STUDIA UBB CHEMIA, LVI, 2, 2011 (p. 5 - 18)

MODEL PREDICTIVE CONTROL OF A DIVIDING-WALL COLUMN

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ABSTRACT. This study explores an optimal model predictive control (MPC) of a dividing-wall column (DWC). Energy minimization is implicitly achieved by using an additional loop controlling the heavy component in the top of the feed side, by using the liquid split as manipulated variable. An industrial case-study is presented based on the separation of the mixture benzene-toluene-xylene (BTX) in a DWC. The results of the dynamic model simulations show that MPC leads to a significant increase in performance – lower overshooting and shorter settling times – as compared to previously reported PID controllers.

Keywords: *DWC, Petlyuk, BTX, MPC, PID, energy efficient control*

INTRODUCTION

Along with reactive distillation, dividing-wall column (DWC) is one of the best examples of process intensification, as it can bring significant reduction in both CapEx and OpEx [1-4]. Classic separations of ternary mixtures developed from direct sequences to thermally coupled columns such as Petlyuk (Figure 1), and the integrated DWC configuration [5-8]. Nonetheless, this process integration leads also to significant changes in the operating mode and ultimately in the controllability of the system [9-12].

In the past decades, the advanced process control received considerable attention in both academia and industry [13-18]. While advanced control strategies made the nonlinear process control more practical, there is still a considerable gap between the control theory and the industrial practice. It is frustrating for the control theory community that elegant and comprehensive frameworks for system analysis and design are rarely implemented in the chemical industry that still applies the well-known PID.

While a variety of controllers are used for binary distillation columns, only several control structures were studied for DWC. In most cases, PID loops within a multi-loop framework were used to steer the system to the desired steady state and reach the goals of dynamic optimization [19-25].

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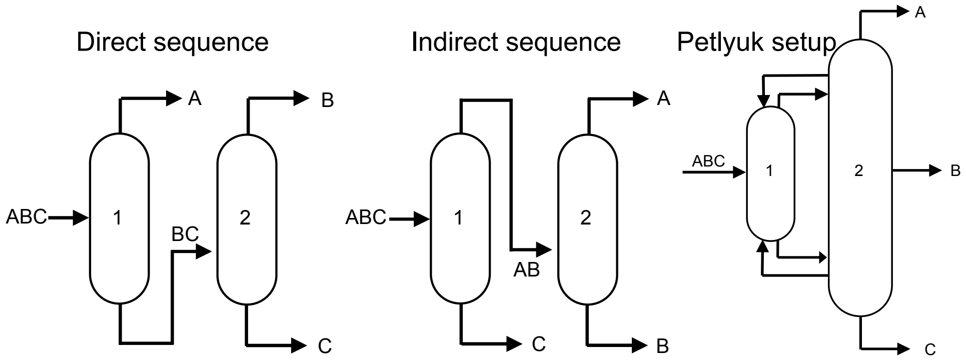

Figure 1. Separation of a ternary mixture via direct and indirect distillation sequences and Petlyuk configuration – thermodynamic equivalent of DWC.

Despite of the complex design and controllability issues, the use of advanced controllers in case of DWC is even more limited. Woinaroschy and Isopescu [26] showed the ability of iterative dynamic programming to solve time optimal control of DWC. Recently, Diggelen et al. [12] published a comparison study of various control structures based on PID loops versus more advanced controllers including LQG/LQR, GMC and high order controllers obtained by H_∞ and μ-synthesis – but no optimal energy control was used. The LQG with integral action and reference inputs was found to deliver the best control performance. When the liquid split is manipulated to achieve minimal energy requirements, the DB/LSV structure was reported as the most effective multi-loop PID control strategy [25].

In few DWC studies reported, MPC outperformed PID while taking into account simultaneously a larger number of manipulated variables [27-29]. Adrian et al. [27] used a black box approach using commercial software was applied in the identification of prediction model and development of the controller, which restricts the understanding to a larger extent.

All these studies investigate different systems and types of disturbances and hence a common conclusion to identify the best controller cannot be withdrawn. In this work we propose an advanced control strategy based on MPC. The control scheme is enhanced by adding an extra loop controlling the heavy component in the top of the feed side, by using the liquid split as manipulated variable, thus implicitly achieving energy minimization. To allow a fair comparison with previously published work, this study considers as industrial case-study the ternary separation of benzene-toluene-xylene (BTX) in a DWC. The results show that MPC leads to a significant increase in performance, as compared to conventional PID controllers within a multi-loop framework. Moreover, the dynamic optimization employed by MPC allows the operation of DWC with minimum energy requirements.

