Journal of Applied Sciences

ISSN 1812-5654

Journal of Applied Sciences 8 (7): 1214-1220, 2008
ISSN 1812-5654

Development of NARX Model for Distillation Column and Studies on Effect of Regressors

K. Ramesh, N. Aziz and S.R. Abd Shukor
School of Chemical Engineering, Engineering Campus, Universiti Sains Malaysia, Seri Ampangan, 14300 Nibong Tebal, Pulau Pinang, Malaysia

Abstract: Development of suitable nonlinear model is the critical step in the application of nonlinear model based controllers to distillation column. Selecting the proper model structure to capture the data relation in terms of regressors is the important aspect in nonlinear modeling. In this study, the wavenet based Nonlinear Auto-regressive with Exogenous inputs (NARX) model is developed using input and output regressors. The model validation and regressor analysis shown that the selected regressors have the potential of capturing the nonlinearity of the process.

Key words: Distillation column, NARX model, regressors, nonlinear dynamics

INTRODUCTION

Distillation accounts for approximately 95% of the separation systems used for refining and chemical industries (Humphrey *et al*., 1991). It needs to be controlled close to optimum operating conditions because of economic incentives. Close control of distillation column improves the product quality, minimizes energy usage and maximizes the plant throughput and its economy. It is a complex multivariable system and exhibit highly nonlinear dynamic behavior due to their nonlinear vapor-liquid equilibrium relationships. A clear and thorough understanding of the nonlinear dynamic characteristics of the system is necessary for selecting an appropriate structure for the nonlinear model.

Development of nonlinear model is the critical step in the application of nonlinear model based control strategies. Nonlinear behavior is the rule, rather than the exception, in the dynamic behavior of physical systems. Most physical devices have nonlinear characteristics outside a limited linear range. In most chemical processes, understanding the nonlinear characteristics is important for designing controllers that regulate the process (Eskinat *et al*., 1991). Many authors (Leontaritis and Billings, 1985; Juditsky *et al*., 1995; Sjoberg *et al*., 1995; Qin and Badgewell, 1998; Pearson, 2003) have noted the difficulty of developing the models required for nonlinear model-based control strategies. With carefully designed data collection experiments, the dominant behavior of plant can be fitted into one of the several possible structures. The main challenge in this task is to select a reasonable structure for the nonlinear model to capture the process nonlinearities. The nonlinear model used in control purposes should be as simple as possible, warranting less computational load and at the same time retain most of the nonlinear dynamic characteristics of the system (Henson, 1998).

The practical difficulty of nonlinear dynamic model development arises from several sources, of which the following two are fundamental. First fact is that model utility can be measured in several conflicting ways and second, the fact that the class of nonlinear models does not exhibit the unity that the class of linear models does. The four extremely important measures of model utility are approximation accuracy, physical interpretation, suitability for control and ease of development (Pearson, 2003). Fundamental models are generally far superior to empirical and semi-empirical models with respect to the first two of these criteria, but they also suffer badly with respect to the last two. At the other extreme, black-box models are purely empirical, based entirely on input/output data. Consequently, these models generally lack of physical interpretation possible for white-box models, on the other hand, the option of choosing convenient model structures that facilitate formulating and solving the associated control problem.

In engineering dynamics, control engineering and many other areas, auto-regressive with exogenous inputs (ARX) models are widely utilized for describing dynamic data regimes for linear and non-linear systems (Erik, 2000;

Corresponding Author: N. Aziz, School of Chemical Engineering, Engineering Campus, Universiti Sains Malaysia, Seri Ampangan, 14300 Nibong Tebal, Pulau Pinang, Malaysia Tel: +604 -5996457 Fax: +604 -5941013

