

Optimal Operation of a Three-Product Dividing-Wall Column with Self-Optimizing Control Structure Design

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ABSTRACT: This paper deals with optimal operation of a three-product Dividing-Wall Column (DWC). The main idea is to design a control structure, through a systematic procedure for plantwide control, with an objective to achieve desired product purities with the minimum use of energy. Exact local method is used to find the best controlled variables as single measurement or combination of measurements based on the idea of self-optimizing control. It concluded that it is possible to have better self-optimizing properties by controlling linear combinations of measurements than by controlling conventional individual measurements. Dynamic validation showed that the proposed control structure with the aid of low-complexity simple PI controller stabilized the plant, rejected the effect of disturbances and made DWC to produce product with desired specifications.

KEY WORDS: Dividing-wall column; Optimal operation; Self-optimizing control; Systematic plantwide control design; Control structure design.

INTRODUCTION

Distillation is one of the most important separation technologies. Despite of its all well-known advantages and the widespread uses, it needs large amount of energy. To be more precise, distillation needs more than 50% of plant operating cost [1]. Process intensification has led to major developments in separation technology during the last decades and has a solution to this problem. The Dividing-Wall Column (DWC) is an important example of process intensification [2]. It is an implementation of the topology of fully thermally coupled Petlyuk column [3], as is shown in Fig. 1. Dividing-wall columns can reduce up to 30% in the capital invested and up to 40%

in the energy costs [4]. Reduced mixing loss via reduction in remixing effect, which happens usually in conventional distillation trains, can make considerable savings [5, 6]. The value of saving is dependent on feed composition, relative volatility and product purity specification and could be higher in the case of separation of mixtures with more components [7]. In this way, DWC overcomes the usual problem of trading-off between reducing operating cost at the expense of higher investment costs [8]. Dunnebier & Pantelides studied the optimal design of DWCs with detailed column models and mathematical optimization and confirmed

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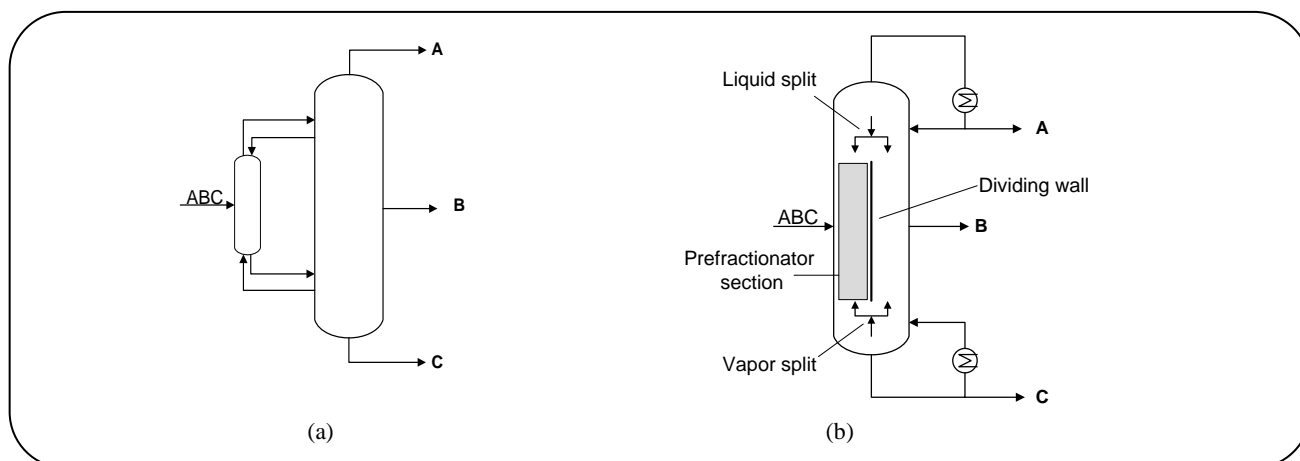


Fig. 1: Separation of ternary mixture with (a) Petlyuk configuration (b) Dividing-wall column.

that substantial benefits in both operating and capital costs can be achieved [9]. Also, DWC reduces space requirements by 40% compared to conventional distillation columns [10]. However, in spite of all these clear advantages, the practical use of DWC at industrial scale is still limited to only a few companies [1].