PROBLEM STATEMENT

Following the brief literature review, it is clear that due efforts are placed into developing reliable control strategies for DWC [24]. As the distillation process is a multivariable process, this leads to a multivariable control problem. Due to its very well-known benefits [14-16], Model Predictive Control is a worthwhile option to control in an optimal way a multivariate, nonlinear and constrained process such as DWC. However, up to this date and to the best of our knowledge, the control of DWC using MPC has been studied only by Adrian et al., but only to a certain degree [27]. Moreover, their results do now allow a fair comparison with other ternary separation systems previously reported in literature.

Therefore, there is a need to further investigate the applicability of MPC to DWC. In this study, we consider an industrially relevant ternary separation system (benzene-toluene-xylene, BTX) and compare the MPC performance with the best multi-loop PID control strategy reported. The internal prediction model used by the MPC in this work is derived from the linearization of the nonlinear distillation model, and not from step-response experiments. Such method is more accurate as the resulting first-principle linear model represents all the states, just as the nonlinear model, and it is not limited to the range of the identification experiments.

All the control strategies are enhanced by adding an extra loop control aimed to implicitly minimize the energy requirements by caring out the dynamic optimization. The goal is to maintain the product purities at their given set point, even in the presence of disturbances, while preserving the minimum energy requirements. It is very important for a distillation column to handle the disturbances in the feed, as its flow rate and composition depends heavily on the up-stream process. The column must also meet the required product purities in order to comply with the on-spec targets. For that reason, we based our investigation on the criteria of disturbance rejection in the feed flow rate and composition, as well as set point tracking of the product purities.

MODEL PREDICTIVE CONTROL

MPC is an optimization-based multivariable control technique using (non-)linear process models for the prediction of the process outputs. The schematic representation of MPC is best shown in Figure 2. At each sampling time the model is updated on the basis of new measurements and state variable estimates. Then the open-loop optimal manipulated variable moves are calculated over a finite prediction horizon with respect to some optimization function (e.g. cost, energy), and the manipulated variables for the subsequent prediction horizon are implemented. Then the prediction horizon into the future and the previous steps are repeated. [14-16].

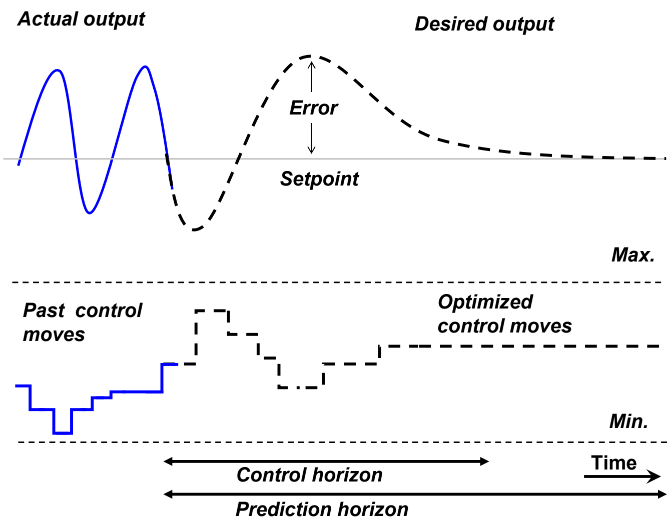

Figure 2. Schematic representation of the Model Predictive Control (MPC)

RESULTS AND DISCUSSION

The dynamic nonlinear model of the column was described in more detail in a previous study by Diggelen et al., dealing with the comparison of control strategies for DWC [12]. Due to the assumptions made, the model is relatively simple but it does capture all the essential elements required to describe and control the DWC system. The following key assumptions were used: 1. constant pressure, 2. constant relative volatility, 3. neglected energy balances, and 4. linear liquid dynamics. The full dynamic model was successfully implemented in Mathworks Matlab and Simulink® [30, 31].

Figure 3 (left) illustrates the modeled DWC, consisting of 6 sections of 8 stages each. The feed stream consisting of benzene-toluene-xylene (noted here as ABC for convenience) is fed into the prefractionator side (feed side of the DWC), between section 1 and 2. Benzene is obtained as top distillate, xylene as bottom product, while toluene is withdrawn as side stream of the column (product side of the DWC, between sections 4 and 5).

