

Continuous-Time Hammerstein Nonlinear Modeling Applied to Distillation

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Nonlinear dynamic predictive models are essential for optimal operation and control of many processes. This work presents the predictive modeling of a simulated high purity distillation column using a continuous-time block-oriented modeling methodology developed by Rollins et al. (1998). The proposed methodology is based on a closed-form exact solution to Hammerstein structure and, hence, referred to as the Hammerstein Block-oriented Exact Solution Technique or H-BEST. The Hammerstein structure consists of a nonlinear static gain function that feeds a linear dynamic function. Thus, input vector u passes through the static gain function to obtain $f(u)$ and then passes through the linear dynamic map $G(s)$ and produces the output vector y .

The use of Hammerstein structure for modeling this particular column had previously been investigated by Eskinat et al. (1991). We will refer to the model proposed by Eskinat et al. as the EJM model in this work. This work compares the EJM model to the H-BEST model and demonstrates the advantages of H-BEST in model development and its higher prediction accuracy for these types of processes. The EJM model is a discrete-time Hammerstein model, where the nonlinear static gain is given by a polynomial in the input u and the dynamics are modeled using a discrete transfer function. Chen and Rollins (2000) have shown that discrete-time models (DTM) can exhibit critical drawbacks when sampling is infrequent, non-constant, or not online, but the continuous-time H-BEST method does not suffer from these limitations.

The steady-state or ultimate response of the distillate composition shows dramatically different behavior for positive and negative changes in reflux rate, the input. A critical advantage of H-BEST is that it has the ability to account for this variation by using separate models for the steady-state distillate response over the input space. More specifically, since the static gain

function f appears explicitly in the model formulation of H-BEST, it can be changed over the input space, as shown in this study.

The procedure that H-BEST relies on for model identification is also very different from the conventional approach used by Eskinat et al. The input signal in the traditional approach is usually a pseudo-random sequence design (PRSD) with varying switching times. In contrast, H-BEST uses an input change sequence in the form of sequential step tests for model development derived from the statistical design of experiment (SDOE). Thus, this methodology is able to obtain very accurate ultimate response models over a well designed input space. Rollins et al. (2003a) show the superiority of SDOE over PRSD through the use of a quantitative measure of information content based on the D-optimality criterion (Bates and Watts, 1988) and Bhandari and Rollins (2003) demonstrates the superiority of SDOE over PRSD in a study involving a continuous stirred-tank reactor.

The main objective of this article is to demonstrate greater accuracy of H-BEST in modeling this high purity distillation column as compared to DTM, which is unable to vary in its structure in the ultimate response over the input space. To this end, this note has the following outline. The next section presents the details of the distillation column. Following this section, details of the EJM model are given. After that, the H-BEST model identification and prediction algorithm are presented. Finally, predictive performance of H-BEST is evaluated using an arbitrary input test sequence and is compared to EJM.

Distillation Process

The distillation process in this study is a binary separation and consists of the dynamic material balances for the trays, the condenser, and the reboiler. The assumptions made include: constant relative volatility, stage efficiency of 100%, perfect level control in the reboiler and the condenser, and no delay in vapor and liquid response. Some properties of the distillation

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Table 1. Properties of the Distillation Column

Number of trays	25	Distillate composition	0.995	Distillate flow rate	0.5
Feed tray	12	Bottoms composition	0.005	Bottoms flow rate	0.5
Relative volatility	2	Reflux rate	1.477	Tray holdup	0.5
Feed composition	0.5	Boilup rate	1.977	Cond. and bot. holdup	0.5

column are given below in Table 1. The other details of the column, including the material balance equations, have not been presented here due to space considerations and are available in Eskinat et al. (1991).

EJL Model

The EJL model is a discrete-time Hammerstein model, where the nonlinear static gain is given by a polynomial and the dynamics are modeled using a discrete transfer function. The input variable is the reflux rate and the output variable is the distillate composition. The EJL model was obtained using a PRSD with a time length of 1,000 units and a sampling time of 10 units. The PRSD is shown in Figure 1. Thus, in all, a set of 100 data points was used to identify the model. The authors had proposed two models with different static gain functions: a third-order polynomial and a fourth-order polynomial. A comparison of the coefficient of determination R^2 values; for the two models, shows that the model with the fourth-order polynomial ($R^2 = 82.8\%$) fits the data better than the model with third-order polynomial ($R^2 = 77.7\%$). Thus, we selected the fourth-order polynomial model for this comparative study and call it the EJL model. It is given by Eq. 1 below.

$$\Delta X_{d,t} = 0.757\Delta X_{d,t-1} + 0.243(1.04\Delta R_{t-1} - 14.11\Delta R_{t-1}^2 - 16.72\Delta R_{t-1}^3 + 562.75\Delta R_{t-1}^4) \quad (1)$$

where t is the current sampling instant, ΔX_d is the deviation variable for distillate composition, ΔR is the deviation variable for reflux rate, and the time between samples is 10.

