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NONLINEAR STATIC COMPOSITION ESTIMATOR FOR DISTILLATION COLUMNS USING OPEN EQUATION-BASED NONLINEAR PROGRAMMING

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Abstract – In distillation column control, secondary measurements such as temperatures and flows are widely used to infer product composition. This paper addresses the development of nonlinear static estimators using secondary measurements for estimating product compositions of distillation columns. An open equation-based optimization problem, which minimizes the differences between the measured outputs and the estimated outputs, has been formulated and solved by using the nonlinear program (NLP) solver, MINOS5. It is shown that the proposed nonlinear estimator is robust and more powerful than the conventional PLS (Partial-Least-Squares) estimator.

Key words : Distillation, Composition Estimator, Open Equation-Based Modeling, Nonlinear Static Estimator

INTRODUCTION

A typical production objective in distillation is to deliver products meeting certain composition specifications, which means that the economics of a distillation process depends heavily on composition control. However, product quality measurement has been one of the major difficulties associated with the composition control of distillation columns. Although on-line analyzers such as gas chromatographs (GC) have the advantage of directly measuring the product quality, composition control by the analyzers has not been preferred because on-line analyzers still suffer from large measurement delays, high investment/maintenance costs and low reliability. One common alternative to the analyzers is to use a single tray temperature. Although this policy has been most popular in process industries, it is generally not reliable especially in high purity columns and multicomponent columns.

For these reasons, many workers [Weber and Brosilow, 1972; Joseph and Brosilow, 1978; Lee and Kim, 1984; Lee et al., 1989; Mejdell and Skogestad, 1991; Kresta et al., 1994; Piovoso and Kosanovich, 1994; Shin et al., 1997, 1998] have studied the inferential models by using multiple secondary measurements and presented some promising results. However, all this work has been limited to linear estimators, whose main restriction is that they cannot properly handle the nonlinearities of distillation columns. As a result, linear estimators are generally valid over a sufficiently small operation range. A different inferential model should be developed and used for a different control structure due to the difference between their operating range [Kresta et al., 1994]. The use of transformed variables seems to be a way to incorporate the nonlinearities, but there is no general guideline of the transformation yet. For example, the logarithmic transformation of the tray temperatures and the product compositions [Mejdell and Skogestad, 1991] is restricted to binary distillation columns. Additionally, it is very hard to find adequate transformation methods for flow variables such as reflux flowrate and other measurable outputs (e.g. the heat duty of the reboiler). The restriction of the linear estimators becomes more severe in the case of the feed composition estimation. Estimation of the feed compositions is crucial for feedforward control and on-line optimization of distillation columns. The relationship between the feed composition and tray temperature can often be neither described as a linear form nor as even a simple non-linear form [Shin et al., 1998].

Sometimes, no fundamental model is available, and in that case the estimator must be designed empirically by an analysis of process data. However, in the case of distillation columns, the fundamental model and parameters are usually well known. Furthermore, current optimization techniques make it possible to solve large and complex optimization problems quickly and reliably enough for real-time purposes. These motivate us to attack the design of the nonlinear estimator more directly by converting the estimation problems to nonlinear optimization problems.

In this work, we formulate and solve the nonlinear optimization problem in order to estimate the product and feed compositions of distillation columns. The formulated problem includes the fundamental mathematical model of the distillation column in the form of an open equation. The problem has been solved by using an NLP solver, MINOS5. The estimation performance of the nonlinear estimator is presented by compar-

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ing it with that of the linear PLS estimator with a binary column case study; finally conclusions are drawn.