The selection of the property model is crucial in any simulation – an issue already recognized in the world of chemical processes modeling by the axiom "*garbage in, garbage out"* meaning that the simulation results have the same quality as the input data and parameters [32]. For the BTX system considered in this work, several reliable property models are available, such as NRTL or UNIQUAC. Figure 3 (right) provides the composition profile inside the DWC by means of a ternary diagram. The bottom, side and top product are close to the left, top and right corners, respectively. For meaningful dynamic responses, the steady state purity of all products is considered to be 97%.

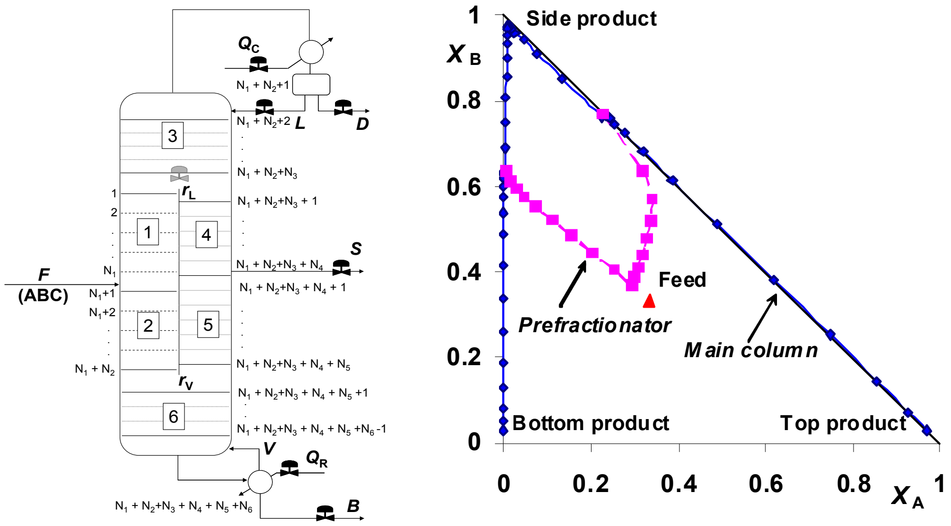

Figure 3. Schematics of the simulated DWC: 6 sections of 8 stages each (left). Composition profile inside DWC, as ternary diagram (right)

In case of DWC, two multi loops are needed to stabilize the column, and another three to maintain the set points specifying the product purities. Based on the results of previous studies [12, 25] – which showed that the DB/LSV structure performed best as compared to all other PID structures – we consider in this work only the best PID configuration as reference case. In this configuration (DB/LSV), the liquid levels in the reflux tank and reboiler are maintained by means of D (distillate) and B (bottoms flow rate) whereas the product compositions are maintained by manipulating L (liquid reflux), S (side product flowrate) and V (vapor boil-up) respectively [12].

An additional optimization loop is added to manipulate the liquid split (r_L) in order to control the heavy component composition in the top of fractionators (Y_{C_PF1}), and implicitly achieving minimization of the energy requirements. Several studies demonstrated that implicit optimization of the energy usage is achieved by controlling the heavy impurity at the top of the prefractionator [23, 25]. The MPC controller was designed to handle a 10×6 system of inputs and outputs. The inputs include the controlled variables – mole fraction of A in distillate (x_A), B in the side stream (x_B), C in the bottom product (x_C) and C in the top of the prefractionator (Y_{C_PF1}), liquid holdups in the reflux tank (H_t), reboiler (H_r) and the disturbance variables. The disturbance variables defines the feed by feed flowrate (F), compositions of benzene ($x_{F,A}$) and toluene ($x_{F,B}$) in the feed and heat quality (q_F). The outputs include the manipulated variables – D, B, L, S, V and r_L. Figure 4 shows the DB/LSV scheme and the MPC alternative proposed in this work.

