Simple Empirical Nonlinear Model for Temperature-Based High-Purity Distillation Columns

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The high-purity distillation column is a very important unit operation in chemical and petrochemical industry. In addition to the usual process interaction problems and possible operation constraints, these columns exhibit very strong asymmetric nonlinear behavior, and tend to be very ill-conditioned. The combination of these attributes makes the control of high-purity columns a very challenging problem for which only partial solutions are available. The major issues involved in modeling and dual composition control of high-purity columns have been studied and reported in several publications: McDonald and McAvoy (1987); McDonald (1987); Georgiou, Georgakis, and Luyben (1988); Skogestad and Morari (1988); Skogestad and Lundström (1990); Eskinat et al. (1991); Jacobsen, et al. (1991); Chang et al. (1992); Wang and Yu (1993); Jacobsen and Skogestad (1994).

With industrial columns, however, tray temperatures are much more readily available on-line than composition measurements. For those rare situations in which on-line composition analyzers are available, the maintenance effort required for obtaining consistently reliable measurements sometimes proves overwhelming, and the measurements themselves, if reliable, may often be subject to large delays. It is therefore currently more customary to base product quality control schemes on tray temperature measurements for the distillation columns separating binary or pseudo-binary mixtures. For this reason, Chien and Ogunnaike (1992) investigated the possibility of using a linear model in a temperature-based control system and found out that the "high frequency" linear models showed less variation with operating conditions. While acceptable closed-loop performance can be obtained using these models in a model-predictive-control (MPC) framework, the residual plant/model mismatch will still be significant enough that the resulting performance may, in fact, be no better than obtainable from a well-tuned set of multiloop PID controllers.

It appears therefore that in order to obtain better controller performance than is routinely possible with multiloop PID controllers, it may be necessary to base the controller design on nonlinear models which are much more representative of the true plant behavior over the entire operating range. In this article, we purpose a very simple empirical nonlinear model for temperature-based high-purity distillation columns. The proposed model is in first-order form with the process "gain" and "time constant" as nonlinear functions depending on operating conditions (where process measurement is currently at) and two limiting high and low temperatures (bottom and top temperatures). A rigorous distillation column simulation will be used to represent the "plant." Some plant dynamic test data will be used to estimate the model parameters. Prediction capability of the proposed model will be compared to some other commonly used nonlinear models.

Process Description

The studies reported in this article were carried out using the distillation column model developed by Weischedel and McAvoy (1980). The column separates mixtures of methanol and ethanol, with 27 theoretical trays and a product split of 0.99/0.01. For more detailed information of the dynamic model, please refer to the above article. The control configuration is the one used by Chien and Ogunnaike (1992) and subsequently used by Sriniwas et al. (1995) in which the temperatures near the top (tray 21) and the bottoms (tray 7) of the distillation column are the controlled variables and reflux flow rate and vapor flow from reboiler are the manipulated variables. The controlled and manipulated variables used are defined in dimensionless form as deviation variables divided by the measurement spans. Please refer to Sriniwas et al. (1995) for the exact definitions.

Figure 1 shows the process open-loop responses for $\pm 1\%$ and $\pm 5\%$ step changes in the dimensionless reflux and steam flows. These step responses illustrate the following facts about this two-point temperature control system:

(1) It exhibits asymmetric nonlinearities (mirror image inputs produce corresponding response that are fundamentally and significantly dissimilar in character);

(2) It is highly interactive (a change in any one input variable affects both temperatures);

(3) It is ill-conditioned (the responses from both inputs are very similar in nature, and thus reduce the independence of these two manipulated variables such as $+5\%$ steam rate changes produce very similar temperature responses as compared to -5% reflux rate changes).

