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Predictive Functional Control Applied to Multicomponent Batch Distillation Column

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Abstract

This work describes the implementation of a Predictive Functional Control (PFC) algorithm on a ternary batch distillation column to control temperature by manipulating the reflux ratio. The PFC is tuned off-line by using simplified models obtained by applying identification techniques. The temperature set point is described by a polynomial related with an optimal dynamic behaviour determined to achieve the composition specifications. The separation performance is closely checked with the help of a soft sensor, based on a non linear Hammerstein model described in a previous work, which input is top temperature and the outputs are the estimated compositions. Additionally the model composition estimations are employed for calculating the accumulated compositions for each tank. Therefore a type of split range control for the corresponding valves of each tank is programmed in order to storage each component under quality requirement. Experiments were performed on a rigorous model developed in HYSYS.Plant® with data of a real pilot column. All concerning to control policy was implemented in MATLAB. Results comparing optimal PID and PFC are presented.

Keywords: Batch distillation columns; Non-linear model; Predictive Functional Control Soft-sensor.

1. Introduction

The Predictive Functional Control (PFC) technique is the third generation of a family of Model Algorithmic Control (MAC), developed by Richalet and coworkers during the last decades (see Richalet, 1993). It resides on representing the plant with certain model, generate the control algorithm for one or more coincidence points with the reference trajectory, solve it and apply the calculated input action. The later can be constrained on its maximum and minimum values and its rate of variation. No report was found in the

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open literature showing the application of this kind of control technology to batch distillation. The internal model, which gives the relationship among top temperature (controlled variable) and reflux ratio (manipulated variable), is obtained by linear identification techniques named N4SID, detailed in Jimenez et al (2002), and used here for predictions.
In addition, a non linear identification technique is used for obtaining a reduced order Hammerstein model working as the soft sensor presented in Ruiz et al. (2004). It can handle the correlations among temperature and compositions of the batch distillation column.
The case study analyzed here consists on an experimental batch column given by Nad and Spiegel (1987) to separate the ternary system of toluene, n-heptane and cyclohexane. The soft sensor is used to correct the temperature set point if the estimated instantaneous compositions do not match with the optimally specified ones. In addition the soft sensor allows to predict the accumulated composition in the different vessels and determine how to manipulate the valves corresponding to the main and off cuts.

2. Case Study: Multicomponent Batch Distillation

The pilot plant shown in Figure 1 which data are taken from Nad and Spiegel (1987) is briefly described here. The distillation column has a 162 mm inner diameter filled with structured packing Sulzer Mellapak 250 Y (packing height of 8.0 m). The system involves a ternary mixture of cyclohexane, n-heptane and toluene. The whole column including reboiler and condenser has 20 theoretical plates. The initial charge is 40.07% of cyclohexane, 39.40% of n-heptane, and 19.90% of toluene. The duration of each step and the corresponding reflux ratio profiles are given in Jimenez et al. (2002).

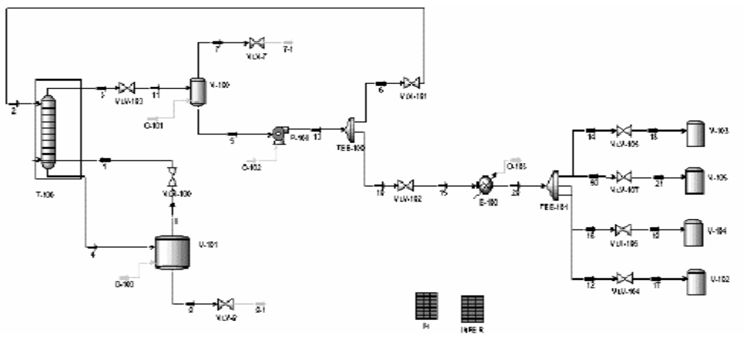

Figure 1. Batch Distillation Column in HYSYS Plant®.

3. Control Project Steps

The main control objective consists in the implementation of PFC for the top temperature of the column which follows an optimally specified set point to achieve the required composition profiles. The control implementation is shown in Figure 2.
This project involves the steps of system identification, controller design and implementation with the basic library of the communication protocols between software. It allows to connect the control routine in MATLAB™ to all other elements of the plant simulated by HYSYS.Plant®.

