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Optimal Operation and Stabilising Control of the Concentric Heat-Integrated Distillation Column

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Abstract: A systematic control structure design method is applied on the concentric heat-integrated distillation column (HIDiC) separating benzene and toluene. A degrees of freedom analysis is provided for identifying potential manipulated and controlled variables. Optimal operation is mapped and active constraints are identified for constructing the supervisory control layer. The fundamental problem of obtaining a stabilising control structure is addressed resulting in the regulatory control layer design. A supervisory control layer is devised and combined with the regulatory control layer. The control structure is finally evaluated by dynamic simulation for proving an acceptable performance.

1. INTRODUCTION

In the heat-integrated distillation column (HIDiC), gradual condensation occurs along the rectifying section and gradual boil-up occurs along the stripping section as heat is exchanged between the sections. This can be realised by operating the rectifying section at a higher pressure by introducing a compression step above the feed stage. One proposal for realisation of the HIDiC arrangement is a concentric HIDiC (Govind, 1987), in which the high-pressure rectifying section is placed within the column shell constituting the low-pressure stripping section (see Figure 1). Each tray are heat-integrated in the same vertical position (e.g. #2 and #33) such that heat is transferred from the inner rectifying section to the outer stripping section. Due to the gradual condensation and boil-up, the column sections change cross sectional areas along their heights as indicated in the figure.

The HIDiC is a result of process intensification (PI) of a conventional distillation column by combining two phenomena (heat and mass transfer) in the column itself. The general operation implications from PI are (Nikačevic et al., 2012) (i) increased operational complexity because of stronger interaction between inputs, (ii) fewer degrees of freedom, (iii) increased sensitivity to disturbances, and (iv) narrower operating windows. Some of the more established distillation column configurations, on which PI has been applied, are the dividing-wall column (DWC) and the reactive distillation column (RDC). In the DWC, more degrees of freedom (DOFs) arise while strong input-output interactions result, which leads to oscillating closed-loop responses for decentralised control (Hernández and Chinea-Herranz, 2012). The same might apply to the HIDiC due to its highly interactive nature.

Many authors consider only dual composition control schemes with dynamic HIDiC models that assume constant pressures (Nakaiwa et al., 2003; Liu and Qian, 2000; Huang et al., 2007). Only few authors consider pressure dynamics for control (e.g. Ho et al. (2009)), despite the large degree of interaction between the column pressures and the separation performance in the HIDiC. This paper addresses the design of a decentralised control structure, using a systematic approach (Skogestad, 2004) on the separation of benzene/toluene by distillation. In the process of designing the control structure, optimal and stable operation is analysed.

2. TOOLS AND METHODS

2.1 Distillation Column Model

A first-principle model of a HIDiC based on the work of Bisgaard et al. (2015) is implemented in MATLAB for simulation. The model consists of dynamic mass and energy balances, and takes into account temperature dependency of physical properties, tray pressure drops, time-varying tray pressures, and liquid and vapour hydraulics. In the following sections, relevant parts of the model are outlined, since these determines the dynamic performance of the concentric HIDiC.
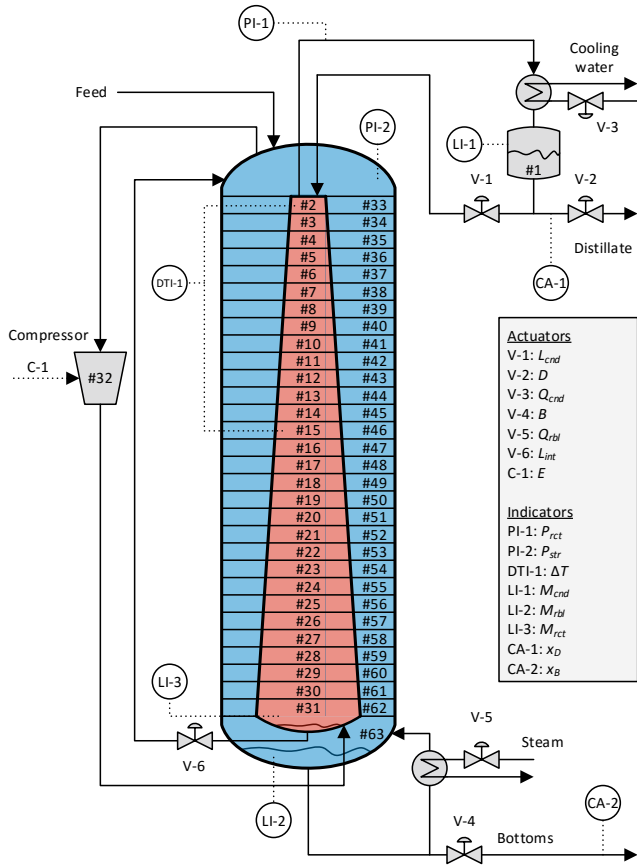
Fig. 1. Concentric heat-integrated distillation column for separating benzene/toluene.