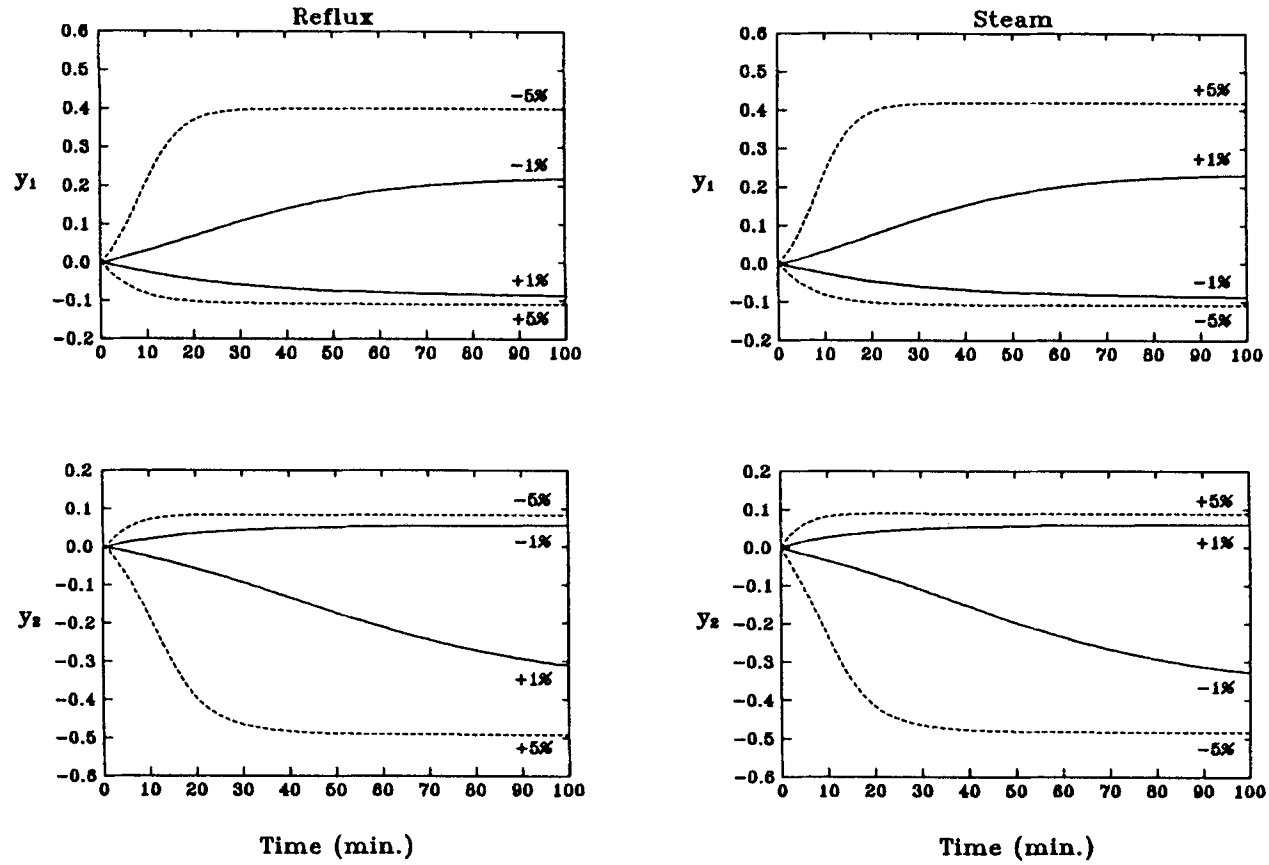

Figure 1. Column open-loop step responses.

These three critical characteristics make the typical simple linear models, which have been used successfully for characterizing low-to-medium-purity columns, no longer appropriate. The strong nonlinearity makes it extremely difficult to characterize high-purity columns with any degree of fidelity using simple linear models. In particular, attempts to characterize column responses by first-order transfer functions often lead to models with ridiculous RGA elements. (cf. Luyben, 1987; Chien and Ogunnaike, 1992; Sriniwas et al., 1995).

The ill-conditioning nature of high-purity distillation columns imposes a severe restriction on the achievable performance of inverse-model based controllers (e.g., model predictive controller). In particular, when the models (whose inverses are approximated as the process controllers) are of the simplest linear form, the extent of plant/model mismatch is usually such that these otherwise high performance controllers must be detuned significantly or closed-loop stability will be jeopardized. The performance may then degrade to a point where it becomes comparable to that obtainable with conventional multiloop PID controllers tuned on the basis of linear "high frequency" (i.e., integrator) process models. The articles by Chien and Ogunnaike (1992) and also by Sriniwas et al. (1995) clearly illustrate this fact.

