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Modelling and Control Analysis of Dividing Wall Distillation Columns

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Abstract: This work aims to study the behavior of fluid mixtures in the dividing wall column, particularly from a controllability point of view. It covers the aspects of design, modeling, and control. A ternary mixture of benzene, toluene, and o-xylene (BTX) is selected as a case study. A controllability analysis for determining and screening the candidate control combinations of the manipulated variables is carried out with the aid of a linearized model using the concept of relative gain array (RGA). The manipulated variables are the reflux (L), the distillate (D), the side stream (S), the bottom (B) and the boilup (V). Based on RGA criterion, two of the candidate combinations are selected to control the column due to the low interaction between control loops. In each combination the manipulated variables are used to control the top level, the bottom level, the top composition, the middle composition and the bottom composition. Finally, the performance of these two combinations is examined and found to be successful in resisting the disturbances.

Keywords: *Dividing wall column; Modelling; Non-linear model; Linear model; control*.

1. INTRODUCTION

The dividing wall column is a new application of the concept of (process intensification) which implies integrating several unit operations into one common apparatus. This configuration is expected to decrease significantly the capital cost and the operating cost of the process due to equipment reduction and lower energy requirements compared to conventional distillation sequences. Consequently, it has the potential to be a promising alternative for the conventional columns sequences used to separate multi-components mixtures.

The dividing wall column is a distillation column for multi-component separation that has a vertical partition wall in the central section (Fig. 1.ii). The feed side of two compartments acts as the prefractionator and the product side as the main column**.**

The column may contain either trays or packing. The dividing wall column (DWC) allows substantial energy savings and reduction in capital cost up to 30-40% [1], while separating in a single body a multi-component mixture into pure products.
The DWC belongs to thermally coupled distillation columns which include the Petyluk column [2] (Fig. 1.i) that was initially introduced by Brugma in 1942 [3]. The petyluk column was named after Petyluk who studied theoretically this configuration in 1965. What is called now the dividing wall column (DWC) is a similar structure to Petyluk proposed by Wright in 1945 and introduced to the industry world in 1987 by Kaibel [4]. The DWC and Petyluk column are believed to be thermodynamically equivalent.

These two full thermally-coupled structures subjected to studies concerning different aspects such as design.[5] controllability and degrees of freedom [6], [7].

Controllability and degrees of freedom of the DWC were investigated by Wolff et al.[6] and Mutalib et al.[7]. In the first paper four point and three point control strategies were proposed while in the second paper it was recommended to exclude the split ratios (L and V) from the set of manipulated variables. Halvorsen et al. [8] gave some guidelines for optimal operation of Petyluk column. Hernandeze et al. [9] investigated the control structure of thermally coupled columns and estimated that the energy gained when using thermally-coupled configurations. Petyluk column was found to be the lowest energy consumer. In the work of van Diggelen et al. [10], the DWC control issues were explored and a comparison of various control strategies, including advanced controllers were made. Using controllers based on temperature measurement instead of composition was the subject of the work of Ling et al. [11]. They proposed a structure of differential temperature control that handled different disturbances more effectively than ordinary temperature control**.**

Adrian et al. [12] investigated the implementation of model predictive control and outlined that additional effort to set up the model predictive control is estimated to be three times higher, the performance of model predictive control however is found to be superior to the use of single loop PI controllers especially when constraints for operating conditions should be taken into account.

