The 30th Annual Conference of the IEEE Industrial Electronics Society, November 2 - 6, 2004, Busan, Korea

Development of Soft Sensor System via Dynamic Optimization

Xuemei Zhu[1,2] , Shuqing Wang[1]

[1]National Key Laboratory of Industrial Control Technology , Institute of Advanced Process Control
Zhejiang University, Hangzhou 310027,P. R. China, e-mail : (xmzhu, sqwang)@iipc.zju.edu.cn
[2] Department of Control Science and Engineering, Information and Control Engineering Technology Research Centre
Nanjing Normal University, Nanjing 210042, P. R. China

Abstract—**In chemical process industry, some variables are difficult to measure on-line due to the limitation of measurement techniques, reliability or high cost to install a hard sensor. Some measurable variables, such as product quality , cannot be used for real-time optimization and control due to the large time delay.The soft-sensing of these variables is considered as an efficient method, and remains as an open problem. A new soft sensor system is developed to solve these problems in this work, which is based on rigorous model by using dynamic optimization to minimize the bias square between the model outputs and the measured outputs. Compared with other soft sensor systems, the proposed soft sensor system accurately employs the nonlinear model and considers the constraints in the optimization. It not only is more efficient in economic but also can be used on-line for real-time optimisation and control. The soft sensor system is successfully applied to estimation of the feed composition of a pilot heat-integrated distillation column system.**

I. INTRODUCTION

It is very important to measure or estimate the operation variables accurately for process optimization, monitoring, fault detection and control. In chemical process industry, some variables are difficult to measure directly (e.g. quality variables, feed composition variables and product concentration variables), either because there are no physical sensors available, or because these are too expensive to install. Gas chromatographs and near-infrared analysers are always used to measure the composition, but gas chromatographs have large measurement time delays and these measurements cannot be used for real-time optimization and control due to the introducing of a time delay. Furthermore, most analysers suffer from high investment and maintenance costs. For example, it spends more than $10 million to equip on-line analyzers, and $0.5 million to support them for a typical modern oil refinery in one year [1].

In the last decade, studies on soft sensors have been resumed due to developments in computer processing capability, which reduced required time for mathematical calculations. Soft-sensing techniques have been considered as efficient methods and key technologies for unmeasured process variables when hard sensors are not available or too expensive to install. Soft sensors are model-based approach to provide on-line estimates of difficult-to-measure variables through calculations of measurable variables (e.g. temperatures, pressures and flow rates). A number of estimators can be used as soft sensors, for example Extended Kalman Filters (EKF) [2] and neural networks [3] are commonly used.

Neural networks are one of the best known black-box soft sensor. Their complex structure makes it possible to establish highly nonlinear correlations between input and output variables, thus being able to represent a wide variety of processes. Nevertheless, neural network soft sensors need a great number of data and long time training, and the extrapolation capacity of these soft sensors is generally very limited.

EKF is by far the most popular algorithm for on-line state and parameter estimation.But it has some drawbacks: inability to handle constraints and to make physical sense of the estimated variables, such as the component must be positive and only between 0 and 1, and the poor use of the nonlinear properties of models. It can also suffer from some numerical problems and convergence difficulties due to approximations of model linearization.

With the development of chemical process knowledge, more attentions have been paid to rigorous model based optimization, monitoring and control. In order to overcome problems that exist in neural networks and EKF soft sensors, rigorous model based nonlinear optimization is extensively used to estimate state and parameter, due to accurately employing the nonlinear model and considering the constraints in the optimization. The objective function is formulated as the sum of squared error between measurement data and model outputs. The best estimation can be obtained by minimizing the objective function subject to constraints of the model equations.

In this paper, a soft sensor system based on rigorous model is developed by using dynamic optimization. The system is described by rigorous model that is a set of large-scale nonlinear differential and algebraic equations (DAEs). The sequential quadratic programming (SQP) and the orthogonal collocation methods are used to solve the dynamic nonlinear optimization problem. The approach is successfully applied to soft-sensing of the feed composition of a pilot heat-integrated distillation column system.