Mahfouf *et al.*, 2002; Karny and Pavelkova, 2007). However, the performance of these linear models for prediction and control has been limited. In particular, the nonlinear nature and strong directionality of the process present problems during identification. NARX model has been considered as alternatives to linear models in a number of chemical process applications such as distillation column (Sriniwas *et al.*, 1995; Verhaegen, 1998), CSTR (Lee and Lee, 2005; Srinivasarao *et al.*, 2006), pH process (Proll and Karim, 1994; Bomberger and Seborg, 1998) etc. Many algorithms have been employed to identify the parameters of the NARX models. Among these algorithms, Prediction Error Minimization (PEM) method (Spinelli *et al.*, 2006), Least Squares (LS) algorithm (Chen *et al.*, 1989; Previdi and Lovera, 2004) and genetic algorithm (Li and Jeon, 1993; Chen *et al.*, 2007) are the most often used.

Sriniwas *et al.* (1995) have used polynomial NARX model for identification and control of a high-purity distillation column and they didn't use any systematic analysis to select the past inputs and past output in the model. Verhaegen (1998) made the comparative analysis of Wiener identification approach and NARX neural network black-box identification method and concluded that former one is better in the identification of the temperature-product quality relationship in a multi-component distillation column. None of the papers have explained about the regressor analysis which is important to capture the data relation in NARX modeling. Hence in this work, new wavenet based NARX model is used to capture the nonlinear dynamics of the distillation column and regressor analysis is carried out to ensure the proper selection of regressors.

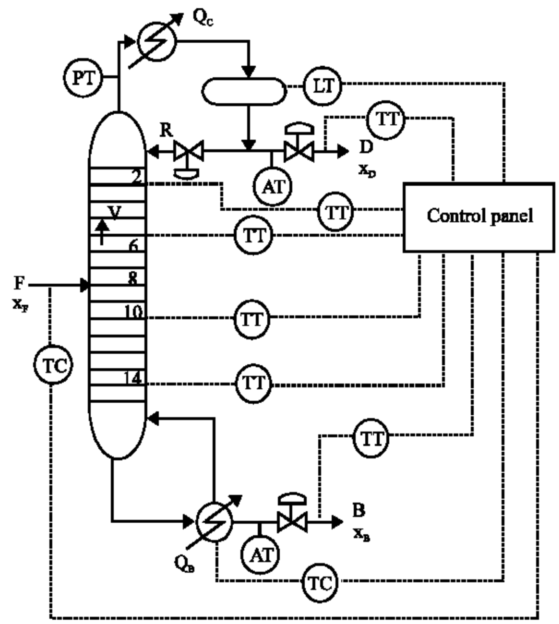

Fig. 1: Pilot plant distillation column

Table 1: Nominal operating conditions and the column parameters

Parameters	Values
No. of trays	15
Feed tray number	8
Column diameter	10.8 cm
Weir height	2 cm
Weir length	8.3 cm
Feed composition	0.308
Feed flow rate	1 kmol h^{-1}
Distillate composition	0.98
Distillate flow rate	0.31 kmol h^{-1}
Bottoms flow rate	0.69 kmol h^{-1}
Reflux flow rate	1.09 kmol h^{-1}
Reflux drum hold up	0.015 m^3
Reboiler hold up	0.007 m^3

DISTILLATION COLUMN CASE STUDY

The schematic of pilot plant distillation column utilized in this study is shown in Fig. 1. The methanol-water binary mixture was used as feed. The top and bottom product compositions are the controlled variables in distillation column. The reflux flow rate and reboiler vapor boil up rate are used as manipulated variables, whereas feed flow rate and feed composition are considered as disturbances. The nominal operating conditions and the column parameters are listed in Table 1. The reboiler and feed temperatures were controlled using separate PID controllers. In all the experiments, tray 2, tray 6, tray 10, tray 14, distillate and bottom product temperatures are measured. The top and bottom product compositions are determined using refractive index analysis.

The experimentally validated first principle model is used as a process model in this work. In the process model, calculation of activity and fugacity coefficients are included in order to account for the non-ideality. The activity coefficients are calculated using UNIFAC model and the fugacity coefficients are calculated using virial equation of state. The detailed first principle model equations and the experimental validation of model were discussed in somewhere else (Ramesh *et al.*, 2007).