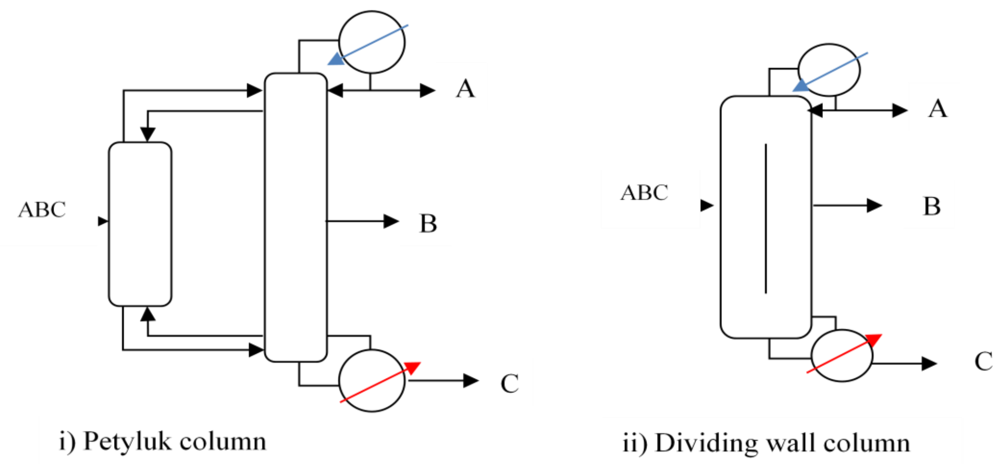

Fig. 1. (i) Petyluk column, (ii) Dividing wall column

This work is aimed to analyse the control loop (PI controllers) pairing for DWC columns and their performance using the RGA method. The performance of the investigated control loop pairing is further tuned through the cohen-coon method and assessed using the Nyquist stability criteria.

2. MATERIALS AND METHODS

2.1 Separation in DWC

For a three component mixture (A the lightest, B the intermediate and C the heaviest), the prefractionator separates the lightest component (A) from the heaviest component (C), while the middle component (B) is distributed. The main column separates (A) from (B) in trays above the middle stream product, and (B) from (C) in trays below the middle stream product. The main column has the three product streams and supplies the reflux and vapor streams required by the prefractionator, resulting in a double thermal coupling between both parts. For a three component mixture (A the lightest, B the intermediate and C the heaviest), the prefractionator separates the lightest component (A) from the heaviest component (C), while the middle component (B) is distributed. The main column separates (A) from (B) in trays above the middle stream product, and (B) from (C) in trays below the middle stream product. The main column has the three product streams and supplies the reflux and vapor streams required by the prefractionator, resulting in a double thermal coupling between both parts.

The idea of the Petlyuk Column and the DWC can be extended to arrangements for the separation of multi-component mixtures with more than three components with only one condenser and one reboiler,

2.2 Case Study

A ternary mixture of, toluene, and o-xylene (BTX) is to be separated in a DWC. The case study data is shown in Table 1. The The behavior of the column is studied in a four step framework as follows.

- Short cut design.
- Non-linear and Linear models simulation.
- RGA analysis of control loops pairings.
- Assessment of disturbance rejection performance of the selected control configurations.

Table 1: Case study data

Feed properties			
Feed flow rate F = 1 kmol/min,			
Feed state, $q_F = 1$			
	Benzene	Toluene	Xylene
Normal boiling point, K	$T_A = 353$	$T_B = 385$	$T_C = 419$
Relative volatilities	$\alpha_{AC} = 7.1$	$\alpha_{BC} = 2.2$	$\alpha_{CC} = 1$
Feed composition	$z_A = 0.3$	$z_B = 0.3$	$z_C = 0.4$
Products specifications			
specifications	Flow rate kmol/min	Purity	
Distillate	0.333	Benzene $x_A = 98\%$	
Side stream	0.333	Toluene $x_B = 98\%$	
Bottom	0.334	Xylene $x_C = 98\%$	

2.3 The DWC design

Serra [5] presented a model of three conventional columns in series to study the design of the DWC as shown in Fig. 2. Table 2 presents specification needed for designing the shortcut model. Fenske-Underwood-Gilliland equations are used for the design of the series of the three columns. The estimated DWC parameters to achieve the desired separation of the BTX mixture are given in detail in Table 3

2.4 Dynamic Model for DWC

According to the process behavior, there are two types of dynamic models: *linear and non-linear.* Linear models allow the easy manipulation of transfer functions which are the principal tools in studying dynamic control. However, non-linear models can be linearized by means of several methods.

2.4.1 Non-linear dynamic model

Simplified stage-by-stage material and energy balances are applied to the column trays to create the non-linear model detailed next.

