Case Report

A port-stream based equation oriented modelling of complex distillation column: A dividing wall column case study

R. Idris, N. Harun, MR. Othman[*]

Process Systems Engineering Research Group, FKKSA, Universiti Malaysia Pahang, Gambang 26300, Pahang, Malaysia. E-mail: rizza@ump.edu.my

ABSTRACT

Dividing wall column (DWC) offers higher degree of freedom in comparison with the conventional column. Furthermore, the different sections configurations within the column are highly interacting with several recycle loops. Facing with such complex unit operation, describing its behaviour encourages the focal point on the resolution of ideal modelling approaches. Equation oriented (EO) modelling of DWC has been studied by several researchers involving complex algorithm and methodology. In this work, a new approach for modelling of DWC is presented. The modelling methodology involves variables connectivity based on ports and streams that is admissible to equation-oriented flow sheet. To verify the functionality of the proposed method, the modelled DWC is validated with two case studies depicted from experimental literature data to separate alcohol mixture and fatty acid fractionation. The model development was performed in MOSAIC, a web-based modelling tool and run in gPROMS. The model shows good convergence and has less than 10% error when compared to the above mentioned case studies. To furthermore extend the model capability, relative gain array (RGA) analysis was conducted for the fatty acid fractionation to determine the best control configuration in DWC. Result shows that L-S-V and L-S-B configurations are the best control configurations. Our analysis also shows that reflux flowrate, side flowrate and vapor boilup are best to control distillate product, side product and bottom product, respectively.

Keywords: Dividing Wall Column; Process Modelling; Relative Gain Array

ARTICLE INFO

COPYRIGHT

1. Introduction

Dividing wall column (DWC) is an intensified design of Petlyuk column which provides a good alternative to conventional distillation column due to possible saving in both energy and capital cost around 30%[1]. A DWC possesses a vertical partition that splits the column shell into a pre-fractionator and main column section as shown in **Figure 1**. Such configuration compensates the impurity of the side product from being mixed with the distillate and bottom products. For ternary mixtures, applying DWC is able to cut down a column, thus reducing the number of condenser and reboiler with reliable product quality achievement. Regardless of its potential advantages, industrial implementation of dividing wall columns was often restricted due to the design, control and operational concern.

Often modelling of DWC was done through sequential modular (SM) based model compared to equation oriented (EO) based model. In SM modelling, two or three column configurations were often used. Four column configurations, however, are more accurate to represent the four sections of DWC[2].
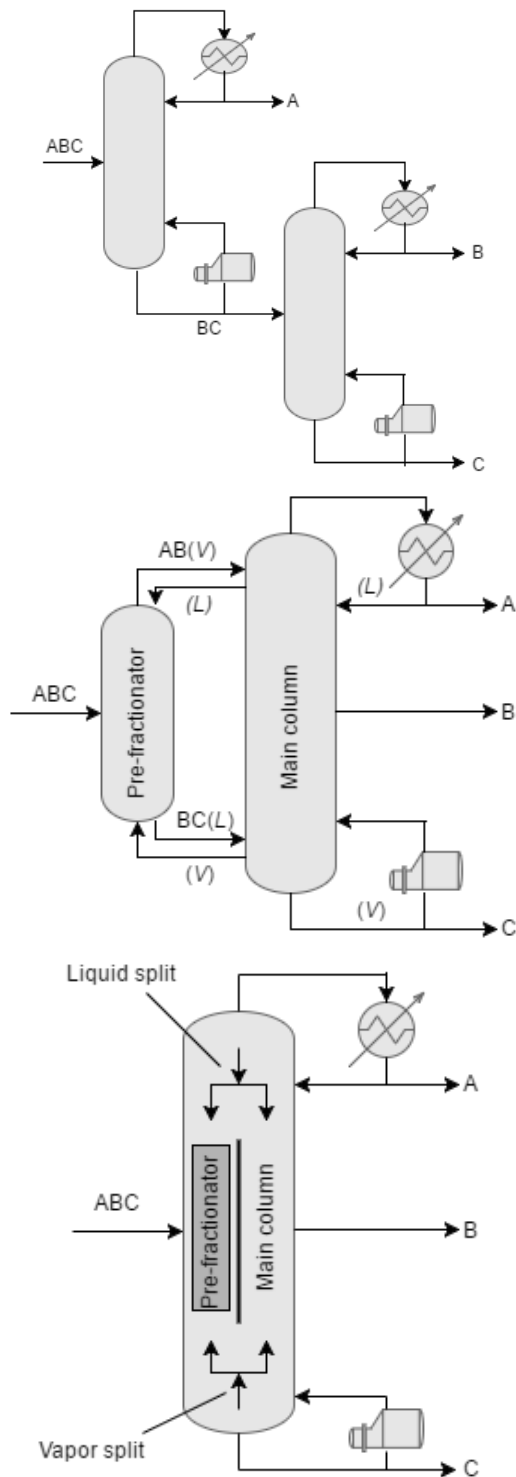
Figure 1. (Left) Conventional distillation column (Middle) Petlyuk column and (Right) Dividing wall column (DWC) configuration.

However, with the existence of internal recycle streams in DWC, due to the interconnecting stream, on all four column sections caused serious convergence problems. EO, on the other hand, offers good solution over SM, especially when dealing with design and optimization problems, solving heat integrated or recycled processes and model tuning

analysis. EO modelling compensates the convergence problem by accumulating all model equations together and solves them at the same time. Modelling of DWC via first principle EO modelling is not an easy task as it is considered as complex non-standard distillation column. One main reason is due to the interconnectivity of input/output variables, especially on the pre-fractionator section and main column section.

Work on EO modelling of DWC is however limited due to its modelling complexity. Dunnebier and Pantelides had considered the modelling of DWC using so called detailed column superstructures based on the State Operator Network formulation[3]. Due to the complexity of the models and mathematical problems, determination of the optimal structure referring to the suggested approach encountered some obstacles in optimization. Pattison *et al.*[4] also presented a new modelling approach based on the Pseudo-transient method. They reformulated the steady-state MESH (material, equilibrium, summation, and heat) equations of DWC as differential-algebraic equation (DAE) system which has the same steady state solution as the original system. These works applied a complicated EO approach to DWC modelling, which is time-consuming to comprehend. As such, we introduced a much simpler and systematic modelling approach. The proposed method solves the input/output variables connectivity of different equation systems by introducing a port and stream concept. Generally, the approach presents an equation system which functionally similar to a unit operation, i.e., column, reboiler, and condenser, with a presence of ports to identify the standardization of input and output variables. In addition, the existence of streams in connects another individual equation system together. To aid the model development, a MOSAIC modelling software will be used as modelling tools and gPROMS to solve the equation systems.

