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Process Optimization of DWC for Fatty Acid Fractionation using Taguchi Methods of Experimental Design

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Experimental design (ED) is a powerful technique for optimizing the performance of a process. Compared to a model-based optimization technique, ED does not require the development of mathematical formulation but nevertheless needs a good model or experimental setup and statistical analysis. This paper presents an ED based optimization approach of a dividing wall column (DWC) model for industrial oleochemical fatty acid fractionation. Taguchi method of ED will be used for the optimization of the control variables for efficient fractionation of fatty acid cuts, namely light-cut (LC), middle-cut (MC) and heavy-cut (HC). The DWC model was developed in Aspen Plus software using a rigorous four-column configuration. It is used to identify sensitive parameters, simulate experimental layout trials and results validation. The process is designed to achieve product purity of >99 mol.% LC and MC, and >90 mol.% for HC. A step-by-step approach to process optimization using Taguchi method is presented along with the statistical analysis results and their interpretation. The ED output will help in understanding the interaction between variables and their effects. With its simple, fast and non-tedious approach, ED using Taguchi method could prove its significance in improving the performance of fatty acid fractionation using DWC for possible industrial application.

1. Introduction

Optimization has been employed in various chemical engineering problems to find the best solution to a process within given bounds and constraints. One approach of optimization is by formulating the problem using model equations. This task requires the elements such as predictive model, objective function, constraints and control variables. Such an approach, however, requires extensive mathematical model development thus prone to modelling error, ill-defined problem, convergence issues and computational complexity. Another approach with less mathematical effort is through the use of a modular based process simulator which helps especially in developing highly interactive and complex processes. However, it still demands robust computational algorithms and prone to convergence problems. ED is an interesting alternative to model or equation based optimization. ED does not require extensive mathematical development; nevertheless, it needs a good model or experimental setup and statistical analysis. It is useful to study and understand process parameters interaction and then optimise the process performance using limited budget and resources. Taguchi method is a powerful ED technique (Antony et al., 2001), and has been applied successfully in many applications that involve complex process interactions. This paper discusses the application of Taguchi method for optimising a rigorous four column DWC model developed in Aspen Plus. A four column DWC configuration is a non-standard model in Aspen Plus and not easily converged. Carrying such a simulation requires experience and is computationally demanding. To achieve optimal design a lot of tuning is needed especially on sensitive parameters; for this, ED comes in handy. By implementing ED based optimization it is expected to minimize the computational complexity compared to model or equation based optimization i.e. Aspen optimization tool. This way, the complex model development using process simulators could be utilised along with a simpler approach for optimization; hence, it provides a simpler and practical approach for optimizing the performance of the process. The general steps for optimization using Taguchi method is illustrated in Figure 1.

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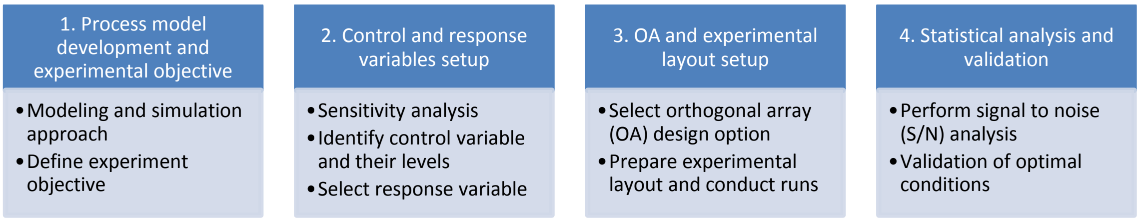


Figure 1: General steps for optimization using experimental design

2. DWC model development and experimental objective

DWCs are advantageous for separating ternary mixtures into pure fractions, especially medium boiling component. Its unique internal configuration reduces the investment and operating costs, which leads to lower carbon dioxide emission (Barroso-Muñoz et al., 2011). Because of these advantages, DWC has attracted many researchers and companies for various applications. To name a few biodiesel fractionation (Cho et al., 2015), azeotropic and extractive distillation process (Kiss et al., 2013), pressure swing absorption (Loy et al., 2015) and methyl acetate production (An et al., 2015). In 2013, crude palm oil (CPO) production in Malaysia recorded an increase of 2.3 % to 19.22 Mt against 18.79 Mt recorded in 2012 (AOTB, 2014). The oleochemical industry in Malaysia is now one of the largest in the world, which currently accounts for 39 % of world palm oil production and 44 % of world exports (MPOC, 2014). There are 18 oleochemical companies in operation in Malaysia; our survey shows that none of them apply DWC for their fractionation process. To show the applicability of DWC in oleochemical industry, an industrial DWC column for fatty acid fractionation is modelled using rigorous four RADFRAC configuration in Aspen Plus. The model is based on the modelling work of Othman and Illner (2014), which will be used to identify sensitive parameters, simulate experimental trials and results validation. The experimental objective is to have the response variable or product purity of >99 mol.% for LC and MC and >90 mol.% for HC with optimal setting of the control variables. Insights on the modelling approach is presented next.