H-BEST and Model Identification

This section gives an exact solution for step input changes to Hammerstein systems. For a series of step changes in input at times t_k, t_{k+1}, \dots , the solution is given by the algorithm in Eq. 2 below

$$t_k \leq t < t_{k+1}$$

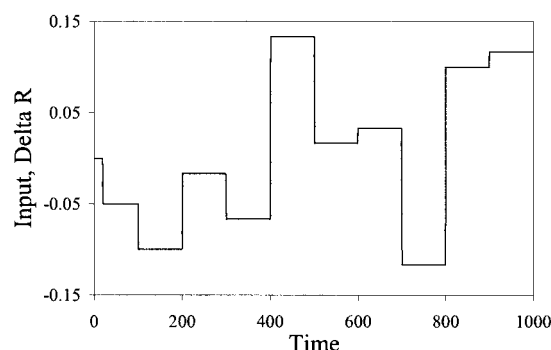


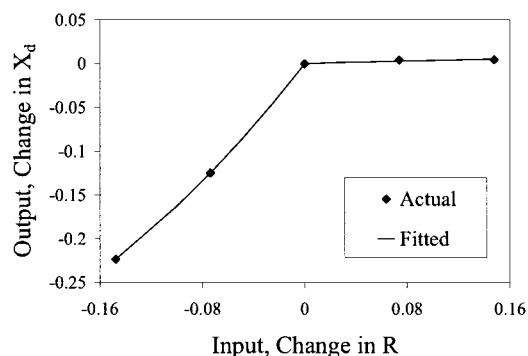
Figure 1. PRSD used for identification of the EJL model.

$$y(t) = y(t_k) + [f(u(t_k); \beta) - y(t_k)] \cdot g(t - t_k; \tau) \quad (2)$$

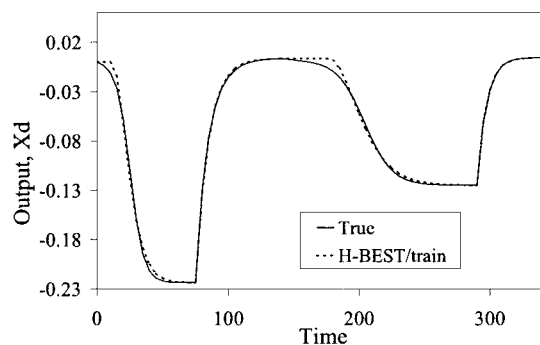
where u and y are deviation variables, $f(u; \beta)$ is the static gain or ultimate response function, $g(t; \tau) = \mathcal{L}^{-1}(G(s)/s)$ with $G(s)$ being the linear dynamic function in the Laplace domain, and \mathcal{L}^{-1} is the inverse Laplace transform operator. The proof of the exactness of the solution and the conditions for which the solution is applicable are given in detail in Rollins et al. (2003a). The solution identifies the functions (f and g) and retains them in their original form.

Methodology and Model Identification

This section presents the methodology to obtain forms of the nonlinear static gain and linear dynamic model and their parameter estimates when modeling physical systems from data. The specific steps for H-BEST model building are as follows:



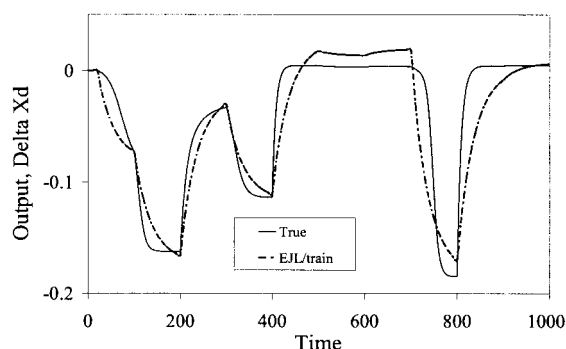
(a)



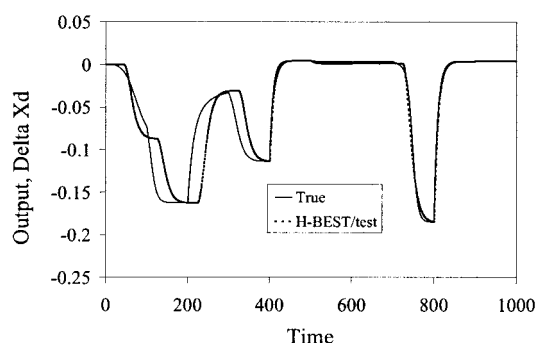
(b)

Figure 2. (a) The actual and fitted response for the steady-state or ultimate change in X_d given by the static gain function $f(\Delta R; \beta)$, that is, Eq. 3; (b) dynamic response of the distillate composition for the four step tests.

The fitted response is given by Eq. 2 in combination with Eqs. 3 and 4.



(a)



(b)

Figure 3. The output responses from the EJL model (a) and H-BEST (b) to the input sequence shown in Figure 1.

This sequence is used to train the EJL model.

(1) Determine the statistical experiment design; (2) Run the experimental design as a series of step tests, allowing steady state to occur after each change and collecting the data over time; (3) Use the steady-state data to determine the ultimate response function, $f(\mathbf{u}; \beta)$; and (4) Use the dynamic data to determine the dynamic function, $g(t; \tau)$, for each output.