2. Modelling methodology

This section describes details of the proposed method. For better understanding, this section starts with definition of equations systems and variables involved in modelling of DWC.

2.1 Equation system and variables of DWC

Equation system is combination of fundamental principle of the underlying process or unit operation under considerations by reformulating the MESH (material, equilibrium, summation, and heat) equations. The DWC models in this work were based on the conventional equilibrium-based models of the distillation column. In this work we are focusing on the product composition and composition along the DWC. Energy balance will be our future work. The following assumptions had been taken into account for the model development:

1) Steady-state equilibrium stage model.
2) Average phase equilibrium constant.
3) Material balance.
4) Constant vapour split ratio as it is fixed by column design.

For the rectifying section, pre-fractionator section, main section, and stripping section the component material balance for component i at stage j is given as:

$$0 = V_{j+1}y_{j+1} + L_{j-1}x_{j-1,i} - V_j y_{j,i} - L_j x_{j,i} + F_j z_{j,i} - S_j x_{j,i} \tag{1}$$

Where, S represents a side stream flow rate. Summation equations is given in equation (2) whereas equilibrium relationship is given in equation (3).

$$\sum_{i=1}^{N} x_{j,i} = 1 \quad \sum_{i=1}^{N} y_{j,i} = 1 \tag{2}$$

$$y_{j,i} = K_{j,i} x_{j,i} \tag{3}$$

For the condenser, the material balance is:

$$0 = V^{(upper)} \cdot y_i^{(upper)} - L_0 \cdot x_{D,i} - D \cdot x_{D,i} \tag{4}$$

Whereas, the summation equation is given as:

$$\sum_{i=1}^{N} x_{D,i} = 1 \tag{5}$$

For the reboiler,

Material balance:

$$0 = L^{(bottom)} \cdot x_i^{(bottom)} - V^R \cdot y_i^R - W \cdot x_{W,i} \tag{6}$$

Equilibrium relationship:

$$y^R = K^R \cdot x_{W,i} \tag{7}$$

Summation equation is:

$$\sum_{i=1}^{N} x_{j,i} = 1 \quad \sum_{i=1}^{N} y_{j,i} = 1 \tag{8}$$

At the intersection of rectifying section with pre-fractionator and main column, the vapor mixing is represented by,

$$V_{j=NS+1}y_{j=NS+1,i} = V^{left}y_i^{left} + V^{right}y_i^{right} \tag{9}$$

$$V_{j=1}y_{j=1,i} = V^{left}y_i^{left} \tag{10}$$

$$V_{j=1}y_{j=1,i} = V^{right}y_i^{right} \tag{11}$$

Whereas, liquid splitting is represented by,

$$\alpha L_{j=NS} = L^{left} \tag{12}$$

$$x_{j=NS,i} = x_i^{left} \tag{13}$$

$$(1-\alpha)L_{j=NS} = L^{right} \tag{14}$$

$$x_{j=NS,i} = x_i^{right} \tag{15}$$

$$L_{j=0}x_{j=0,i} = L^{upper}x_i^{upper} \tag{16}$$

On the other hand, at the intersection of pre-fractionator and main with stripping sections vapor splitting is represented by,

$$V_{j=NS+1}y_{j=NS+1,i} = V^{bottom}y_i^{bottom} \tag{17}$$

$$\beta V_{j=1} = V^{left} \tag{18}$$

$$y_{j=1,i} = y_i^{left} \tag{19}$$

$$(1-\beta)V_{j=1} = V^{right} \tag{20}$$

$$y_{j=1,i} = y_i^{right} \tag{21}$$

And liquid mixing is represented by,

$$L_{j=0}x_{j=0,i} = L^{left} \cdot x_i^{left} + L^{right} \cdot x_i^{right} \tag{22}$$

$$L_{j=NS}x_{j=NS,i} = L^{left}x_i^{left} \tag{23}$$

$$L_{j=NS}x_{j=NS,i} = L^{right}x_i^{right} \tag{24}$$

The connection between rectifying and condenser unit are given by,

$$V_{j=1}y_{j=1,i} = V^{out}y_i^{out} \tag{25}$$

$$L_{j=0}x_{j=0,i} = L^{in}x_i^{in} \tag{26}$$

Meanwhile, stripping and reboiler connectivity is given by,

$$L_{j=NS}x_{j=NS,i} = L^{out}x_i^{out} \tag{27}$$

$$V_{j=NS+1}y_{j=NS+1,i} = V^{in}y_i^{in} \tag{28}$$

The subscripts NS and $NS+1$ indicate that liquid and vapour flow on the last stage of each section will be connected to other section. The superscripts in and out are known to be the inlet and outlet flow which happen between stripping/reboiler and rectifying/condenser, while superscript of upper, left, right, and bottom are referring to rectifying, pre-fractionator, main, and stripping section respectively. Next, α indicates a liquid splitting factor and β is for vapour split factor.

2.2 Unit block and ports

The challenge in modelling of DWC is to accommodate the internal flows between the partition walls. In this work, we treated rectifying section, pre-fractionator, main, and stripping section as individual unit block along with the condenser and reboiler. A unit block model consists of sets of mathematical equation systems to describe the

phenomenon occurring inside the unit. This creates a convenient way to model the DWC as a group of 6 sub-unit bocks with underlying equation systems. **Table 1** indicates the underlying classification of equation system involved in the respective unit block.