MODELING AND OPTIMIZATION USING OPEN EQUATIONS

With the large, fast computers of today, "open" equation-based models are more efficient than the traditional internally converged models for simulation and optimization of chemical processes. The technique is suitable for modeling many forms of systems, and the models can be used for solving a variety of design, control and logistics problems [Gallun et al., 1992]. In the open equation approach, all of the model equations are written in the form

$$\mathbf{F}(\mathbf{x}) = \mathbf{0} \quad (1)$$

where $\mathbf{F}$ is an m dimensional vector of the equations and $\mathbf{x}$ an n dimensional vector of the variables. In the case where m is less than n, optimization is performed. If m equals n, instead of optimization the entire system equations are solved simultaneously. This approach, which is also called as "equation-oriented" approach, has many advantages for modeling and optimization, such as flexibility in the formulation and solving [Biegler, 1989]. There exist different types of problems for Eq. (1): If we know the values of the parameters (e.g. heat transfer coefficients of a heat exchanger), then with a set of given inputs we can calculate the response of the model. This is a simulation problem. On the other hand, sometimes we know the parameters and the responses and we may wish to estimate the inputs. This is known as data reconciliation, which sometimes also includes the reconciliation of some of the response measurements. Sometimes we may know the response and the inputs, and we may wish to determine the values of the parameters. This operation is usually termed regression or parameter estimation. Finally, the values of the parameters may be known and it may be desirable to find the values for the manipulated variables, which in some way optimizes the operation. All of these different modes of analysis can be accommodated very naturally in the open equation approach of $\mathbf{F}(\mathbf{x}) = \mathbf{0}$.

The estimation of the product compositions can be classified into the data reconciliation case. In estimating the product compositions of distillation columns, process responses such as tray temperatures and various flow rates, so called secondary measurements, are known and we want to estimate the product compositions using the secondary measurements.

PROBLEM FORMULATION AND SOLUTION METHOD

1. Formulation

The following nonlinear optimization problem (NLP) is formulated in order to estimate the product compositions and the feed compositions. The set of fundamental equations of the distillation column are well known as MESH equations in Eq. (2) and are considered as the equality constraints of the formulation. All available measurements such as flows, pressures and the heat duties of the condenser and the reboiler as well as the tray temperatures can be included in the objective function, but for the sake of convenience, only the tray temperatures are used.

Note that the resulting estimator is totally independent of the operation range and the operation mode (e.g. manual, cascade and so on). Furthermore, since the estimator by the above approach estimates not only the product composition but also all other variables (e.g. the compositions, temperatures, and flow rates of all internal streams, and so on) simultaneously, it can be also applied to monitoring the column status. For example, we monitor flooding condition of the column with the estimated values of internal traffic.

$$\text{Min } \Phi = \sum_{i=1}^{N} (T_i - T_i)^2 \quad (2)$$

subject to

Mass Balance Equations

$$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} = 0 \quad \text{for } i = 1,2,\Lambda, N (i \neq N_F)$$

$$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} - F z_{F,j} = 0 \quad \text{for } i = N_F$$

$$(L_N + D) x_{D,j} - V_{N-1} y_{N-1,j} = 0 \quad \text{for condenser}$$

$$B x_{B,j} + V_1 y_{1,j} - L_2 x_{2,j} = 0 \quad \text{for reboiler}$$

Equilibrium Relationships

$$y_{ij} - K_{ij} x_{ij} = 0 \quad \text{for } i = 1,2,\Lambda,N$$

Summation Equations

$$\sum_j^{N_c} y_{ij} - 1 = 0 \quad \text{for } i = 1,2,\Lambda,N$$

$$\sum_j^{N_c} x_{ij} - 1 = 0 \quad \text{for } i = 1,2,\Lambda,N$$

Heat Balance Equations

$$L_i h_i + V_i H_i - L_{i+1} h_{i+1} - V_{i-1} H_{i-1} = 0 \quad \text{for } i = 1,2,\Lambda,N (i \neq N_F)$$

$$L_i h_i + V_i H_i - L_{i+1} h_{i+1} - V_{i-1} H_{i-1} - F H_F = 0 \quad \text{for } i = N_F$$

$$(L_N + D) h_N - V_{N-1} H_{N-1} - Q_c = 0 \quad \text{for condenser}$$

$$B h_1 + V_1 H_1 - L_2 h_2 - Q_B = 0 \quad \text{for reboiler}$$

2. Solution Method

The optimization problem in Eq. (2) can be classified as a nonlinear constrained optimization problem. The MESH equations in Eq. (2) are treated as the equality constraints and the bounds of the variables are also specified by their physically meaningful values. In this (e.g. $0 \le x_{ij} \le 1$, $0 \le y_{ij} \le 1$, and $T_L^b \le T_i \le T_H^b$) work we solved the problem by using the nonlinear optimization solver MINOS5 in the modeling language GAMS [Brooke et al., 1992].