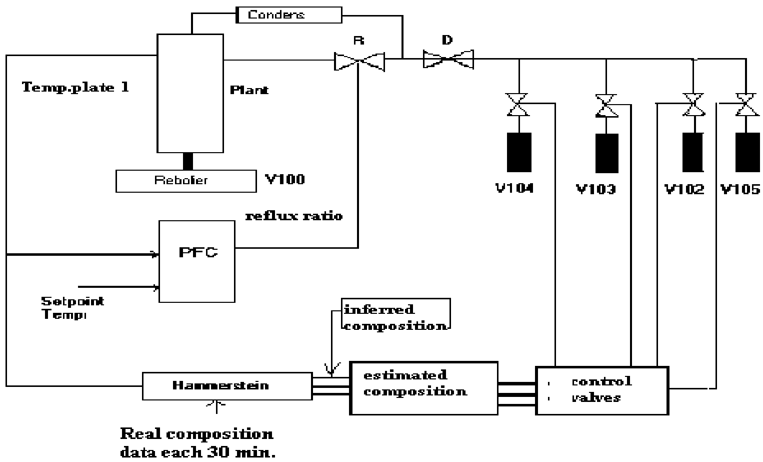

Figure 2. control structure applied to the batch distillation.

3.1 Identification Techniques Applied to Obtain the Internal Model

In this section will be given the fundamental equations used for implementing the predictive control structure over the plant shown in Figure 2. A reliable state-space model, obtained following the 4SID methods, which considers a LTI system with n inputs and m outputs is described by

$$\begin{aligned} x_{k+1} &= Ax_k + Bu_k + w_k \\ y_k &= Cx_k + Du_k + v_k \end{aligned} \tag{1}$$

where x_k is the state vector, u_k is the input vector (RR), y_k is the output vector (T), and w_k and v_k are the process noise and output measurement noise vectors respectively. The estimated matrices were given in Ruiz et al. (2004) and are detailed in eq. 2.

$$\begin{aligned} &A = \begin{bmatrix} 1.0009 & -0.0618 \\ 0.0006 & 0.9324 \end{bmatrix}; \quad B = \begin{bmatrix} 0.1679 \\ 0.1716 \end{bmatrix}; \quad D = 0 \\ &C = \begin{bmatrix} -0.1328 & -0.3651 \end{bmatrix}; \quad X0 = \begin{bmatrix} 0.1679 \\ 0.1716 \end{bmatrix} \end{aligned} \tag{2}$$

The system given by eq. 2 can be transformed in a discrete transfer function available for implementing the internal model of the PFC which consists on a first order with integrator model:

$$G = \frac{-0.08495\,z + 0.08487}{z^2 - 1.933\,z + 0.9333} \tag{3}$$

3.2 Controller Design

The main PFC controller elements are: a) independent model approach which predicts the dynamic behavior of the plant on a prediction horizon given by eq. 3; b) for this case, where the plant transfer function presents an integrative element, decomposition principle for unstable system must be considered; c) exponential reference trajectory corresponding to first order closed loop response; d) polynomial structuration of the future manipulated variable that minimize the difference between reference trajectory and model prediction at one or most coincidence points; f) constraints on manipulated variable (MV) and state variables; g) tuning in time and frequency domain.

3.3 Mathematical Calculations for PFC Design

Since the identified transfer function was of first order plus integrator it is decomposed as shown in Figure 3.

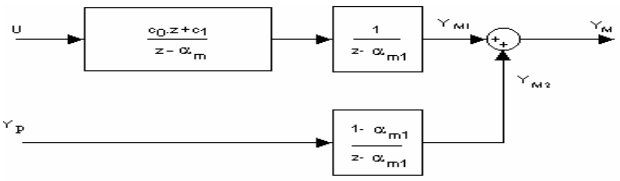

Figure 3. Decomposition of the integrator term.

$$\alpha_{m1} = \exp\left[-\frac{Ts}{\tau_{desc}}\right] \tag{4}$$

τ_{desc} is the decomposition time generally considered equal to the closed loop time response.

$$y_m(n+h_j) = y_{m1}(n+h_j) + y_{m2}(n+h_j) \tag{5}$$

$$\hat{y}_P(n+h_j) = y_m(n+h_j) + \hat{e}(n+h_j) \tag{6}$$

The control law is calculated by minimizing the difference between predicted output ($\hat{y}_P$) and reference trajectory (y_R).

$$D = \sum_{j=1}^{nh} \left\{ \hat{y}_P(n+h_j) - y_R(n+h_j) \right\}^2 \quad \text{so,} \; \frac{\partial D}{\partial \mu} = 0 \tag{7}$$

$$c(n+h_j) - y_R(n+h_j) = \lambda^{hj}.(c(n) - y_p(n)) \tag{8}$$

Where C represents the set point, and h_j each coincidence point considered then

$$c(n+h_j) = \sum_{i=0}^{P} c_j(n)\ i^j \tag{9}$$

P indicates the total number of extrapolation terms to describe the set point trajectory based on specific number of its past values. By doing the calculations, D becomes