Table 1. Unit block and its associated equation systems

| Unit block	Equation systems involved
Rectifying	1, 2, 3, 9, 12, 13, 14, 15, 25, 26
Pre-fractionator	1, 2, 3, 10, 16, 17, 23
Main	1, 2, 3, 16, 17, 24
Stripping	1, 2, 3, 18, 19, 20, 21, 22, 27, 28
Condenser	4, 5
Reboiler	6, 7, 8

In order to properly connect different unit blocks together, the application of port is introduced into the unit block. Port is used to provide reconciliation of different input and output variables of a unit block to or from another unit block. To further describe the concept, an example to rectifying unit is considered (referring to **Figure 2**). Rectifying unit is located at the top section of the DWC internal configuration. Vapour from the pre-fractionator section and main section will be mixed at the last stage of the rectifying unit, whereas, liquid flow at the last stage will be split into both side of pre-fractionator section and main section. To describe this phenomenon, equation (9) represents the vapour mixing occurred at the last stages of the rectifying section. Port 1 (P1) signifies the vapour flow from the first stage of the pre-fractionator section (Equation (10)), whereas, P5 signifies the vapour flow from the first stage of the main section (Equation (11)). Thus, the input variables involved for the vapour mixing are $V^{left}, V^{right}, y_i^{left}$ and y_i^{right}. Equation (12) to equation (15) on the other other hand signify the splitting of liquid flow flowing down from the last stage of rectifying section into pre-fractionator section and main section. P2 denotes the liquid split to the pre-fractionator represented by equation (12) and equation (13), whereas, P4 denotes the liquid split to the main section represented by equation (14) and equation (15). Therefore, the output variables for the liquid split are $L^{left}, x_i^{left}, L^{right}$, and x_i^{right}. In addition, P6 denotes the liquid flow from condenser to the first stage of the rectifying unit which describes by equation (26). P3, on the other hand, denotes the

vapour flow from the first stage as described by equation (25). Therefore, V^{out} and y_i^{out} are the output variables of the vapour flow, whereas, L^{in}, and x_i^{in} are the input variables of the condenser.
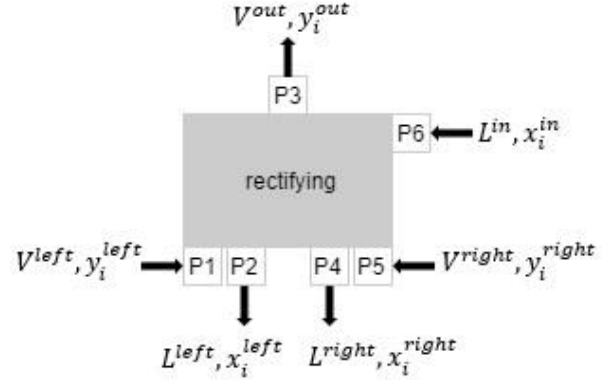
Figure 2. Rectifying Unit Block Model with Ports**.**

For the port to be reconciled, it needs to have an interface variable. An interface consists lists of identified independent variables to restrict the accessibility of the other unrelated variables in the overall equation system. In this example, f and c_i were used as interface variable to represent vapour/ liquid flowrate and composition of component i, respectively. Overall, f will represent variables $V^{out}, L^{in}, V^{left}, L^{left}, V^{right}$ and L^{right}, whereas, c_i will represent variables $y_i^{out}, x_i^{in}, y_i^{left}$, x_i^{left}, y_i^{right}, and x_i^{right}. The port and interface application are visualized in **Figure 3.**
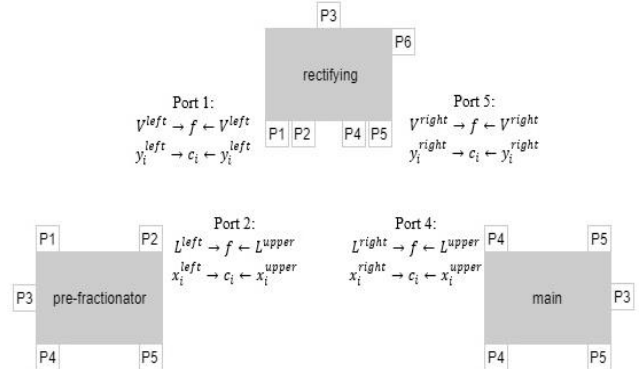

Figure 3. Port and interface application in DWC sub-units block**.**

2.3 Unit block connectivity using stream

When all the unit blocks and its associated ports have been created, they are then ready to be connected to each other using streams. The purpose of stream is to connect two different units block that provides ports to work jointly in a flowsheet. The

implementation of a stream requires list of identified variables in the interface along with ports in order to be combined together. The flow direction of the stream, either "output" port or "input" port indicator needs to be specified for smooth connectivity. The output port represents the start of the stream while input port indicates the end of the streams, depending on how the flow direction works. **Figure 4** exhibits the complete model of DWC with ports and streams application. The dotted and solid lines indicate the flow of liquid and vapor respectively inside DWC.
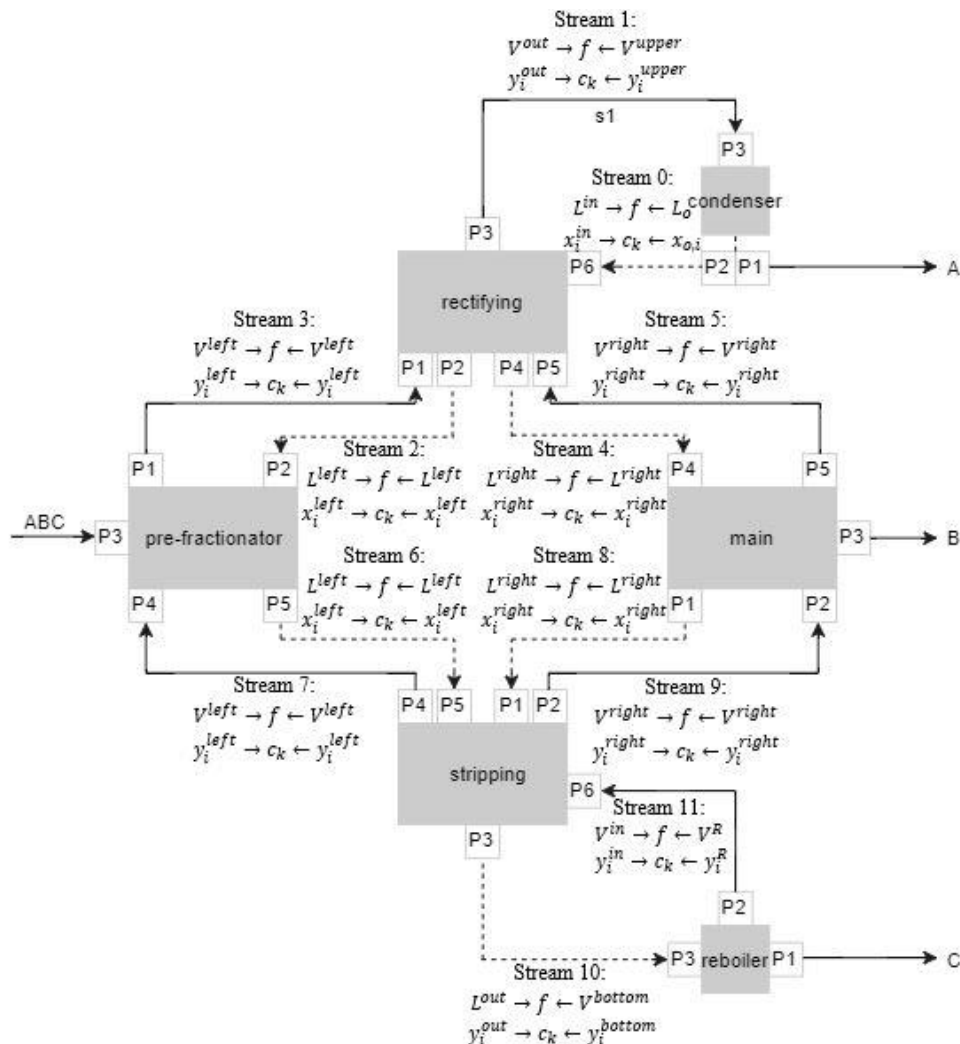
Figure 4. Model of DWC with port-stream application.

