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Thermodynamic Equivalence Validation of New Fpdwcs with Two Partition Walls

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Four-product dividing wall columns (FPDWCs) with two partition walls is shown to be energy efficient compared with conventional column sequence for multi component separation. However, its industrial implementation is restricted due to two uncontrollable vapor splits. To handle this obstacle, the vapor-liquid thermal coupling streams between column sections were transferred into liquid-only stream and the derived configuration is thermodynamic equivalent to original ones in minimum vapor flow condition. The main advantage of the synthesized configurations is featured with none vapor splits or with vapor split controlled by means outside the column and is encouraging for industrial use. Moreover, to validate the thermodynamic equivalent feature in practical conditions, sequential optimization method was used for optimal design and rigorous simulations were performed.

1. Introduction

As a kind of energy efficient distillation technology, dividing wall column has been widely implemented industrially, e.g. hydrocarbons, alcohols, aromatics, acetals, ketones and cryogenic air separations. Obviously, there are no restrictions on the type of chemicals.(Asprion et al., 2010) Moreover, combination with reactive distillation, azeotropic distillation, extractive distillation and batch distillation, R-DWC (Ehlers et al. 2017), A-DWC (Le et al. 2015), E-DWC (Staak et al. 2017) and B-DWC (García-Ventura et al. 2016) could be derived. Recently, four-product dividing wall column (FPDWC) has received attention both in industrial and academic research.(Halvorsen et al. 2013, Dejanović et al. 2011)

There has been no application for FPDWCs, except Kaibel column in BASF.(Dejanović et al. 2014, Tututi-Avila et al. 2017) The main reason resists in the multiple uncontrollable vapor splits. Usually, the energy efficiency is contradicted with design simplicity and operation stability. Designers have to sacrifice energy efficiency to make the system more controllable, (Luyben 2018a,b) which results in the simplest FPDWC-Kaibel column. However, for further increasing energy-efficiency in chemical industry, it is incentive to study FPDWCs with multiple partition walls and put them in use.

Although some instruments (patent in China) have been invented to control the vapor split at the bottom of partition wall, by regulating the flow resistance in the two sides of partition wall, there is no equipment put into industrial use because of complexity and non-sensitivity. In order to solve the uncontrollable vapor split, Rakesh Agrawal (Agrawal 2000) converted the liquid-vapor thermal coupling streams to liquid-only thermal coupling stream by adding parallel column sections. In this way, configuration with vapor split controlled by means external to the column and configurations without vapor split could be derived. In their recent work, they extended the idea to fully thermally coupled arrangement for FPDWCs (extended Petlyuk) and enumerate the number of new configurations.(Ramapriya et al. 2014, 2016) Furthermore, they applying the method to any thermally coupled column by extending the partition wall all the way to the top and bottom of the column.(Ramapriya et al. 2017a,b) However, the main drawback of the above-mentioned work resists in two aspects: firstly, the easy-to-operate configuration is only thermodynamic equivalent to the original one with uncontrollable vapor split under minimum vapor flow conditions. In practical conditions, there is no pinch at the thermal coupling position and their thermodynamic equivalence should be validated. The second aspect is that

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in terms of industrial use, the dividing wall columns with more than three partition wall are too complex for implementation. Up to now, there has been no DWC with two partition walls implemented, so easy-to operate FPDWCs with two partition walls need to be proposed.

In our previous work, FPDWCs with two partition walls could be synthesized from extended petlyuk arrangement, by moving the separation task from middle column forwards to prefractionator.(Ge et al. 2017) The two derived configurations are shown Figure 1. For convenience, B-D represents that non-sharp split is conducted in the prefractionator for hypothetical four components mixture. In the present work, by converting the vapor-liquid thermal coupling streams to liquid-only stream, six new configurations with prospect of industrial application were derived, which features two partition walls and adjustable vapor splits (or no vapor split). Optimal design of new derived FPDWCs is conducted and its thermodynamic equivalence to original one is validated by rigorous simulation in practical operation conditions.