$$D(n) = \sum_{j=1}^{N} \left[\underbrace{\mu(n)^T . y_B(h_j) + \alpha_m^{hj} . y_{mi}(n) + e(n) + \sum_{j=1}^{d_e} e_j(n).(-i)^j \,|.h_j}_{\hat{y}_p(n+h_j)} \; - \underbrace{c(n+h_j) + \lambda^{h_j}.(c(n) - y_p(n))}_{y_R(n+h_j)} \right]^2 \tag{10}$$

$$d(n) = \alpha_m^{hj}.y_{mi}(n) + e(n) + \sum_{j=1}^{d_e} e_j(n).(-i)^j.h_j - c(n+h_j) + \lambda^{h_j}.(c(n) - y_p(n)) \tag{11}$$

$$\mu(n) = Y_{BC} \cdot Y_B \cdot d(n) \tag{12}$$

Y_B and Y_{BC} values are known because they correspond to the output information for selected U_B input base functions such as steps, ramps or parabolas.

$$Y_{BC} = \left\{ \sum_{j=1}^{N} y_B(h_j).y_B(h_j)^T \right\}^{-1} \tag{13}$$

$$Y_B = [y_B(h_1)\ y_B(h_2)\ ....\ y_B(h_N)] \tag{14}$$

3.4 Temperature Set Point Configuration

The last point is to configure a proper temperature set point which is based on the composition specification. The proposed problem is to maximize the amount of distillate for a given time (4.5 hours) and a 0.98 molar fraction for cyclohexane because it is considered to be the most important product to obtain. It is solved taking into account the following relationships:

$$\underset{Rt}{\text{maximize}} \left(j = \int_0^T \frac{dD}{dt}.dt = \int_0^T \frac{V}{R_t + 1}.dt \right) \tag{15}$$

$$\text{subjected to: } x_{Dav} = \frac{\int_0^T \frac{V}{R_t + 1}.x_D^{(1)}.dt}{\int_0^T \frac{V}{R_t + 1}.dt} = x^* \tag{16}$$

4. Results

In Figure 4 the instantaneous temperature and the set point values are presented when PFC is implemented together with the reflux ratio given by the control algorithm of eq. 12. Results indicate that a good servo-behaviour with smooth movements of the manipulated variable, except at the initial interval of the distillation, are achieved. In Table 1 the accumulated composition and level on each tanks of main cuts for both PFC and PID, respectively.

Table 1. Accumulated composition on each tank and % level after first batch time.

Component/% level	PID	PFC
Cyclohexane (V104)	0.984	0.982
Level (V104)	49.84	48.83
N-heptane (V102)	0.2103	0.2772
Level (V102)	20.73	33.5
Toluene (reboiler)	0.4656	0.4692
Level reboiler	8.62	8.5

Data for PID was taken from a previous work (Ruiz et. al., 2004) where the composition from soft sensor estimation was the controlled variable. Table 2 shows the same as Table 1 but for the slop cuts where it is clear that less reprocessing material is needed when PFC is implemented.

Table 2. Accumulated composition on each tank and level after the first batch time for both slop cuts.

	First slop cut (V103)		Second slop cut (V105)	
	PID	PFC	PID	PFC
Cyclohexane	0.95772	0.96141	0.53556	0.38764
n-heptane	0.00185	0.00177	0.11452	0.16741
Toluene	0.04043	0.03682	0.34991	0.44495
Level (%)	18.23	6.29	44.37	22.27

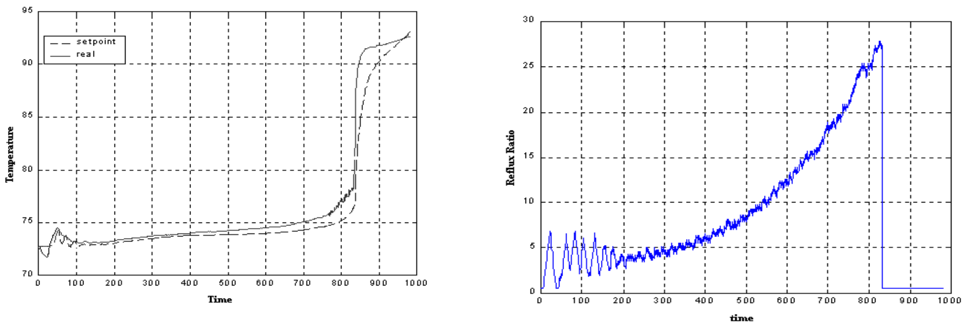

Figure 4. Simulation results with HYSYS.Plant® and MATLAB™ of temperature and its corresponding reflux ratio for optimal cyclohexane recovery.

5. Conclusions

PFC tuning involves several parameters, obtained by off-line optimization using both N4SID and Hammerstein simplified models, which help significantly to reduce the computational time. It allowed a good setpoint tracking with smooth movements for the manipulated variable during the first batch time. In addition, a comparison with the optimal PID is included remarking that PFC allows to achieve a better profitability by reducing the reprocessing operation time.

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