Modeling a Nonlinear Binary Distillation Column

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Abstract: Because the process dynamics tend to become too complex to be efficiently controlled, there is always a need to develop innovative control technologies, in order to obtain high economic performance. A way to achieve this objective is to use one of the control strategies which rely on the controlled process model such adaptive control, model predictive control, internal model control, robust control. In order to use one of these control techniques, the process model has to be obtained. The purpose of this paper is to present a model identification method, based on Markov parameters, for a nonlinear chemical process, the propylene/propane binary distillation column.

Keywords: binary distillation, process modelling, identification, Markov parameters.

1. INTRODUCTION

The fundamental problem in control is to find a technically feasible way to act on a given process (system) so that the process (system) adheres, as closely as possible to some desired behaviour. (Goodwin, *et al.*, 2001)

Traditionally, for chemical processes, a way to accomplish this requirement is using model based control strategies. In order to apply one of these control strategies the model of the process has to be known (obtained). This model can be a nonlinear one, with the advantage of being more precise and the disadvantage of increasing the algorithm complexity and the computing effort, or a linear one, with the advantage of simplicity and the disadvantage of not being too precise.

For this work a middle solution was chosen, which combines the two main advantages of linear and nonlinear models: the distillation column model will be a nonlinear one, but represented as a reunion of linear models, one linear model for each operating point and process channel.

2. THE BINARY DISTILLATION COLUMN

The distillation column (Fig. 1) has the L-B, Shinskey controlled structure approach (Marinoiu and Paraschiv, 1992) (the reflux flow is used to control the top (propylene) composition and the bottom product flow is used to control the bottom (propane) composition).

The process (Fig. 2) has two outputs (the propylene (top) and propane (bottom) compositions) and four main inputs, two controlled variables (the reflux and bottom product flows) and two disturbances (the feed flow and feed composition).

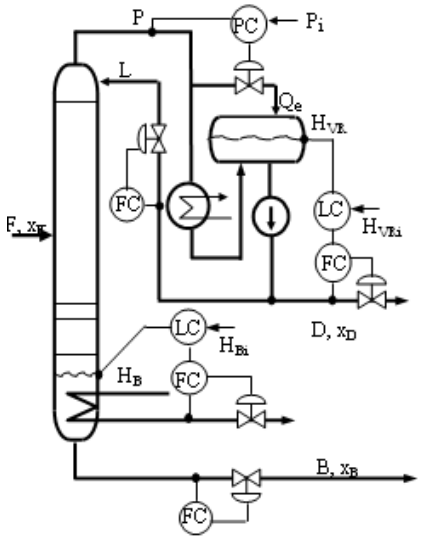

Fig. 1. Propylene(C3')/propane(C3) distillation column: PC – pressure controller, FC – flow controller, LC – level controller, L – reflux flow, P - pressure, Pi – pressure setpoint, B – bottom product flow, H_{VR} – reflux tank level, H_{VRi} – reflux tank level setpoint, H_B – bottom column level, H_{Bi} – bottom column level setpoint, F – feed flow, x_F – feed composition, x_B – bottom composition, x_D – top composition.

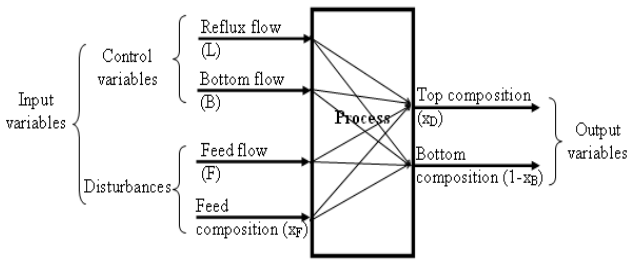

Fig. 2. Distillation process block diagram.

Using data from an industrial column the process was simulated using HYSYS® simulation environment, observing that it has a nonlinear behaviour, characterized by different gains and transient times for each operating point and each process channel (Fig. 3 and 4).