II. PROBLEM FORMULATION

The soft sensor is a model-based approach to infer the process unmeasured variables. Several types of soft sensors can be developed according to different process models. The models may be black box or white box. If the system states are operating over a wide range, e.g. the operation is respect to flexible conditions and real-time optimization with economic benefit, continuous processes with grade transitions and the batch process then a mechanistic model

0-7803-8730-9/04/$20.00 ©2004 IEEE

or rigorous model might be the best choice. Rigorous model represents a unique insight into the behaviour of the process, and applicability for advanced non-linear control such as nonlinear model predictive control and real-time optimization strategies. More and more attentions have been paid to rigorous model based control and optimization. In chemical process industry, the dynamic rigorous system models are based on chemical and physical principles, and prior knowledge. It can be described by a set of nonlinear DAEs.

$$\mathbf{g}(\dot{\tilde{\mathbf{x}}}, \tilde{\mathbf{x}}, \hat{\mathbf{u}}, \boldsymbol{\theta}) = 0 \quad (1)$$

where $\mathbf{g} \subseteq \Re^{n+m}$ is the vector of model equations, $\dot{\tilde{\mathbf{x}}}$ denotes the time derivatives of the total state variables, $\tilde{\mathbf{x}} = [\mathbf{x},\mathbf{y}]^T, \mathbf{x} \in \mathbf{X} \subseteq \Re^n$ is the unmeasured part of system state variable, $\mathbf{y} \in \mathbf{Y} \subseteq \Re^m$ is the measured part of state variable or output variable, $\hat{\mathbf{u}} \in \mathbf{U} \subseteq \Re^k$ is the vector of the given measured input variables, $\boldsymbol{\theta} \in \boldsymbol{\Theta} \subseteq \Re^p$ is the vector of the variables to be estimated by soft sensors. For the pilot plant, $\mathbf{y}$ involves the measured temperatures on some trays and the distillate or bottom flow rate. $\hat{\mathbf{u}}$ includes the measured feed flow rate, reboiler duty, reflux flows and column pressure. $\mathbf{x}$ represents unmeasured state variables in the model, i.e. compositions of liquid and vapor phases, vapor and liquid flow rates and the holdups on the trays inside the column. $\boldsymbol{\theta}$ is the unmeasured feed composition which is estimated by the soft sensor.

If we suppose that the unknown model parameters are theoretical identifiable, the soft sensor is to adjust the model parameters $\boldsymbol{\theta}$ until reaching the minimum of the bias between the sampled system outputs and the model simulation outputs, as is shown in equation (2).

$$\min_{\boldsymbol{\theta}} \int_{t_0}^{t_f} (\mathbf{y}-\hat{\mathbf{y}})^T \mathbf{W}(\mathbf{y}-\hat{\mathbf{y}}) d\tau \quad (2)$$

s.t

$$\mathbf{g}(\dot{\tilde{\mathbf{x}}}, \tilde{\mathbf{x}}, \hat{\mathbf{u}}, \boldsymbol{\theta}) = 0 \quad (3)$$

$$\boldsymbol{\theta}^{\mathrm{L}} \le \boldsymbol{\theta} \le \boldsymbol{\theta}^{\mathrm{U}} \quad (4)$$

To solve this problem numerically, it is necessary to discretize the DAEs and transform them into algebraic equations. Collocation on finite elements and multiple shooting are two common methods for the discretization[4]. In this approach, discretization of the DAEs is by orthogonal collocation on finite elements [5]. After this discretization, problem (2) is now transformed to (5):

$$\min_{\boldsymbol{\theta}} f = \min_{\boldsymbol{\theta}} \sum_{i=1}^{I} (\mathbf{y}_i - \hat{\mathbf{y}}_i)^T \mathbf{W}_{\mathbf{Y}} (\mathbf{y}_i - \hat{\mathbf{y}}_i) \quad (5)$$

s. t.

