} + \mathbf{F_m m} \tag{1}$$
$$\mathbf{c} = \mathbf{G_u u} + \mathbf{G_m m} \tag{2}$$

where $\mathbf{c}$, θ, $\mathbf{u}$, and $\mathbf{m}$ mean the unmeasured outputs, the measured outputs, the unmeasured inputs, and the measured inputs, respectively.
What we call the linear estimator design is to find a matrix $\mathbf{K}$ which estimates $\hat{\mathbf{y}}^\mathbf{T}$ (i.e., $[\hat{\mathbf{u}}^\mathbf{T} \vdots \hat{\mathbf{c}}^\mathbf{T}]$) from optimally selected secondary measurements $\mathbf{x}^\mathbf{T}$ (i.e., $[\theta^\mathbf{T} \vdots \mathbf{m}^\mathbf{T}]$) :

$$\hat{\mathbf{y}} = \mathbf{Kx} \tag{3}$$

In the projection estimator(Weber and Brosilow, 1972; Joseph and Brosilow, 1978), $\hat{\mathbf{y}}$ are obtained as

$$\hat{\mathbf{u}} = \mathbf{F_u^\dagger}(\theta - \mathbf{F_m m}) \tag{4}$$
$$\hat{\mathbf{c}} = \mathbf{G_u F_u^\dagger}(\theta - \mathbf{F_m m}) + \mathbf{G_m m} \tag{5}$$

where $\mathbf{F_u^\dagger}$ means the general pseudoinverse of $\mathbf{F_u}$.
In the regression estimators, the estimator matrix $\mathbf{K}$ is obtained directly from the data matrices $\mathbf{X}^{n\times q}$ and $\mathbf{Y}^{n\times p}$. The estimator matrix by MLR(Multiple Linear Regression) is

$$\mathbf{K_{MLR}} = \mathbf{Y^T}(\mathbf{X}^\dagger)^\mathbf{T} \tag{6}$$

To avoid the singularity problem due to collinearities in the MLR , PCR(Principal Component Regression) and PLS(Partial Least Square) methods can be used as

$$\mathbf{K_{PCR}} = \mathbf{Y^T T (T^T T)^{-1} P^T} \tag{7}$$

$$\mathbf{K_{PLS}} = \mathbf{Q}\left(\mathbf{P^T W}\right)^{-1}\mathbf{W}^T \tag{8}$$

where $\mathbf{T}^{n\times k}$ is the score matrix and $\mathbf{P}^{q\times k}$ and $\mathbf{Q}^{p\times k}$ are the loading matrices.
Since only the first k terms may be distinguished from measurement noise, the matrices include only these k most important directions.

RELATIONSHIP BETWEEN THE ESTIMATORS

PROJECTION AND MLR

Consider the case where (1) there is no measured inputs, i.e., $\mathbf{m} = 0$ and $\mathbf{x} = \theta$, (2) $\dim(\theta) < \dim(\mathbf{u})$, (3) only the unmeasured outputs are estimated, i.e., $\mathbf{y} = \mathbf{c}$, then the projection estimator can be written by

$$\hat{\mathbf{c}} = (\Phi_{\mathbf{c}\theta^T}\Phi_{\theta\theta}{}^{-1})\theta \tag{9}$$

The covariance matrix $\Phi_{\theta\theta}$ and the cross correlation matrix $\Phi_{\mathbf{c}\theta}$ can be expressed in terms of Θ and $\mathbf{C}$ as

$$\Phi_{\theta\theta} = \mathbf{F_u F_u^T} = (1/n)\Theta^T\Theta \tag{10}$$

$$\Phi_{\mathbf{c}\theta} = \mathbf{G_u F_u^T} = (1/n)\mathbf{C}^T\Theta \tag{11}$$

Therefore, eq.(9) can be expressed

$$\hat{\mathbf{y}} = \mathbf{Y^T X (X^T X)^{-1} x} \tag{12}$$

Therefore, it is clear that in the case where $\dim(\theta) < \dim(\mathbf{u})$ and $\mathbf{m} = \mathbf{0}$, the MLR estimator is equivalent to the projection estimator, and thus it can not estimate the unmeasured variables exactly.
Since eqs. (10) and (11) are still valid in the case where $\dim(\theta) \geq \dim(\mathbf{u})$, it is also clear that the inversion problem in the MLR estimator is inherent in the case where $\dim(\theta) > \dim(\mathbf{u})$ because $\text{rank}(\mathbf{F_u}) = \text{rank}(\Theta) = \dim(\mathbf{u})$. One may try to use the PCR method in order to overcome the inversion problem instead of the MLR method. The number of factors used in the PCR method should be $k \leq \dim(\mathbf{u})$. If $k = \dim(\mathbf{u})$, the resulting estimator provides the exact estimate of the product composition and the estimator gain matrix using the PCR method is the same as the projection estimator using eq. (4). This result is obvious because the number of factors needed to describe a model is equal to the model dimensionality if the relationship between the variables is linear.