The dynamic non-linear model can be represented by the following compressed formula of an ordinary differential equations system [10]:

$$x' = f(\mathbf{x}, u, d, t) \tag{1}$$

$$\mathbf{Y} = g(\mathbf{x}, u) \tag{2}$$

where x = the states vector consisting of compositions and liquid holdups,
$u=[L\ S\ V\ D\ B\ R_L\ R_V]$ is the input vector,
$d = [F\ z\ q_F]$ is the disturbance vector,
$\mathbf{Y} = [x_A\ x_B\ x_C\ M_T\ M_R]$ is the output vector (selected states),

The Livermore Solver for Ordinary Differential Equations (LSODE), a built-in-function in Octave, is used to solve the system assuming that all initial compositions inside the column are equal to those of the feed.
The results obtained through the non-linear simulation of the proposed structure are very close to the desired specifications (Table 1). The calculated products compositions are: $[x_A\ x_B\ x_C]$ = [0.987 0.975 0.989 product compositions at steady state (time $\rightarrow \infty$).

Table 2. Specification needed for designing the shortcut model

The column	Specifications
Column 1	Recoveries of A and C (arbitrarily chosen, 0<recovery<1)
Column 2	Distillate and bottom purities
Column 3	Distillate and bottom purities

Table 3. DWC design parameters and internal flows

Structure parameters	
Total number of trays	38
The prefractionator	
No. of trays in the Prefractionator	13
Feed tray	6
The main column	
No. of trays in the main column	25
Reboiler stage	1
First common tray below wall	10
Side stream tray	16
First common tray above wall	22
Condenser stage	25
Internal flowrates	
Reflux L (kmol/min)	2.78
Boilup V (kmol/min)	3.11
Liquid split	0.33
Vapour split	0.32

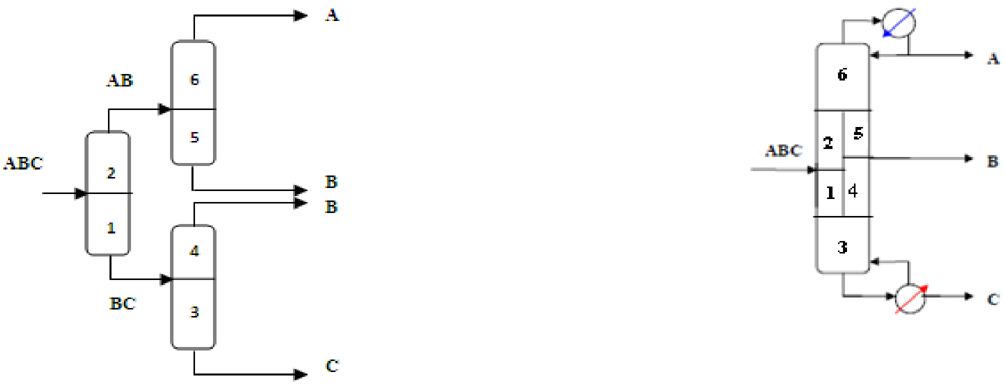

Fig. 2. Equivalent shortcut model to DWC

2.4.1 Linear dynamic model

Using Taylor expansion and keeping only the first order terms, the equivalent linear representation for the DWC non-linear dynamic model [13] described by equations (1) and (2) is:

$$\mathbf{x}' - \mathbf{x}_0' = A(\mathbf{x} - \mathbf{x_0}) + B(u - u_0) \quad (3)$$

$$\mathbf{Y} - \mathbf{Y}_0 = C(\mathbf{x} - \mathbf{x_0}) + D(u - u_0) \quad (4)$$

where ($\mathbf{x_0}, u_0$) is the steady state

Laplace transformation of the linear model described by equations (3) and (4) gives the corresponding representation in *s domain*

$$\boldsymbol{X} = \boldsymbol{G(s)U_{\blacksquare}} \quad (5)$$

$$\boldsymbol{Y} = \boldsymbol{C}(s\boldsymbol{I} - \boldsymbol{A})^{-1}\boldsymbol{B}_{\blacksquare} + \boldsymbol{D}_{\blacksquare}\boldsymbol{U}_{\blacksquare} \quad (6)$$