3. Model development

The DWC development based on the proposed methodology was performed in MOSAIC. MOSAIC is a web-based equation oriented modelling environment for modelling of chemical processes, which developed by the Process Dynamics and Operations Group at Technische Universitaet Berlin. One of the MOSAIC features is modelling at the documentation level[5]. The model equations in MOSAIC are entered using LaTeX style and saved in MathML which provide higher readable model to the user. MOSAIC additionally works as a code generator which is able to export the developed model into certain programming language code.

3.1 Variable Specification and Classification

One of the important features of EO modelling is the variables' specification required as input data and generated as output predictions. Each variable in the equations will be specified by fixing the value or enabling the modeling tool to manipulate the value[6]. Those variables are classified as design and iteration values. Design variables indicate the fixed value variables, whereas, iteration variables mean calculated variables in the equation systems.

72

Those variables can be changed either from iteration variables to design variables or vice versa until the DOF becomes zero. For the case of the DWC model, the vapor composition, constant phase equilibrium, liquid and vapor flow in respective unit are assigned as design variables. Meanwhile, the liquid composition and products stream composition are set to be iteration variables. Another important issue to be considered is the initial value for the iteration variables. It should be noted that, in modeling solving, good initial values are crucial since the developed model would work well when all variables near the solution[7]. One may be used SM software, i.e., Aspen Plus is used to aid initilization values estimation for a good convergence.

3.2 DWC model structural analysis

To guarantee that the equation systems of DWC model are well formulated, the degree of freedom (DOF) analysis is carried out to determine if the equation systems are well, under, or over determined. **Figure 5** shows the structural analysis of mixed DOF of the DWC model. The consequences of inaccurate chosen of design variables in the DWC system lead to the insufficient structure analysis (referring to **Figure 5**), and unsolved problems in the compiler or solver.
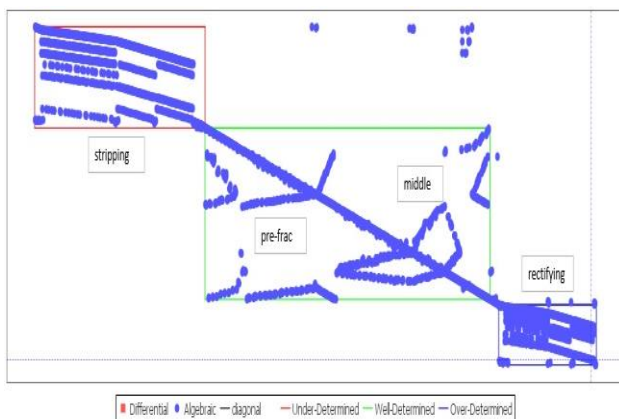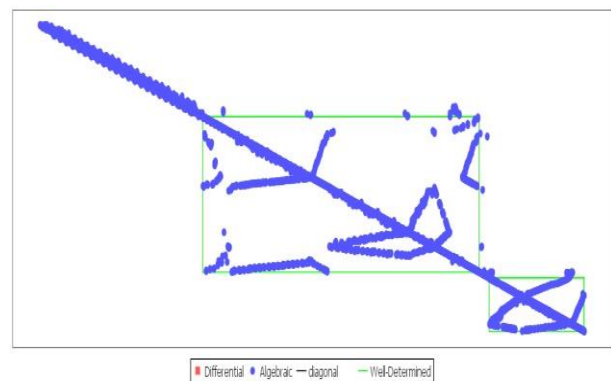

Figure 5. Unstable structure analysis of DWC system.

The insufficient structure analysis generates three different colours of rectangle/line which are green, blue, and red. The under-determined equation system represented in blue rectangle line is due to more equations being provided than calculated variables, while the red rectangle line exhibits under-determined equation system caused by less equation being provided than variables to be calcu-

lated. From the figure, the equation systems for pre-frac and middle are well determined. Stripping section and reftifying equation systems on the other hand are under-determined and over-determined, respectively.

From the **Figure 5**, it visualized that the structure of the equation systems is affected by the chosen degree of freedom[8]. In other words, to achieve a well-posed problem, the needs in change of design variable and calculated variable specifications are compulsory to preserve DOF. To ensure that all equation systems are well determined, selection of design and iteration variables is important to solve the given problem, to identify the product stream compositions. Based on the whole structure analysis of DWC, further observation shows that some of the design variables on rectifying equation system are set as iteration variables and likewise some of the iteration variables on stripping equation system are set as design variables. Therefore, to fix this problem, the classification of design and iteration variables should be restructured.

After proper assignments of design and iteration variables, **Figure 6** shows that the overall six sub-equation systems of DWC model are "well determined", which means the model is solveable. Other than that, the structure analysis also gives the information on the type of equations. In this case, the structure analysis indicates that the whole equations system of DWC involved with algebraic equations with non-existing of ordinary differential equations (ODEs) as well as non-existing differential algebraic equations (DAEs).

Figure 6. Well determined structure analysis of DWC system.

4. Model validation

The completed DWC model simulation in

MOSAIC was exported to gPROMS ModelBuilder to solve the compositions in the column. To demonstrate the capability of the modelling approach and to increase the acceptance of the model, the modelled DWC is validated with two case studies. Case Study 1 refers to open literature experimental data depicted from Nguyen et al.[9], whereas, Case Study 2 refers to fatty acid fractionation from Illner and Othman[2]. For Case 1, the model will be compared with the second data set of the experimental work. Furthermore, in Case 2, the model will be compared to a simulated case study for fractionating fatty acid in DWC.