Liquid and Vapour Hydraulics. The liquid flow rate is described by the Francis weir formula (Wittgens and Skogestad, 2000):

$$L_i = \begin{cases} C_i^L \rho_i^L H_{oW,i}^{3/2}/MW_i^L, & H_{oW,i} > 0 \\ 0, & H_{oW,i} \leq 0 \end{cases} \quad (1)$$

$$H_{oW,i} = H_{cl,i} - H_W \quad (2)$$

$$h_{cl,i} = M_{T,i} MW_i^L / \left(\rho_i^L A_{a,i} \right) \quad (3)$$

where

C_i^L = constant depending on the liquid loading of tray i [m$^{-0.5}$s^{-1}]
ρ_i^L = liquid phase density [kg m^3]
MW_i^L = molecular weight of the liquid [kg mol^{-1}]
H_{oW},i = liquid height above the weir [m]
$A_{a,i}$ = active area of stage i [m^2]
H_W = weir height [m]
$H_{cl,i}$ = clear liquid height [m]
$M_{T,i}$ = Total tray liquid holdup [mol]

Note that both $A_{a,i}$ and H_W are dimensional parameters of the column internals. C_i^L is calculated from Eq. (1) from the steady state liquid flow profile.

The vapour flow through perforated plates can be described as done by Kolodzie and van Winkle (1957). In this work, the volumetric flow rate is simplified to be proportional to the square root of the pressure gradient:

$$V_i = C_i^V (\rho_i^V)^{0.5} (P_i - P_{i-1})^{0.5} / MW_i^V \quad (4)$$

where

C_i^V = constant depending on the vapour loading of the individual trays [m^2]

Internal Heat Integration. The internal heat transfer rate is given by

$$q_s = UA(T_r - T_s) \quad (5)$$
$$q_r = -q_s$$

where

U = overall heat transfer coefficient [kW m^{-2} K^{-1}]
A = heat transfer area (assumed constant on every tray) [m^2]
T = temperature of a tray in the rectifying section (r) or the stripping section (s) [K]

Applying Eq. (5) on the concentric HIDiC (Figure 1) gives $q_{33} = UA(T_2 - T_{33})$ and $q_2 = -q_{33}$ and so on.

2.2 Control Structure Design Procedure

The control structure design procedure is outlined by Larsson and Skogestad (2000) and Skogestad (2004) and rules for this method are collected by Minasidis et al. (2015). The procedure deals with the structural decisions that are required for the controller design. This includes the selection of manipulated variables (MVs), the selection of controlled variables (CVs), the selection of measurements for control, and the selection of their interconnection, which is termed the control configuration. The procedure consists of systematic steps, which will be applied on the concentric HIDiC. The procedure can be divided in two major steps: The top-down analysis (steady state considerations) and bottom-up (dynamic considerations).