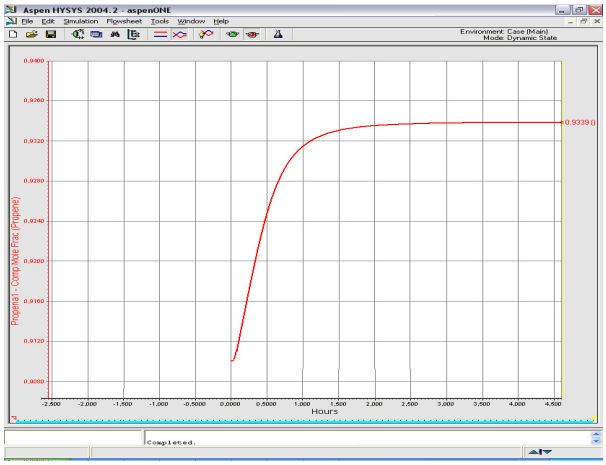

Fig. 3. The top composition x_D trend when the reflux flow L increases with 5%; x_D increases from 0.91 mol. fr. to 0.9339 mol. fr..

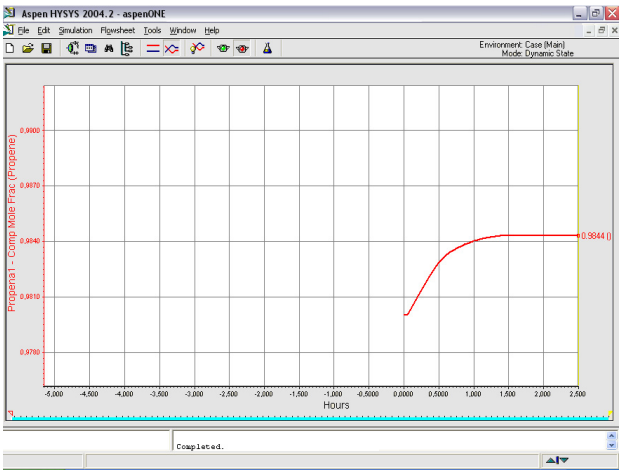

Fig. 4. The top composition x_D trend when the reflux flow L increases with 5%; x_D increases from 0.98 mol. fr. to 0.9844 mol. fr..

3. MARKOV PARAMETERS IDENTIFICATION METHOD - THEORETICAL ISSUES

The Markov parameters identification procedure is used to obtain the parametric model of a process using nonparametric models such Dirac pulse response.

Let us consider a linear, discrete system $\sum = (A, B, C, D)$, characterized by the input-state-output (I-S-O) model: (Cîrtoaje, 2004)

$$\begin{cases} x_{k+1} = Ax_k + Bu_k \\ y_k = Cx_k + Du_k \end{cases}, \tag{1}$$

in which x_k is the state variable vector (n dimensional); u_k - the input variable vector (m dimensional); y_k - the output variable vector (p dimensional); A - matrix having nxn size; B - matrix having nxm size; C - matrix having pxn size; D - matrix having pxm size.

This system is characterized by the observability matrix, O_n (Ryoung, *et al.*, 1998)

$$O_n = \begin{bmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{bmatrix}, \tag{2}$$

the controllability matrix, R_n

$$R_n = \begin{bmatrix} B & AB & \dots & A^{n-1}B \end{bmatrix} \tag{3}$$

and the Hankel matrix, H_r

$$H_r = \begin{bmatrix} CB & CAB & \dots & CA^{r-1}B \\ CAB & CA^2B & \dots & CA^rB \\ \vdots & \vdots & \ddots & \vdots \\ CA^{r-1} & CA^rB & \dots & CA^{2r-2}B \end{bmatrix}. \tag{4}$$

Using the notation g_k for $CA^{k-1}B$, $k \geq 1$, the matrix H_r becomes

$$H_r = \begin{bmatrix} g_1 & g_2 & \cdots & g_r \\ g_2 & g_3 & \cdots & g_{r+1} \\ \vdots & \vdots & \ddots & \vdots \\ g_r & g_{r+1} & \cdots & g_{2r-1} \end{bmatrix}, \tag{5}$$

In which g_k is the system weight function (the system response to a Dirac pulse), for $k \geq 1$. (Julius, 2007)

The expressions $CA^{k-1}B$, $k \geq 1$ are named *Markov parameters.*

Using (5), if the system order *n* and the functions g_k are experimentally known, the Hankel matrix can be obtained without knowing the model parameters A, B, C and D, like in (4).

