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Advanced Control of a Reactive Distillation Column

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Abstract

The paper presents a detailed analysis of the dynamic behavior of a reactive distillation column. A control relevant dynamic model is derived using first-principles modeling and it is used to study the dynamic behavior of the process at high and low purity operating regimes. The results are used to analyze the performance of linear and nonlinear model predictive control in comparison to coupled PID control.

Keywords: reactive distillation, nonlinear model predictive control.

1. Introduction

Reactive distillation processes have received a tremendous industrial interest over the last decade. Reactive distillation combines both separation and reaction in one unit, offering significant economic advantages in some systems, particularly for reversible reactions, which are limited by equilibrium. Despite the complex nonlinear dynamics of these systems caused by the coupling between the reaction and separation processes, research has been focused mainly on the steady-state design of the reactive distillation system [1,2]. Several control approaches have been proposed based on linear [3], or nonlinear control approaches [4]. The objective of the paper is to evaluate the feasibility of different control techniques from both linear and nonlinear controllers by considering the application of nonlinear model predictive control (NMPC), linear model predicative control (LMPC) and coupled PI control to a sample reactive distillation process. The main contribution of the paper besides the simulation of the different control strategies consists in the systematic analysis of the control performances based on the detailed open-loop analysis of the dynamic behavior of the system at low and high purity operating conditions.

2. Mathematical model of the reactive distillation column

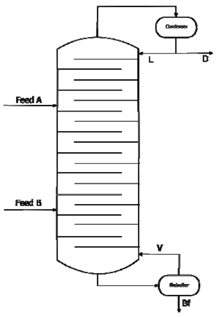

Fig. 1. Reactive distillation column

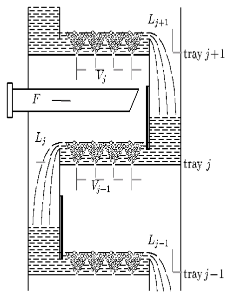

Fig. 2. Tray-by-tray model of the column

This case study is based on a general mathematical representation of a reactive distillation column (Fig. 1), where a reaction of the form:

$$A + B \xleftrightarrow{\;r\;} C + D \tag{1}$$

takes place in the liquid phase. The column is considered to have 41 theoretical trays. The feed of component A and B enter the column in tray number 10 and 30, respectively. The products C and D are removed as top and bottom products, respectively. The process control objective is to maximize conversion of the reactants and separation of the products. As manipulated variables the reboiler vapor flow and the liquid reflux in the condenser are used. The distillate flow and the bottom liquid flow are used to control the total liquid holdup in the reboiler and the condenser, respectively. The reaction is assumed to take place only in the liquid phase. The tray-to-tray model equations (Fig. 2) for the column trays are given by:

$$\frac{dM_i^l}{dt} = F_i + L_{i+1} + V_{i-1} - L_i - V_i + Vol_i \sum_{j=0}^{NC} \mu_j r_i \tag{2}$$

$$\frac{d(M_i^l x_{i,j})}{dt} = F_i x_f + L_{i+1} x_{i+1,j} + V_{i-1} y_{i-1,j} - L_i x_{i,j} - V_i y_{i,j} + Vol_i \mu_j r_i \tag{3}$$

for $i = \{2,\cdots,40\}$, $j = \{1,\cdots,4\}$. Here, $x_{i,j}$ and $y_{i,j}$ are the mol fractions of component j in the liquid and in the vapour of tray i. M_i^l is the total molar liquid hold-up of a tray i. The model equations for the condenser and the reboiler are as follows:

$$\frac{dM_b^l}{dt} = L_2 - Bf - V_b + Vol_b \sum_{j=1}^{NC} \mu_j r_b \tag{4}$$

$$\frac{d(M_c^l)}{dt} = V_{40} - L_c - Df + Vol_c \sum_{j=1}^{NC} \mu_j r_c \tag{5}$$

$$\frac{d(M_b^l x_{i,j})}{dt} = L_2 x_{2,j} - Bf x_{b,j} - V_b y_{b,j} + Vol_b \mu_j r_b \tag{6}$$

$$\frac{d(M_c^l x_{c,j})}{dt} = V_{40} y_{40,j} - L_c x_{c,j} - Df x_{c,j} + Vol_c \mu_j r_c \tag{7}$$

where Bf and Df are the product flow from the reboiler and the condenser, respectively. The reaction rate is given by:

$$r_i = k_{or} \left(x_{i,A} x_{i,B} - \frac{1}{k_{eq}} x_{i,C} x_{i,D} \right) \tag{8}$$