Noting that [4]:

$$\boldsymbol{G}(s) = (s\boldsymbol{I} - \boldsymbol{A})^{-1}\boldsymbol{B}_{\blacksquare} \quad (7)$$

where $\boldsymbol{G}(s)$ is the transfer function matrix, $\boldsymbol{I}$ is the unity matrix, $\boldsymbol{A}, \boldsymbol{B}_{\blacksquare}, \boldsymbol{C}, \boldsymbol{D}_{\blacksquare}$ are the coefficients matrices

When looking at the two models, the profiles produced by the two models initially diverge but these deviations occur within the first 5 minutes and disappear soon after. The profiles almost coincide at steady state, the state around which the model is linearized and will be further analyzed. Due to the short period of deviation the linear model can be considered as a reasonable approximation for the non-linear model.

3. RESULTS AND DISCUSSION

3.1 Controllability analysis of DWC column

The relative gain array (RGA) method is used to select the most feasible pairs of input output variables (i.e. manipulated/controlled variables) [14][15]. ***RGA*** of a system with a transfer function matrix ***G(s)*** is calculated as follows:

$$\boldsymbol{RGA}(\boldsymbol{G}(s))|_{s\to 0} = (\boldsymbol{G}(s).\times(\boldsymbol{G}(s)^{-1})')\big|_{s\to 0} \;\ldots\ldots\ldots . (8)$$

According to the model described, given the feed properties (flow rate, quality and composition), the DWC has seven operation DOF corresponding to seven candidate manipulated variables in the process [10].

These are: [L V S D B Rl Rv]

The variables to be controlled are: [x_A x_B x_C MT MR]

Accordingly only five manipulated variables will be selected. When investigating the variation of the two splits Rl and Rv they are excluded because of their weak effect on the nearby composition and to avoid their similar simultaneous effect on the middle composition that might lead the loops to interact significantly.

Table 4. RGA for different control schemes

scheme	Controlled variables	Manipulated variables		
		L	***S***	***V***
DB/LSV	x_A	58.75	−0.004	−57.74
	x_B	−21.32	0.341	21.97
	x_C	−36.43	0.663	36.76
		D	***S***	***V***
LB/DSV	x_A	0.650	−0.004	0.353
	x_B	0.132	0.341	0.526
	x_C	0.217	0.662	0.120
		L	***S***	***B***
DV/LSB	x_A	0.357	0.419	0.223
	x_B	0.523	0.534	−0.057
	x_C	0.119	0.046	0.834
		D	***S***	***B***
LV/DSB	x_A	-59.4×10^8	39.0×10^8	20.5×10^8
	x_B	48.8×10^8	-69.2×10^8	20.5×10^8
	x_C	10.7×10^8	30.3×10^8	-41.0×10^8

The proposed control configurations are DB/[L S V], DV/[D S V] , LB/[L S B] and LV/[D S B]. In each combination the manipulated variables are used to control the top level, the bottom level, the top composition x_A, the middle composition x_B and the bottom composition x_C respectively.

The values of the RGA are included in Table 4 below. According to the RGA criterion, it is recommended to associate controlled and manipulated variables to yield a corresponding positive value of relative gains and close to unity. The values in Table 4 show that LB/DSV (scheme 2) and DV/LSB (scheme 3) can be considered as the best choices due to the lower interaction between the separate control loops. Whereas, it is obvious that DB/LSV and LV/DSB configurations seem to be worse.

Moreover, some sort of cross pairing between variables, although not presented here, may be beneficial, that is to manipulate x_A with S and x_B with D in LB/DSV configuration and pairing x_B with B and x_C with S in DV/LSB configuration.

3.2 Controller tuning

Controller parameters along with the control loop direction obtained from steady state gain array are listed in Table 5; the controller reverse the effect of the disturbance this is why the proportional parameter takes the opposite sign of the corresponding element in the steady state gain array .