$$\mathbf{g}_i(\mathbf{x}_i, \mathbf{y}_i, \hat{\mathbf{u}}_i, \boldsymbol{\theta}_i) = \mathbf{0}, \ (i=1,\dots, I) \quad (6)$$

$$\boldsymbol{\theta}^{\mathrm{L}} \le \boldsymbol{\theta} \le \boldsymbol{\theta}^{\mathrm{U}} \quad (7)$$

where $\hat{\mathbf{y}}_i \in \hat{\mathbf{Y}} \subseteq \Re^m$ is the measurement process data, and $\mathbf{y}_i \in \mathbf{Y} \subseteq \Re^m$ is the model output at the same sampling instants i. f is the objective function to be minimized of the soft sensor system with a moving horizon window(MHW) of I time intervals. I is the length of the MHW. The performance of soft sensor will improve when the horizon length I increases. However, the computational cost also increases. The diagonal matrix $\mathbf{W}_y \in \Re^{m \times m}$ is the collection of weighting factors. $\mathbf{W}_y$ is the known covariance matrix of the measurement errors. $\boldsymbol{\theta}^{\mathrm{L}}$ and $\boldsymbol{\theta}^{\mathrm{U}}$ are the given lower and upper bounds of the soft-sensing variables according to the prior information.

III. COMPUTATIONAL METHOD

Due to the relationship $\mathbf{y} = \boldsymbol{\Psi}(\boldsymbol{\theta})$ is not known explicitly, equation (5) shows that it is a nonlinear dynamic optimization problem with constraints of model equations and the lower and upper bounds. Approaches to solve dynamic optimisation problem usually use a discretization method to transform the dynamic system to a nonlinear programming (NLP) [4]. The approaches to solve such problem can be classified into simultaneous strategy [6], in which the discretization and optimization are performed simultaneous and a huge NLP is included, and sequential strategy, in which a simulation step is used to compute the dependent variables and so that only the independent variables are solved by NLP [7]. In our problem, the sequential strategy is employed to solve the NLP for the soft sensor system. Only the estimated parameters are included in SQP algorithm to reduce the number of variables in SQP, while the $I*(m+n)$ dependent variables can be obtained by solving the model equations (6) with the estimation value of the parameter, the gradients of objective function and the sensitivities of dependent variables to estimation parameter are computed via the simulation step solution. The two-level structure, optimization level and simulation level, computation approach is proposed, as shown in Fig. 1.

These suppositions are made that in every time interval i the soft-sensing value of $\boldsymbol{\theta}_i$ and the inputs $\hat{\mathbf{u}}_i$ are constant to analysis this problem. There are $I*p$ variables to be estimated by the soft sensor in one MHW. Objective function and gradients are the two key components in SQP algorithm. The objective function $f(\boldsymbol{\theta})$ is differentiated

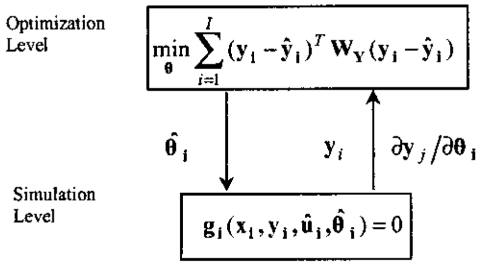

Fig. 1 A two-level calculation structure

with respect to each unknown parameter, to yield the gradients:

$$\varphi_i(\boldsymbol{\theta}) = \frac{\partial f(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}_i} = 2\sum_{j=i}^{I} \frac{\partial \mathbf{y}_j}{\partial \boldsymbol{\theta}_i} \mathbf{W}_Y(\mathbf{y}_j - \hat{\mathbf{y}}_j) = 2\sum_{j=i}^{I} \mathbf{S}_i(\boldsymbol{\theta}) \mathbf{W}_Y(\mathbf{y}_j - \hat{\mathbf{y}}_j), \quad (i=1,\dots,I) \tag{8}$$

where

$$\mathbf{S}_i(\boldsymbol{\theta}) = \left[\frac{\partial \mathbf{y}_j}{\partial \boldsymbol{\theta}_i}, j = i,\dots,I\right], (i=1,\dots,I) \tag{9}$$

Equation (8), (9) mean that we should consider the effect of the variation of the preceding time interval estimated parameters on the subsequent state variables, so j, the subscript of y, is only from i to I.