Dividing-wall columns have the coupling effect of the various phenomena such as mass and energy flows of vapour and liquid, which meet above and below the wall and heat transfer across the dividing wall. It makes DWC comparatively complex multivariable system [11] and understanding its operability and controllability issues still a growing matter [4]. However, studies have already proved that the DWC is not difficult to control providing that an appropriate control structure is selected [1]. Wang & Wong studied controllability and energy efficiency of a high-purity DWC and with a temperature-composition cascade structure could handle feed disturbance and internal disturbances such as changes in liquid and vapour split ratio [12]. Cho *et al.* proposed profile position control scheme and showed that it had better control performance and shorter settling time than conventional temperature-composition cascade control scheme [13]. Adrian *et al.* used different types of PI controller concepts and compared the structures with Model Predictive Control (MPC) and found that MPC gives a better control performance [14]. Serra *et al.* studied the application of dynamic matrix control (DMC) and concluded that DMC has a quite limited ability to control DWC in compare with PI controller [15]. Wolf & Skogestad studied the operation and control of three

product Petlyuk column and proposed control structures for product composition control [16].

Operation at a pre-designed nominally optimal point may not necessarily be actually optimal due to real-time disturbances, measurement and controller errors, and uncertainties. In a DWC with fixed vapour and liquid split fraction, disturbances may move the optimum to a region in the solution surface with a sharp optimum where the system may be unstable or at least impossible to obtain reasonable energy savings if we keep both vapour and liquid split fraction below and above the wall constant [17]. Thus it seems difficult to achieve the potential energy savings compared to conventional approaches in a DWC without a good control strategy. However, only very few control structures have the function of control product purities and in the meantime minimize energy consumption, which is the concern of this paper. Ling & Luyben proposed a new control structure that controlled product purities and also minimized energy consumption via composition control of the heaviest component in vapour phase over the prefractionator section [18]. Kiss & Bildea [1] gave an overview of the available control strategies for DWC and they used the proposed method of Ling & Luyben [18] to achieve optimal operation. Ling & Luyben, in other work, also proposed a temperature control structure for DWC [19]. Kiss & Rewagada studied several conventional control structures based on PID control loops and showed that DB/LSV configuration was the most stable control structure [4] and, like the work of Ling & Luyben [18], an additional loop was used

to implicitly achieve minimization of energy requirements. *Ghadrdan* [20] proposed control structure for a four product Kaibel column for special cases with relatively cheap energy where the product purities do not play a vital role, or when there is a bottleneck in the process [21]. *Dwivedi* studied a three product DWC and in order to minimize energy consumption simply control the two compositions in the two prefractionator ends to make prefractionator operate close to its preferred split [22]. *Dwivedi* in the other work, for the first time, proposed a control structure for a four product extended Petlyuk column [23].

Traditionally, Controlled Variables (CVs) have been selected based on intuition and process knowledge. *Skogestad* [24] presented a method for selecting “self-optimizing” controlled variable in the form of some function of the measured variables in such a way that keeping this controlled variable constant makes the process operate close to economically optimal steady state operation in the presence of disturbances and implementation errors. In other word, optimal operation is achieved by designing a “smart” control structure with the aid of an offline process model to support decision making in control structure design.

Based on the concept of self-optimizing control for selecting CVs, various methods have been proposed. The first local approach was the approximate Minimum Singular Value (MSV) or the maximum gain rule described by *Skogestad & Postlethwaite* [25]. *Halvorsen et al.* presented the exact local method with the worst-case loss which leads to nonlinear optimization problem [26]. This work was reformulated as a quadratic optimization problem with linear constraints by *Alstad et al.* [27] which is easier to solve numerically. *Yelchuru & Skogestad* [28] proposed a simpler and more practical calculation. *Alstad & Skogestad* [29] devised a method in which combination matrix simply located in the left null space of optimal sensitivity matrix without the consideration of implementation error. *Kariwala et al.* [30] proposed exact local method with average loss for self-optimizing control which leads to super optimal solution. The usefulness of the concept of self-optimizing control for the selection of CVs has been shown through several case studies [31-33].

The main goal of our paper is to design a control structure by applying the concept of self-optimizing technique for a three product DWC with common case of operation objective. The rest of this paper is organized as follow. The theoretical section will describe process under study and

will propose self-optimizing control structure for the selected DWC plant which is supported with numerical simulation. Theoretical section is followed with results and discussion section and conclusions are in the final section.

THEORITICAL SECTION

Process description

In this paper separation of 1 kmol/s mixture of benzene/toluene/o-xylene with the relative volatility of 7.1/2.2/1 is studied. Feed enters to the DWC at the temperature of 358K and with the concentration of 30/30/40 mol% B/T/X. Chao-Seader in the Aspen Plus simulator is used as physical property package. DWC is simulated using two absorbers, a stripper and a rectifier column [18]. There are 24 stages in prefractionator and in sidestream section, 9 stages in rectifier section and 13 stages in stripper section. Feed enters at stage 21 and sidestream withdraws at stage 20 as is shown in Fig. 2. Product purities are 99 mol %. Condenser pressure is 0.37 atm and tray pressure drop is 0.0068 atm. The reflux ratio is 2.85 and reboiler heat duty is 35.6 MW.