3. SEPARATION OF BENZENE/TOLUENE

3.1 System Description

Consider the separation of 83.3 mol s^{-1} of an equimolar, saturated liquid mixture of benzene/toluene by distillation. It is desired to obtain benzene (in distillate) and toluene (in bottoms) with purities of minimum 99%. A HIDiC design with 30 trays in both sections and all being heat-integrated in the same vertical height as illustrated in Figure 1. A heat exchange area of 15 m^2 per heat-integrated pair is used, which is assumed to be achieved by installing heat transfer panels (de Rijke, 2007). A conservative overall heat transfer coefficient of 0.60 kW m^{-2} K^{-1} is employed, giving $UA = 9.0$ kW K^{-1} in Eq. (5). Conventional column sizing has been employed, leading to a gradually increasing cross sectional area in the rectifying section from the top, while the stripping section cross sectional area is gradually decreasing. The combined cross sectional area (i.e. the outer column diameter) is constant. As a result, the nominal tray liquid holdups vary along the column as illustrated in Figure 2. This liquid holdup profile strongly deviate from conventional distillation columns, in which the holdup usually is approximately constant. The column dimensional parameters are provided in Table 1, while the physical parameters are accessible in the DIPPR database (AIChE, 2014). The constants C_i^L and C_i^V are calculated based on the nominal steady state liquid and
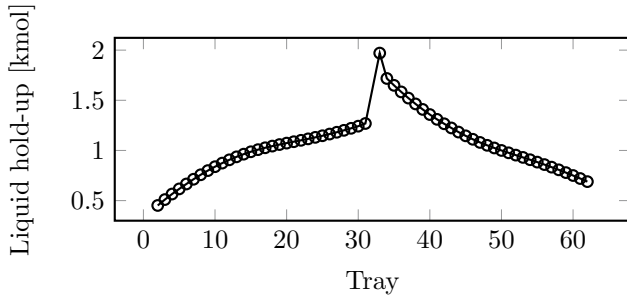
Fig. 2. Nominal tray holdup profile.

Table 1. Model parameters.

Parameter	Value
Tray pressure drop*	0.0070 bar
Liquid height over weir*	12.5 mm
Tray type	Sieve
Weir height	50 mm
Internal heat transfer area per tray	15 m^2
Downcomer area per tray area	0.07
Liquid holdup time in condenser and reboiler	300 s

*Used for estimating constants C_i^L and C_i^V in Eq. (1) and (4)

vapour flow rate profiles, the specified tray pressure drops, and the liquid heights over the weirs (Table 1). Ideal liquid and vapour phases are assumed for the vapour-liquid equilibrium relations. In addition to the concentric HIDiC, a conventional distillation column (CDiC) with the same specifications and parameters is considered in order to compare the optimal performance of the HIDiC.

3.2 Top-down Analysis

Degrees of Freedom Analysis. The operational degrees of freedom (actuators) are illustrated in Figure 1 with feed flow rate given. Seven steady state degrees of freedom correspond to the seven operational degrees of freedom. From the seven steady state degrees of freedom, the three holdups M_{cnd}, M_{rbl}, and M_{rct} have no impact on the steady state operation (and on the cost function). Thus, four variables are available for optimisation.

Definition of Optimal Operation. Assuming an electricity price of 0.14 \$ kWh^{-1}, a pressure dependent steam price starting at 22.39 ·10^{-3}\$ kg^{-1} for 2 bar steam, a cooling water price of 0.080 · 10^{-3} \$ kg^{-1}, a distillate (distillate) price of 1.04 \$ kg^{-1} ICIS (2015), a bottoms (toluene) price of 0.853 \$ kg^{-1} ICIS (2015), and a feed price of 0.50 \$ kg^{-1}, the objective function (J) becomes

$$\min J = [0.50 m_F - 1.04 m_D - 0.853 m_B$$
$$+ \left(1.99 + 20.4 (P_{steam} - 1.01325)^{0.05}\right) m_{steam}$$
$$+ 0.080 \cdot 10^{-3} m_{cw} + 3.89 \cdot 10^{-5} E] / m_F \quad (6)$$
$$s.t. \; 0.99 \leq x_D$$
$$0.99 \leq 1 - x_B$$
$$E \leq 500 \text{kW}$$
$$1.013 \, \text{bar} \leq P_i \leq 6.0 \, \text{bar}$$
$$0.01 F_0 \leq L_i \leq 200 \; \text{mol s}^{-1}$$
$$0.01 F_0 \leq V_i \leq 150 \; \text{mol s}^{-1}$$

where

Table 2. Nominal, optimal operation points.