4.1 Case study 1: Separation of ternary mixture: Methanol/ 1-Propanol/ 1-Butanol

The verification data were based on the experimental work by Nguyen et al.[9] Their work involved separation of ternary mixtures of alcohol namely methanol, 1-propanol, and 1-butanol using DWC pilot plant.

Table 2. Operating parameter of alcohol ternary mixture for data set 2

| Parameter	Specification
Feed flowrate (kg/h)	5.77
Feed temperature (°C)	85.4
Feed composition (wt%)	
Methanol	0.29
1-propanol	0.46
1-butanol	0.25
Liquid split	0.5
Vapor split	0.5
Reboiler duty (kW/h)	5.1
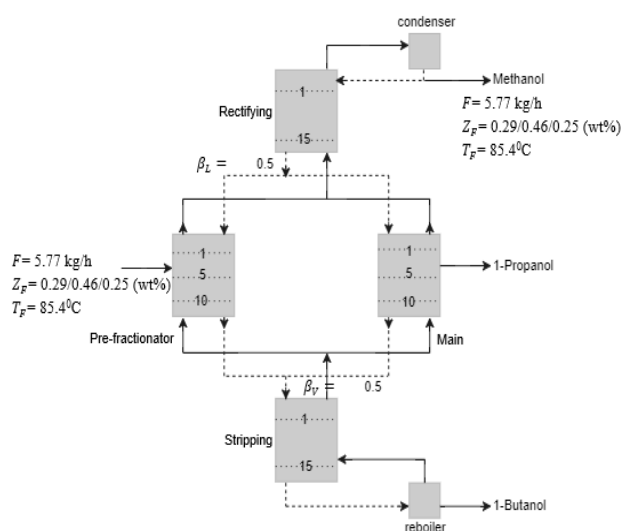
Figure 7. Schematic DWC configuration for the alcohol fractionation.

According to the volatilities of the components,

methanol is withdrawn as a distillate product, while 1-propanol and 1-butanol are collected as side stream and bottom product, respectively. The column structure consists of 15 stages on the rectifying and the stripping section, and 10 stages on the pre-fractionator and main section. The schematic configuration is shown in **Figure 7.** The liquid split was set up to be 0.5 and so does with vapor split as cross sectional areas of pre-fractionator and main column are the same. **Table 2** indicates the operating parameter used in the experimental work.

4.1.1 Initialization value

Good initial values are crucial since the developed model would work well when all variables near the solution[7]. Therefore, to aid the initialization value estimation, Aspen Plus was used in this work. **Figure 8** shows a DWC configuration in Aspen plus flowsheet. A DWC model does not exist in Aspen Plus library due to its customized model. Therefore, an equivalent model of DWC with four rigorous RADFRAC model, two units of mixer and splitter for liquid and vapor internal mixing and splitting purpose were implemented. The results of simulation generated in Aspen Plus were used to provide the initial value of all the unknown variables in the DWC equation systems to gain a good convergence of output value prediction. Once the initialization value was given, the model is ready to be translated into gPROMS code.
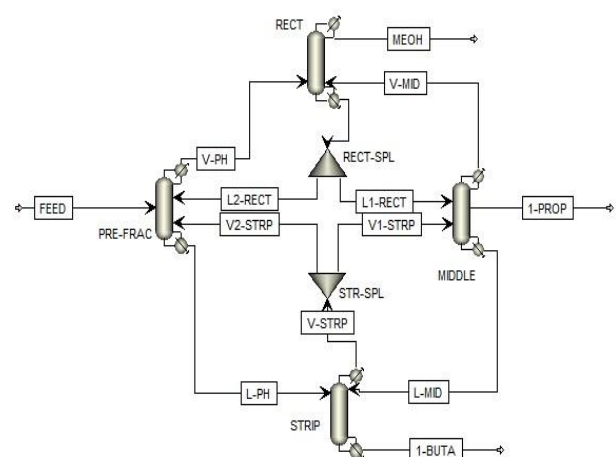
Figure 8. Column configuration of DWC for alcohol mixture.

4.1.2 Model solver

The complete process model of DWC involved large sets of nonlinear algebraic equation (NLE)

and was numerically solved using differential-algebraic solver (DASolver) in gPROMS solution algorithm. This includes Block Decomposition Non-Linear Solver (BDNSOL) and SPARSE solver, which is able to solve the restricted iteration variables that lie within specified lower and upper bound. BDNSOL solver resolves the non-linear equation, according to an individual unit block of rectifying, pre-fractionator, main, stripping, condenser, and reboiler. The variables in each unit blocks were solved using SPARSE through Newton-type iterative method, which resulted on a prediction of component variable in each stage.

4.1.3 Value comparison

The relative error between EO simulation results and literature data was calculated as follows:

$$\text{Relative error (\%)} = \frac{\text{initial} - \text{final}}{\text{initial}} \times 100 \qquad (29)$$

In this study, the relative error which is less than 10% is considered reasonable due to small value of the experimental data from Nguyen *et al.*[9] Moreover, the process characteristic of DWC, such as pressure, energy, and heat transfer were not considered in the modeling work. The verification results are shown in **Table 3**.

Table 3. Relative error between literature data and EO simulation results for data set 2

Parameters	Unit	Literature data	EO simulation	Relative error (%)
Distillate flowrate	(kg/h)	2.00	2.00	0
Methanol composition	(wt%)	0.85	0.93	9.41
Side stream flowrate	(kg/h)	2.17	2.17	0
1-propanol composition	(wt%)	1.00	1.00	0
Bottom stream flowrate	(kg/h)	1.70	1.69	0.58
1-butanol composition	(wt%)	0.89	0.90	1.12