Design of control layers

A process plant includes thousands of measurements and control loops. In term of time scale, it can be divided generally into several layers, as illustrated in Fig. 3. The control layer is subdivided into two layers: supervisory control (advanced control) which is responsible for keeping primary (economic) controlled variables at specific setpoints and regulatory control (base control) which is responsible for stabilizing the plant [25].

In this paper, the systematic procedure of control structure design for complete process plants (plantwide control) by *Skogestad* [34] is followed. In accordance to Fig. 3, the control structure design includes the two main steps; (1) a top-down, mainly steady-state (economic), analysis to identify degrees of freedom and corresponding primary Controlled Variables (CV1) with the objective of optimal plantwide operation, and (2) a bottom-up, mostly dynamic, analysis to identify the structure of the regulatory (stabilizing) control layer and choice of secondary Controlled Variables (CV2).

Top-down design

Definition of the objective function, degrees of freedom and optimization

The objective is to minimize reboiler energy consumption to produce product with desired specification. This is common case and because of

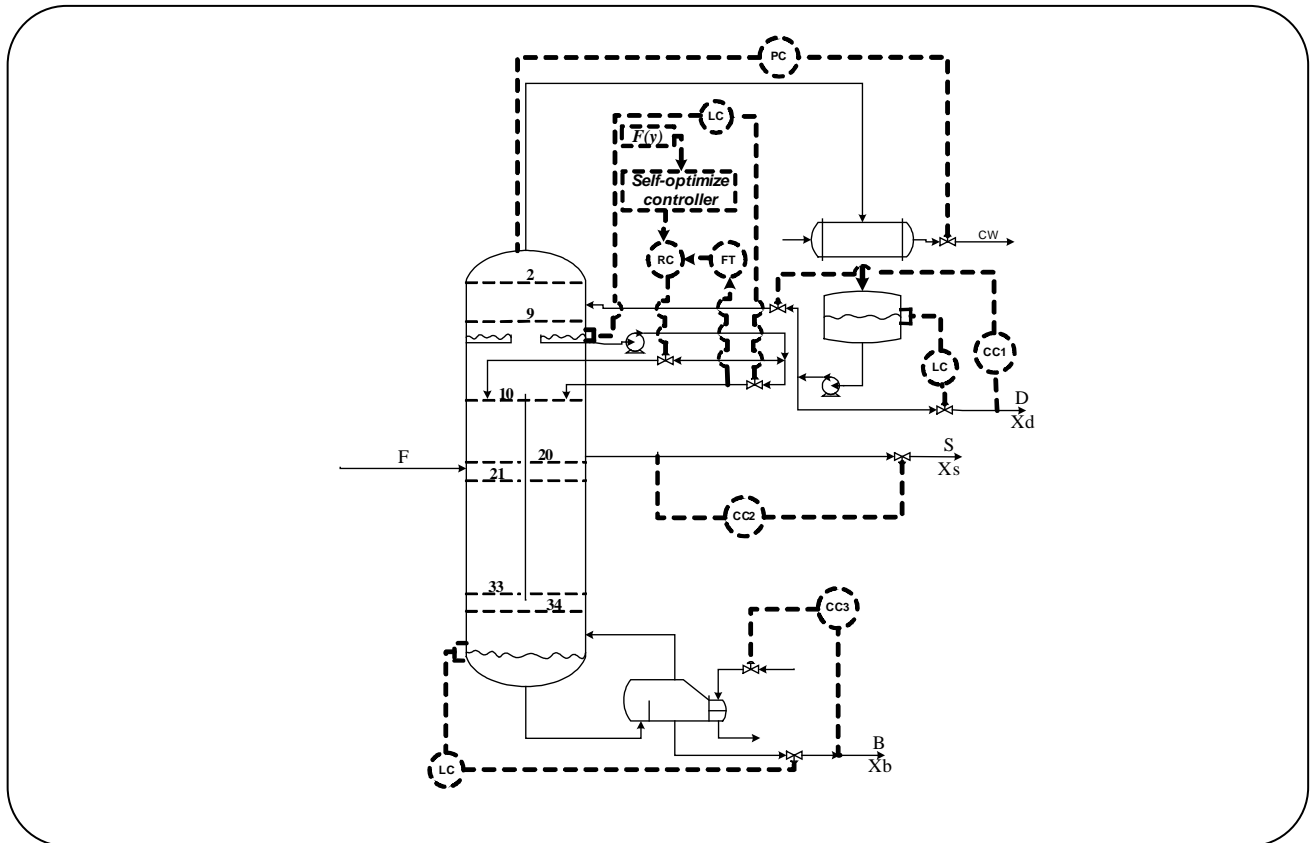


Fig. 2: Dividing-wall column flowsheet with proposed control structure.