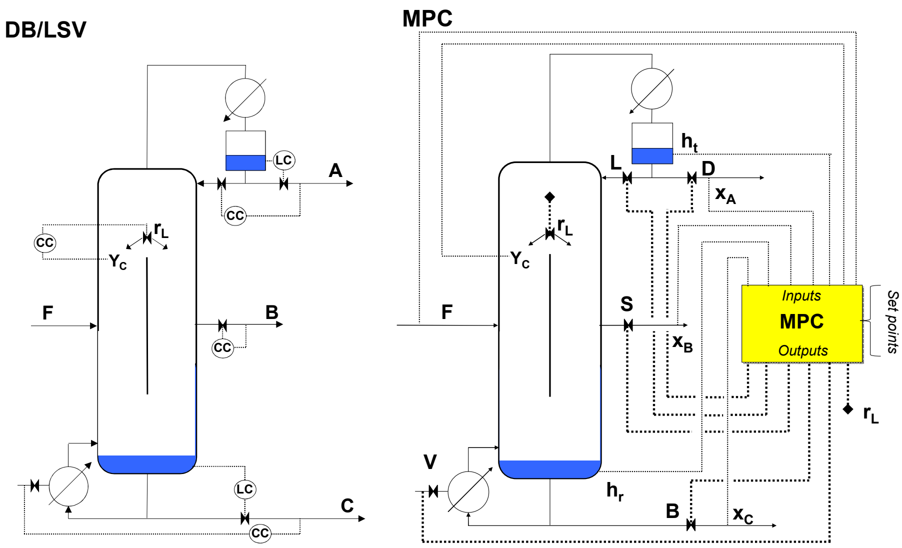

Figure 4. Control structures based on PID loops (left) and MPC (right)

The full nonlinear process model was linearized in order to obtain the continuous state space model. The resulting state space model has 156 states (96 compositions for A and B, C being calculated as the remaining difference; 8 compositions of A and B in the vapor and liquid splitters, reflux tank and reboiler; 48 liquid hold ups on trays; 4 hold ups for the vapor and liquid splitters, reflux tank and reboiler), 10 inputs and 6 outputs representing the controlled and manipulated variables chosen. Prior to the deployment of the controller, the best practices of control engineering require to check the quality of the linearization In order to avoid any mismatch between the models representing the plant and controller. Such a mismatch may cause serious instability in the operation of the plant.

Consequently, the quality of the linearization was evaluated by performing a closed loop simulations while exerting disturbances. The feed flowrate (F) was subjected to a step change of +10% compared to its nominal value, and the deviations in the product compositions were analyzed. This disturbance and the test variables were selected due to its dominant first-order time constant. Thus it serves as a worst case scenario. To validate the linearization in a closed loop, only the level controllers were used to control the inventory in the column and the rest of the multi-loops were kept open. As a result, Figure 5 confirms that a close match exist between the nonlinear and linearized model used in this study. Remarkably, only minor differences can be observed between the linear and the non-linear models.

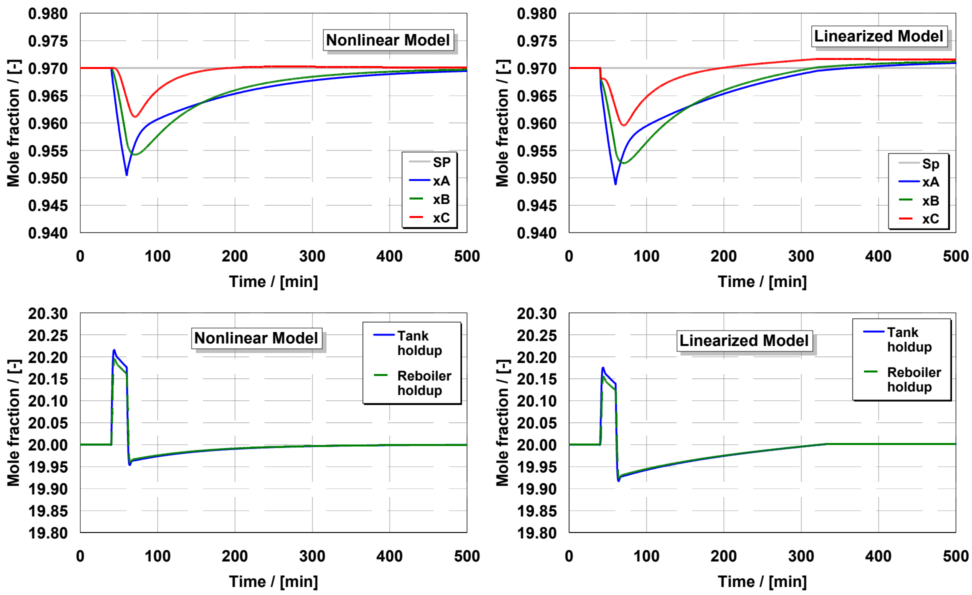

Figure 5. Comparison between nonlinear and linearized system: dynamic response after a step change of +10% in feed flowrate for 20 min.