PROJECTION AND PCR OR PLS

Firstly, let's consider the estimators which use only the measured outputs like tray temperatures as the secondary measurements. In this case, all inputs are considered as the unmeasured inputs regardless of whether they are actually measurable or not. Thus, eqs. (1) and (2) can be expressed by augmenting the matrices $\mathbf{F_u}$, $\mathbf{F_m}$, $\mathbf{G_u}$, and $\mathbf{G_m}$:

$$\theta = \mathbf{F}\begin{bmatrix}\mathbf{u}\\ \mathbf{m}\end{bmatrix} \tag{13}$$

$$\mathbf{c} = \mathbf{G}\begin{bmatrix}\mathbf{u}\\ \mathbf{m}\end{bmatrix} \tag{14}$$

where $\mathbf{F} = [\mathbf{F_u} \vdots \mathbf{F_m}]$ and $\mathbf{G} = [\mathbf{G_u} \vdots \mathbf{G_m}]$.
If $\dim(\theta) \geq \dim(u) + \dim(m)$ and $\text{rank}(\mathbf{F}) = \dim(\mathbf{u}) + \dim(\mathbf{m})$, $\mathbf{u}$ and $\mathbf{m}$ can be estimated from eq.(13) by

$$\begin{bmatrix}\hat{\mathbf{u}}\\ \hat{\mathbf{m}}\end{bmatrix} = \mathbf{F}^{\dagger}\theta \tag{15}$$

Therefore, the product compositions $\mathbf{c}$ are estimated by

$$\hat{\mathbf{c}} = \mathbf{K}_\theta\theta \tag{16}$$

where $\mathbf{K}_\theta = \mathbf{G}\mathbf{F}^{\dagger}$.
Note that the estimator using eq.(16) is unique regardless of the estimation methods. Both the projection estimator and the PCR or PLS estimator of which number of factors are equal to system dimensionality give the same estimator gain matrix.
Now let's consider the estimators which use both the measured outputs and the measured inputs as the secondary measurements. The form of the estimator can be written by

$$\hat{\mathbf{c}} = \mathbf{K}_{\theta\mathbf{m}}\begin{bmatrix}\theta\\ \mathbf{m}\end{bmatrix} \tag{17}$$

The matrix $\mathbf{K}_{\theta\mathbf{m}}$ is composed as follows:

$$\mathbf{K}_{\theta\mathbf{m}} = [\ \mathbf{K}_1 \vdots \mathbf{K}_2\ ] \tag{18}$$

The matrix $\mathbf{K}_1$ is for the measured outputs θ and the matrix $\mathbf{K}_2$ is for the measured inputs $\mathbf{m}$.
One can easily find that the matrix $\mathbf{K}_{\theta\mathbf{m}}$ is not unique (there are infinite numbers of sets for $\mathbf{K}_1$ and $\mathbf{K}_2$): since the matrix $\mathbf{K}_\theta$ in eq.(16) is unique (Stewart, 1973), the following relation can be obtained from eqs. (16) and(18).

$$\mathbf{K}_\theta\theta = \mathbf{K}_1\theta + \mathbf{K}_2\mathbf{m} \tag{19}$$

The above relation should be valid for arbitrary inputs. Thus, by substituting eq.(1), we can get

$$(\mathbf{K}_\theta - \mathbf{K}_1)\mathbf{F_u} = \mathbf{0} \tag{20}$$

$$(\mathbf{K}_\theta - \mathbf{K}_1)\mathbf{F_m} - \mathbf{K}_2 = \mathbf{0} \tag{21}$$