For distillate product stream, the result acquired from EO simulation for Methanol composition was 0.93 wt% which differs about +0.08 wt% from reference literature data and led to 9.41% relative error. The side product stream, 1-propanol demonstrates an equivalent of convergence value with literature data in regards to product flowrate and composition. For bottom stream flowrate, a different about +0.1 kg/h in comparison to literature experimental data was recorded which resulted in 0.58% relative error. Whereas, the composition of 1-butanol generated from EO simulation appeared to have a slightly different about +0.01 wt% and makes the relative error of 1.12%. Therefore, from the table, the proposed model shows a good convergence in term of products flowrate and compositions and has less than 10% relative error which shows applicability of the proposed approach.
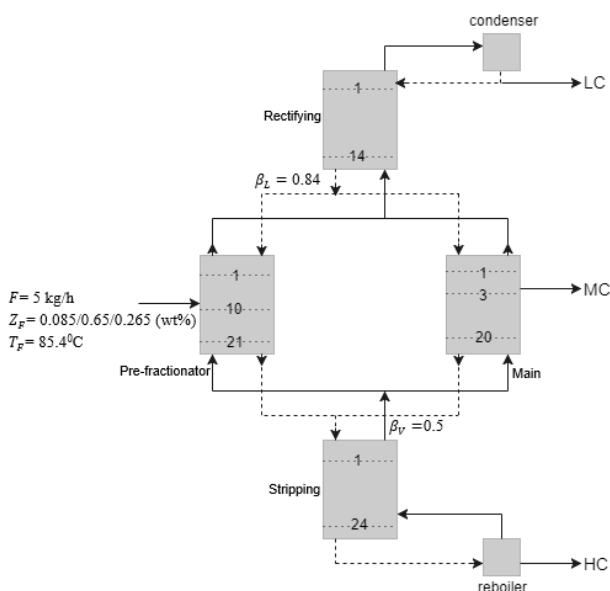
4.2 Case study 2: Fatty acid fractionation

The validated DWC model was then tested to a fatty acid (FA) fractionation. By far, in the oleo-chemical industry particularly for FA, the mixture had only been studied by[2] since most of the industry still using a conventional distillation columns to separate FA mixture[1,10,11]. The configuration of the dividing wall column for fatty acid fractionation was designed similarly using four columns sequence proposed by the authors. Fatty acid fractionation was separated into three cuts light-cut (LC), middle-cut (MC), and heavy cut (HC) according to their boiling points. The boiling point of LC which represented by C_{10} is 269 ℃, while the boiling point of MC (C_{14}) and HC (C_{16}) are 326 ℃ and 350 ℃, respectively. Since C_{10} is the most volatile component, it will be withdrawn as a distillate product. The least volatile component (C_{16}) will be withdrawn at the bottom of the column due to high boiling point, while the side stream goes to component C_{14}. The design parameter input was based on the simulation work done by Illner and Othman[2], but with slide modification that suits the pilot plant design capacity of 5kg/hr.

Figure 9 shows the schematic DWC configuration for fatty acid fractionation. The rectifying section consists of 14 stages, while pre-fractionator section has 21 stages, main section and stripping section have 20 and 24 stages, respectively. The condenser is at stage 0 and reboiler at the last/bottom stage of the column. Feed stream enters at stage 10 from the top in the pre-fractionator section and the side product is withdrawn at stage 3 in the main section. The liquid split ratio is 0.84, and the vapor split ration is 0.5. Thus the wall is located at the middle of the column.

Using the same relative error calculation in

equation (29), **Table 4** compares the product specification value in Aspen Plus and the developed model. Result shows that the highest relative error is 0.88% for bottom stream flow rate. The bottom flowrate from model was -0.01 lower than the initial reference data which is 1.13 kg/h, while for the HC composition, the model shows 0.999 wt% which led to 0% of relative error. For both side stream flowrate and MC product composition, the value indicates zero difference between initial reference data and the model which was 3.451 kg/h and 0.942 wt%, respectively. Same goes to distillate flowrate composition which represented by LC, where the initial input data and final value output prediction was identical. The results conclude the applicability of the developed model.

Figure 9. Schematic DWC configuration for fatty acid fractionation.

**Table 4.** Comparison between specified product value in Aspen Plus and EO simulation

Parameters	Unit	Aspen Plus	EO simulation	Relative error (%)
Distillate flowrate	(kg/h)	0.420	0.420	0
LC composition	(wt%)	0.999	0.999	0
Side stream flowrate	(kg/h)	3.451	3.451	0
MC composition	(wt%)	0.942	0.942	0
Bottom stream flowrate	(kg/h)	1.130	1.120	0.88
HC composition	(wt%)	0.999	0.999	0

4.2.1 FA composition trend in DWC

Figure 10 gives the composition profiles in the rectifying, main, and stripping sections. **Figure 10** (**a**) shows the composition trend for the rectifying section. It can be seen that the highest composition of LC was at stage 1 and remain consistent up to stage 10 with 0.999 to 0.995 wt%. At stage 11 up to stage 13, the composition begins to decrease gradually and became 0.076 wt% at stage 14. Meanwhile, the side component, MC starts to increase slowly from stage 11 at 0.037 wt% to 0.867 wt% at stage 14, while the HC product almost remains at 0.0 wt% at the last stage of rectifying column.

Figure 10 (**b**) shows the trend for LC, MC, and HC product composition in main section. From the graph, as LC component starts to enter the first stage of the main column, the composition indicates 0.0 wt%. On the contrary, MC composition remains constant around at composition of 0.93 wt% at stage 15 until it reached stage 31 and starts to decrease to 0.645 wt% at the last stage of the main column. For HC component, the composition remains constant at stage 15 up to stage 31 with 0.057 wt% and increases slowly at 0.355 wt% when reached the last stage of the main section.

Figure 10 (**c**) shows the composition trend in the stripping column. From the graph, LC component composition remains at 0 wt% along the stripping column, which means zero existence of distillate product on the stripping section, while for MC component, it starts to decrease steadily as it enters the first stage from 0.237 wt% to almost 0.0 wt% until the last stage of stripping section. On the other hand, the composition of HC component begins to increase slowly starting from the stage 35 up to stage 41, and reached the highest composition with 0.999 wt% at the last stage of the stripping section. Therefore, these graphs clearly shows that LC and MC components are separated at the upper stage of the main column, meanwhile, MC and HC components are separated at the bottom stage of the main column.