The PID control loops were tuned by the direct synthesis method proposed by Luyben [13]. Table 1 shows the tuning parameters of the PID controller. As fairly accurate evaluations of the process time constants τ, 20, 40 and 60 min were used, respectively. For the level controllers, a larger reset time τ_i = 100 min was chosen as no tight control is required.

As no reliable design rules are available in the literature for tuning MPC controllers [14-16], heuristics combined with a trial and error method were used – dependent on a number of factors related to the controller and the process: prediction (p) & control (m) horizon, input (w_u) & ouput (w_y) weights, sampling time (Δk), operating constraints on inputs and outputs as well as the rate of change rate of inputs (Δu). Table 2 shows the tuning parameters for the MPC control structure proposed here (Figure 4, right).

Table 1. Tuning parameters of the PID controllers of the DB/LSV structure

DB/LSV	P (%/%)	I (min)	D (min)	Control direction
$x_A \rightarrow L$	3	40	0	–
$x_B \rightarrow S$	3	20	0	+
$x_C \rightarrow V$	3	40	0	–
$y_C \rightarrow r_L$	1	20	0	+
Tank level → D	1	100	0	+
Reboiler level → B	1	100	0	+

Table 2. Tuning parameters of the MPC controller

	Manipulated variables						Controlled variables						
Weights	D	B	L	S	V	r_L	x_A x_B x_C	y_{C_PF1}	h_t	h_r	F	$x_{F,A}$ $x_{F,B}$	q_F
w^y	1	0.8	0.3	0.9	0.3	0.1	–	–	–		–	–	–
w^y	–	–	–	–	–	–	1	1	0.3	0.5	1	1	0.5
$w^{\Delta u}$			0.2							0.1			
Constraints			[kmol/min]			[-]	[-]		[m]	[kmol/min]		[-]	[-]
(±)	0.2	0.2	0.3	0.2	0.3	0.15	0.02	0.005	0.1	0.1	0.1	0.02	0.5

Prediction horizon *p*	Control horizon *m*	Sampling time Δk
30	5	3 min

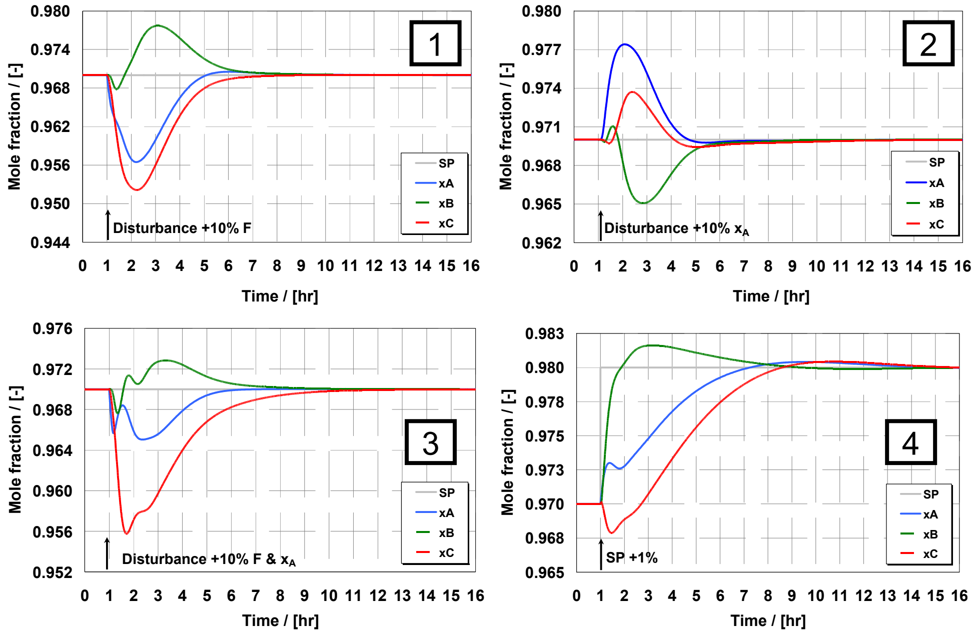

Figure 6. Dynamic response of DB/LSV PID control structure, at a persistent disturbance of +10% in the feed flow rate (1), +10% x_A in the feed composition (2), +10% in both feed flow rate and composition (3) and +1% increase of setpoint (4)

In the dynamic simulations performed in this study, the purity set points (SP) are 97% for all product specifications. Persistent disturbances of +10% in the feed flow rate (F) and +10% in the feed composition (x_A) were exerted either alone or simultaneously for the dynamic scenarios. The ability of the controllers to track the set point is also tested by changing all purity set points from 0.97 to 0.98. The chosen disturbances are either measured (MPC), or unmeasured (PID) in which case the controllers are relying only on the feedback action. Such disturbances and set point changes resemble the most common transitory regimes arising in practice, due to planned changes or unexpected disturbances in actual operation.