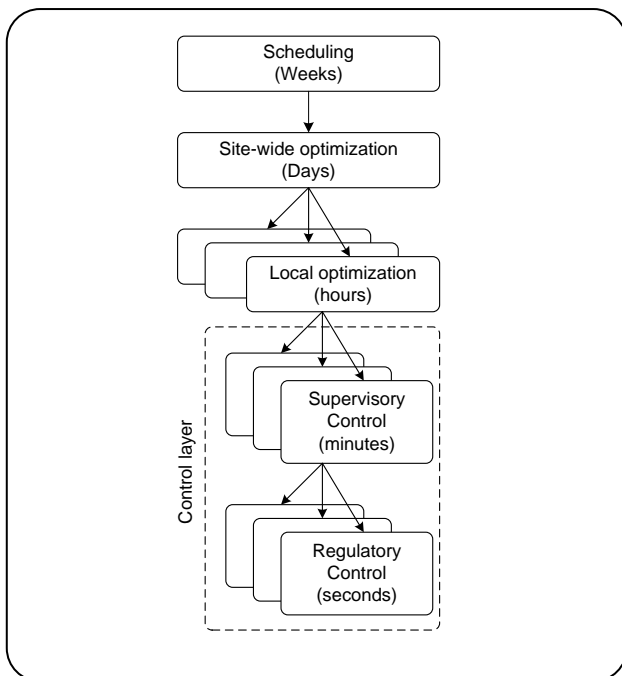


Fig. 3: Typical control hierarchy in a process plant [25].

the narrow optimal region it is a difficult case to control, but guarantees product specifications [21]. With the constant feed flow rate and pressure, there are 7 dynamic degrees of freedom and with taking into account two liquid level inventories there are 5 steady state degrees of freedom. This is an important number because it is equal to the number of primary controlled variables that we need to select. Three product purities are the three active constraints that maintained by three steady state freedom degrees. So, two unconstrained degrees of freedom, namely as vapour (R_v) and liquid (R_l) split fraction, are left to minimize energy. Reboiler heat duty at the nominal point changes with these two unconstrained degrees of freedom as the surface plot in Fig. 4. With minimization of heat input duty, vapour and liquid split fractions at bottom and top of the wall are 0.625 and 0.353, respectively.

Owing to the fact that the location of the wall is fixed, vapour split ratio is also fixed during the operation of the column [1, 4]. From practical point of view, it is more realistic case where the vapour split is not a degree of freedom [22]. In this paper we also consider the vapour

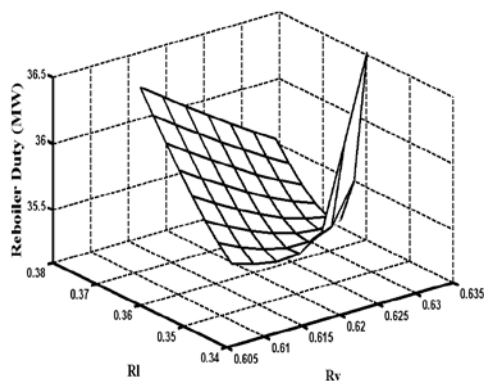


Fig. 4: Surface plot of the reboiler heat duty.

split is not a degree of freedom and demonstrate the usefulness of the proposed self-optimizing control structure for the practical use of DWC. But manipulating vapour split fraction is a new and open topic [35]. Therefore, there is one remaining unconstrained degree of freedom which can be used to control a self-optimizing control variable. In addition, active constraints (product composition) and also feed composition considered as important disturbances.

Identification of candidate CVs

It is common to use stage temperature as measurement in distillation columns. So, all of the DWC stage temperatures are selected as candidate measurements. Thus, it has 70 candidates (stages 1 to 24 in prefractionator, 25 to 33 in rectifier, 34 to 57 in sidestream and 58 to 70 in stripper section).

Self-optimizing control

To quantify optimal operation a scalar cost function, J , is considered, which should be minimized for optimal operation. Generally, the original independent variables, u_0 , is divided into the constrained variables, u' , which are used to satisfy active constraints $g'(x,u,d) = 0$ and the remaining unconstrained variables, u ($u_0 = \{u', u\}$). It is assumed that these optimally “active constraint” have been implemented, so that u_0 includes only the remaining unconstrained steady-state degree of freedom, u . Finally, the objective is to achieve optimal steady-state operation, where the degree of freedom, u , are selected such that the scalar cost function, $J(u,d)$, is minimized in the “reduced space” optimization problem for any given disturbance, d , by solving the following problem.