The vapour mol fraction is calculated based on constant volatilities by:

$$y_{i,j} = \frac{\alpha_j \cdot x_{i,j}}{1 + \sum_{j=1}^{NC} (\alpha_j - 1) \cdot x_{i,j}} \tag{9}$$

Finally, the change in component composition is given by:

$$\frac{dx_{i,j}}{dt} = \frac{1}{M_i} \left(\frac{d\left(M_i^l x_{i,j}\right)}{dt} - x_{i,j} \frac{dM_i^l}{dt} \right) \tag{10}$$

The reactive distillation column model was implemented in the Matlab/Simulink environment. The column is represented by a Simulink S-Function, which is written in C-language and compiled with the Watcom compiler to a *dll* file for fast simulation.

3. Open-loop dynamic analysis

Reactive distillation is an extremely nonlinear process with highly interacting dynamics. The characteristics of the process change under different operating conditions, thus, linear models are only good approximations of the real process for very small deviations of the steady state. Prior to design a controller we have done several simulations to characterize the sensitivity of the control variables with respect to small input changes and disturbances. Steady state deviations have been analyzed starting from two different steady states.

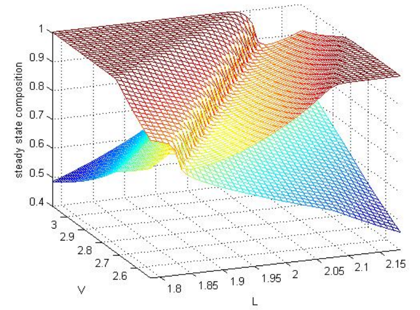

Fig. 3. Steady state analysis within the low purity operating regime (0.79, 0.81) (open loop simulations). Small changes in the input result in significant steady state changes.

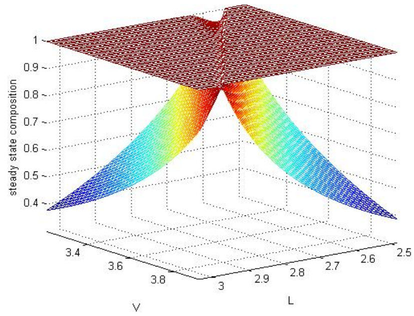

Fig. 4. Steady state analysis within the high purity operating regime (0.99, 0.99) (open loop simulations). Small changes in the input result in drastic steady state changes.

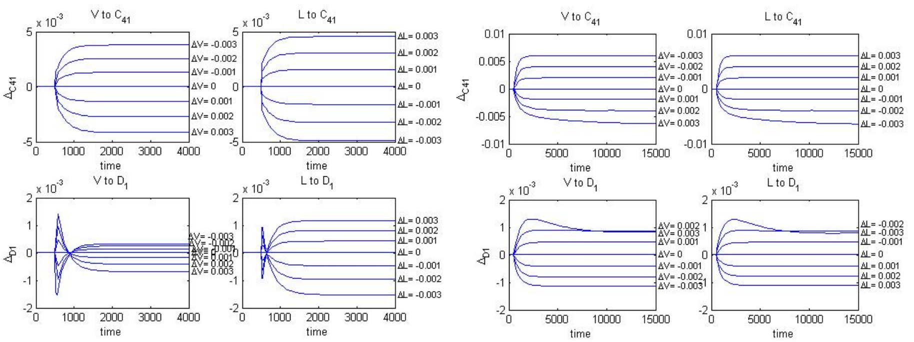

Fig. 5. Step response of the reactive distillation column for very small steps in the inputs in the low purity operating region (left) and high purity region (right).

The reboiler vapour flow V and the condenser reflux L have been varied with ± 10% of the respective steady stated values. Figures 3 and 4 show new steady states resulting from the input variation. The trend is different for small regions of the steady state for operation in a low purity region and a high purity region, however the overall trend for larger input changes are similar. A high composition for both C_{41} in the condenser and D_1 in the reboiler is achievable only in a narrow regime, thus, disturbances are expected to have high influences in the composition of the outflows. Figure 5 presents the step responses of the column w.r.t. very small steps (at t=1000 min) in the vapour and liquid flow. The responses are completely different in the two operating regimes. Note the sign reversal in the gain, also the longer response time for the high purity regime. This already suggests, that a linear controller would have to be tuned quite *sluggish* if it is to be used in the whole operating region.