Empirical Low-Order Nonlinear Model Development

In order to obtain improved performance from model predictive controllers (or any such inverse-model based controllers), it is clear that, among other things, the models must be at least more representative of the process. The key focus is the reduction of the plant/model mismatch, so that tighter controller tuning can be tolerated without sacrificing stability.

Model structure

For the foregoing reasons, we now propose a simple empirical nonlinear model structure for our example temperature-based system. The model has the following first-order differential equation form

$$\tau(y)\frac{dy}{dt} = -y + K(y)u \tag{1}$$

where $y = \text{col}[y_1, y_2]$, controlled variable vector; $u = \text{col}[u_1, u_2]$, manipulated variable vector; $dy/dt = \text{col}[dy_1/dt,\ dy_2/dt]$ is the first-order derivative of controlled variable; $\tau(y)$ is a diagonal process time constant matrix, a nonlinear function of y; $K(y)$ is a process gain full matrix, also a nonlinear function of y.

The process gain and time constant variations are represented explicitly by the following empirical expressions suggested by the observed characteristics of the step responses displayed in Figure 1

$$k_{ij} = k_{ij}^0 + k_{ij}^1 \Delta y_i^{\text{top}} + k_{ij}^2 \Delta y_i^{\text{bot}} \tag{2}$$

$$\tau_{11} = \tau_{11}^0 + \tau_{11}^1 \Delta y_1^{top} \quad (3)$$

$$\tau_{22} = \tau_{22}^0 + \tau_{22}^1 \Delta y_2^{bot} \quad (4)$$

where the "driving force" terms show the relative difference in temperatures of measured tray temperatures to the two limiting high and low temperatures in the distillation column (T_{bot} and T_{top}) are defined as

$$\Delta y_1^{top} = \frac{T_{21} - T_{21ss}}{T_{21} - T_{top}} \quad (5)$$

$$\Delta y_1^{bot} = \frac{T_{21} - T_{21ss}}{T_{bot} - T_{21}} \quad (6)$$

$$\Delta y_2^{top} = \frac{T_7 - T_{7ss}}{T_7 - T_{top}} \quad (7)$$

$$\Delta y_2^{bot} = \frac{T_7 - T_{7ss}}{T_{bot} - T_7} \quad (8)$$

Parameter estimation

The fundamental parameters of this empirical nonlinear low-order model are: k_{ij}^0, k_{ij}^1 and k_{ij}^2, associated with the process gains, and τ_{ii}^0, τ_{ii}^1 associated with the time constants. While these parameters can be estimated from process data via several different techniques, the following procedure, based on open-loop step response data, is perhaps one of the simplest:

(1) Implement step input changes in each u_i, one at a time, making sure that in each case, both positive and negative changes of varying magnitudes are implemented such that enough of the operating region is covered;

(2) From y_i, the individual output response to each input change in u_j obtained in the usual manner, estimates the process gain, k_{ij}. For example, several different magnitudes of positive and negative changes in u_1 will give rise to several y_i responses from which corresponding estimates of k_{i1} associated with the specific u_1 input will be obtained.

(3) Using Eq. 2, and the "data" obtained in step 2, the empirical parameters may then be estimated by simple regression technique such as multiple linear regression.

(4) Once the twelve steady-state parameters are obtained, the remaining four τ_{ii}^0, τ_{ii}^1 parameters associated with the dynamic behavior of the system can be estimated by employing techniques for nonlinear parameter estimation in ordinary differential equations along with the dynamic step response data.

An alternative procedure to obtain the model parameters is to treat the model in Eqs. 1–8 as a unit, and employing same techniques as in step 4 of the above procedure. The difference is that the number of the estimated parameters is much larger in this case (total of 16 parameters), thus, it will be much more computationally involved. However, this procedure has an added advantage in that the type of input excitation experiment does not need to be limited to step responses.