NONLINEARITY STUDIES

The nonlinear dynamic characteristic of the system is necessary to select an appropriate structure of the nonlinear model along with an input and output variables for the nonlinear model. The dynamic behavior of the process is studied by giving positive and negative step changes in reflux flow rate, vapor boil up rate, feed flow rate and feed composition.

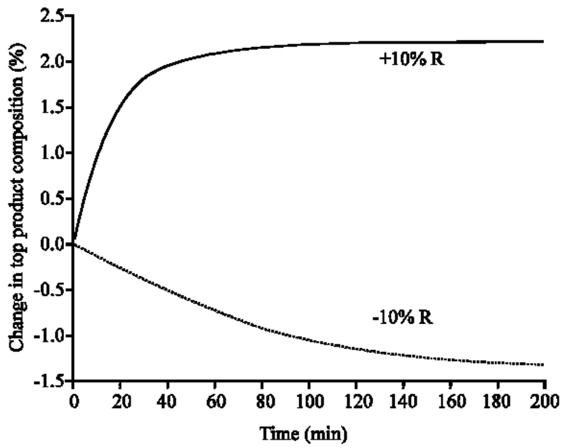

Fig. 2: Responses in top product composition for ±10% change in R

The response in top product composition change for ±10% change in reflux flow rate (R) is shown in Fig. 2. It was observed that the magnitude of % change in top product composition for +10% R is different compared to -10% change in R, i.e., asymmetric responses to symmetric input changes and it clearly indicated the violation of odd symmetry of the linear systems. The similar types of responses were obtained for top product composition for ±10% change in vapor boil up rate (VB), feed flow rate (F) and feed composition. All the dynamic simulation studies have indicated that the violation of odd symmetry of the linear systems. The asymmetric responses to symmetric input changes in the dynamic behavior specified the necessity of nonlinear model (Pearson, 2003) for distillation column.

NARX MODEL

The nonlinear ARX structure models dynamic systems using a parallel combination of nonlinear and linear blocks, as shown in the Fig. 3.

The nonlinear and linear functions are expressed in terms of variables called regressors, which are functions of measured input-output data. The predicted output $\hat{y}(t)$ of a nonlinear model at time t is given by the following general equation.

$$\hat{y}(t) = F(u(t)) \tag{1}$$

where, u(t) represents the regressors. F is a nonlinear regression function, which is approximated by the nonlinearity estimators. The function F can include both linear and nonlinear functions of u(t), as shown in Fig. 3.

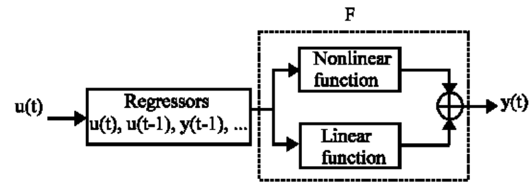

Fig. 3: NARX model structure

The past output regressors are represented as:

$$y(t-1), y(t-2), \ldots, y(t-na) \tag{2}$$

The past input regressors are represented as:

$$u(t-nk), u(t-nk-1), \ldots, u(t-nk-nb+1) \tag{3}$$

Where:

na = Number of past output terms used to predict the current output.

nb = Number of past input terms used to predict the current output.

nk = Delay from input to the output in terms of the number of samples. This value defines the least delayed input regressor.

The meaning of na and nb is similar to the linear-ARX model parameters in the sense that na represents the number of output terms, nb represents the number of input terms and, nk represents the minimum input delay from an input to an output.