$$\mathbf{S}(\boldsymbol{\theta}) = \begin{bmatrix} \frac{\partial \mathbf{y}_1}{\partial \boldsymbol{\theta}_1} & 0 & 0 & 0 \;\dots & 0 & 0 \\ \frac{\partial \mathbf{y}_2}{\partial \boldsymbol{\theta}_1} & \frac{\partial \mathbf{y}_2}{\partial \boldsymbol{\theta}_2} & 0 & 0 \;\dots & 0 & 0 \\ \dots & \dots & \dots & \dots \;\dots & 0 & 0 \\ \dots & \dots & \dots & \dots \;\dots & \dots & \dots \\ \frac{\partial \mathbf{y}_{I-1}}{\partial \boldsymbol{\theta}_1} & \frac{\partial \mathbf{y}_{I-1}}{\partial \boldsymbol{\theta}_2} & \frac{\partial \mathbf{y}_{I-1}}{\partial \boldsymbol{\theta}_3} & \dots \;\dots & \frac{\partial \mathbf{y}_{I-1}}{\partial \boldsymbol{\theta}_{I-1}} & 0 \\ \frac{\partial \mathbf{y}_I}{\partial \boldsymbol{\theta}_1} & \frac{\partial \mathbf{y}_I}{\partial \boldsymbol{\theta}_2} & \frac{\partial \mathbf{y}_I}{\partial \boldsymbol{\theta}_3} & \dots \;\dots & \frac{\partial \mathbf{y}_I}{\partial \boldsymbol{\theta}_{I-1}} & \frac{\partial \mathbf{y}_I}{\partial \boldsymbol{\theta}_I} \end{bmatrix} \tag{10}$$

The matrix $\mathbf{S}(\boldsymbol{\theta}) = \lfloor \mathbf{S}_i^T(\boldsymbol{\theta}), i = 1,\dots,I \rfloor$, defined by equation (10), is so called sensitivity matrix. As shown in equation (10), $\mathbf{S}(\boldsymbol{\theta})$ is always a triangle matrix. $\mathbf{S}_{ij}$ are sensitivity coefficients. The sensitivity matrix coefficient is the first derivative of the dependent state variable $\mathbf{y}$ with respect to the unknown parameters $\boldsymbol{\theta}$. Due to the relationship $\mathbf{y} = \boldsymbol{\Psi}(\boldsymbol{\theta})$ is not known explicitly, the sensitivity coefficients are implicitly calculated with the following method.

The objective function and the gradients of the objective function are computed in each iteration calculation. Sensitivity coefficients of the dependent variables to estimation parameters are computed via the simulation model. The model equations are computed by the Newton-Raphson algorithm. To calculate the gradients of the objective function, only $\partial \mathbf{y}_j / \partial \boldsymbol{\theta}_i$ is needed to compute, which can be obtained by the partial derivative of equation (6) about $\boldsymbol{\theta}_i$:

$$\frac{\partial \mathbf{g}_i}{\partial \boldsymbol{\theta}_i} + \frac{\partial \mathbf{g}_i}{\partial \tilde{\mathbf{x}}_i} \frac{\partial \tilde{\mathbf{x}}_i}{\partial \boldsymbol{\theta}_i} = \mathbf{0} \tag{11}$$

Then

$$\frac{\partial \tilde{\mathbf{x}}_i}{\partial \boldsymbol{\theta}_i} = -\left(\frac{\partial \mathbf{g}_i}{\partial \tilde{\mathbf{x}}_i}\right)^{-1} \frac{\partial \mathbf{g}_i}{\partial \boldsymbol{\theta}_i} \tag{12}$$

where $\partial \mathbf{g}_i / \partial \tilde{\mathbf{x}}_i, \partial \mathbf{g}_i / \partial \boldsymbol{\theta}_i$ are the Jacobin matrixes of the system equation to $\tilde{\mathbf{x}}_i$ and $\boldsymbol{\theta}_i$, respectively. For the system with a high dimension of state variables, the calculation of the inversion of the Jacobian matrix $\partial \mathbf{g}_i / \partial \tilde{\mathbf{x}}_i$ will be time consuming and ill-condition. In the practical numerical implementation, the sensitivity coefficient is computed by Gauss elimination of equation (13), rather than by matrix inversion and multiplication of equation (12).

$$\frac{\partial \mathbf{g}_i}{\partial \tilde{\mathbf{x}}_i} \frac{\partial \tilde{\mathbf{x}}_i}{\partial \boldsymbol{\theta}_i} = -\frac{\partial \mathbf{g}_i}{\partial \boldsymbol{\theta}_i} \tag{13}$$

Because the last collocation point of the dependent variable is the starting point of the next time interval, the other sensitivity coefficients can be computed by iteration [8].