The constants of the level controllers are arbitrarily chosen (the value proposed in the model 'column A' is adopted) [16], while the reaction curve method is applied to obtain the parameters of the composition controllers. A step change is introduced in the manipulated variable and the response of the controlled variable is plotted.

Table 5. Controllers parameters sets

Control loop	Kc		τ_i	
LB/DVS				
Top level-L	+10		-----	
Bottom level-B	+10		-----	
	Initial estimates	Final adjustment	Initial estimates	Final adjustment
x_A-D	7.4	8	3.75	8
x_B-V	7.4	8	3.75	8
x_C-S	7.4	8	3.75	8
DV/SLB				
Top level-D	+10		-----	
Bottom level-V	+10			
	Initial estimates	Final adjustment	Initial estimates	Final adjustment
x_A-S	8.4	8	1.78	20
x_B-L	8.4	8	1.78	10
x_C-B	8.4	8	1.78	10

In both configurations it is only the x_B loop (the middle loop) that fulfills the condition required to apply the reaction curve method; that is simulating a first order system with time lag. The parameters of this loop are calculated based on the reaction curve tuning method. Although this method only give initial guesses for the middle loop parameters, the same values are assumed for the parameters of the two other loops and further readjustments are made until the best performance is reached.

3.3 Control configurations assessment

The closed-loop response of the DWC for the two control configurations LB/DVS and DV/SLB, after cross pairing the variables, is analyzed through exerting disturbances of +10% in the feed flow rate (*F*) and -10% in the feed quality (q_F). The responses are plotted in Fig. 3 and Fig. 4 respectively.

Proportional (P) controllers are used to control liquid level in the reboiler and the condenser since they are capable to absorb fluctuations of liquid levels in the large tanks of the reboiler and the condenser [5]. Whereas, the tighter proportional-integral (PI) controllers are used to control compositions [17].

The reaction curve tuning method (Cohen-Coon method) is used to determine the first estimates of the controller parameters then these values will be refined and readjusted until the desired performance and stability is obtained [18].

Table 6. Settling time and maximum offset for LB/DVS and DV/ LSB schemes

Scheme	**10% feed disturbance**			
	Settling time, min	**Max. offset %**		
		$\mathbf{x_A}$	$\mathbf{x_B}$	$\mathbf{x_C}$
LB/DVS	511	0.158	0.626	0.469
DV/ LSB	661	0.425	0.476	0.219
	10%composition disturbance			
LB/DVS	470	$2.8x10^{-3}$	$8x10^{-3}$	$1.7x10^{-3}$
DV/ LSB	602	$2.5x10^{-3}$	$7.4x10^{-3}$	$6.5x10^{-4}$