2.1 Modelling and simulation approach

Sequential-modular (SM) based modelling of DWC using commercial simulators typically involves rigorous simulation of two columns (Kiss and Ignat, 2012); prior to rigorous simulation, Premkumar and Rangaiah (2009) employed three shortcut columns for estimating number of stages for rigorous simulation. A four column configuration has been employed by Dejanovic et al., (2011) for an aromatics processing plant. Recently, Othman and Illner (2014) employed four column configuration for fatty acid fractionation as shown in Figure 2. A four column configuration offers few advantages including flexibility in dimensioning the column sections and suitable for control system study in dynamic simulation (Dejanovic et al., 2011). Conversely, it requires extensive computational effort because of the complex interactions between different blocks that involves several recycle loops and more interconnected streams. This lead to lack of proper initialization and therefore prone to convergence error. Simulating the model is not straightforward compared to a standard distillation block in Aspen Plus. A lot of tuning need to be done for the model to converge and modelling experience could help a lot.

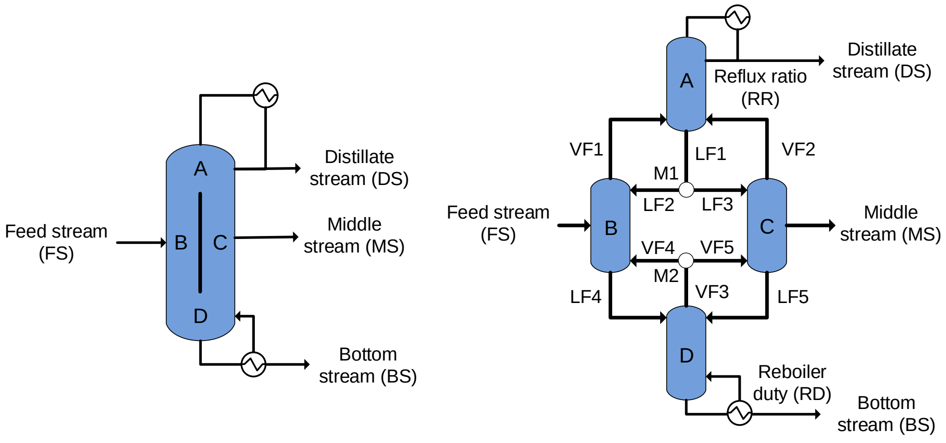


Figure 2: (Left) Typical DWC configuration (Right) Equivalent 4-column DWC configuration