			CDiC	HIDiC
Design degrees of freedom	P_{rct}	bar	1.01	1.01
	CR	-	-	2.28
	L_{cnd}	mol s^{-1}	60.25	0.8333
	Q_{rbl}	kW	3329	1194
Cost function	J	\$ kg^{-1}	-0.4323	-0.4345
Constraints (bold: active)	x_D	-	**0.9900**	**0.9900**
	$1 - x_B$	-	0.9997	0.9915
	min L_i	mol s^{-1}	55.76	**0.8333**
	max L_i	mol s^{-1}	143.0	137.3
	min V_i	mol s^{-1}	97.84	36.0
	max V_i	mol s^{-1}	102.3	111.8
	min P_i	bar	**1.01**	**1.01**
	max P_i	bar	1.45	2.31
	E	kW	-	348.7
	$T_{cnd} - T_{cw,out}$	K	45.48	71.10

$J =$ net cost per feed flow rate [\$ kg^{-1}]
$m =$ mass flow rate [kg s^{-1}]
$P_{steam} =$ steam pressure (minimum 2 bar) [bar]

The four optimisation DOFs are L_{cnd}, Q_{rbl}, P_{str}, and P_{rct}. The expected disturbance range in terms of nominal values are for the feed flow rate $0.8 F_0 \leq F \leq 1.4 F_0$ and benzene feed composition $0.8 z_0 \leq z \leq 1.2 z_0$.

Optimal Operation (Active Constraints). The solver "fmincon" in MATLAB is used for the optimisation using the sequential quadratic programming algorithm. The solution to the optimisation problem (Eq. (6)) is listed in Table 2. For comparison, the optimal operating point of a conventional distillation column (CDiC) is presented. The cost function is lower for the HIDiC, which illustrates its capability of reducing the operating cost by employing internal heat integration. Furthermore, negative objective functions are obtained, which means that profits are achieved. The nominal solution of the HIDiC has three active constraints involving x_D, P_{str}, and L_{cnd} as indicated with boldface numbers (Table 2). Hence, (free DOFs)=4-3=1. In this case, one variable for self-optimising control can be used, since the active constraints must be controlled for optimum economic performance. The loss, of maintaining the bottom composition (x_B) or the compression ratio (CR) constant, are evaluated. It is found that x_B should be used as the remaining primary controlled variable since the economic loss is the least when keeping x_B constant. Thus, the primary controlled variables ($\mathbf{CV}_1$) are $\mathbf{u_{CV}} = [P_{str}, x_D, x_B, L_{cnd}]$. This result shows that the reflux flow rate (L_{cnd}) must be kept at its minimum and can, thus, not be used for temperature or composition control in the rectifying section, which typically is the case in conventional distillation. The minimum value of L_{cnd} is chosen as a safety (back-off) value such that the upper trays do not dry out.

Optimal Operation. The active constraint regions are identified by the brute-force method for various disturbances. A grid of 30 nodes is used to represent the disturbance space. For each node, an optimisation is carried out and the obtained active constraint regions and objective function contours are illustrated in Figure 3.
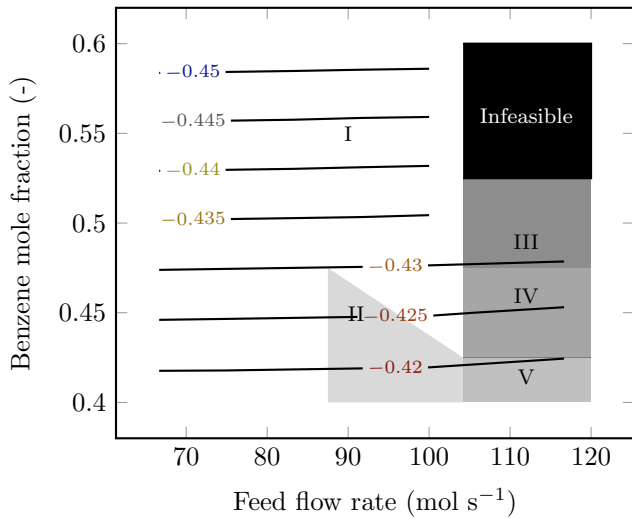
Fig. 3. Active constraint regions: I: x_D, P_{min}, L_{min}, II:$x_D, x_B, P_{min}, L_{min}$, III: $x_D, x_B, P_{min}, V_{max}$, IV: $x_D, x_B, V_{max}, E_{max}$, V: $x_D, x_B, L_{max}, E_{max}$.