(a)

(b)

(c)
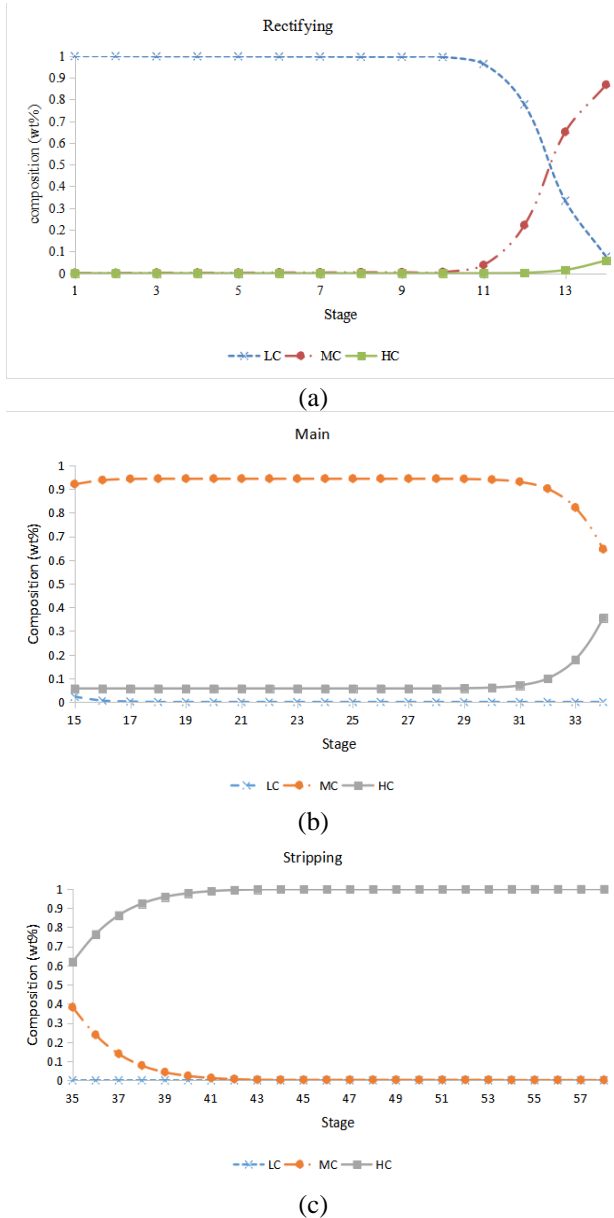
Figure 10. Components trend along **(a)** Rectifying, **(b)** Main, and **(c)** Stripping section.

4.2.2 Relative Gain Array (RGA)

To further exploit the developed model, RGA analysis was conducted to the DWC FA fractionation model. Based on the model, RGA analysis could be used to determine suitable control scheme at steady-state. For DWC, a multi-input-multi-output (MIMO) control scheme was used due to the possibility of multiple interaction between manipulated and controlled variables[12].

According to Koko and Barakat[13], there are seven DOF corresponding to seven manipulated variables in DWC. However, the liquid split (β_L) and vapor split (β_V) are not suggested to be a manipulated variables, because they could cause a se-

rious problem in the operation and controllability of DWC[14,15]. Therefore, five available manipulated variables namely reflux flowrate (L_o), distillate flowrate (D), side flowrate (S), bottom flowrate (B), and vapor boilup (V) were used to analyze its interaction to the controlled variables which are distillate, side, and bottom product compositions. For DWC, a combination of three manipulated variables was chosen. Thus, based on the five manipulated variables, there are four possible control scheme configurations namely L-S-V, D-S-V, L-S-B, and D-S-B. To determine the best control scheme configurations, the four control schemes were analyzed.

Table 5 consists of the base case values for the FA fractionation. The open-loop gain was calculated from the step changes on each manipulated variables. The step changes were carried out by changing one manipulated variables at a time while putting the rest of manipulated variables constant at their base case value. For each control schemes configuration, a 10% step change of the base case value on each manipulated variables was applied. The results of the steady-state gain array and its calculated RGA value are presented from **Table 6** up to **Table 9**.

Table 5. FA fractionation base case values

Manipulated variables	Value	Controlled variables	Value
Reflux flowrate, Lo (kg/h)	25.74	LC (wt%)	0.999
Distillate flowrate, D (kg/h)	0.42	MC (wt%)	0.942
Side flowrate, S (kg/h)	3.45	HC (wt%)	0.999
Bottom flowrate, B (kg/h)	1.13		
Vapour boilup, V (kg/h)	35.13		

Table 6. Steady state gain matrix and RGA for L-S-V scheme

CV	Steady state gain			Relative Gain Array (RGA), λ		
	MV$_1$ = L	MV$_2$ = S	MV$_3$ = V			
X$_{LC}$	-0.03559	0	0.00006	0.99999	0	0.00001
X$_{MC}$	-0.00081	-0.01151	-0.00081	0.00001	0.99421	0.00578
X$_{HC}$	0	0.00006	-0.00070	0	0.00579	0.99421

Table 7. Steady state gain matrix and RGA for D-S-V scheme

CV	Steady state gain			Relative Gain Array (RGA), λ		
	MV$_1$ = D	MV$_2$ = S	MV$_3$ = V			
X$_{LC}$	0.04524	-0.00551	-0.00077	1.22945	-0.26012	0.03067
X$_{MC}$	0.02143	-0.01206	0.00032	-0.26089	1.25206	0.00883
X$_{HC}$	-0.00095	-0.00009	-0.00075	0.03143	0.00807	0.96050

77

Table 8. Steady state gain matrix and RGA for L-S-B scheme

CV	Steady state gain			Relative Gain Array (RGA), λ		
	MV$_1$ = L	MV$_2$ = S	MV$_3$ = B			
X$_{LC}$	-0.03561	0	0	1.00000	0	0
X$_{MC}$	0.00042	-0.05197	0.00531	0	0.97339	0.02661
X$_{HC}$	-0.00059	0.00672	0.02513	0	0.02661	0.97339

Table 9. Steady state gain matrix and RGA for D-S-B scheme

CV	Steady state gain			Relative Gain Array (RGA), λ		
	MV$_1$ = D	MV$_2$ = S	MV$_3$ = B			
X$_{LC}$	0.10476	-0.00029	0	1.11392	-0.11392	0
X$_{MC}$	0.12976	-0.00490	0.01142	-0.10542	1.43829	-0.33288
X$_{HC}$	0.00714	0.00075	-0.00779	-0.00851	-0.32437	1.33288

According to the RGA principles, it is strongly recommended to choose the value of relative gains array λ_{ij}, (which are positive and closed to one[13,16]. This shows that the control loop between controlled variable i and manipulated variable j has a strong interaction and did not be effected by the other control loops.

Table 7 and **Table 9** show the RGA value for D-S-V and D-S-B configurations. The values of λ_{11} are 1.22945 and 1.11392, respectively. For the first manipulated variable, it indicates that the manipulation of distillate flow did not only affect the distillate composition (x_{LC}), but also experience an interaction with other controlled variables (x_{MC} and x_{HC}) as well. For the second manipulated variable, which is side flowrate, these configurations show the value of λ_{22} equals to 1.25206 for D-S-V and 1.43829 for D-S-B. This shows that the interaction between side flowrate on side composition (x_{MC}) does have an interference from other controlled variables (x_{LC} and x_{HC}) too. Finally, for the third manipulated variable, the interaction between vapor boilup in D-S-V and bottom flowrate in D-S-B on bottom composition (x_{HC}) give the λ_{33} value of 0.96050 and 1.33288. It means that the interaction of control loop under consideration was provoked by the other control loops (x_{LC} and x_{MC}).