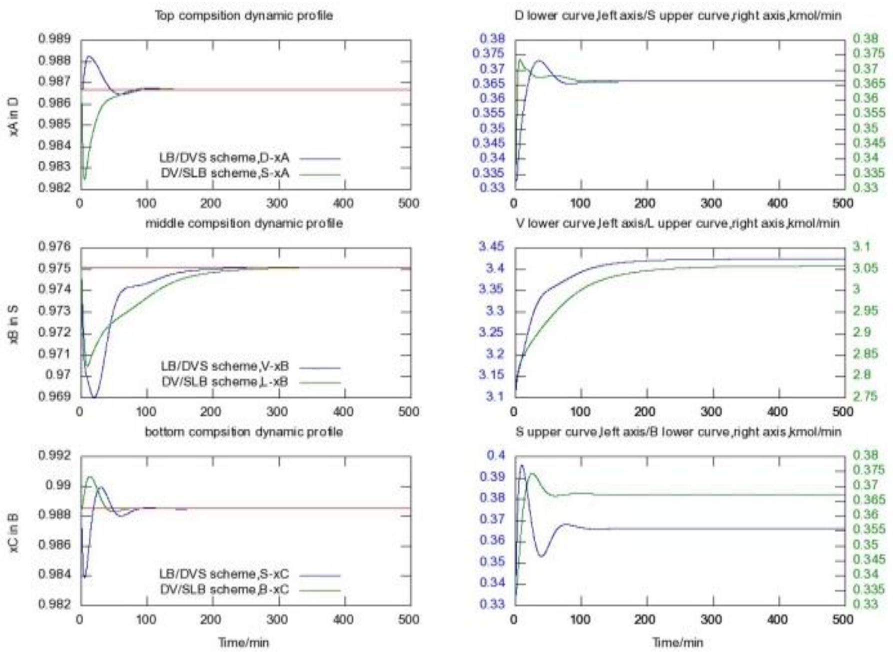

Fig. 3. Dynamic response of the products composition (left) and the manipulating flows rate (right) to 10% feed flow rate disturbance.

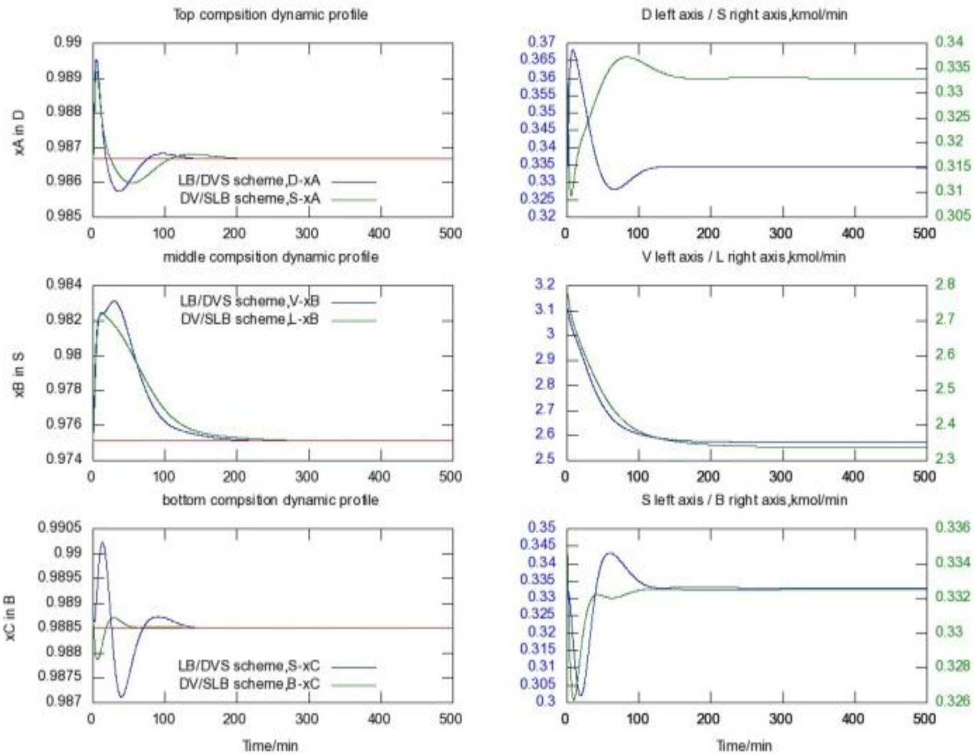

Fig. 4. Dynamic response of the products composition (left) and the manipulating flows rate (right) to -10% feed quality q_F