$$\min_{x,u} J(x, u, d)$$

$$\text{Subject to } f(x, u, d) = 0 \text{ and } g(x, u, d) < 0 \quad (1)$$

Where $x \in \mathbb{R}^{n_x}$, $u \in \mathbb{R}^{n_u}$ and $d \in \mathbb{R}^{n_d}$ are the states, disturbances, respectively; f is the set of equality constraints corresponding to the model equation; g is the set of inequality constraints that limits the operation. The objective is to find an optimal measurement combination, $c = Hy$, such that a constant setpoint, c_s , policy, in which u is adjusted to keep c constant on c_s , yields near optimal operation in accordance with Eq. (1) where

$$c_s = Hy^{\text{opt}} \quad (2)$$

To quantify the difference between alternative choices of c , the loss is defined as the difference between the actual (economic) cost and the optimal cost [25]

$$L = J(u, d) - J(u^{\text{opt}}, d) \quad (3)$$

Where for a given d , solving Eq. (1) gives $u^{\text{opt}}(d)$. The cost mainly depends on the steady-state behavior, which is a good assumption for most continuous plants in the process industry. In the reduced space after implementing active constraints and elimination of the states, the model equation is as follow;

$$y = f_y(u, d) \quad (4)$$

In a local linearized model around nominal operating point (*) the measurement variables are

$$y = G^y u + G_d^y d \quad (5)$$

Where $G^y = \left(\frac{\partial f_y}{\partial u}\right)^{*T}$, and $G_d^y = \left(\frac{\partial f_y}{\partial d}\right)^{*T}$. The controlled variable c is selected function of y

$$c = h(y) \quad (6)$$

Where the function h is free to choose. By substituting Eq. (4) into Eq. (6)

$$c = h[f_y(u, d)] = f_c(u, d) \quad (7)$$

The linearized model in the reduced space is

$$y = Gu + G_d d \quad (8)$$

Where $G = \left(\frac{\partial f_c}{\partial u}\right)^{*T}$ and $G_d = \left(\frac{\partial f_c}{\partial d}\right)^{*T}$.

The implementation error, n , has two sources; (1) the steady-state control error, n^c , and (2) the measurement error,

Table 1: Expected magnitude of individual disturbances

i	Disturbance	$W_d(i,i)$
1	Toluene mole fraction in F	0.12
2	Benzene mole fraction in D	0.2
3	Toluene mole fraction in S	0.2
4	Xylene mole fraction in B	0.2

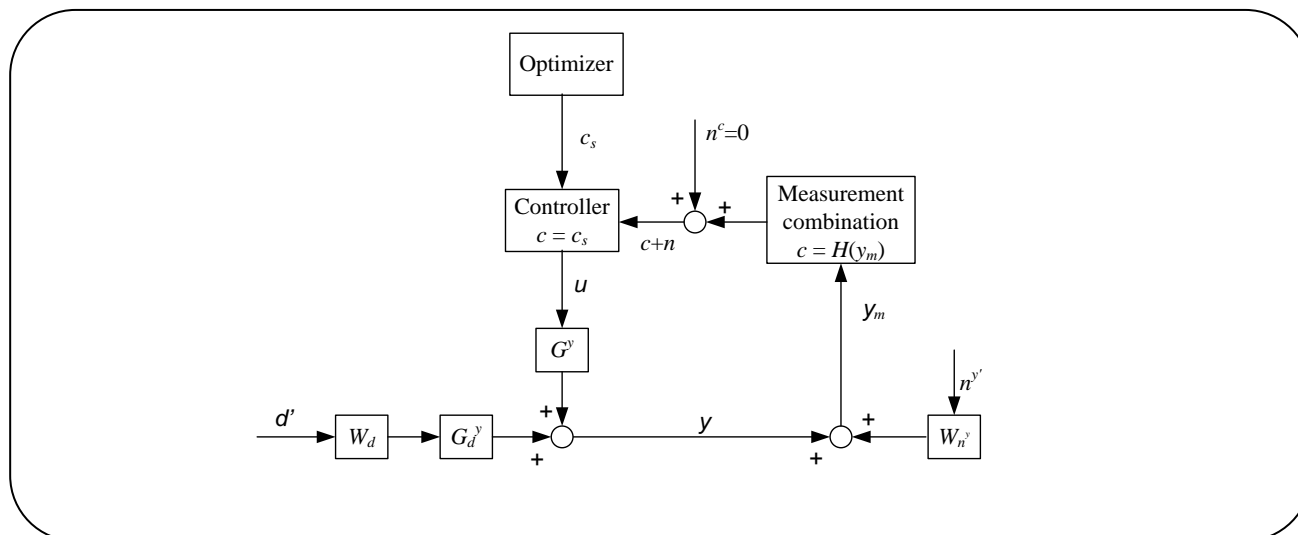


Fig. 5: Block diagram of feedback control structure including an optimizer layer.

n^y ; ($n = n^c + Hn^y$). In Fig. 5, the control error is shown as an exogenous signal; although in reality it is determined by the controller. In any case, we assume here that all controllers have integral action, so we can neglect the steady-state control error, i.e. $n^c = 0$.