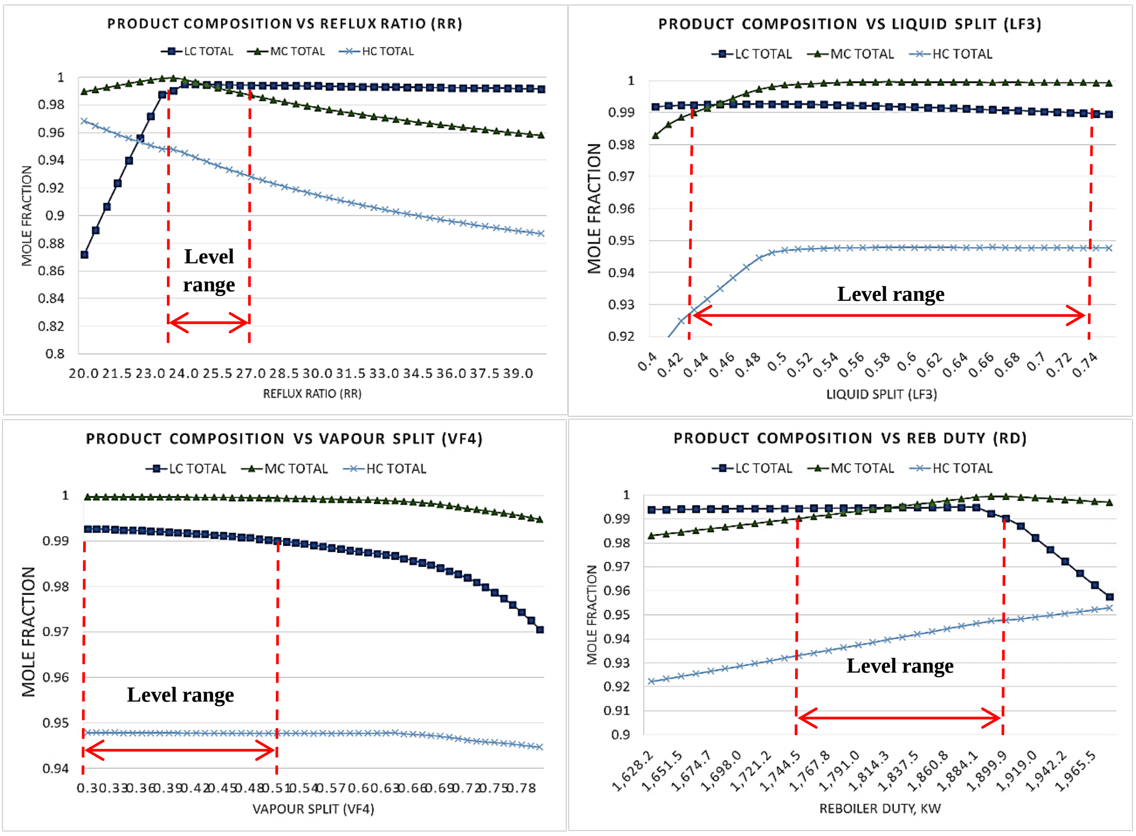


Figure 3: Effect of different control variables on product composition

Table 1: Control variable and corresponding levels

Control variable	**Level**				
	1	2	3	4	5
Reflux ratio (RR)	23.6	24.3	25.1	25.8	26.5
Liquid split (LF3)	0.43	0.503	0.575	0.648	0.72
Vapour split (VF4)	0.30	0.353	0.405	0.458	0.51
Reboiler duty (RD)	1,733 kW	1,775 kW	1,817 kW	1,858 kW	1,900 kW

3. Control and response variables setup

The next step in ED procedure is to define the control and response variables. In this work, several control variables were selected based on work by Dohare et al. (2011), they include reflux ratio (RR), liquid split to section C (LF3), vapour split to section B (VF4), and reboiler duty (RD) as shown in Figure 2. These control variables were varied to investigate their effect on the response variables, which are the product compositions, namely, LC at the distillate stream, MC at the middle stream and HC at the bottom stream. These effects can be investigated by applying sensitivity analysis approach. In Aspen Plus, sensitivity analysis can be done either in sequential-modular (SM) mode or equation-oriented (EO) mode. In this work, sensitivity analysis based on SM mode was employed using the model analysis tool in Aspen Plus. During sensitivity analysis, all the variables were kept constant except the control variable under study. Apart from observing the variables interactions, sensitivity analysis is also used to identify possible range for the control variable levels. It is recommended to choose the range, which is able to meet the desired design value. The sensitivity results and its corresponding control variable level range are shown in Figure 3. The control variables and its corresponding levels are then given in Table 1.

4. Orthogonal array and experimental layout design and run

Orthogonal array (OA) is a simple and useful tool to design an experiment that helps the designer to study the influence of multiple controllable factors on the average of quality characteristics and the variations in a fast and economic way (Panda and Singh, 2013). The selection of OA depends on several factors including number of interactions, number of factors, time and cost (Antony et. al, 2001). For the present study, the experimental design was based on the L25 orthogonal array of Taguchi method. The OA layout is shown in Table 2. The simulation was conducted according to the experimental layout. For physical experiment, it is necessary to repeat the experimental run several times in order to have adequate degrees of freedom for the error term (Antony et al., 2001). However, in the present work, the case is modelled and simulated using process simulators. Therefore, a single unrepeated run is sufficient since the initialization value is the same. The product composition for each cut corresponding to each run is also shown in Table 2. It can be seen from this table that not all runs produce the desired product specification. This is due to the variation of control variables setting in the OA matrix that significantly affects the response variable unlike sensitivity analysis approach whereby only one control variable was varied while the rest were kept constant.