Further, the Hankel matrix decomposition, using single values decomposition procedure, (Hajdasinski and Damen, 1979) can be written:

$$H_r = USV^t, \tag{6}$$

in which S is a diagonal matrix having same order with matrix H_r, with the diagonal elements nonnegative, (which are also singular values) in crescent order; U – is a matrix having the singular vectors of the matrix $H_r \cdot H_r^t$, as columns; V^t – is a matrix having the singular vectors of the matrix $H_r^t \cdot H_r$, as lines.

Using the matrices U, S and V, obtained from (6), the controllability and observability matrices, R_n and O_n, are: (www, 2008)

$$R_n = \sqrt{S}V^t, \; O_n = U\sqrt{S}. \tag{7}$$

Further, from (7) the system's matrices A, B, C and D can be computed, using (2) and (3), obtaining the system model having the I-S-O form (1).

4. MARKOV PARAMETERS IDENTIFICATION METHOD - PRACTICAL ISSUES

Using the Markov parameters identification procedure (Fig. 5), models of the process can be determined for every process channel (Fig. 2). From the control operation point of view, these models have to be simpler, but robust. (Mikles and Fikar, 2000) A way to express the model of a process is by a second order transfer function with dead time:

$$G = \frac{k_m e^{-\tau s}}{T_2 s^2 + T_1 s + 1}, \tag{8}$$

where k_m is the process gain, τ is the dead time and $\sqrt{T_2}$ and T_1 are time constants.

The Markov parameters identification method uses as input an experimental data set, represented as a system response to a Dirac pulse input, and as output data, the I-S-O (input-state-output) model (1).

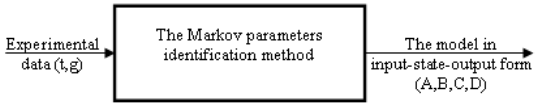

Fig. 5. The identification method block diagram.

Because the available experimental data, obtained from process simulations using HYSYS, are represented by the response *h* in time *t* of the process to a step change in input (as in Fig. 3 and 4), in order to apply the identification method these set of data have to be converted to a pulse response *g* – *step*1 of the identification procedure. (Fig. 6)

Because the result of the identification procedure is the model in I-S-O form, using a conversion method this is converted into an input-output (I-O) model (transfer function) – *step* 3 of the identification procedure. (Fig. 6) Further, this I-O model (8) can be used in a process control stage.

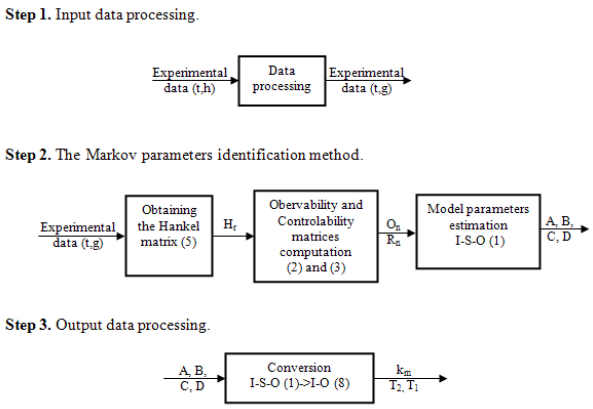

Fig. 6. The identification method steps: t – time, g – system pulse response, h – system step response, H_n – Hankel matrix, (5), O_n – observability matrix, (2), R_n – controllability matrix, (3), A, B, C, D – the parameters of the I-S-O model, equation (1), k_m, T_2 and T_1 – the parameters of the I-O model, equation (8).

5. MODELING THE BINARY DISTILLATION COLUMN

From the dynamic simulation results (Fig.3, 4) it can be observed that the process has a nonlinear behavior, with the operating point.