IV. COMPUTATION RESULTS

The above technique is used for soft-sensing of feed composition of an industrial size pilot plant—a heat-integrated distillation column system. All calculations are carried out on a personal computer using the COMPAQ VISUAL FORTRAN 6.1 compiler. To solve the dynamic optimization, a standard SQP solver of the IMSL library of routine NCONG is used.

Heat-integrated distillation columns are commonly used in the chemical industry to reduce the energy consumption of distillation processes. In the industrial practice, both the feed flow rate and feed composition of such columns change significantly and frequently. It is well known that an on-line composition measurement is usually not possible. Since advanced control strategies, such as dynamic real-time optimization (RTO) and nonlinear model predictive control (MPC), need the real-time value of the feed composition, it has to be estimated based on a model and measurable variables such as temperatures, pressures and flow rates.

A. Process Description

Fig. 2 shows that the pilot plant consists of a high pressure (HP) column and a low pressure (LP) column both with the same diameter of 100 mm. They have a central down-comer with 28 and 20 bubble-cap trays, respectively. The plant can be operated in downstream, upstream and parallel arrangements. In our problem, the plant is constructed as parallel arrangements for separation of a binary mixture of methanol and water. The overhead vapour of HP column is used as the heating medium to the reboiler of LP column. Temperature, pressure, level and flow rate measurement instruments are equipped with the plant, and all the signals are connected with the computer control system.

The nominal operating conditions of the plant are listed in Table 1.

To reach the optimal operation and satisfy the quality constraints, four control variables are optimized on-line, which are heat supply to the HP column, HP column reflux rate, reflux rate and feed rate of the LP column. The unmeasurable feed composition should be estimated on-line by the soft sensor.

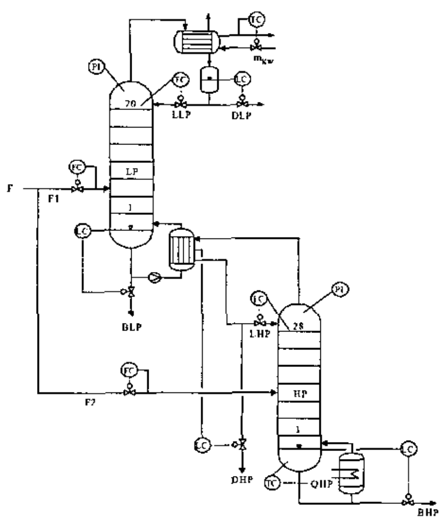

Fig. 2 Flow sheet of the heat-integrated distillation column system

Table 1 Nominal operation conditions

	HP column	LP column
The number of tray, NST	30	22
Feed composition, x_F[mol/mol]	0.4	0.4
Feed rate, F [l/h]	19	16
Feed tray, N_F	20	16
Feed temperature, T_F [°C]	60	60
Overhead composition, x_D	0.99	0.99
Bottoms composition, x_B	0.01	0.01
Top pressure [bar]	4.659	1.028
Heat input, Q [kW]	9.95	

B. Modelling

The dynamic model of the system is developed according to vapour-liquid equilibrium, overall and component material balances and energy balance for each tray j where the trays are numbered from the reboiler ($j=1$) to the condenser ($j=NST$). The non-ideal liquid phase is computed by Wilson model. The component compositions of vapour and liquid phases, the vapour and liquid flow rates, the temperature, the pressure, and the liquid holdup are the state variables of each tray. The total number of state variables of each tray is $NK*2+5$ (NK the number of components). For one column the whole number of state variables is $(NK*2+5)*NST$. The DAEs model is based on the following assumptions:

- Negligible vapour holdup,
- Ideal vapour behaviour on each tray,
- No heat loss,
- Total condenser without subcooling.