Application

The simpler procedure enumerated above was applied to the high-purity column described above. By implementing $\pm 1\%$ and $\pm 5\%$ step changes in the manipulated variables. The result of the estimation exercise is summarized below:

For Process Gains

$$k_{11}^0 = -23.3; \quad k_{11}^1 = -21.8; \quad k_{11}^2 = 40.4$$
$$k_{12}^0 = 23.9; \quad k_{12}^1 = 22.6; \quad k_{12}^2 = -38.5$$
$$k_{21}^0 = -31.0; \quad k_{21}^1 = -49.5; \quad k_{21}^2 = 45.8$$
$$k_{22}^0 = 32.5; \quad k_{22}^1 = 49.2; \quad k_{22}^2 = -42.4$$

For Time Constants

$$\tau_{11}^0 = 75.1; \quad \tau_{11}^1 = -71.9$$
$$\tau_{22}^0 = 121.2; \quad \tau_{22}^1 = 104.6$$

The fitting of the "true plant" dynamic step response by this simple empirical nonlinear model is excellent. For the purpose of further illustrating the ability of this simple empirical nonlinear model to predict process characteristics, several different input excitation sequences that the model has not seen in the parameter estimation stage will be used to test the model. Figure 2 shows the comparison between the "plant data" and the open-loop model prediction when there are $\pm 2\%$ and $\pm 10\%$ step changes in the reflux and steam flow rates. This simple nonlinear model captures very well the three important process characteristics of the high-purity distillation column. The common pitfall of the empirical models while predicting process behavior outside of the operating region defined at the identification stage has not been seen at all. On the contrary, the model gave excellent extrapolated prediction results. Also note that the initial response (high frequency portion) of the model agrees with the plant very well indicating good control-relevant property of this nonlinear model.

Another input excitation experiment that we have used to test the nonlinear model is proposed by Leontaritis and Billings (1987) and utilized by Sriniwas et al. (1995) in their development of another nonlinear model. They proposed that the input should be a random variable taken from a uniform distribution with the appropriate range. We choose to have u_1 and u_2 lie between $\pm 5\%$—a range determined from step responses being large enough to produce output data which capture the essence of the true process dynamics. The specific stochastic characteristics of the input sequences are obtained by allowing each input variable to change at each sampling instant (every minute in this case) to a new value with a predetermined probability (switching probability). If the input is to change, the new value is drawn from a uniform distribution over the interval $(-0.05, 0.05)$. This input excitation experiment is called "nonlinear excitation" hereafter.

Two sets of input excitation were generated to represent low and high frequency components of the system (similar as Figures 8 and 9 in Sriniwas et al. (1995)). The output predictions are shown in Figures 3 and 4 with switching probability of 0.1 and 0.8, respectively. Notice that the model only knows the input sequence in this 500-min time period and needs to