3.3 Bottom-up Design

Design of Regulatory Control Layer. Single-loop controllers are used in the regulatory control layer. The HIDiC has three integrating variables that require control, namely the condenser holdup (M_{cnd}), the reboiler holdup (M_{rbl}) and the rectifying section holdup (M_{rct}). Furthermore, it is generally important to control pressures, as these closely resemble integrating variables. Hence, the rectifying section pressure (P_{rct}) and the stripping section pressure (P_{str}) must be controlled. In addition to these five variables, the temperature profile must be controlled by either controlling a sensitive stage temperature or a sensitive temperature difference in a part of the column (Skogestad, 2007). Due to the nature of the HIDiC, significant pressure variations might occur and thus controlling a temperature difference between two trays in the same section (ΔT) is desired. It is also desired to use the temperature measurement to indirectly control a product purity of the most valuable component. In particular, the mentioned temperature loop is strongly emphasised by Skogestad (2007) as it provides several benefits as e.g. indirect level and composition control and reduces interaction in composition control loops. One relatively insensitive tray temperature (T_2) was selected for providing indirect pressure compensation, while a sensitive tray temperature (T_{15}) was selected such that the resulting temperature difference ($\Delta T = T_2 - T_{15}$) is sensitive to disturbances and input changes. Finally, the six identified secondary controlled variables are

$$\mathbf{y}_2 = [M_{cnd}, M_{rbl}, M_{rct}, P_{rct}, P_{str}, \Delta T]. \tag{7}$$

One of the most important criteria of the regulatory level is that it must be fast. Thus, the "pair close" rule (Minasidis et al., 2015) is essential for designing this control layer. As a result, the rectifying section holdup should be controlled by the intermediate liquid flow rate ($L_{int} \to M_{rct}$). This loop has no impact on the remaining control decisions or the steady state, and it will thus not be considered further. It also follows that the condenser holdup should be controlled by the distillate flow rate ($D \to M_{cnd}$) and the reboiler holdup should be controlled by the bottoms flow

rate ($B \to M_{rbl}$). Steady state relative gain array (RGA) (Bristol, 1966) is used to pair the remaining secondary controlled and manipulated variables. Steady state was ensured after 10 hours when imposed to a +1% step changes in the individual input:

$$\mathbf{G}(s=0) = \begin{bmatrix} \frac{\Delta P_{rct}}{\Delta Q_{cnd}} & \frac{\Delta P_{str}}{\Delta Q_{cnd}} & \frac{\Delta(\Delta T)}{\Delta Q_{cnd}} \\ \frac{\Delta P_{rct}}{\Delta Q_{rbl}} & \frac{\Delta P_{str}}{\Delta Q_{rbl}} & \frac{\Delta(\Delta T)}{\Delta Q_{rbl}} \\ \frac{\Delta P_{rct}}{\Delta E} & \frac{\Delta P_{str}}{\Delta E} & \frac{\Delta(\Delta T)}{\Delta E} \end{bmatrix}$$

$$= 10^{-3} \begin{bmatrix} 4.2653 & 2.1645 & -63.4868 \\ 3.8781 & 1.9449 & 7.4990 \\ 5.2909 & 0.8490 & 2.2554 \end{bmatrix} \Rightarrow \tag{8}$$

$$\mathbf{\Gamma} = \mathbf{G} \otimes (\mathbf{G}^{-1})^T = \begin{bmatrix} -0.0168 & 0.1332 & \mathbf{0.8836} \\ -0.4534 & \mathbf{1.3366} & 0.1168 \\ \mathbf{1.4702} & -0.4698 & -0.0004 \end{bmatrix}$$