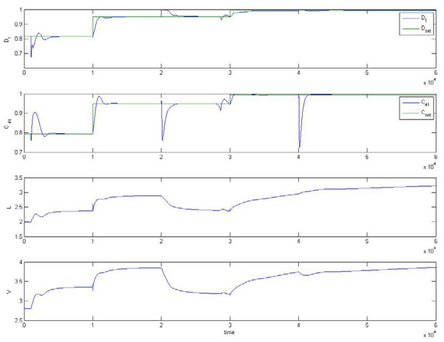

Fig. 6. Performance of the coupled PI control for setpoint changes and various disturbances using coupled PID control. Disturbances in feeds A and B occurred at times 1000, 20000 and 40000 minutes (+20%, -20%, -20% disturbance in the nominal flow).

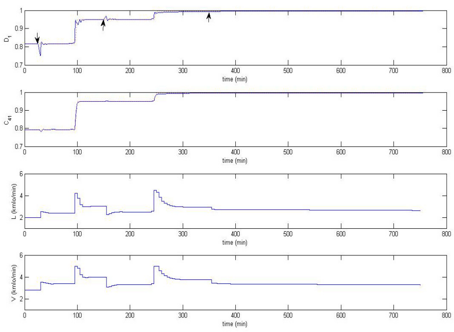

Fig. 7. NMPC performance for setpoint change from low purity to high purity performed in two steps. Arrows indicate unmeasured disturbances in the flow rate for feeds A and B: +20%, nominal, -20%.

4. Comparative simulation of coupled PI, LMPC and NMPC of the system

Different controller and control structures have been tested. Among them, decentralized PID, coupled PID, linear and nonlinear model predictive control. The decentralized PID couldn't cope with large setpoint changes and any disturbances in the high purity region. The PID-like control structure was based on open-loop analysis, RGA calculations and trial and error simulations (intuition) with the nonlinear model. The controller parameter found by considerations of a linear model (Taylor approximation around a steady state) failed to stabilize the system over the whole operating regime. Since we want to operate the column under different conditions, we have analysed two different steady states: one at low product purity (0.8, 0.8) and one at high product purity (0.99, 0.99). Linear models were derived by first order power series expansion and controllability analysis performed using RGA. The values of the entries in the RGA were quite large and negative at frequency zero (steady state), indicating difficult control problem. In addition, we observed sign reversal and inverse response. For systems with negative entries in the RGA it is not recommended to choose diagonal PID, since the system might be unstable if a loop becomes open (e.g. due to saturation). Interaction is taken into account using a coupled PID structure. Problems due to saturation were handled by considering anti-windup structure and less aggressive tuning. If the controller is tuned more aggressive, problems with saturations are more pronounced, and for different cases (e.g. large disturbances or setpoint changes), the controller fails. The control performance of the best PI structure and tuning (coupled with anti-windup) is shown on Figure 6. The closed-loop response is very slow, however a faster controller would lead to a highly oscillating response and even instability of the closed system. LMPC is regarded as more advanced control technique than simple PID's, however for such a highly nonlinear process with a wide operating regime and large disturbances, the LMPC is not able to stabilize the process at the desired setpoint using a single linear model. Multiple linear models, identified in different operating conditions, or a model of the measured disturbances can be employed to enhance the performance, but since the effects are expected to vary over the operating regime, this control technique has been abandoned in favour to the NMPC, where the aforementioned problems are inherently considered in the controller. The NMPC controller uses a multiple shooting optimisation solver called HQP (huge quadratic programming) and an optimization package OptCon. Due to the multiple shooting approach a much larger optimisation problem arises which is, however, highly structured. Therefore sparse techniques can be applied, such that the optimisation problem is solved very fast. The excellent control performance achieved by the NMPC controller is shown in Figure 7. The results evidence that in comparison with a well-tuned linear controller the nonlinear model predictive controller shows a superior performance, by keeping a tight product composition, with respect to setpoint-changes and disturbances.

5. Conclusions

The application of several advanced control approaches have been illustrated in the case of a reactive distillation column. The dynamic and steady state analysis of the open loop system illustrates the difficulty of the control depends on the operating regime. Linear MPC was not able to control the system, whereas a coupled PID gave acceptable results, with very slow response time in the high purity operating zone. A nonlinear MPC based on efficient multiple shooting algorithm and the software package OptCon has been implemented, which showed excellent control performance.

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