As illustrated by the next figures, the mole fractions of components A in the top distillate (x_A), B in the side stream (x_B) and C in the bottom product (x_C) are returning to their set point (SP) within reasonable short settling times. Figure 6 show that the control structure DV/LSB exhibits overshooting mainly in the toluene composition.

The dynamic response of the MPC controller is shown in Figure 7, being characterized by low overshooting and short settling times. The MPC steer the system to the given set points under the specified constrains unlike the PID controller that cannot be directly subjected to constrains.

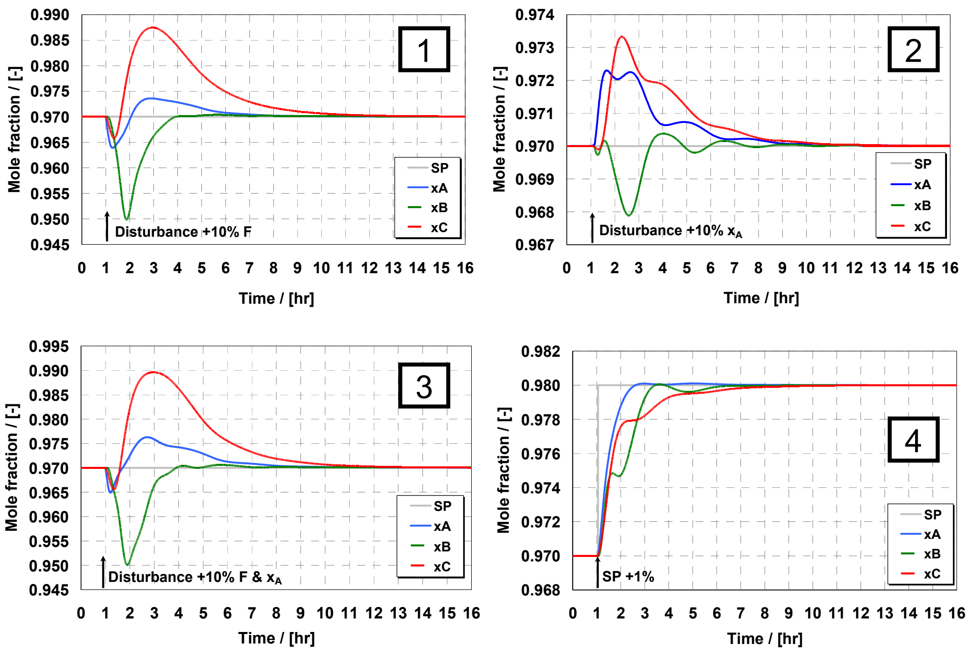

Figure 7. Dynamic response of MPC control structure, at a persistent disturbance of +10% in the feed flow rate (1), +10% x_A in the feed composition (2), +10% in both feed flow rate and composition (3) and +1% increase of setpoint (4)

In case of +10% F and +10% x_A disturbances illustrated by Figure 7, it can be observed that the composition profiles of MPC are identical in nature. However, these profiles are inverted for the PID controller in case of the same disturbances as seen in Figure 6. This demonstrates the ability of MPC to deliver a consistent performance. Such consistency would be valuable in actual plant operation to accommodate the resultant changes and their retentive effects over time. For example, in any case of the disturbances, one can expect the average value of the purity of toluene to be reduced over time if the MPC is in action.

Both PID and MPC control structures exhibit short settling time of less than 10 hours for all components. The performance of these controllers is compared in Figure 8, in terms of the integral absolute error (IAE) that conveniently accounts for both overshooting and settling times. IAE is defined here as the integral of the SP error (e) over the settling time period (t). Accordingly, MPC is the most stable control structure with low values of IAE. Moreover, the performance of MPC for set point tracking is excellent as clearly demonstrated by Figure 7.