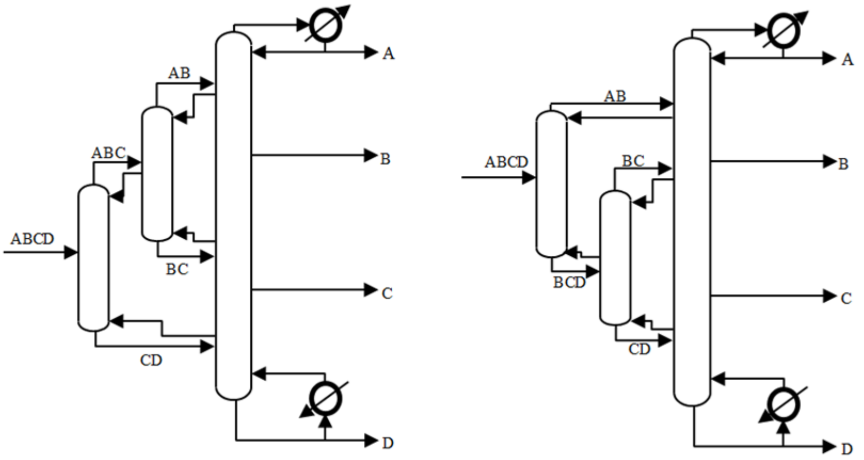

Figure 1 FPDWCs with two partition walls: B-D and A-C configuration

2. Optimal design method for four-product dividing wall column

Optimal deign of distillation system based on shortcut method (e.g. use the total minimum vapor flow) has been employed by some researchers, which could provide initial guess about the minimum energy consumption.(Nallasivam et al. 2013, 2016) However, optimized variables for FPDWCs include both integer variables (such as stage number in each column section) and continuous variables (reboiler duty, reflux ratio, distillate, side stream flow rate and multiple vapor and liquid split ratios) and the relationship between these variables is non-linear, which makes the optimization problem to be mixed-integer nonlinear programming problem rigorously (MINLP). The optimization problem could be formulated as:

$$\begin{aligned} &\min TAC = f(N_i, r_{li}, r_{vi}, Q_{\mathrm{reb}i}, RR_i, F_{si}) \\ &s.t.\quad g(N_i, r_{li}, r_{vi}, Q_{\mathrm{reb}i}, RR_i, F_{si}) \geq x_{product,i} \end{aligned} \tag{1}$$

Where N_{i} represents the stage number in each column section; r_{li} and r_{vi} is the liquid and vapor split ratio, respectively; $Q_{\mathrm{reb}i}$ and RR_i is the reboiler duty and reflux ratio of each column; F_{si} is multiple side product flow rate. By sufficiently using the simulation ability from commercial software, there are mainly two methods to solve this MINLP, one is to use outer stochastic optimization algorithm such as GA (Genetic Algorithm) to connect with simulation software, which terms global optimization;(Tututi-Avila et al. 2017) the other is sequential optimization, i.e., using the SQP (successive quadratic program) embedded in simulation software to optimize the continuous variables and use sensitivity analysis to optimize integer variables.

From our experience, there is no significant difference between the results from the two kinds of method. The main drawbacks of the global optimization resists in the computation load and convergence problem. Therefore, sequential iteration optimization procedure was used to optimize the FDDWCs, which was shown in our previous work. In the developed optimization procedure, sequential iteration method was employed to optimize structural variables, i.e. stage number in each column section. In each iteration, the sub-optimization problem turns to be non-linear programming problem (NLP) and could be formulated as:

$$\begin{aligned} &\min \sum_{i} Q_{\mathrm{reb}i} = f(r_{li}, r_{vi}, Q_{\mathrm{reb}i}, RR_i, F_{si}) \\ &s.t. \quad g(r_{li}, r_{vi}, Q_{\mathrm{reb}i}, RR_i, F_{si}) \geq x_{product,i} \end{aligned} \tag{2}$$

This NLP turns to be a self-optimization problem with $Q_{\mathrm{reb}i}$ as objective and variables simultaneously.