Pairing on negative steady state RGA-elements is undesired, while RGA elements of unity are preferred. Thus, it is clear that the pairing should be ($E \to P_{rct}$), ($Q_{cnd} \to \Delta T$) and ($Q_{rbl} \to P_{str}$). With this pairing, RGA elements close to unity are obtained (indicated in boldface numbers in Eq. (8)). Control of the stripping section pressure by the reboiler duty can be realised as follows: When the reboiler duty is reduced below the nominal value by the means of the controller, the net vapour flow rate through the stripping section is reduced due to the fact that the compressor dictates the flow rate of the outlet vapour.

Design of the Supervisory Control Layer. The supervisory layer may use the setpoints to the regulatory layer as degrees of freedom to control the primary (economic) variables. As for the regulatory control layer, single-loop controllers are used for the supervisory control layer, leading to cascade controllers. The primary controlled variables were identified previously. The setpoint of the temperature profile (ΔT) is used to control the distillate composition (x_D), since the distillate contains the more valuable component. Due to the close relation between the section pressures and the product compositions, the stripping section pressure setpoint is used to control the bottom composition (x_B). As the stripping section pressure is a primary controlled variable, an additional control loop is added that controls the setpoint of the stripping section pressure to the optimal value. The final resulting control structure is illustrated in Figure 4.

Controller Tuning and Evaluation. The SIMC tuning (Skogestad, 2003) is adopted for the tuning of the controllers. Only PI-controllers were used in this study. However, some rather complex open-loop responses are observed in the responses of the full-order model (Figure 5), making the tuning of the controllers a challenging task if oscillations are to be avoided. The tuning is carried out sequentially for the loops using the desired closed-loop time constant (τ_c) as the tuning parameter. The tuning sequence is based on the expectation/selection of τ_c such that the fast loops are tuned and closed first. However, the two liquid holdup control loops were closed first (($L_{int} \to M_{rct}$) is assumed ideally controlled). Based on insights in the conventional distillation column dynamics, the tuning sequence was derived for the control structure illustrated in Figure 4. The following sequence was used after the liquid holdup loops were closed: ($Q_{rbl} \to P_{str}$), ($Q_{cnd} \to \Delta T$), ($E \to P_{rct}$), ($\Delta T^{set} \to x_D$), ($P_{str}^{set} \to x_B$),
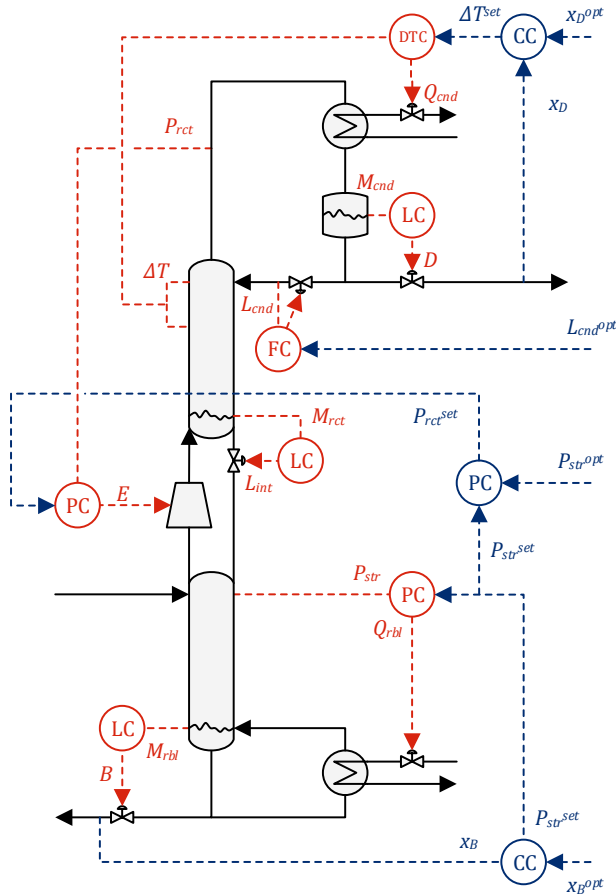
Fig. 4. Control structures for a HIDiC separating benzene/toluene. Red lines represent the regulatory control loops and blue lines represent the supervisory control loops (cascade).