This study proved that MPC based on linear prediction model is very well able to control the highly nonlinear DWC process. Although the application of nonlinear based controllers is appealing, only a minor improvement in the performance is expected because of the precise linearization of the nonlinear model. With today's powerful computational infrastructure and accurate linearization methods, a linearized model of the process can be updated on-line in the MPC controller's hardware. Any large changes in the operating points and capacity will require the re-linearization around the new nominal conditions in order to ensure the robustness of the controller. By approximating a nonlinear system as a family of affine systems, the analysis of the nonlinear system can be transformed into an analysis of several linear systems.

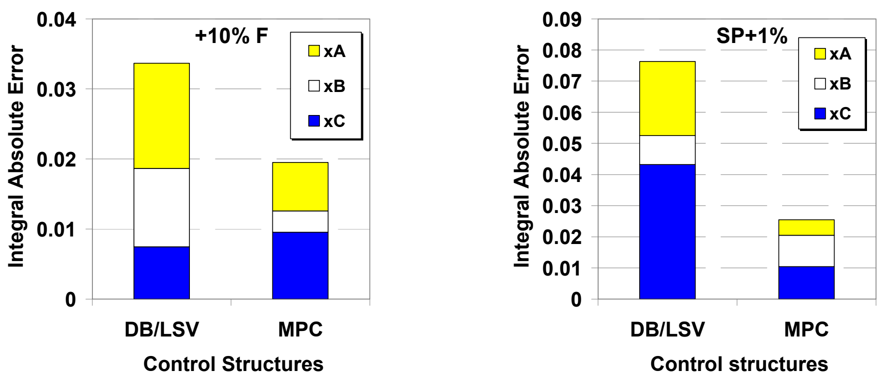

Figure 8. Comparison of controllers performance in terms of integral absolute error (IEA), at a persistent disturbance of +10% x_A in the feed composition (left), and +1% increase of the setpoint (right)

CONCLUSIONS

The full-size nonlinear model used for a DWC in this work, is truly representative of industrial applications. The quality of the linearized model used for the predictions inside MPC is derived from and tested against the full nonlinear model. The variables were selected to achieve the aim of regulatory and inventory control in the column, at the same time minimizing the energy requirements in a very simple, yet practical way. The optimal energy control is based on a simple strategy to control the heavy component composition at the top of the prefractionator side of the DWC by manipulating the liquid split. The performance of the MPC was effectively evaluated against a conventional PID control structure (DB/LSV) that was previously reported to be the best performing in DWC operation.

MPC delivers an outstanding overall performance in case of different industrially relevant disturbances and set point tracking. The integral absolute error (IEA) measured for MPC performance is the lowest. The major reason for this excellent feature of MPC is its ability to act simultaneously and consistently on all the manipulated variables when the disturbances are exerted. The consistent performance delivered by MPC can be very useful in actual plant operation to accommodate the resultant changes over time.

This study proves the ability of linear MPC to control a non-minimal phase and nonlinear process, such as DWC. The significant match in the open loop response of the linearized and nonlinear model suggests that nonlinear MPC is not expected to deliver a significantly better performance. The functionality of the proposed MPC control scheme demonstrated in this study provides an excellent platform for its easy transfer to other DWC applications, such as ternary separations.

ACKNOWLEDGMENTS

We thank Ben H. L. Betlem (University of Twente, NL) for the very constructive discussions. The financial support given by AkzoNobel to Rohit Rewagad, University of Twente, during his MSc internship is also gratefully acknowledged.

NOTATION

ABC	– Ternary mixture of components A, B and C
BTX	– Benzene-toluene-xylene
B	– Bottoms product
D	– Distillate stream
DWC	– Dividing-wall column
F	– Feed stream
H_T	– Reflux tank level
H_R	– Reboiler tank level

IEA	– Integral absolute error
L	– Liquid flow
MPC	– Model predictive control
m	– Control horizon
N_j	– Tray number j
Q_C	– Condenser duty
Q_R	– Reboiler duty
PF	– Pre-fractionator
PID	– Proportional-integral-derivative controller
p	– Prediction horizon
R	– Reflux rate
r_L	– Liquid split
r_V	– Vapor split
S	– Side stream
V	– Vapor flow
w^v	– Weight of variable *v*
x_i	– Molar fraction of component *i* in liquid phase
y_i	– Molar fraction of component *i* in vapor phase
Δk	– Sampling time
τ	– Time constant

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