Wavenet structure based nonlinear function x = F(u) is used to represent the static nonlinearity of the Hammerstein model.

$$\begin{aligned} F(u) = {} & (u-r)PL + as_1 f(bs_1((u-r)Qcs_1)) \\ & + \ldots + as_k f(bs_k((u-r)Qcs_k)) \\ & + aw_1 g(bw_1((u-r)Q - cw_1)) \\ & + \ldots + aw_k g(bw_k((u-r)Q - cw_k)) + d \end{aligned} \tag{4}$$

where, f(u) is the scaling function given by

$$f(u) = \exp(-0.5u'u) \tag{5}$$

g(u) is the wavelet function given by

$$g(u) = (\dim(u) - u'u)\exp(-0.5u'u) \tag{6}$$

P is a m×p matrix
Q is a m×q matrix
u is a regressors vector
r is a 1×m vector
L is a p×1 vector
cs_k is a 1×q vector
cw_k is a m×q matrix
d, as_k, bs_k, aw_k and bw_k are scalars

Parameters with the s are scaling parameters and with the w are wavelet parameters.

In this study, two past outputs (na = 2), current input and one past input (nb = 2) without delay (nk = 0) were used as regressors in the fourth order nonlinear function. The parameters of the NARX model were estimated using standard prediction error method similar to that one described by Eskinat *et al*. (1991). The model parameters are given as follows.

The values of nonlinear subspace P and linear subspace Q associated with wavenet function model are same for this case.

$$P = Q = 1\times10^{3}\begin{bmatrix} 0.1231 & 0.0722 & -3.0130 & 0.2539 \\ 0.1230 & -0.0684 & 2.9863 & -0.2982 \\ -0.0032 & 0.3584 & -0.2362 & -1.1151 \\ 0.0019 & 0.3624 & 1.3979 & 0.9960 \end{bmatrix}$$

$$\text{Linear term coefficient } L = \begin{bmatrix} 0.0040 \\ 0.0009 \\ -0.0003 \\ 0.0002 \end{bmatrix}$$

The values of other nonlinear parameters are given by

The output offset d = 4.9427×10^{-4}

Regressor mean r = $[-5.0717\times10^{-4}\ -4.9979\times10^{-4}\ 2.5621\times10^{-5}\ 3.119\times10^{-5}]$

$$aw_k = 1\times10^{-4}\begin{bmatrix} -0.2951 \\ -0.2293 \\ -0.1526 \\ 0.1076 \end{bmatrix},\ bw_k = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \text{ and } cw_k = \begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & -1 & 0 \\ -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

The different sets of data generated from validated first principle model were used for parameter estimation and model validation. The data used in the NARX model validation is the one which is not used in the parameter estimation. The multilevel changes were made in reflux flow rate to generate u(t) which is the input to the NARX model. u(t) is the difference between the steady-state value and the value of the reflux flow rate in the particular time instant. The input signal u(t) used for model validation was shown in Fig. 4.

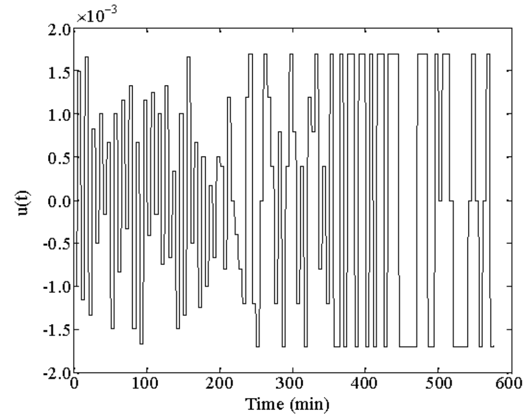

Fig. 4: Input u(t) for multilevel changes in reflux flow rate

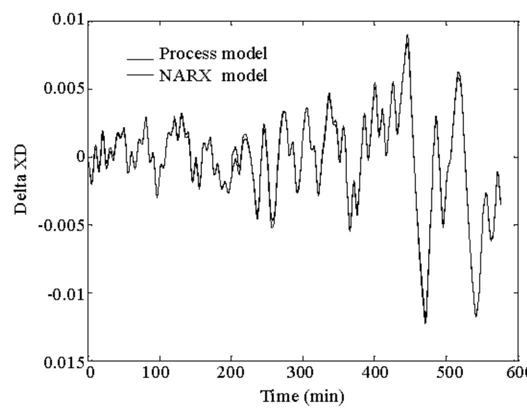

Fig. 5: Comparison of the output of the NARX model and process model

y(t) is the output of the NARX model which is the difference between the steady-state value and the current value of the top product composition in the particular time instant. The comparison of the NARX model output and the experimentally validated first principle model (process model) output was shown in Fig. 5. It has been found that the NARX model results have shown 92.46% agreement with the process model results. The results proved that the wavenet based NARX model was capable of capturing the nonlinear dynamics of distillation column.