3. Thermodynamic equivalent FPDWCs without uncontrollable vapour split

3.1 Converting the vapor-liquid thermal coupling to liquid-only transfer stream

The pressure drop in the two sides of partition wall is an important consideration for its onsite operation. The pressure drop in the two parallel column sections is constrained to equal. Subject to this constraint and the mechanical resistances in the two sides of partition wall, there is a natural uncontrolled vapor split, which implies that the relative vapor flow rates cannot be manipulated during operation. Though methods to address the control of the vapor split problem during the design and dimensioning phase of dividing wall column have been proposed, there is no industrial application during online operating except for an experimental setup using valve to adjust the vapor split ratio. However, the vapor split ratio can have a significant effect on the product purities, energy consumption, and has implications on how far the dividing wall column deviates from its optimal operation.(Ge et al. 2014) Though the liquid split ratio at the top of the partition wall also can have similar effects, it could be well controlled during operation, using collectors and distributors external to the column. Distillation configurations with liquid transfers between different column sections are easier to operate and control than configurations with vapor transfers between column sections. Based on this fact, the bidirectional vapor and liquid transfer stream can be converted to a liquid-only transfer stream by adding a corresponding reboiler or condenser,(Agrawal et al. 1999) however, in this way, the vapor and liquid flow rate across the common rectifying or stripping column sections definitely decrease, which results in the increase of total energy requirement for given stage number in each column section. Another method for converting the liquid-vapor thermally coupled distillation column is to add parallel column sections to solve the deficiency associated with the vapor split. This method has been used to generate more operable configurations for three-product dividing wall column and extended Petlyuk column. The above-discussed practical column with two partition walls can also be translated to the more operable configuration. Figure 2 displays the procedure for converting the bidirectional vapor-liquid thermally coupled stream containing submixture ABC and AB to liquid-only stream. After converting the liquid split associated transfer stream, the new configuration could be derived with each vapor split controllable by means external to the column, e.g. by adjusting condenser duty, the flow resistance in each side of partition walls could be manipulated. Moreover, the vapor split associated bidirectional transfer stream could also be converted to liquid-only transfer stream. In this way, the configuration without vapor split could be obtained.

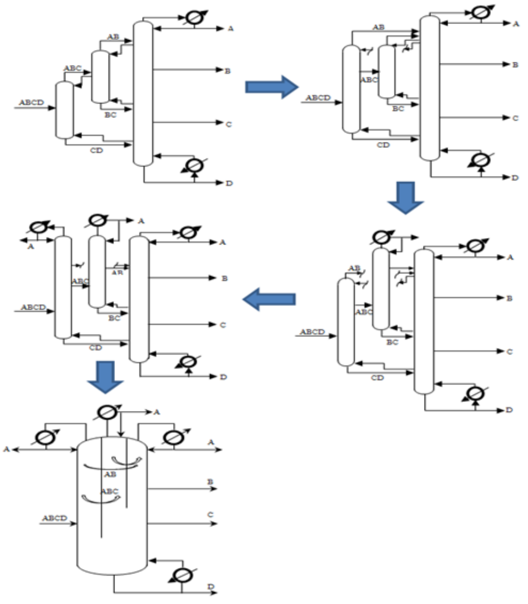

Figure 2 The procedure for converting the vapour-liquid thermal coupling to liquid-only transfer stream

Figure 3 shows the series of operable configurations generated from the two practical four products dividing wall column. In Figure 3(a) and (d), the corresponding vapor splits can be controlled by manipulating the condenser's pressure. While in Figure 3(b), (c), (e), and (f), there is no vapor exchange between column sections. As mentioned above, these easy to operate configurations are thermodynamically to original arrangement on the condition that the column operated at minimum vapor flow conditions.

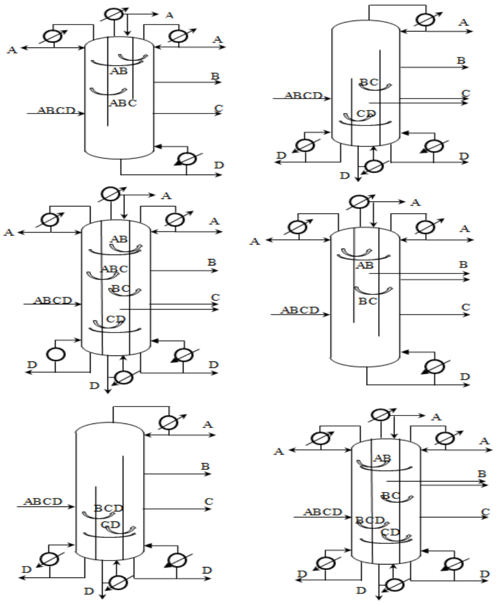

Figure 3 FPDWCs without uncontrollable vapour split derived from B-D and A-C arrangement