Reboiler : ($j=1$, $i=1,\ldots,NK$)

Component balance:

$$\frac{dHU_1 x_{i,1}}{dt} = L_2 x_{i,2} - L_1 x_{i,1} - V_1 y_{i,1} \tag{14}$$

Vapour-liquid equilibrium:

$$y_{i,1} = k_{i,1} * x_{i,1} \tag{15}$$

Summation equation:

$$\sum_{i=1}^{NK} x_{i,1} = 1 \tag{16}$$

$$\sum_{i=1}^{NK} y_{i,1} = 1 \tag{17}$$

Energy balance equation:

$$\frac{dHU_1 H_1^L}{dt} = L_2 H_2^L - L_1 H_1^L - V_1 H_1^V + Q_r \tag{18}$$

Internal trays : ($j=2, NST-1$, $i=1,\ldots,NK$)

Component balance:

$$\frac{dHU_j x_{i,j}}{dt} = L_{j+1} x_{i,j+1} + V_{j-1} y_{i,j-1} - L_j x_{i,j} - V_j y_{i,j} + FF_j x_{Fi,j} \tag{19}$$

Vapour-liquid equilibrium:

$$\eta_j = \frac{y_{i,j} - y_{i,j+1}}{y^*_{i,j} - y_{i,j+1}} \quad (20)$$

where

$$y^*_{i,j} = k_{i,j} * x_{i,j} \quad (21)$$

Summation equation:

$$\sum_{i=1}^{NK} x_{i,j} = 1 \quad (22)$$

$$\sum_{i=1}^{NK} y_{i,j} = 1 \quad (23)$$

Holdup equation:

$$HU_j = 10^3 * (WEIRH + HOW_j) * AR * EPS / VXX_j \quad (24)$$

Hydraulics and the pressure drop equation:

$$P_j = P_{j+1} + DPD_j + DPH_j \quad (25)$$

Energy balance equation:

$$\frac{dHU_j H^L_j}{dt} = L_{j+1} H^L_{j+1} + V_{j-1} H^V_{j-1} - L_j H^L_j - V_j H^V_j + FF_j HLF_j \quad (26)$$

Total condenser: ($j = NST$, $i = 1,\ldots,NK$)
Component balance:

$$\frac{dHU_{NST} x_{i,NST}}{dt} = V_{NST-1} y_{i,NST-1} - (L + D) x_{i,NST} \quad (27)$$

Summation equation:

$$\sum_{i=1}^{NK} x_{i,NST} = 1 \quad (28)$$

Energy balance equation:

$$\frac{dHU_{NST} H^L_{NST}}{dt} = V_{NST-1} H^V_{NST-1} - (L + D) H^L_{NST} \quad (29)$$

The rigorous system model is a set of DAEs. To solve this problem numerically, it is necessary to discretize the DAEs and transform them into algebraic equations. Now, three-point collocation on finite elements method is used. In every time interval, each state variable has three values. For $NK = 2$, the number of state variables in one tray is 9. With three collocation points, 27 state variables should be calculated in one time interval. The whole state variables number in the heat-integrated distillation column system is 1404 $(27*(NST1+NST2) = 27*52 = 1404)$. So, it's a large-scale nonlinear system and can be solved by conventional Newton-Raphson algorithm. Details about this model can be found in literature [5].

C. Parameters Estimation

The available measurements of the temperatures along two columns and some flow rates are used to estimate the parameters. Three time scales of parameters and variables exist in the numerical computation. The smallest one is the three orthogonal collocation points in one time interval of the measurement variables and the state variables obtained by the simulation step. The middle one is the time interval, in which the estimate parameters and the independent variables are constants. The biggest one is the MHW with I time intervals. In this example, the number of time interval I in a MHW is 20. The time interval is 600s; and three orthogonal collocation points are at time 76.2s, 338.1s, and 600s in one time interval. In this work, 6 tray temperatures of the HP column and 5 tray temperatures of LP column in the top, middle, and bottom of the columns, respectively, and the distillates of the two columns are used as measurements. The objective function is:

$$f = \sum_{i=1}^{20} f_i = \sum_{i=1}^{20}\sum_{l=1}^{3} f_{i,l} = \sum_{i=1}^{20}\sum_{l=1}^{3} (\mathbf{y}_{i,l} - \hat{\mathbf{y}}_{i,l})^T \mathbf{W}_\mathbf{Y} (\mathbf{y}_{i,l} - \hat{\mathbf{y}}_{i,l}) \quad (30)$$

The feed composition soft sensor is examined in two cases. Case A is that the feed composition keeps constant at 0.3 mol/mol. Case B is that the feed composition has a great change from 0.4 to 0.3(mol /mol) at 11th time interval. Fig.3 and Fig. 4 show the results of the soft sensor for feed composition of two cases.