REGRESSOR ANALYSIS

The regressor analysis plot displays the characteristics of model nonlinearities as a function of one or two regressors and this will helpful in identify which regressors have the strongest effect on the model output.

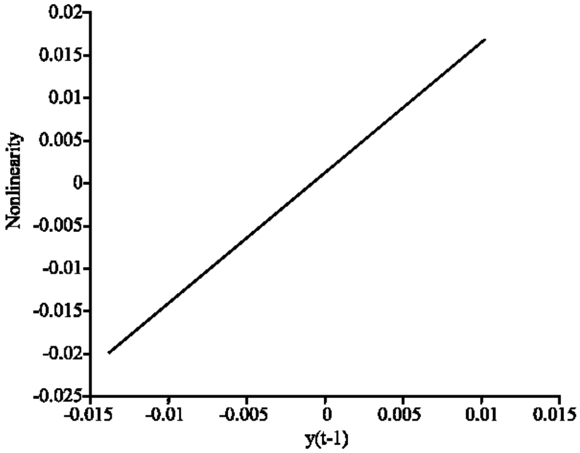

Fig. 6: Effect of regressor y(t-1) on nonlinearity

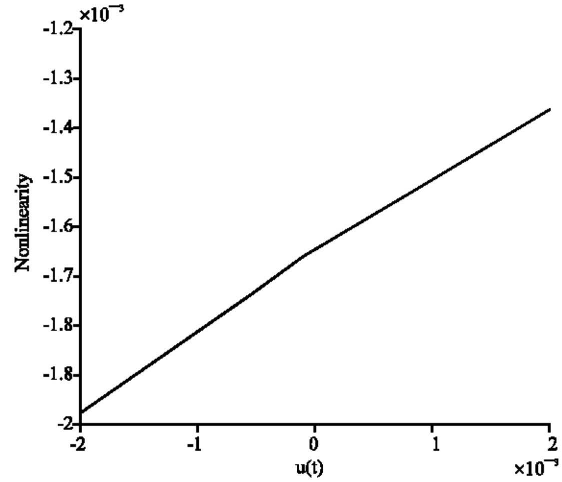

Fig. 8: Effect of regressor u(t) on nonlinearity

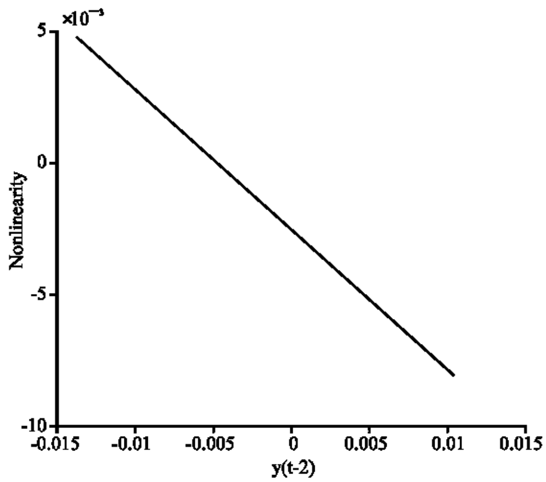

Fig. 7: Effect of regressor y(t-2) on nonlinearity

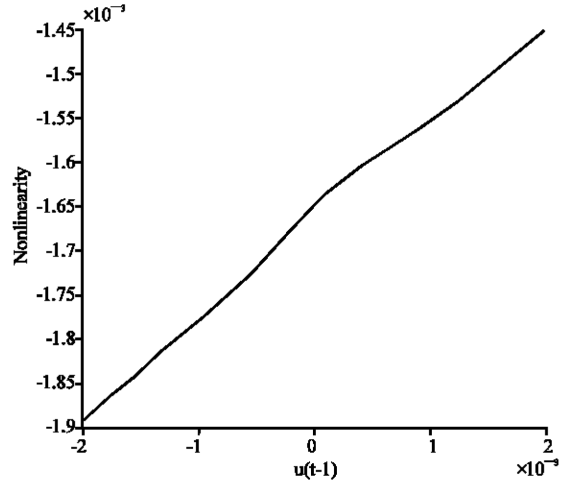

Fig. 9: Effect of regressor u(t-1) on nonlinearity

Understanding the relative importance of the regressors on the output is needed to know which regressors should be included in the nonlinear function. The linear relationship between the regressor and nonlinearity reveal better performance of the regressor in capturing the nonlinearity.

In this research four regressors namely current input regressor u(t), past input regressor u(t-1), past out put regressors y(t-1) and y(t-2) were used. The other regressors like u(t-2) and y(t-3) were studied and their inclusion doesn't show any significant effect in the model results, but increased the complexity of the model. So only above mentioned four regressors were used in this NARX model and their effect on the nonlinearity of the process was discussed below.

The effect of regressor y(t-1) on nonlinearity of the process was shown in Fig. 6. It has been seen from the graph that the relationship between the nonlinearity of the process and the value of regressor y(t-1) is linear and proportional to each other. So the nonlinearity of the process can be better captured by the immediate past output of the process.

The effect of regressor y(t-2) on nonlinearity of the distillation column was shown in Fig. 7. It has been observed that the nonlinearity decreases with increase in regressor y(t-2) although the relationship is linear. The effect of current input regressor u(t) on nonlinearity of the process was shown in Fig. 8. It can be evident from the graph that the relationship is