Table 2: L25 orthogonal array of Taguchi experimental layout, its response and S/N results

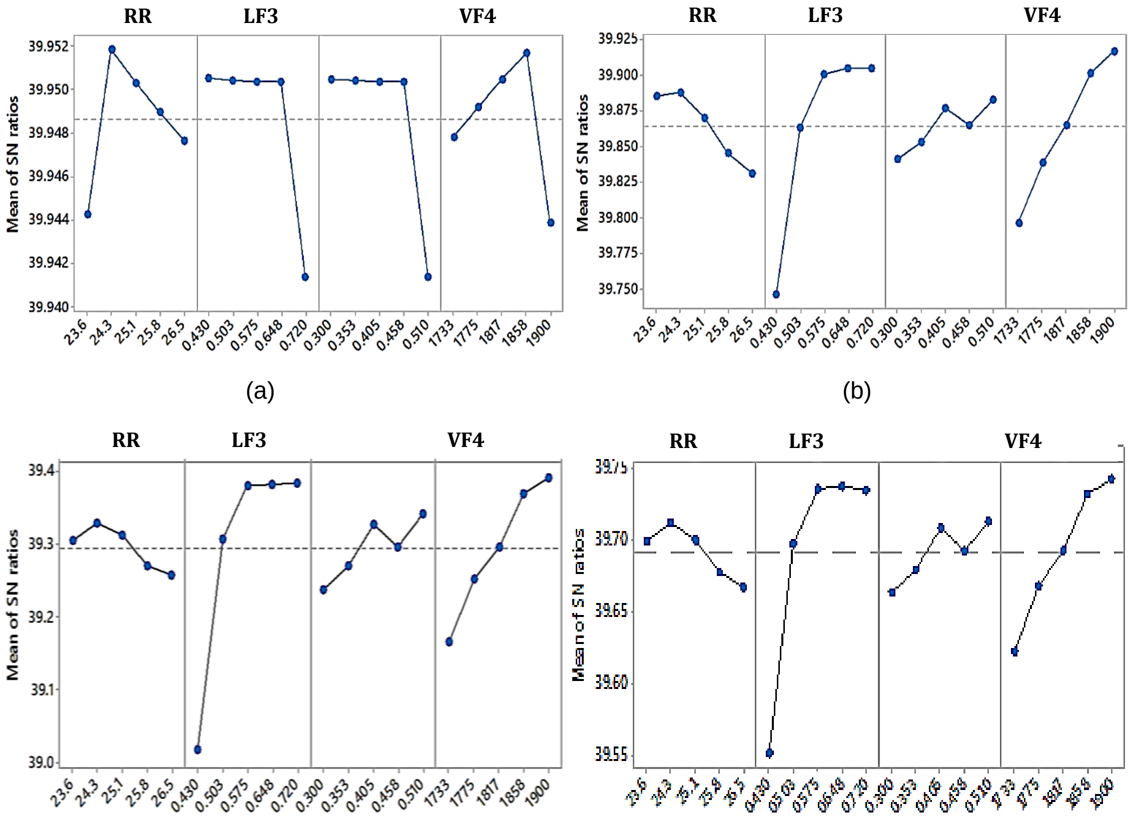
Run	**RR**	**LF3**	**VF4**	**RD**	**Mole %**			**S/N ratio**			
					LC	MC	HC	LC	MC	HC	Overall
1	23.6	0.430	0.300	1733	99.44	95.99	86.59	39.95	39.65	38.75	39.42
2	23.6	0.503	0.353	1775	99.45	98.42	92.08	39.95	39.86	39.28	39.69
3	23.6	0.575	0.405	1817	99.46	99.42	93.96	39.95	39.95	39.46	39.78
4	23.6	0.648	0.458	1858	99.48	99.74	94.39	39.95	39.98	39.50	39.80
5	23.6	0.720	0.510	1900	98.98	99.93	94.78	39.91	39.99	39.53	39.81
6	24.3	0.430	0.353	1817	99.45	97.17	89.17	39.95	39.75	39.00	39.55
7	24.3	0.503	0.405	1858	99.46	99.11	93.45	39.95	39.92	39.41	39.76
8	24.3	0.575	0.458	1900	99.48	99.69	94.32	39.95	39.97	39.49	39.80
9	24.3	0.648	0.510	1733	99.42	98.68	92.79	39.95	39.88	39.35	39.72
10	24.3	0.720	0.300	1775	99.43	98.94	93.17	39.95	39.91	39.39	39.74
11	25.1	0.430	0.405	1900	99.46	98.14	91.34	39.95	39.84	39.21	39.66
12	25.1	0.503	0.458	1733	99.40	97.81	91.33	39.95	39.81	39.21	39.64
13	25.1	0.575	0.510	1775	99.42	98.61	92.71	39.95	39.88	39.34	39.72
14	25.1	0.648	0.300	1817	99.43	98.87	93.09	39.95	39.90	39.38	39.74
15	25.1	0.720	0.353	1858	99.44	99.12	93.46	39.95	39.92	39.41	39.76
16	25.8	0.430	0.458	1775	99.40	96.70	88.80	39.95	39.71	38.97	39.52
17	25.8	0.503	0.510	1817	99.42	98.47	92.56	39.95	39.87	39.33	39.71
18	25.8	0.575	0.300	1858	99.43	98.78	93.02	39.95	39.89	39.37	39.73
19	25.8	0.648	0.353	1900	99.44	99.11	93.43	39.95	39.92	39.41	39.75
20	25.8	0.720	0.405	1733	99.38	98.16	92.02	39.95	39.84	39.28	39.68
21	26.5	0.430	0.510	1858	99.42	97.62	90.74	39.95	39.79	39.16	39.62
22	26.5	0.503	0.300	1900	99.43	98.39	92.29	39.95	39.86	39.30	39.69
23	26.5	0.575	0.353	1733	99.37	97.81	91.62	39.94	39.81	39.24	39.65
24	26.5	0.648	0.405	1775	99.38	98.16	92.03	39.95	39.84	39.28	39.68
25	26.5	0.720	0.458	1817	99.40	98.40	92.37	39.95	39.86	39.31	39.70