Let the elements in the positive diagonal matrices W_d and W_{n^y} are the expected magnitudes of the disturbances and the control errors, i.e.

$$\Delta d = W_d d' \quad (9)$$

$$n^y = W_{n^y} n^{y'} \quad (10)$$

where the scaled disturbances, d' , and error, $n^{y'}$ are any vectors satisfying

$$\left\| \begin{bmatrix} d' \\ n^{y'} \end{bmatrix} \right\|_F \leq 1 \quad (11)$$

Where $\|\cdot\|_F$ is the frobenius norm. The expected magnitudes of individual disturbance for toluene mole fraction in feed and for three product mole fraction are as Table 1. The implementation errors are also considered to be 1.0 degree Celsius.

The worst-case loss over expected set of disturbances

and implementation errors is defined as follow [26]

$$L_{\text{worst}} = \max_{\left\| \begin{bmatrix} d' \\ n^{y'} \end{bmatrix} \right\|_F \leq 1} L = \frac{1}{2} \bar{\sigma}^2(M) \quad (12)$$

Where $\bar{\sigma}$ is the maximum singular value and

$$M = [M_d \quad M_{n^y}] \quad (13)$$

$$M_d = -J_{uu}^{1/2} (HG^y)^{-1} HFW_d \quad (14)$$

$$M_{n^y} = -J_{uu}^{1/2} (HG^y)^{-1} HFW_{n^y} \quad (15)$$

Where $J_{uu} = \frac{\partial^2 J}{\partial u^2}$, and $F = \frac{\partial y^{\text{opt}}}{\partial d^T}$. So, in the “exact local method” to minimize the worst-case loss, the value of $\bar{\sigma}(M)$ with respect to H is minimized [26], or

$$H_{\text{opt}} = \arg \min_H \bar{\sigma}(M) \quad (16)$$

Since Eq. (16) has no unique solution, Alstad *et al.* [27] solved it with linear constraint

Table 2: Subsets of Candidate measurement with optimal combination

No. of selected measurement	Best combination	worst-case loss (MW)
Individual measurement	T_{50}	7.670
2	$-1.049T_{12} + 0.483T_{55}$	1.431
3	$-0.154T_2 - 0.200T_{42} + 1.006T_{56}$	0.620
4	$-0.105T_2 - 0.465T_{13} + 0.567T_{22} + 0.342T_{55}$	0.361
5	$-0.119T_2 - 0.390T_{13} + 0.360T_{22} + 0.358T_{23} + 0.262T_{53}$	0.266
6	$-0.331T_1 + 0.077T_{29} - 0.164T_{42} + 0.325T_{55} + 0.299T_{56} + 0.276T_{57}$	0.214
7	$-0.290T_1 + 0.242T_{24} + 0.100T_{36} - 0.120T_{41} + 0.246T_{54} + 0.247T_{56} + 0.242T_{57}$	0.179

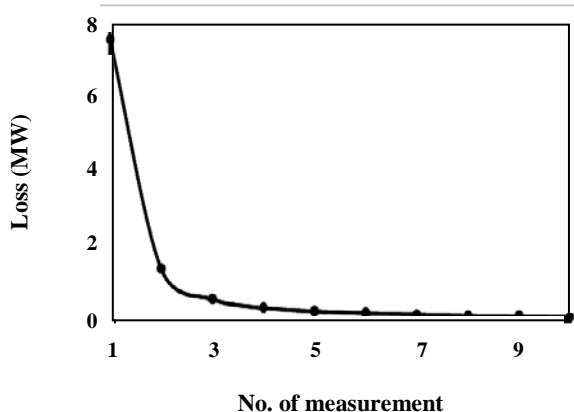


Fig. 6: Minimum local worst-case loss with different number of measurements.

$$\begin{cases} H_{\text{opt}} = \arg \min_H \bar{\sigma}(H\tilde{F}) \\ \text{Subject to: } HG^y = J_{uu}^{1/2} \end{cases} \quad (17)$$

Which leads to the following explicit solution

$$H^T = (\tilde{F}\tilde{F}^T)^{-1}G^y(G^y{}^T(\tilde{F}\tilde{F}^T)^{-1}G^y)^{-1}J_{uu}^{1/2} \quad (18)$$

Where

$$\tilde{F} = [FW_d \ W_{n^y}] \quad (19)$$

To find a subset of, for example, 7 measurements with the best self-optimizing property, there are $\binom{70}{7} = \frac{70!}{7!63!} = 1.1988 \times 10^9$ possible ways. Clearly, an analysis of all of them is intractable. Bidirectional branch and bound method with the exact local method to minimize worst-case loss for self-optimizing control, which is proposed by *Kariwala & Cao* [36], is used to avoid enumeration of all possible alternatives

in the subset selection problem. Table 2 shows that increasing the number of measurements from individual measurement to combination of more measurements leads to lower local worst-case loss. It is obvious from Fig. 6 that with 7 measurements, the loss is reasonably small.