Because the goal of this paper is to obtain a simplified process model, which can be further used in a control application, the main idea is that this model has to be a nonlinear one but represented as a reunion of linear models, one for each process channel and operating point.

The model was chosen to be a second order transfer function, (8), so that the requirements regarding the model precision and the computing effort to be optimum. In the first order model case we have deviations of the model response from the real process response, and in the third order model case the computing effort increases without significant precision changes.

Using the presented identification procedure, models of the process were obtained for different process channels and different operating points.

For L-x_D process channel (Fig. 2) the values of the model parameters k_m, T_2 and T_1 are presented, for different operating points, in table 1. These values were obtained using the experimental data recorded from HYSYS process

simulations, for different operating points (eg. x_d=0.8, 0.85, 0.88 etc. mol. fr.) and applying the Markov identification procedure as in Fig.6.

Using the values for the obtained parameters, a function between these parameters and the operating point was obtained, for each process channel. It has the form (Băieşu, 2008)

$$model\_parameter = m \cdot composition + n, \quad (9)$$

in which *model_parameter* represents one of the k_m, T_2 or T_1 model parameters; composition is the x_D or $(1\text{-}x_B)$ composition; *m*, *n* are the linear dependence parameters.

Table 1. Model parameters values for L –x_D process channel, with the operating point.

x_D[mol. fr.]	k_m[mol. fr./%]	T_2[sec^2]	T_1[sec]
0.8	0.0109	2465	1835
0.85	0.0085	2204	1683
0.88	0.0065	2080	1621
0.9	0.0058	2003	1587
0.92	0.0042	1887	1522
0.93	0.0036	1839	1487
0.95	0.003	1723	1423
0.98	0.0009	1598	1353

Because the dependence between the operating points and one of the three model parameters (k_m, T_2 or T_1) is approximately linear (table 1), for each channel, the values of *m* and *n* were found by linear regression. The results are presented in table 2, for L-x_D and B-$(1\text{-}x_B)$ process channels.

Table 2. M and n values, for L-x_D and B-$(1\text{-}x_B)$ channels.

		L-x_D
k_m	m	-0.0557
	n	0.0556
T_2	m	-4814
	n	6313
T_1	m	-2654
	n	3956
		B-$(1\text{-}x_B)$
k_m	m	-0.0275
	n	0.0149
T_2	m	$1192 \cdot 10^2$
	n	-86216
T_1	m	47750
	n	-34525

Further, using (9), the model parameters km, T_2 and T_1 can be found also for any x_D or $(1\text{-}x_B)$ values.

Accordingly, the process model will be adapted at each input variable change, depending of the operating point by computing the model parameters.

6. MODEL VALIDATION

A mathematical model is considered valid if it reflects, with an imposed precision, the real process behavior.

The model validation stage consisted in estimated data validation, by computing the error (10) between the real data and the estimated data, using the obtained model.

The error is computed using the equation

$$e(i) = y_{experim}(i) - y_{estim}(i), \quad (10)$$

in which i is the current time instant, $y_{experim}$ is the experimental output value, and y_{estim} is the model estimated output value.

Figures 7 and 8 present the trends of the computed error (10) for different process channels and different operating points, to an input variables change.

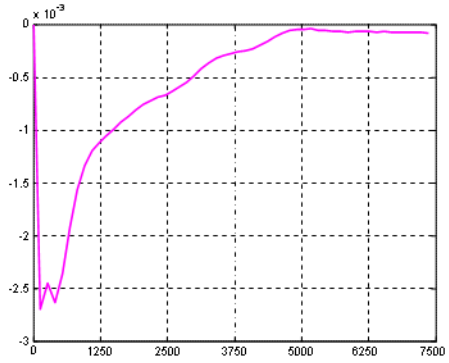

Fig. 7. The error variation [mol. fr.] in time [min] for the operating point x_D=0.95 mol. fr., when the reflux flow increases with 5%. (L - x_D channel)