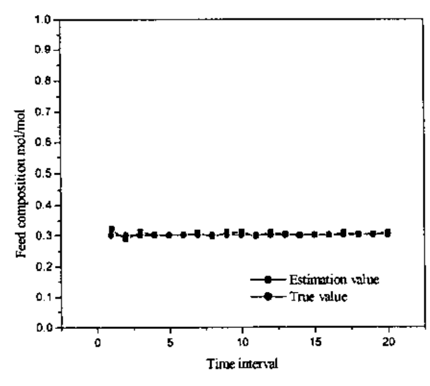

Fig. 3 Feed composition estimation results in case A

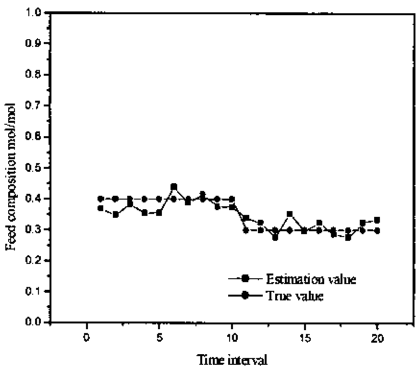

Fig. 4 Feed composition estimation results in case B

V. CONCLUSION AND DISCUSSION

In this paper a nonlinear soft sensor system has been proposed based on rigorous dynamic system model. The soft sensor is to find the unmeasurable parameter value that minimizes the bias between the model outputs and the measurement outputs. It is a dynamic optimization problem that is solved by SQP and the orthogonal collocation. For realizing the numerical evaluation, suitable numerical methods for the optimization and the calculation of sensitivity coefficients are proposed. Compared with other soft sensor systems, the proposed soft sensor system accurately employs the nonlinear model and considers the constraints in the optimization. It can be used on-line for real-time optimization and control. The soft sensor system is successfully verified in the estimation of the feed composition of a pilot heat-integrated distillation column system.

To fulfill the parameter estimation by nonlinear dynamic optimization, a major issue should be taken into account. That is the identifiability of the model parameter. From the point of view of optimization, it is a problem whether the convergence to the global minimum under different initial guesses of the model parameters. In the practical application, the optimal selection of measurements is difficult and important. In our problem, the estimation accuracy is improved by using not only tray temperatures but also distillate rates.

For nonlinear dynamic rigorous model, the theoretical investigation of parameter identifiability is an open problem in the future.

VI. REFERENCES

[1] I. Wadi, "Neural network model predicts naphtha cut point," *Oil & Gas Journal*, vol.94, Iss. 48, Nov. 25, 1996, 67-70.

[2] D.I.Wilson, M.Agarwal and D.W.T. Rippin, "Experiences implementing the extended Kalman filter on an industrial batch reactor, " *Comp. Chem. Engng.*, vol.22, No. 11, 1998, 1653-1672.

[3] A.T.Assis and R.M.Filho, "Soft sensors development for on-line bioreactor state estimation," *Comp. Chem. Engng.*, vol.24, 2000, 1099-1103.

[4] G.Wozny, P.Li, and M.Wendt, "Optimization in process engineering: state of the art and future trends," *Inzynieria Chemiczna I Procesowa*, vol.22, 3A, 2001,137-163.

[5] P.Li, H.P.Hoo and G.Wozny, "Efficient simulation of batch distillation processes by using orthogonal collocation," *Chem. Eng. Technol.*, vol.21, 1998, 853-862.

[6] A.Cecrvantes and L.T.Biegler, "Large-scale DAE optimization using a simultaneous NLP formulation," *AICHE J.*, vol.44, 1998, 1038.

[7] J.S.Longsdon, and L.T.Biegler, "Decomposition strategies for large-scale dynamic optimization problems," *Chem. Eng. Sci.*, vol.47, 1992,851.

[8] P.Li, H.A.Garcia, and G.Wozny, "Optimization of a semibatch distillation process with model validation on the industrial site," *Ind. Eng. Chem. Res.*, vol.37, 1998, 1341-1350.