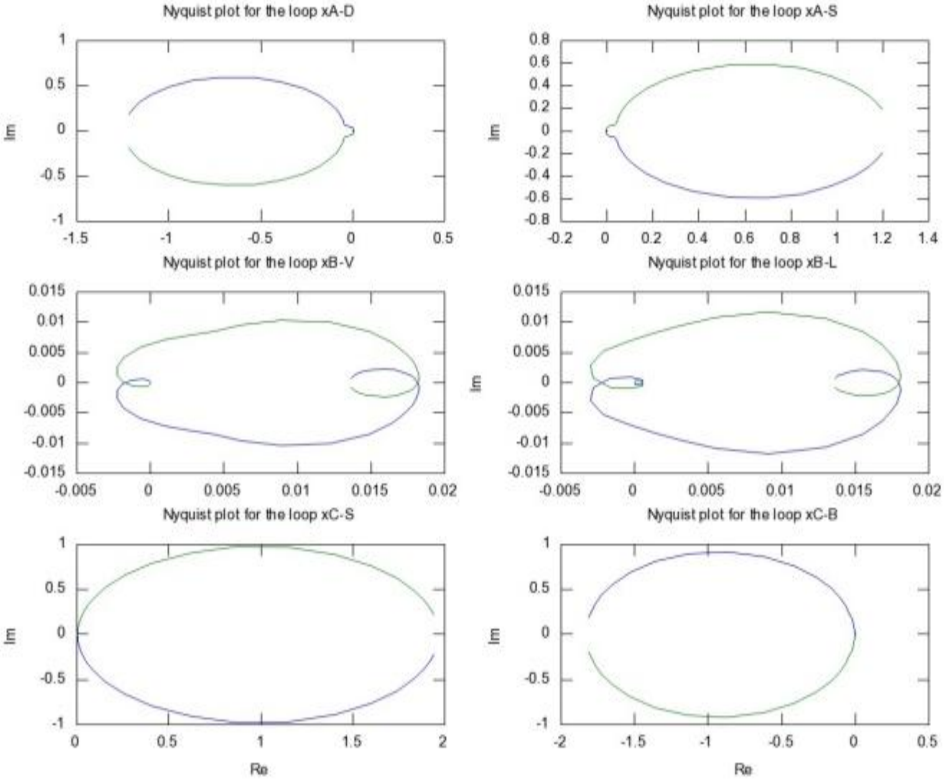

Fig. 5. Nyquist plot for the open-loop system

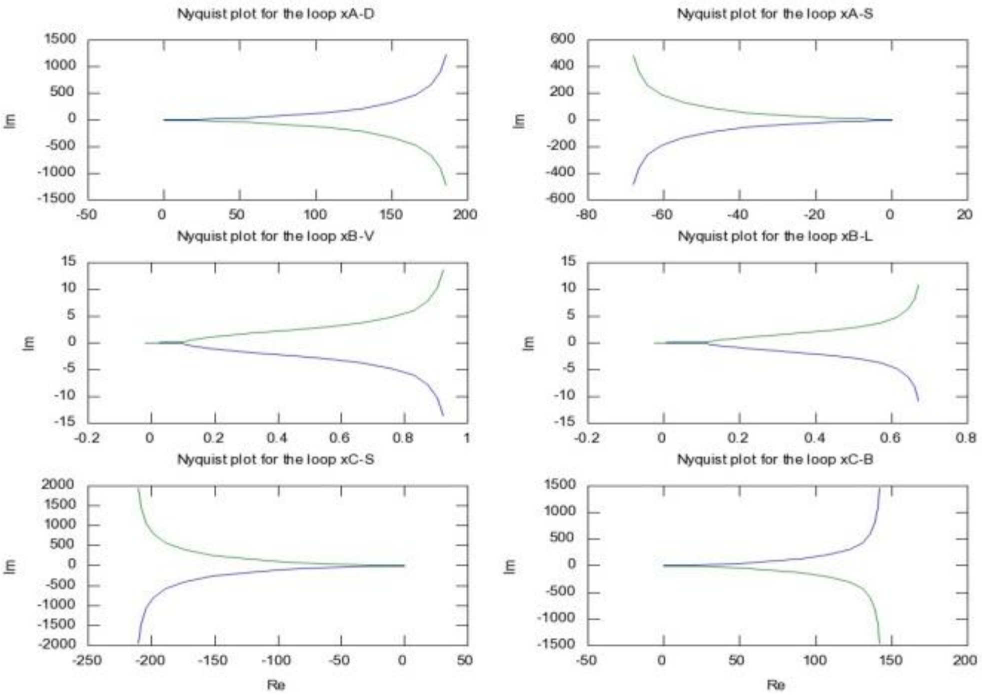

Fig. 6. Nyquist plot for LB/DVS scheme (left) and DV/SLB scheme (right)

Examining the responses it can be seen that both schemes succeed in resisting the disturbances introduced.