3.2 Thermodynamic equivalent validation in practical conditions

To validate the thermodynamic equivalence of the derived configuration with original ones at reflux ratio above the minimum condition, rigorous simulation is should be conducted. After determining the structural and operating variables for B-D and A-C configuration, the added column sections for the new derived configuration are designated to have same stage number with the original parallel column sections. However, the operating variables including the communicating streams between each column sections require to be optimized again, with the SQP method. By employing the aromatic mixture with equimolar composition as case study, the optimal design parameters for original and derived FPDWCs without uncontrollable vapor split are obtained by sequential optimization procedure. By converting the bidirectional vapor-liquid thermally coupled transfer stream to liquid-only stream, all of the vapor and liquid split ratios in the derived configurations are between 0 and 1, which imply that all of the vapor and liquid flow in the column sections are sustainable. Therefore, feasible designs could be ensured by appropriately locating each dividing wall.The energy consumption for each configuration without uncontrollable vapour split is displayed in Table 1.

Table 1: Rigorous simulation results for the derived easy to operate four products dividing wall column

	B-D	(a)*	(b)*	(c)*	A-C	(d)*	(e)*	(f)*
Q_{C1}(KW)	3819	851	3849	1143	3807	1116	3818	1147
Q_{C2}(KW)		790		741		1028		1159
Q_{C3}(KW)		2164		2118		1716		1536
R_1	4.61	4.83	4.65	5.20	4.44	4.41	4.45	3.93
R_2		4.68		5.38		4.23		3.85
R_3		4.38		4.34		4.71		5.78
Q_{B1}(KW)	5327		1172	1172	5316	5366	1484	1169
Q_{B2}(KW)			571	747			900	1194
Q_{B3}(KW)			3614	3590			2942	2985
Q_B**(KW)	5327	5313	5357	5509	5316	5366	5326	5348
Q_C** (KW)	3819	3805	3849	4002	3807	3860	3818	3842

*configuration shown in Figure 3(a),(b),(c),(d),(e) and (f)

**total reboiler or condenser duty for series generated easy to operate and original configuration

Less than 5% difference exists between these configurations.

The FPDWCs without uncontrollable vapor split is thought to be easy to operate. The above-mentioned FPDWCs could be classified into three categories: (1) extending upper side of the entire partition walls to the top while keeping the lower side of the partition walls remain; (2) extending the lower side of the entire partition wall to the bottom while keeping the upper side of partition walls remain; (3) extending the upper and lower end of entire partition walls to the top and bottom simultaneously. However, there exists easy to operate FPDWCs with two partition walls which do not belong to the above-mentioned categories. The example is shown in Figure 4. In this new arrangement, the lower side of the two partition walls is extended to the bottom while the first partition wall is extended to the thermal coupling stream with sub-mixture AB. As for the B-D configuration with two partition walls, by extending each partition wall at least to top and bottom, 4*4 candidates without uncontrollable vapor split could be obtained including the three configurations belonging to the above-mentioned categories.

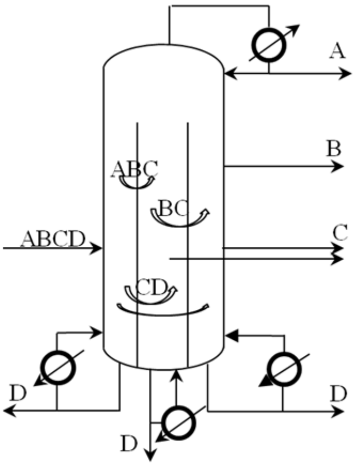

Figure 4 FPDWCs featured with the lower side of two partition walls extending to the bottom and the first partition wall is extended to the thermal coupling stream with sub-mixture AB: derived from B-D configuration

Besides B-D and A-C configurations, some new arrangements with two partition walls are proposed in our previous work, the corresponding configurations by converting the vapor-liquid thermal coupling stream to liquid-only transfer stream could also be derived. Moreover, by optimal design and rigorous simulation, the thermodynamic equivalence in practical operating conditions was validated.

4. Conclusions

The FPDWCs with two partition walls proposed in the present work is shown to be energy efficient compared to the conventional distillation column sequence. By converting the vapor-liquid thermal coupling stream to liquid-only transfer, the uncertainty of the FPDWCs could be reduced for eliminating the uncontrollable vapor split and the thermodynamic equivalence has been validated in practical operating conditions. Moreover, a series of easy to operate FPDWCs with two partition walls were enumerated by converting the vapor-liquid thermal coupling to liquid-only transfer stream, which shows encouraging for the multi-product distillation.

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