Bottom-up Design

Structure of control layer

Pairing of manipulated and controlled variables forms a simple multiloop decentralized structure (DB/LSV) for DWC which is used frequently in literatures such as *Kiss & Rewagada* [4], and *Vandiggelen et al.* [37]. So, the concentration of distillate product, side product and bottom product are controlled with reflux flow, side stream flow and reboiler heat duty, respectively. The control structure is shown in Fig. 2. Proportional-Integral (PI) controller is used in the control structure. A 5 minute dead time is added to all composition loops.

Controller tuning

The PI controllers are tuned with SIMC method [38].

$$K_c = \frac{1}{k} \frac{\tau}{\tau_c + \theta} \quad (20)$$

$$\tau_i = \min[\tau, 4(\tau_c + \theta)] \quad (21)$$

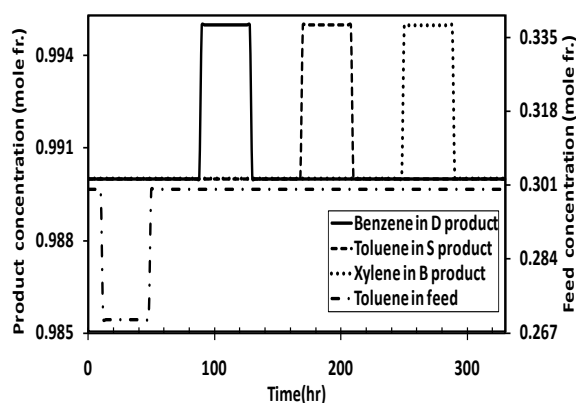
Where k , τ , and θ are the process gain, time constant, and effective time delay, respectively. K_c , τ_i , and τ_c are also the controller gain, integral time constant, and desired closed-loop time constant (tuning parameter), respectively. In our case, we choose $\tau_c = \theta$ to ensure tight control subject to having good robustness for product concentration loops which are active constraints. The controller parameters are in Table 3. The level controllers are proportional only with the gain value of 2.

Table 3: Controllers tuning parameters

Controller	Controlled variables	Manipulated variable	K_c (%/%)	τ_i (min)
CC1	X_D (Benzene)	L	11	170
CC2	X_S (Toluene)	S	9	100
CC3	X_B (Xylene)	Q_R	6.5	200
SOC Controller	Self-optimize control	Liquid split fraction	0.33	310

Table 4: Nonlinear analysis of the proposed self-optimizing structure and corresponding loss.

Disturbance	Loss (percent of nominal value)
d_1 : decrease Toluene mole fraction in F to 0.27	0.88
d_2 : increase Benzene mole fraction in D to 0.995	0.035
d_3 : increase Toluene mole fraction in S to 0.995	0.68
d_4 : increase Xylene mole fraction in B to 0.995	0.59

**Fig. 7: Disturbance trajectory.**

Dynamic validation

The proposed control structure is studied in rejecting the disturbances entered into the plant according to the Fig. 7.

Fig. 8 shows the dynamic responses of proposed control structure. In all cases, the flowsheet is optimized for each disturbance and the corresponding losses from nonlinear model are shown in Table 4.

RESULTS AND DISCUSSIONS

Table 2 shows alternative self-optimizing CVs with different number of measurements and its corresponding local loss. It is clear that the combinations of measurements have imposed lower local loss in compare with conventional single measurement (in the first row of the table). Fig. 6 results that combination of

7 measurements, as self-optimizing controlled variable, is satisfactory and makes loss reasonably small.

Fig. 8 shows that the proposed control structure based on the designed self-optimizing CV with the aid of low-complexity simple PI controller stabilizes the plant, rejects the effect of disturbances and makes DWC produce product with desired specifications. Here “stabilization” means that the process does not “drift” too far away from the designed nominal point when there are disturbances[34]. The product concentrations, as active constraints, are also tightly controlled on desired specification. In all cases the flowsheet is optimized for each disturbance to find the corresponding loss and the flowsheet converges without reaching a new constraint. Thus, the same set of active constraint is considered for entire region of operating condition in this study. In the case of changing active constraint, new CVs for each set of active constraints can be obtained from offline calculation and with the aid of some logic it is possible to switch between suitable CVs.