and ($P_{rct}^{set} \to P_{str}^{set}$). Complex dynamic phenomena are observed, including negative and positive zeros, where the latter leads to inverse responses (Figure 5, loop $P_{str}^{set} \to x_B$). These responses are used to identify process transfer functions. The process transfer functions were reduced to first-order transfer functions using Skogestad's "half rule" (Skogestad, 2003). Furthermore, the numerator time constants (if any) were converted into time delays. Model mismatch of the low-order transfer functions are obtained due to the non-linearity of the system. The tuning parameters (τ_c) for the controllers in the regulatory control layer are chosen such that fast control actions are obtained. However, it is undesirable to have fast control action of the compressor, why this is chosen as 60 seconds. The tuning parameters of the controllers in the supervisory control layer are chosen such that loop interactions are avoided. In particular, τ_c of the master control loops (in the case of cascade) were chosen minimum ten times the values of the corresponding slave control loops. The tank holdups act as pure integrators and were allowed to be controlled relatively sluggishly ($\tau_c = 120$s). The values of τ_c for the remaining control loops are listed in Figure 5.

The control structure is evaluated under various disturbance scenarios of which one is illustrated in Figure 6. The illustrated disturbance scenario contains both regulatory and servo responses:

$t \geq 0$ h: $+20\%\ F$
$t \geq 2.5$ h: $+10\%\ z$
$t \geq 5$ h: $L_{cnd}^{set} = 1.6667$ mol s^{-1}
$t \geq 7.5$ h: $x_D^{set} = 0.985$
$t \geq 12.5$ h: $x_B^{set} = 0.01$

All controlled variables are kept close to their setpoints in the simulation (Figure 6). In particular, the secondary controlled variables (ΔT and P_{str}) are following the setpoint trajectories, dictated by the supervisory control layer. As expected, the distillate composition is more tightly controlled than the bottoms composition, since the temperature control loop is located in the same column section of the distillate. In addition, input saturation is observed, and thus, anti-windup is included in the simulation.

4. CONCLUSION

Based on rigorous distillation column simulations of the concentric heat-integrated distillation column (HIDiC) separating a binary mixture of benzene/toluene, the following main conclusions can be extracted:
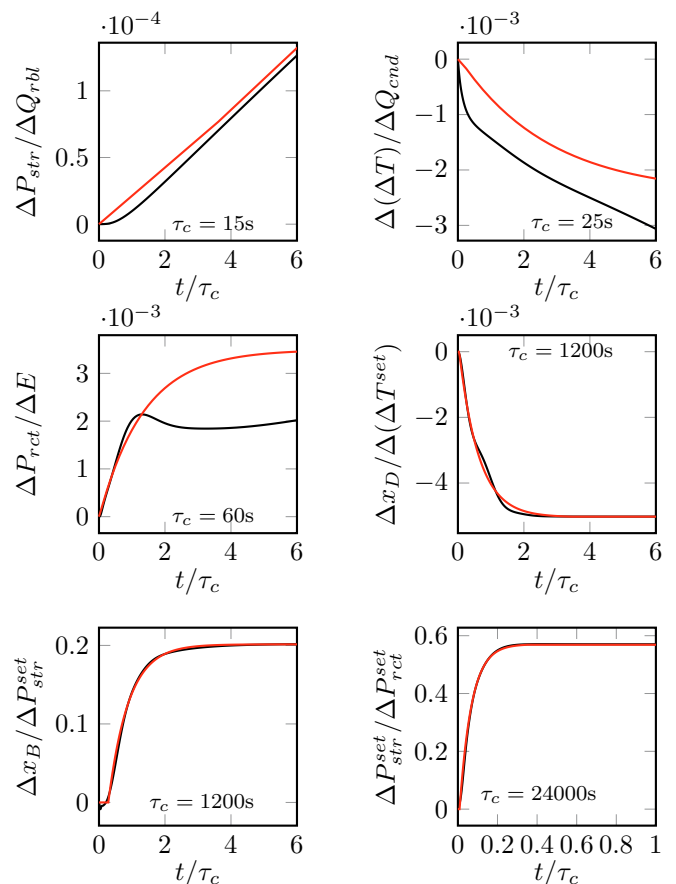