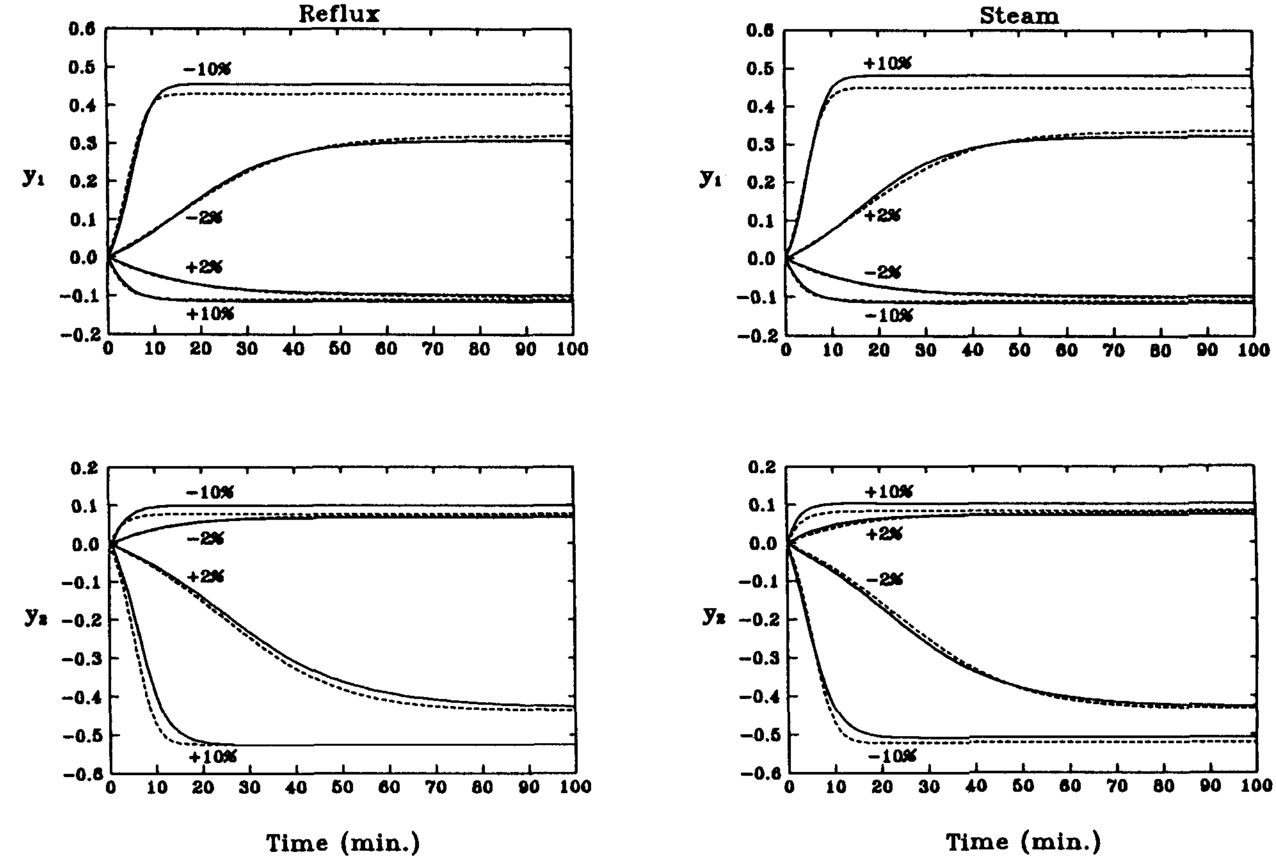

Figure 2. Model prediction for step inputs.

predict the output response for the entire time period. The prediction is not corrected by using the previous plant measurements as one-step ahead prediction does, so the test is much more severe. The prediction performances as illustrated in Figures 3 and 4 are excellent.

Comparison to Other Nonlinear Models

In what follows, the prediction ability of this simple nonlinear low-order model will be compared to some other nonlinear models proposed for high-purity distillation columns reported in the literature. The various nonlinear models used for comparison are as follows:

Logarithmic transformation: model A

By far the most recommended strategy for building reliable models for high-purity column control involves using logarithmic compositions rather than the raw composition measurements themselves (cf. Koung and Harris, 1987; Georgiou et al., 1988; Skogestad and Morari, 1988), and various arguments have been advanced for this recommendation. Recently, Mejdell and Skogestad (1991) have suggested a similar logarithmic transformation for tray temperature measurement.

Chien and Ogunnaike (1992) studied this distillation column and defined the following transformed temperature measurement

$$\theta = \ln\left(\frac{T - T_{\text{top}}}{T_{\text{bot}} - T}\right) \tag{9}$$

They identified a linear second-order model for the column using these transformed variables. We will use this model to compare with the simple nonlinear model proposed in this article. Please refer to Chien and Ogunnaike (1992) for more detailed information about this logarithmic transformed model.

Nonlinear autoregressive model with exogenous input (NARX): model B

Sriniwas et al. (1995) uses NARX structure to develop nonlinear model for this distillation column. A total of nine models were identified using the generated data from several different input switching probabilities and different model orders. Some statistical model validation tests were performed to determine the best NARX model for this column. The resulting best model is from input switching probability of 0.3 and the model is in discrete form with sampling time of one minute

$$\begin{aligned} y_1(k+1) = {} & 1.4\times10^{-4} + 0.98y_1(k) - 0.27u_1(k) + 0.21u_2(k) \\ & - 1.91y_1(k)u_1(k) + 1.44y_1(k)u_2(k) + 5.96y_1^2(k-1)u_1(k) \\ & - 3.71y_1^2(k-3)u_2(k) - 0.11y_1^2(k-2) \end{aligned} \tag{10}$$