Table 4 clearly shows that nonlinear loss is less than 1 percent which is approximately zero from practical point of view. So, the proposed method has removed the need for complex intensive Real-Time Optimization (RTO) computations. This means that the proposed control structure based on the selected self-optimizing CV makes control structure meet changes in operating condition and keep the plant close to optimal operation.

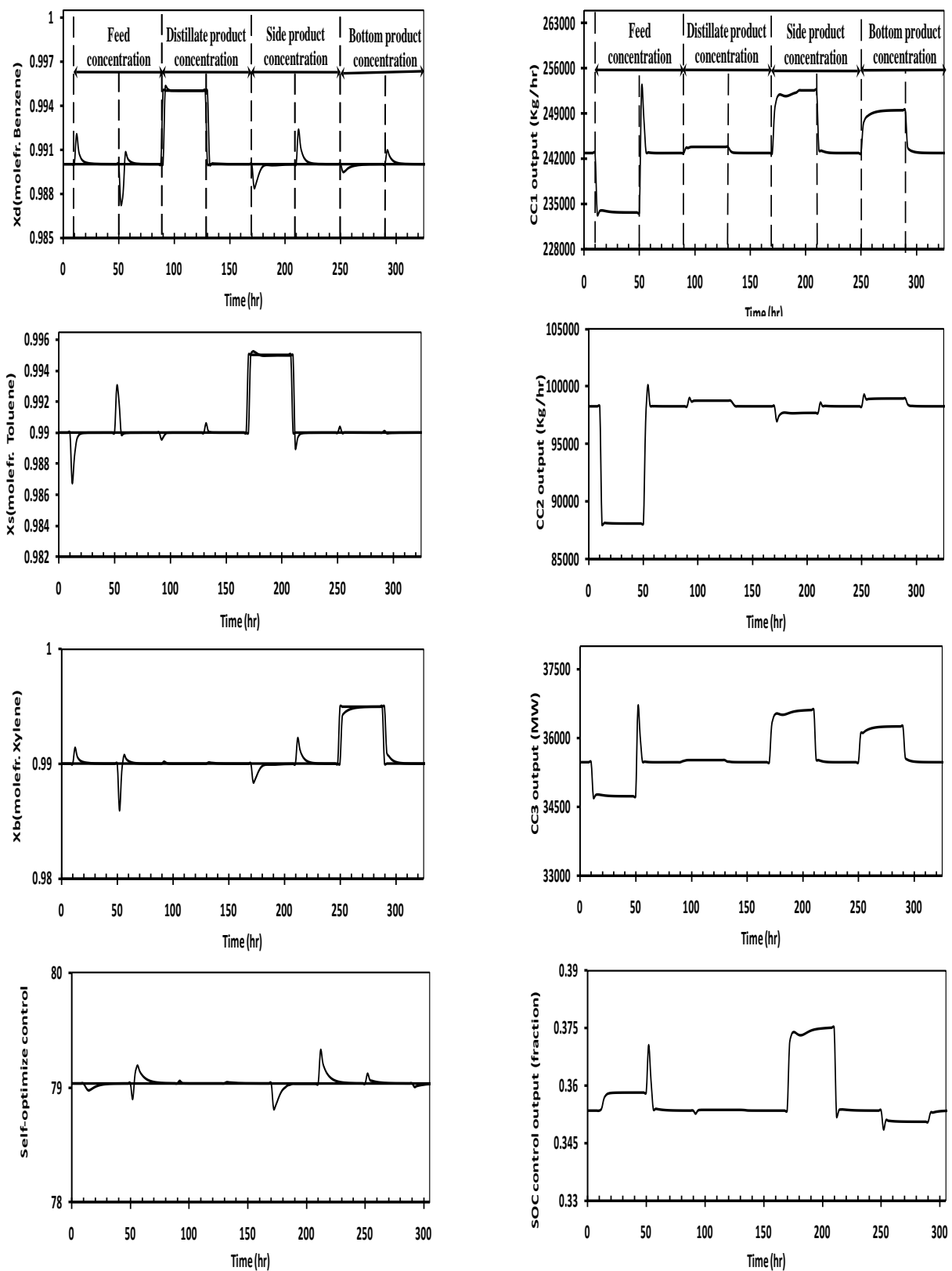


Fig. 8: Dynamic responses of proposed self-optimize control structure.

CONCLUSIONS

In this paper, a control structure based on the systematic procedure by applying the concept of self-optimizing technique was developed. It showed that linear combination of measurements, led to a lower loss in compare with controlling conventional individual measurement. In addition to close to optimal operation, the dynamic simulation showed that the proposed control structure, with the aid of low-complexity simple PI controller, stabilized the plant, rejected the effect of disturbances and made DWC produce product with desired specifications.

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