linear, however the effect of regressor u(t) on nonlinearity is not significant compare to regressor y(t-1). The effect of input regressor u(t-1) on nonlinearity of the process was shown in Fig. 9. It can be seen from the graph that the relation between regressor u(t-1) is slightly nonlinear compare to other three regressors. The study of effect of each regressor in the NARX model on nonlinearity of the process has concluded that the regressors of past outputs having more effect on nonlinearity of the process compare to input regressors.

CONCLUSION

The studies on nonlinear dynamic characteristics of the distillation column using the experimentally validated first principle model have proven the necessity of nonlinear model for the distillation column. The wavenet based NARX model using input and output regressors was developed and applied to distillation column. The model validation results and the regressor analysis have concluded that the selected regressors have the potential of capturing the nonlinearity of the process.

ACKNOWLEDGMENT

The authors gratefully acknowledge the financial support by Ministry of Science, Technology and Innovation (MOSTI), Malaysia through the IRPA-8 project No: 03-02-4279EA019.

NOMENCLATURE

as_k : Scaling coefficient
AT : Analysis transmitter
aw_k : Wavelet coefficient
bs_k : Scaling dilation
bw_k : Wavelet dilation
cs_k : Scaling translation
cw_k : Wavelet translation
D : Distillate flow rate (kmol h^{-1})
d : Output offset
f(u) : Scaling function
FL : Feed flow rate (kmol h^{-1})
g(u) : Wavelet function
LC : Level controller
na : Number of past outputs
nb : Number of past inputs
nk : Delay from input to the output
P : Linear subspace matrix
PT : Pressure transmitter
Q : Nonlinear subspace matrix
R : Reflux flow rate (kmol h^{-1})
R : Regressor mean vector
TC : Temperature controller
TT : Temperature transmitter
u(t) : Input to the NARX model
VB : Vapor boilup rate (kmol h^{-1})
XB : Bottom product composition
XD : Top product composition
XF : Feed composition
y(t) : Output of the NARX model

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