Since $\dim(\theta)$ is greater than $\dim(\mathbf{u})$, it is clear that there are infinite numbers of sets for $\mathbf{K}_1$ which satisfy eq.(20) for given $\mathbf{F_u}$ and $\mathbf{K}_\theta$.
The projection estimator in eq.(5) is one of them. In

the projection estimator, $\mathbf{K}_1$ and $\mathbf{K}_2$ are obtained separately and $\mathbf{K}_1$ is the matrix by which the unmeasured inputs are estimated from the measured outputs compensated by the measured inputs. On the other hand, in the regression estimators $\mathbf{K}_1$ and $\mathbf{K}_2$ are obtained simultaneously and they are the matrices by which the unmeasured outputs are estimated from both the measured inputs and outputs. In the projection estimator, the measured outputs such as temperatures are used only for estimating the unmeasured inputs rather than the unmeasured outputs. The effects of the measured inputs on the unmeasured outputs is directly described in terms of the measured inputs. It is easy to understand if considering the extreme case where there is no unmeasured disturbances, i.e.,($\mathbf{u} = 0$). The estimation of the projection estimator is done by $\hat{\mathbf{c}} = \mathbf{G}_{\mathbf{m}}\mathbf{m}$. On the other hand, if we construct the PCR or PLS estimators using both θ and $\mathbf{m}$ as the secondary measurements, the estimator use both θ and $\mathbf{m}$ even when $\mathbf{u} = 0$. This structural difference between the regression estimators and the projection estimator results in quite different estimation characteristics. Since the projection estimator highly depends on the information of a few measured inputs, it is very sensitive to process noise in measured inputs. Furthermore, if the measured inputs have nonlinearities and/or different dynamic characteristics from the unmeasured outputs to be estimated, which is often the case in high purity distillation columns, the estimation performance severely decreases. On the other hand, since the regression estimators such as PCR and PLS equally use both the measured outputs and inputs, they are relatively insensitive to the process noise and the nonlinearities of the measured inputs. The comparisons of two approaches will be presented by considering a linear case study in later section.

RESULTS OF CASE STUDY

Simulation studies for several columns were performed using the rigorous steady state simulator, Aspen-Plus. The tray temperatures are used as the measured outputs while R and Q_B as the measured inputs. When both θ and $\mathbf{m}$ are used as the secondary measurements, the projection estimator is not equivalent to the regression estimators(PCR and PLS) as shown in Fig. (1). The model coefficients of θ for the top product composition are almost the same in magnitude in each type of the estimator. But the model coefficients of $\mathbf{m}$(i.e., R and Q_B) are very different as :

$$\mathbf{K}_2 = [-0.1604\ 0.9455\ ]^{\mathbf{T}} \text{ for projection estimator}$$
$$\mathbf{K}_2 = [\ 0.0599\ 0.0680\ ]^{\mathbf{T}} \text{ for PLS estimator}$$

Since the effect of $\mathbf{m}$ on the product composition is described by only $\mathbf{m}$ itself in the projection estimator, the performance of the estimator is very sensitive to

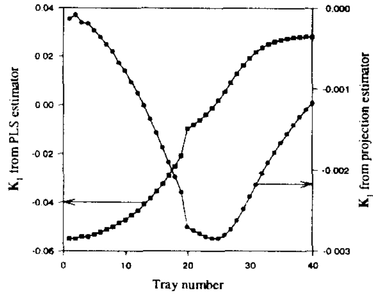

Figure 1. Comparison of the model coefficients of the projection and PLS estimator.

the noise in $\mathbf{m}$ while the performance of the regression estimators is relatively robust. Fig. 2 shows the performances of the projection and PLS estimators when the standard deviation of the noise in $\mathbf{m}$ is 10% of the signal. This structural dependency may also cause the degradation of the estimation performance in the real situation due to different dynamics and nonlinearities of the measured inputs $\mathbf{m}$. If the system is linear, the

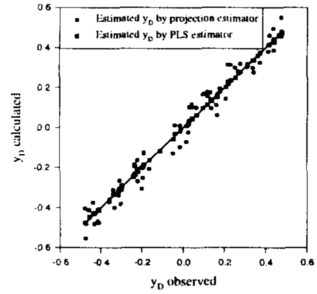

Figure 2. Comparison of the predictions of the top product composition using the projection and PLS estimator when the noise is present in the measured inputs.

estimator does not depend on the control structure of the system and the inferential model obtained from any control structure can be directly used in the others. However, since distillation systems are generally nonlinear, different inferential models will be obtained from different control structures. Therefore, it is important that the model to use will be the one based on data collected under conditions closest to those expected in the final application.