5. Statistical analysis and validation

The simulation data were analysed using signal to noise (S/N), which measures the functional robustness of product or process performance in the presence of undesirable external disturbances (Kapur and Chen, 1988). The larger-the-better (LB) response was applied to ensure adequate product purity. Using this response, the S/N ratio was calculated using the following equation:

$$\frac{S}{N} = -10\ \log\frac{1}{n}\sum_{k=1}^{n}\frac{1}{y^2} \tag{1}$$

Here, *n* is the number of repeated experiments and *y* is the response of the experiment. Note that *n* is considered 1 for computational modelling. Calculation of S/N ratio was done in Minitab vr17. The calculated S/N ratio is shown in Table 2, and its main effect plot is illustrated in Figure 4. The main effect plot elucidate the interaction of different control factor levels to the responses output. Generally, the highest peak of S/N ratio in the graph is the optimum condition for robust process performance. In Figure 4a, RR and RD have major contributions to LC purity, and LF3 and VF4 have minor effect except at the end of the levels range. The optimum design variables for LC was found to be 24.3 for reflux ratio, 0.43 for liquid split, 0.30 for vapour split and 1,858 kW for reboiler duty. With this setting, the purity of LC is 99.46 %. Interestingly, it is found that the main effect plots for MC and HC (in Figure 4b and 4c) have the same trend. Whereby, LF3 and RD contributes the most in controlling the product purity of both streams. RR and VF4 contribute moderately. Figures 4b and 4c show the main effects plot for MC and HC. Both figures show almost identical effect. For MC the optimal setting was 24.3 for reflux ratio, liquid split and vapour split were 0.648 and 0.51, the reboiler duty was 1,900 kW. This setting achieves MC purity of 99.70 %. HC purity achieved is 94.33 % with optimum setting of 24.3 for reflux ratio, 0.72 and 0.51 for liquid and vapour split and 1,900 kW for reboiler duty. For overall response, the analysis takes into account the multiple response parameters, namely LC, MC and HC purity. Such analysis is possible due the same unit of measurement. Overall response result in Figure 4d shows that the most contributing variables out of the selected control variables were LF3 and RD whereas RR and VF4 contribute moderately. It is also found that increase of RR reduces the product purity especially MC and HC whereas increase of LF3, VF4 and RD increases the product purity especially the MC and HC. The overall optimum setting was 24.3 for reflux ratio, liquid split and vapour split were at 0.648 and 0.510, and reboiler duty was 1,900 kW. With this setting, the process able to achieve the desired purity: 99.98 mol.% for LC, 99.70 mol.% for MC and 94.33 mol.% for HC.