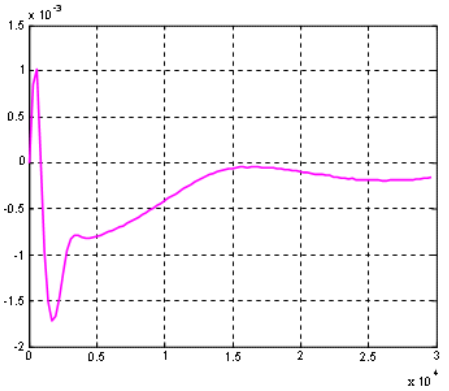

Fig. 8. The error variation [mol. fr.] in time [min] for the operating point 1-x_B=0.83 fr. mol., when the bottom product flow increases with 5%. (B – (1-x_B) channel)

The maximum error values, computed for each process channel, are presented in table 3.

Table 3. The maximum error values.

Channel	L - x_D	F - x_D	x_F - x_D
|e_max|[mol.fr.]	$3.2 \cdot 10^{-3}$	$2.25 \cdot 10^{-3}$	$2.1 \cdot 10^{-3}$
Channel	B – (1-x_B)	F – (1-x_B)	x_F – (1-x_B)
|e_max|[mol.fr.]	$2.5 \cdot 10^{-3}$	$1.8 \cdot 10^{-4}$	$1.7 \cdot 10^{-4}$

As it can be observed, from table 3, the obtained process model is adequate for its purpose, to be used in some model based control algorithms, because the modeling errors are insignificant. This conclusion is also sustained by the resolution of the devices which generates the experimental data or by the resolution of the numerical/analogical conversions and by the trends from figures 9 and 10.

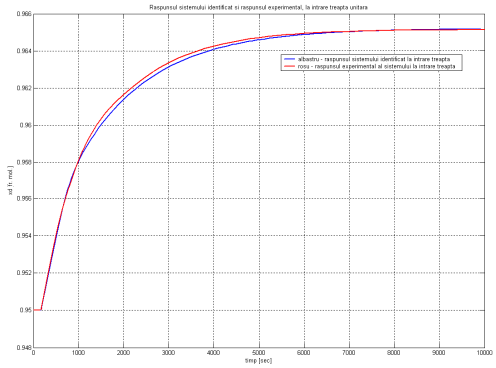

Fig. 9. The real process response and the process model response, to a step input change, for the operating point x_D=0.95 mol. fr., when the reflux flow increases with 5%.

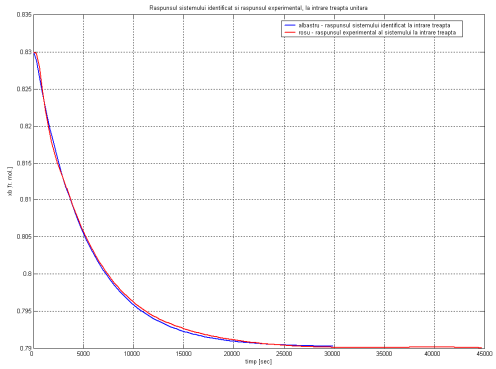

Fig. 10. The real process response and the process model response, to a step input change, for the operating point 1-x_B=0.83 mol. fr., when the bottom product flow increases with 5%.

The trends from Fig. 9 and 10 present the real process response and the process model response, for L-x_D and B-(1-x_B) process channels, to a step change of the input variables L and B, respectively. As it can be observed from the two trends, the process model response is approximately the same as the real process response.

Taking into account the results from the model validation step, the conclusion is that the model is a valid one, and can be used in further control applications.

7. CONCLUSIONS

This paper presents a method for modeling a nonlinear binary distillation column using Markov parameters identification technique.

The process is a multivariable one, with two outputs (the propylene and propane compositions) and four main inputs, two controlled variables (the reflux and bottom product flows) and two disturbances (the feed flow and feed composition).

The main idea and contribution of this paper was to obtain a set of local transfer-function models, using available input/output data and the Markov parameters identification procedure, to represent the dynamic system for different operating points and process channels, and then to connect the set of local models to form a global dynamic model.

The obtained process model is a nonlinear one, but represented as a reunion of linear models, described by second order transfer functions with dead time.

The model was validated and can be used in further control applications.

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