3. Example

In this section, the estimation performance of the proposed nonlinear estimator will be compared to that of the conventional PLS estimator for the binary column. More details of the PLS method are available in many articles [Geladi and Kowalski, 1986; Lorber et al., 1987].

4. Process Description

A rigorous steady state simulation for the binary column of normal-hexane and cyclo-hexane with 40 theoretical stages (in-

Table 1. Simulation conditions for the binary distillation column

	Base case conditions	Variation in steady state reference set
F	1000.0 kmol/hr	Constant
T_F	347.3 K	Constant
z_F	0.5	0.4–0.6
P	1 atm	Constant
y_D	0.98	0.97-0.9997
x_B	0.02	0.0003-0.03

cluding reboiler) is performed. The feed stream enters the column at stage 20 as saturated liquid. The nominal operation conditions and the variation of the inputs of the binary column are given in Table 1. It is assumed that the phase equilibrium of the system is ideal. Rault's law is used for the phase equilibrium relationships in Eq. (2).

5. Evaluation Criteria

For the PLS estimator, a cross validation procedure is adopted by splitting the data into two parts: the calibration data and the prediction data. The calibration data are used to build the regression model, and the prediction data are then used to evaluate the predictive ability of the model. The Prediction Error Sum of Squares (PRESS) [Montgomery, 1992] is used to evaluate the absolute performance. For the estimation of the distillate composition, the PRESS can be calculated by

$$\mathrm{PRESS} = \sum_{k=1}^{M} (y_{D,k} - \hat{y}_{D,k})^2 \quad (3)$$

where M is the number of data sets (here, M=64).

In the same way, we can check the estimation performance for the bottom composition x_B and the feed composition z_F. The PRESS value of the nonlinear estimator is calculated and compared with that of the PLS estimator.

RESULTS

For our binary column example, the design of the PLS estimator was based on the guidelines suggested by Shin et al. [1997]: (1) the number of factors used in the PLS estimator is three (the system dimensionality of our binary column is three); (2) only the tray temperatures are used as the secondary measurements; (3) the transformations $L_{T,i} = \ln\{(T_i - T_L^b)/(T_H^b - T_i)\}$ and $Y_D = \ln\{y_D/(1-y_D)\}$ are adopted for estimating the top and bottom product compositions [Mejdell and Skogestad, 1991] and no transformation for the feed composition. Additionally, the performance of the PLS estimator with no transformation is also compared. In order to check the sensitivity of the estimators, random noise is added to the tray temperatures.

The PRESS values of various estimators for the distillate composition are listed in Table 2. As shown in Table 2, the proposed nonlinear estimator yields far better results than the PLS estimator both in the noise-free case and the noise-corrupted cases. Similar results were obtained for the case of the bottom product composition (not seen here). Fig. 1 compares the estimation performances of the two estimators when the noise level is 0.2 °C. It should be noted that the proposed nonlinear estimator especially yields very accurate estimates for the estimation of the feed composition, while the PLS estimator gives meaningless results (the PRESS value is about 0.182 in all