Table 6 includes settling time and maximum offset for both schemes. Settling time is determined to be the longest time at which max $(\|[x_A\ x_B\ x_C]- [x_{A0}\ x_{B0}\ x_{C0}]\|)=10^{-7}$

When introducing a disturbance to the feed flow rate the LB/ DVS scheme shows better performance as it needs less time to restore the system to the original state, actually it is 1.3 times faster.

The stability of the open-loop system and the closed-loop system for both schemes is checked using Nyquist plots. The middle loop in the open-loop system violates the stability condition of Nyquist criterion (Fig. 5). However it is obvious that implementing the PI controllers converts the system to a completely stable system (Fig. 6).

4. CONCLUSIONS

The dividing wall column is a fruit of searching energy-efficient systems in distillation process.
Focusing on control, the DWC design and modeling are also studied in this work by means of the traditional methods used to study the conventional columns.

The well-known Fenske-Underwood-Gilliland equations applied to a series of three conventional columns representing the DWC give proper estimations of the DWC structure and internal flow rates.

A non-linear model simulating the DWC depending on simplified assumptions is created in Octave. However, this model gives a general comprehension of the DWC behavior. In addition, using conservation laws of mass and energy, a stage by stage model does not seem to converge. Alternatively, the DWC is divided into two linked columns that have been separately modeled.

The non-linear model undergoes a linearization process to produce the linear model which is an essential requirement for performing the controllability analysis. Comparing the data calculated through the linear model to those resulted from the non-linear one shows that linear model can be a reasonable approximation.

To analyze the DWC controllability and to determine the best control configuration the relative gain array RGA concept is used. According to this concept, the two configurations DV/ LSB and LB /DSV show signs of superior performance.
Cohen-Coon tuning method (reaction curve method) gives reasonable initial guesses for the parameters of the PI controllers controlling the top level, the bottom level, the top composition, the middle composition and the bottom composition.

Introducing 10 % disturbance in feed flow rate and feed quality both control schemes are capable to absorb the disturbances effect. However, DV/ LSB scheme shows better performance when introducing the feed flow rate disturbance, which has more significant effect compared to that of composition, as it is 1.3 times faster to return the system to the steady state. Both schemes operate within the limits of stability that is checked via the closed loop response of the Nyquist stability criterion.

The study confirms that the traditional methods used in the design and the control of conventional distillation columns work well and give reasonable results when applied to the DWC.

These conclusions, combined with the potential benefits of capital and operating costs reduction, make of the DWC a promising arrangement for multi-component separation.

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NOMENCLATURE

- ***A*** coefficient matrix of linear model
- B bottom stream
- ***B*** coefficient matrix of linear model
- $\boldsymbol{B}_{\blacksquare}$ modified coefficient matrix
- *C* number of components
- ***C*** coefficient matrix of linear model
- **D** distillate of the dividing wall column
- ***D*** coefficient matrix of linear model
- $D_{\blacksquare}$ modified coefficient matrix
- d disturbances vector
- F feed flow rate
- ***G*** transfer function
- ***I*** unit matrix
- L reflux in the dividing wall column
- M_R reboiler holdup
- M_T condenser holdup
- q_F feed quality
- *Re* real part of a complex number
- R_L liquid split ratio
- R_V vapour split ratio
- S side stream
- ***s*** Laplace domain variable
- T toluene
- *t* time
- $U_{\blacksquare}$ modified input and disturbance vector
- *u* input vector in time domain
- $u_{\blacksquare}$ input and disturbance vector in time domain
- u_o input vector at steady state
- V boilup in the dividing wall column
- ***X*** the states vector in Laplace domain
- X xylene
- x the states vector in time domain
- x_A benzene concentration in top product
- x_B toluene concentration in top product
- x_C xylene concentration in top product
- ***x*** liquid fraction for a component
- x_0 steady-state value of states vector
- x' vector containing the states time derivative
- x'_0 vector containing the steady-state value of the states time derivative
- *Y* output vector in Laplace domain
- Y output vector in time domain
- ***y*** vapour fraction
- z feed fraction