There is an optimal model dimension which minimizes the prediction error. The recommended number of factors is equal to the number of inputs which have independent and dominant influence on the measured output profile. Therefore, three factors were used for the binary column. Since the directions of the temperature profile cannot be explained in terms of R and Q_B in the linear form, the use of R and Q_B is not preferred. The value of PRESS was 0.263×10^{-4} when R, Q_B and tray temperatures were used while it was 0.588×10^{-5} when only tray temperatures were used.

In the case of no noise, the results with unit-variance scaling are better than those with no scaling. But the estimator becomes more sensitive to noise because the weight on the temperature measurement, which has small variance (e.g. T_1), is large. When the transformation $\ln(y_D/(1-y_D))$ on y_D is applied, the performance is not good(EPV=92.698, PRESS=0.531×10^{-3} with k=3.). The performance of the estimator is improved by using the logarithmic transformation both on the composition and temperature by $\ln(y_D/(1-y_D))$ and $\ln((T_i-T_L^b)/(T_H^b-T_i))$. The EPV with no noise is close to 100 % after only 3 factors due to the linearizing effect of the transformation. But the transformation is somewhat sensitive to noise because $(T_i-T_L^b)/(T_H^b-T_i)$ term becomes zero or infinite at the end of the column.

CONCLUSIONS

Two approaches (i.e., projection estimator and regression estimator) for the design of the estimator have been discussed. The inversion problem in the MLR estimator has been shown from the equivalency with the projection estimator in the special case. The projection estimator using measured outputs only is equivalent to the PCR or PLS estimator with proper number of factors. When both the measured outputs and inputs are used as the secondary measurements, the projection estimator is not equivalent to the PCR or PLS estimator any more. In this case, the structural dependency on the measured inputs makes the two estimators to have very different characteristics. It makes the projection estimator more sensitive to measurement noise, thus the projection estimator does not fully take the main benefit for using multiple measurements with a high degree of redundancy by averaging effect of the process measurement noises. Furthermore since the relationship between the inputs and outputs are generally nonlinear, the high dependency on the inputs in the projection estimator leads to performance deterioration in the actual case. The control structure has no effects on the inferential model in the linear case but gives different results in the actual case due to nonlinearity.

Based on the analysis, the guidelines on the design of composition estimator via PLS have been presented: The recommended number of factors is equal to the system dimensionality, i.e., the number of independent variables (e.g. z_F, y_D, x_B, and column pressure P) which uniquely affect the temperature profile. The additional factors does not consistently cope with nonlinearity while they lead to severe performance deterioration in the presence of noise. The relationships between the auxiliary measured inputs (R and Q_B) and the product composition cannot be described in the linear form. Thus, the estimation using the measured inputs is not desirable. Both variable transformation and scaling have effects on on the performance of the estimator by giving a different weighting. The performance of the logarithmic transformation only on the composition is not good if the change of z_F is frequent. The transformation $\ln(y_D/(1-y_D))$ and $\ln((T_i-T_L^b)/(T_H^b-T_i))$ is most effective but also most sensitive to measurement noise. Unit variance scaling gives good insights into the collinearities among the measurements by making the collinear measurements with T_1 have the same information as T_1. It also enhances the estimation performance but makes the estimators sensitive to noise.

ACKNOWLEDGEMENT

Financial support from the Korea Science and Engineering Foundation through the Automation Research Center at Postech is gratefully acknowledged. This work was also supported by Korea Research Foundation.

References

Weber, R. and C. B. Brosilow, "The Use of Secondary Measurements to Improve Control.," *AIChE*, vol. **18**, no. 3, pp. 614-623, 1972.

Joseph, B. and C. B. Brosilow, "Inferential control of processes : Part I. steady state analysis and design.," *AIChE*, vol. **24**, no. 3, pp. 485-492, 1978.

Kresta, J. V., T. E. Marlin, and J. F. MacGregor, "Development of inferential process models using pls.," *Computers chem. Eng.*, vol. **18**, no. 7, pp. 597-611, 1994.

Mejdell, T. and S. Skogestad, "Estimation of distillation compositions from multiple temperature measurements using partial-least-squares regression.," *Ind. Eng. Chem. Res.*, vol. **30**, pp. 2543-2555, 1991.

Piovoso, M. J. and K. A. Kosanovich, "Application of multivariate statistical methods to process monitoring and controller design.," *Int. J. Control*, vol. **59**, no. 3, pp. 743-765, 1994.

Stewart, G. W., "Introduction to Matrix Computation.," Academic Press, Inc., Orlando, 1973.