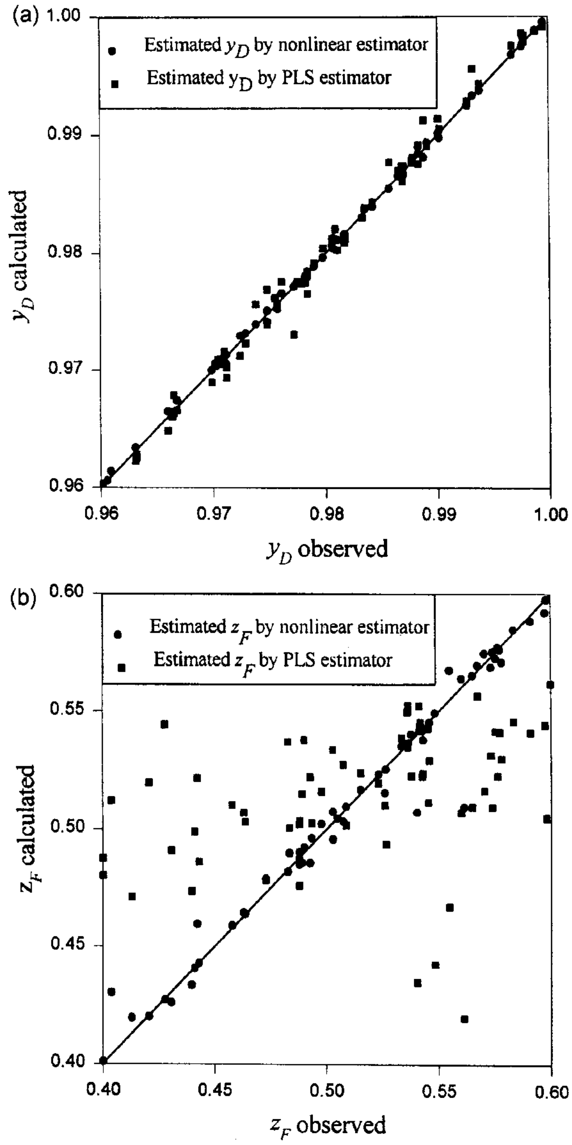

Fig. 1. Comparison of the performance of the proposed nonlinear estimator and the linear PLS estimator.

Table 2. PRESS values of various estimators for distillate composition y_D

Estimation methods	Noise level (°C)		
	0.0	0.1	0.2
Nonlinear estimator	0.248×10^{-9}	0.210×10^{-7}	0.817×10^{-7}
PLS (with $L_{T,i}$ and Y_D)	0.554×10^{-4}	0.516×10^{-4}	0.907×10^{-4}
PLS without transformation	0.343×10^{-3}	0.345×10^{-3}	0.351×10^{-3}

cases). The PRESS values of the nonlinear estimator are 5.632×10^{-5}, 3.886×10^{-3}, and 5.663×10^{-3} for the noise levels 0.0, 0.1, and 0.2 °C, respectively. Considering the fact that several important applications such as feedforward control, on-line optimization, and monitoring in the distillation area have been mainly restricted by difficulty in measuring or estimating the feed composition, the result has very important meaning in practice.

CONCLUSIONS

For distillation columns the main difficulty in using linear estimators is the nonlinearity in the process. In order to overcome this problem, the nonlinear static estimator using open equation-based nonlinear programming has been proposed. The estimation problem can be converted to a nonlinear optimization problem by proper formulation. The formulated problem is solved by using an NLP solver, MINOS5. It is fast and reliable enough for real-time purposes. The proposed nonlinear estimator shows much better prediction performance and robustness than the linear PLS estimator. In addition, the proposed estimator can also be used for other important applications such as process monitoring, feedforward control, and on-line optimization. Finally, the proposed approach is theoretically sound because it includes the fundamental mathematical model of the distillation systems. The proposed approach to the estimator design can be directly extended to other systems as long as their fundamental models are available.

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NOMENCLATURE

h : specific enthalpy of liquid mixture
H : specific enthalpy of vapor mixture
K : K factor (or value)
L : liquid flow rate
R : reflux ratio
Q_B : heat duty of reboiler
T : temperature
V : vapor flow rate
x : liquid composition
x_B : bottom product composition
y : vapor composition
y_D : distillate composition
Y_D : logarithmic distillate composition
z_F : feed composition

Greek Letter

Φ : objective function

Superscripts

b : boiling point pure component
∃ : estimated variable

Subscripts

i : tray number
j : index for component
H : heavy component
L : light component

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