Fig. 5. Dynamic response to $+1\%$ step change and sequential tuning (ordered from top left to bottom right) with previous loops closed. Legend: Full-order model response (——), fitted low-order model response (——).
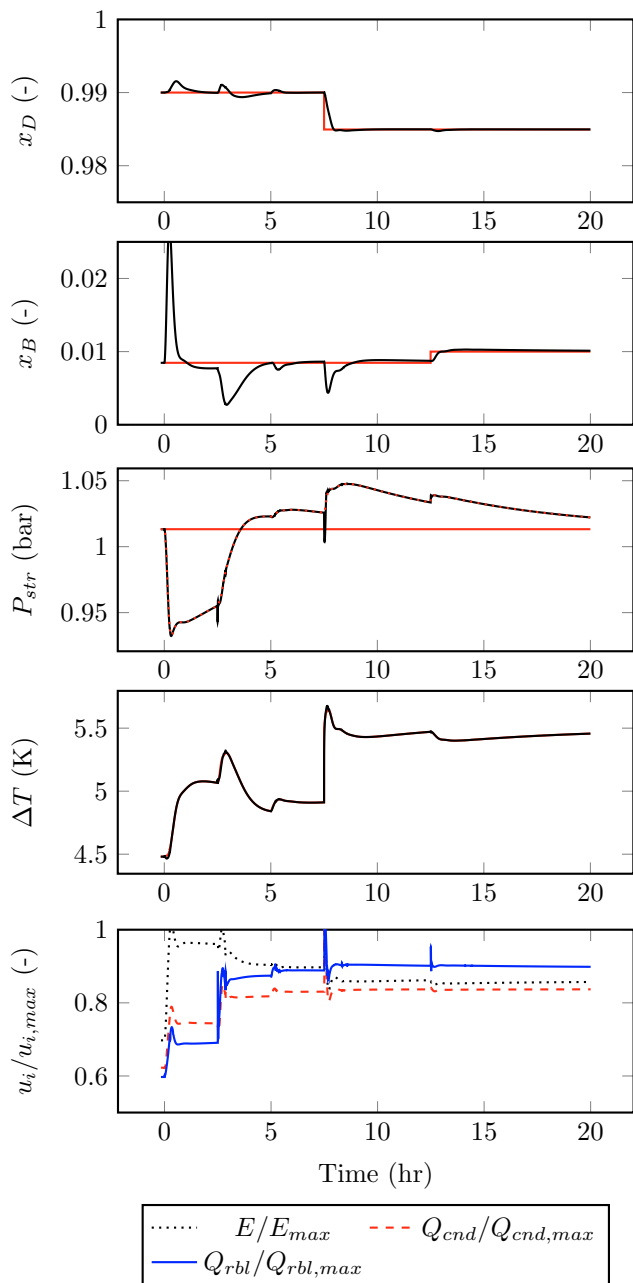
Fig. 6. Selected responses of CVs and MVs to the five step disturbances. $Q_{cnd,max} = -Q_{rbl,max} = -2000$ kW and $E_{max} = 500$ kW.

i. A control structure consisting of a regulatory and a supervisory layer has been systematically derived and evaluated for a separation with a more valuable distillate product, resulting in an acceptable performance.

ii. Deriving a stabilising control system is challenging. However, in simulation we found that it can be operated steadily under realistic disturbance scenarios.

iii. There are significant interactions in both the regulatory and the supervisory layer control loops, thereby encouraging the use of e.g. multi-variable pressure control.

iv. The overall dynamics are complex giving evidence of non-linear behaviours.

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