The other two configurations, L-S-V and L-S-B, on the other hand, were selected due to small interaction between the loops. Based on **Table 6** and **Table 8**, for L-S-V and L-S-B configurations, the value of λ_{11} equals to 0.9999 and 1.0000,

which show that distillate composition (x_{LC}) only responds to the manipulation of distillate flowrate and did not respond with other manipulated variables (x_{MC} and x_{HC}). For the second manipulated variable for both configurations, which is side flowrate, the values of λ_{22} are 0.99421 and 0.97339, which are close to unity and these indicate that the side flowrate can control the side composition (x_{MC}) with a very small interference from other controlled variables (x_{LC} and x_{HC}). Same goes to λ_{33}, the effect of manipulated variables of vapor boilup in L-S-V and bottom flowrate in L-S-B on bottom composition (x_{HC}) is substantial compared to other controlled variables with the value of 0.99421 and 0.97339, respectively.

Based on the RGA analysis results, the effect of interaction in the D-S-V and D-S-B configurations was higher than unity compared to the L-S-V and L-S-B configurations. In other words, it can be concluded that L-S-V and L-S-B configurations are the best options. With regards to manipulated and controlled variable pairings, the RGA analysis shows that no cross pairing should be implemented on the L-S-V and L-S-B configurations. As a result, the reflux flowrate will control the distillate product (x_{LC}), side flowrate will control the side product (x_{MC}), and bottom vapor boilup would control the bottom product (x_{HC}).

5. Conclusion

In this paper, a systematic approach of modelling complex distillation column with port and stream connectivity was introduced. The method has been applied to modelling of DWC. The proposed method provides a simpler way to model an EO based process by defining the input/output variables of the unit block and standardizing the variables through the existing unit block equation system. However, some aspects should be thoroughly reviewed particularly in solving a large mathematical problem such as verification/classification of variables, DOF, and model structure. Failure to do so leads to errors and unsolved problems. The developed approach had been compared with two case studies for verification and validation purpose and shows good convergence. This approach can be applied on other process system and does not only

applicable on DWC. The model was also extended to RGA analysis. For the fatty acid fractionation, L-S-V and L-S-B configurations are the best control configurations. The analysis also shows that reflux flowrate, side flowrate and vapor boilup are best to control distillate product, side product and bottom product, respectively.

Conflict of interest

The authors declare that they have no conflict of interest.

Acknowledgements

References

1. Aly G, Ashour I. Applicability of the perturbed hard chain equation of state for simulation of distillation processes in the oleochemical industry. Part I: Separation of Fatty Acids. Separation Science and Technology 1992; 27(7): 955–974. Available from: http://doi.org/10.1080/01496399208019735
2. Illner M, Othman MR. Modelling and simulation of a dividing wall column for separation of fatty acid in oleochemical industries; 2014 Oct 29; Kuala Lumpur. Taylor's University & IChemE, Kuala Lumpur: SOMChE & RSCE 2014 Conference; 2014. p. 1–9.
3. Dunnebier G, Pantelides CC. Optimal design of thermally coupled distillation columns. Industrial & Engineering Chemistry Research 1999; 38(1): 162–176.
4. Pattison RC, Gupta AM, Baldea M. Equation-oriented optimization of process flowsheets with dividing-wall columns. AIChE Journal 2015; 62(3): 704–716. doi: 10.1002/aic.15060
5. Kuntsche S, Barz T, Kraus R, *et al.* MOSAIC a web-based modeling environment for code generation. Computers & Chemical Engineering 2011; 35(11): 2257–2273. Available from: http://doi.org/10.1016/j.compchemeng.2011.03.022
6. Marchetti M, Rao A, Vickery D. Mixed mode simulation — Adding equation oriented convergence to a sequential modular simulation tool. Computer Aided Chemical Engineering 2001; 9: 231–236. Available from: http://doi.org/10.1016/S1570-7946(01)80034-1
7. Pantelides CC, Nauta M, Matzopoulos M, *et al.* Equation-oriented process modelling technology: recent advances & current perspectives; 2015 Feb; Abu Dhabi, UAE. Abu Dhabi, UAE: 5th Annual TRC-Idemitsu Workshop; 2015.
8. Gani R, Cameron IT, Lucia A, *et al.* Process Systems Engineering, 2. Modeling and Simulation. Ullmann's Encyclopedia of Industrial Chemistry 2012. Available from: http://doi.org/10.1002/14356007.o22_o06
9. Nguyen TD, Rouzineau D, Meyer M, *et al.* Design and simulation of divided wall column: Experimental validation and sensitivity analysis. Chemical Engineering and Processing: Process Intensification 2016; 104: 94–111. Available from: http://doi.org/10.1016/j.cep.2016.02.012
10. Chemtech S, Acid A, Separation A, *et al.* Separation technology for the chemical process industry [Internet]. Switzerland: Sulzer Ltd.; 2017. Available from: https://www.sulzer.com
11. IPS Engineering. Oleochemical processing plant. Angers, France: IPS Engineering; 2014. Available from: https://www.ips.engineering
12. Sankaranarayanan D, Deepakkumar G. Implementing the concept of relative gain array for the control of MIMO system: Applied to distillation column. Annals University Regional Centre, Coimbatore, India 2015; 4648–4653.
13. Koko IOM, Barakat TAM. Modelling and control analysis of dividing wall distillation columns. University of Khartoum Engineering Journal (UofKEJ) 2015; 5(1): 18–25.
14. Mutalib MIA, Smith R. Operation and control of dividing wall distillation columns. Chemical Engineering Research and Design 1998; 76(3): 319–334. Available from: http://doi.org/10.1205/026387698524965
15. Cho Y, Kim B, Kim D, *et al.* Operation of divided wall column with vapor sidedraw using profile position control. Journal of Process Control 2009; 19(6): 932–941. Available from: http://doi.org/10.1016/j.jprocont.2008.12.003
16. Chansomwong A, Zanganeh KE, Shafeen A, *et al.* A decentralized control structure for a CO_2 compression, capture and purification process: An uncertain Relative Gain Array approach. IFAC Proceedings Volumes (IFAC-Papers Online) 2011; 18: 8558–8563. Available from: http://doi.org/10.3182/20110828-6-IT-1002.00663