As mentioned previously, the input variable is the reflux rate (ΔR) and the output variable is the distillate composition (ΔX_d). The input range is between $\pm 10\%$ of its steady-state value. Since the ultimate response behavior is expected to be nonlinear, the experimental design consisted of four step tests in the following order: -10% , $+5\%$, -5% , and $+10\%$. The data were sampled every five units, and the total time for the tests was 350 units. The steady-state or ultimate response behavior is shown in Figure 2a, where the fitted ultimate response models are given by Eq. 3 below. The dynamic response from the step tests are shown in Figure 2b, and the fitted dynamic models for g are given by Eq. 4 below.

$$f(\Delta R; \beta) = \Delta X_d = \begin{cases} 1.863\Delta R + 2.369\Delta R^2, & \Delta R \leq 0 \\ 0.0006 + 0.031\Delta R, & \Delta R > 0 \end{cases} \quad (3)$$

Table 2. Comparison of Prediction Accuracy Using SSPE Values

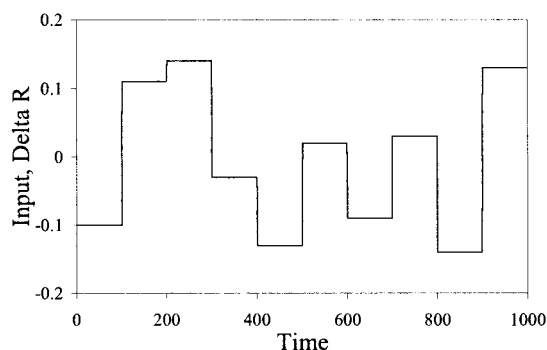
Model	SSPE for Sequence in Fig. 1 (N = 100)	SSPE for Sequence in Fig. 4 (N = 300)
H-BEST	0.04	0.09
EJL	0.07	0.28

$$g(t; \tau) = \begin{cases} \left(1 - e^{-(t-\theta)/\tau} \left[1 + \frac{1}{t} + \frac{1}{2} \left(\frac{t}{\tau} \right)^2 \right] \right); & \tau = 7.91, \theta = 11.24, \text{ for } \Delta R \leq 0 \\ (1 - e^{-(t-\theta)/\tau}); & \tau = 9.54, \theta = 0.86, \text{ for } \Delta R > 0 \end{cases} \quad (4)$$

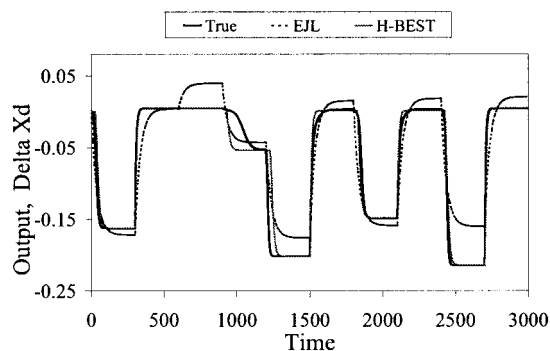
Comparison Study

In this section we compare the predicted responses for H-BEST and EJL. The first comparison is for the EJL training sequence shown in Figure 1. For H-BEST, this sequence is a test sequence. In Figure 3 the performance of H-BEST is shown to be more accurate in fitting the EJL training data than EJL. To quantitatively assess the closeness of agreement between the true and predicted values, we define a term called the sum of squared prediction error (SSPE) given by Eq. 5 below

$$\text{SSPE} = \sum_{i=1}^N (y_i - \hat{y}_i)^2 \quad (5)$$



(a)



(b)

Figure 4. An arbitrary test input sequence (a) and the predicted output responses from H-BEST and EJL (b).

where y_i and \hat{y}_i are the i^{th} true and the i^{th} predicted values and N is the number of points. The SSPE values for the predictions in Figure 3 are given in Table 2.

For an objective comparison of the predictive performances of H-BEST and EJM, an arbitrary test input sequence is used, as shown in Figure 4. From the predictions shown in Figure 4, it is seen that H-BEST is more accurate than EJM. The SSPE for this new sequence, which is a test sequence for both methods, is also given in Table 2. As indicated, the SSPE for EJM is about three times greater than SSPE for H-BEST.

Closing Remarks

We have presented a continuous-time predictive modeling technique and shown its higher accuracy in modeling high purity distillation. The EJM prediction error is about three times larger than the H-BEST prediction error for the case examined. One major strength of H-BEST is its ability to vary in its structure in the ultimate response over the input space. Other advantages of H-BEST include a simple procedure for model identification with shorter test duration. The use of SDOE instead of PRSD allows one to estimate the behavior of the steady-state or ultimate response function (f), as well as dynamic function (g), over the entire input space. Hence, if these forms vary over the input space, then separate functions can be identified and incorporated by H-BEST, as shown in this

work. This ability is critical for processes such as high purity distillation, which can have drastic form changes from low to high distillate purity as column inputs change.

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