(a) (b)

(c) (d)

Figure 4: Main effect response plot for S/N ratio (a) Light-cut (b) Middle-cut (c) Heavy-cut (d) Overall

6. Conclusions

In this paper, an experimental design based on Taguchi method was applied to optimize the control variables of a complex four column DWC model for fatty acid fractionation. Analogous to physical experiment, the model was used to identify sensitive parameters, simulate experimental trials and validate results. The paper also illustrated sensitivity analysis approach to identify suitable range for selection of the control variable levels. It is suggested to select control variable range that lies within the desired product purity for significant selection of level values. Data analysis on the experimental design layout was conducted using S/N ratio. Overall it is found that the most contributing variables that affect the product purity were LF3 and RD. The selected optimal design variable values were found to be reflux ratio of 24.3, liquid split and vapour split were 0.648 and 0.510, and reboiler duty of 1,900 kW. With this setting, the experimental design was able to obtain the desired purity for all products. It will be interesting to apply the approach for optimizing the operation and installation cost of DWC, which will be our future work. Use of ED significantly reduces the extensive effort of mathematical development especially for complex processes. Other than that, fewer runs and iteration were needed, thus avoiding computational complexity. However, ED might not be as accurate, precise and extensive as mathematical model based optimization since the latter accounts for process phenomenon through mass, equilibrium, summation and enthalpy (MESH) equations. Overall, our study demonstrates the successful integration of Taguchi method to a complex model developed using process simulators, for simple, fast and non-tedious approach of process optimization.

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References

An D., Cai W., Xia M., Zhang X., Wang F., 2015, Design and control of reactive dividing-wall column for the production of methyl acetate, Chemical Engineering and Processing: Process Intensification, 92, 45-60

Antony J., Warwood S., Fernandes K., Rowlands H., 2001, Process optimisation using Taguchi methods of experimental design, Work Study, 50(2), 51-58.

AOTB (Advanced Oleochemical Technology Division), 2015. Oleochemical Industry in Malaysia <portal.mpob.gov.my/aotd/industry.htm>, accessed 06.08.2015.

Barroso-Muñoz F.O., Hernandez S., Segovia-Hernández J.G., Hernández-Escoto H., Rico-Ramírez V., Chávez R.H., 2011, Implementation and operation of a dividing-wall distillation column, Chemical Engineering & Technology, 34(5), 746-750.

Cho H.J., Choi S.H., Kim T.Y., Kim J.K., Yeo Y.K., 2015, Design of a dividing wall column for fractionation of biodiesel, Korean Journal of Chemical Engineering, 32(7), 1-14.

Dejanovic I., Matijasevic L., Jansen H., Olujic Z., 2011, Designing a packed dividing wall column for an aromatics processing plant, Industrial and Engineering Chemistry Research, 50, 5680-5692.

Dohare R.K., Singh K., Kumar R., Upadhyaya S., Gupta S., 2011, Dynamic model of dividing wall column for separation of a ternary system, In CHEMECA -2011, September 2011. New South Wales, Australia.

Kapur K.C., Chen G., 1988, Signal-to-noise ratio development for quality engineering, Quality and Reliability Engineering International, 4, 133-41.

Kiss A. A., Ignat R. M., 2012, Enhanced methanol recovery and glycerol separation in biodiesel production – DWC makes it happen, Applied Energy, 99, 146-153.

Kiss A.A., Suszwalak D.J.C., Ignat R.M., 2013, Breaking azeotropes by azeotropic and extractive distillation in a dividing-wall column, Chemical Engineering Transactions, 35, 1279-1284.

Loy Y.Y., Lee X.L., Rangaiah G.P., 2015, Bioethanol recovery and purification using extractive dividing-wall column and pressure swing adsorption: An economic comparison after heat integration and optimization, Separation and Purification Technology, 149, 413-427.

MPOC (Malaysian Palm Oil Council), <www.mpoc.org.my/Malaysian_Palm_Oil_Industry.aspx>, accessed 06.08.2015.

Othman M.R., Illner M., 2014, Modelling and simulation of a dividing wall column for separation of fatty acid in oleochemical industries, In SOMChE & RSCE 2014, 29-30 October 2014. Kuala Lumpur, Malaysia.

Panda A.K., Singh R.K., 2013, Optimization of process parameters by Taguchi method: Catalytic degradation of polypropylene to liquid fuel, Int. J. of Multidisciplinary and Current research, Sept/Oct 2013, 50-54.

Premkumar R., Rangaiah G.P., 2009, Retrofitting conventional column systems to dividing-wall columns, Chemical Engineering Research and Design, 87(1), 47-60.