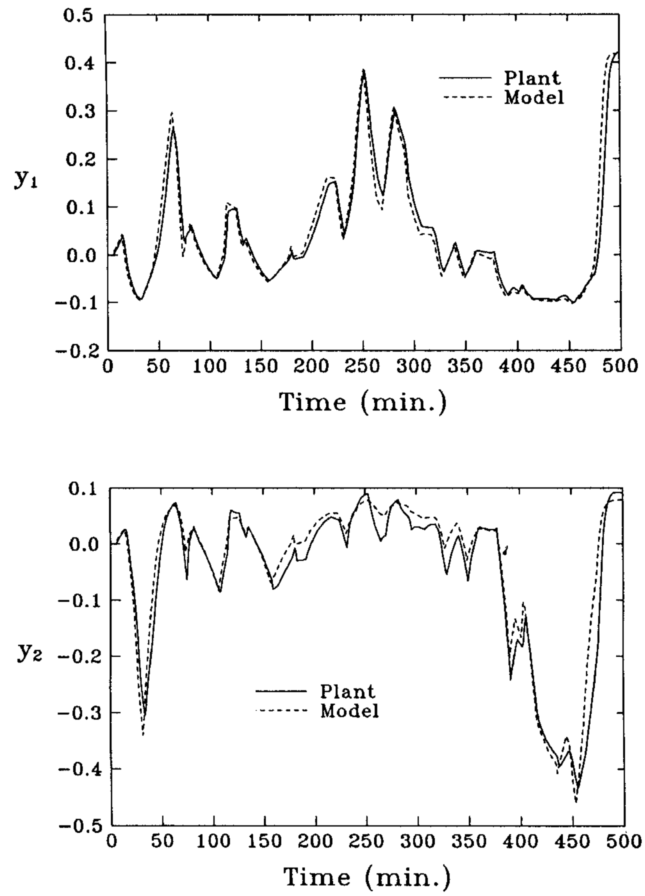

Figure 3. Model prediction for nonlinear input excitation with switching probability of 0.1.

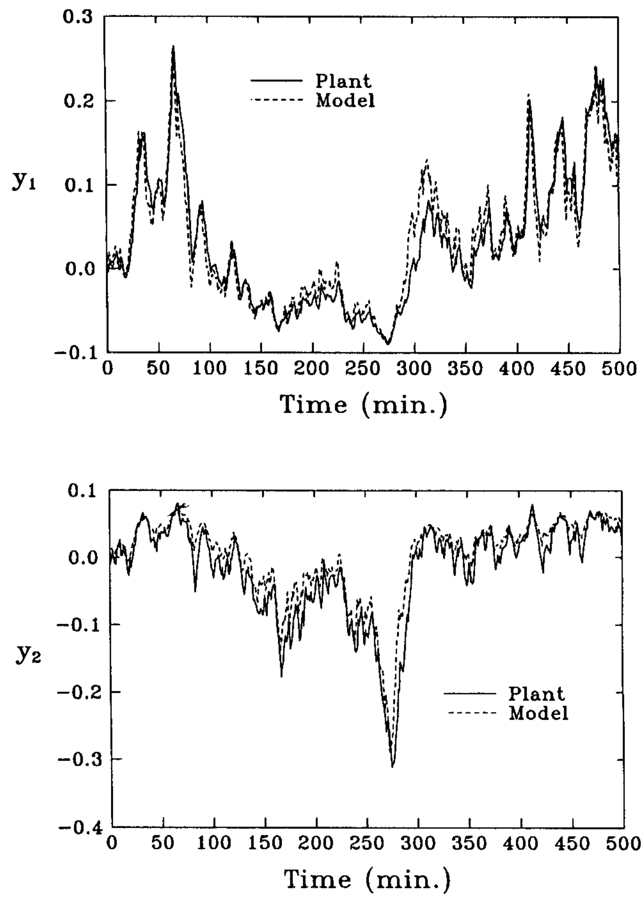

Figure 4. Model prediction for nonlinear input excitation with switching probability of 0.8.

$$y_2(k+1) = -1.7\times 10^{-3} + 0.99y_2(k) - 0.32u_1(k) + 0.31u_2(k) + 0.76y_1(k)u_1(k) - 1.02y_1(k)u_2(k) - 1.22y_2^2(k)u_2(k) - 12.1y_2(k-1)u_2^2(k) \quad (11)$$

We will also use this model for comparison.

Wong and Seborg's empirical nonlinear low-order model: C

Wong and Seborg (1986) have proposed a similar model structure as Eq. 1 for composition control. The process gain and time constant matrices are also functions of the process output vector y. We extend their idea into the temperature-based system. The difference between our proposed model to Wong and Seborg's model is in the definition of process gain matrix. Their process gain elements are defined as

$$k_{ij} = k_{ij}^0 + k_{ij}^1 \Delta y_1^{\text{top}} + k_{ij}^2 \Delta y_2^{\text{bot}} \quad (12)$$

where Δy_1^{top} and Δy_2^{bot} are defined previous as Eqs. 5 and 8.

Notice that every element in the process gain matrix are all functions of the same "driving force" (Δy_1^{top} and Δy_2^{bot}), thus limiting the achievable nonlinear behavior of the column. Also in the model, one controlled variable, say y_1, is not only dependent on the value of y_1 but also dependent on where the other controlled variable y_2 is currently at what value. This assumption will become unreasonable under the condition when the temperature-based control system is actually a single-input, single-output system. On the other hand, the proposed model form in this article (Eqs. 1–8) can also apply to a single-input, single-output system without any modification in the model form. The controlled variables y is dependent on the relative difference in temperature of the measured tray temperatures to the two limiting high and low temperatures (T_{bot} and T_{top}) in the column.

Table 1 shows the summary of the comparison for the simple empirical nonlinear model proposed in this article with the alternative nonlinear models described earlier in this section. For comparison purpose, the sum of the square prediction errors will be used as an indication of how good the pure open-loop prediction is without any knowledge of the previous process measurements. The proposed model is superior in all the input excitation experiments.

Conclusions

A very simple empirical nonlinear low-order model has been proposed for high-purity distillation columns. The model captured very well the three critical process characteristics of the high-purity distillation column which cannot be characterized by any simple linear models. There is a straightfor-

Table 1. Comparison of Pure Prediction Errors for Various Nonlinear Models

Pure Prediction Errors, SSE $(y_1 + y_2)$/No. of data points				
Input Excitation	Proposed Model	Model (A)	Model (B)	Model (C)
$u_1 + 2\%$	0.000234	0.00880	0.00179	0.0689
$u_1 - 2\%$	0.0000937	0.00954	0.0115	0.0753
$u_1 + 10\%$	0.000525	0.136	1.40	0.0647
$u_1 - 10\%$	0.00103	0.190	0.0501	0.0668
$u_2 + 2\%$	0.000149	0.0240	0.0196	0.0483
$u_2 - 2\%$	0.0000937	0.00954	0.0115	0.0753
$u_2 + 10\%$	0.00131	0.171	0.0330	0.0750
$u_2 - 10\%$	0.000329	0.165	0.0569	0.0592
PRBS in u_1	0.0000384	0.000171	0.000122	0.000246
PRBS in u_2	0.0000558	0.000313	0.000125	0.000330
Nonlinear Excitations				
p = 0.1	0.00216	0.0106	0.00453	0.0282
p = 0.3	0.00157	0.0151	0.00938	0.0200
p = 0.8	0.00135	0.00136	0.00422	0.00930

ward procedure to follow in order to obtain the model parameters from several open-loop step tests; thus, this method can be widely applicable to any industrial column. Another advantage of this model form is that both two-point and single-point temperature control structures can utilize this simple model to describe the dynamic behavior of temperature response without any modification.

The model prediction comparison to other nonlinear dynamic models such as logarithmic transformation, NARX model, and other empirical nonlinear models clearly shows the superior agreement of this model to the true process under various input excitations. The low-order model structure is also simple enough so the model can be easily implemented in a model predictive control framework or used for another control system design purpose.

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