Chapter

Heat Integration of Reactive Divided Wall Distillation Column

Rajeev Kumar Dohare and Parvez Ansari

Abstract

In this chapter, the esterification reaction of methyl acetate with methanol and acetic acid is proposed by the new column configuration that is a reactive divided wall distillation column (RDWC). The heat integration of the proposed column configuration is studied and found that heat integration techniques are efficient to save energy up to 14.23% in comparison to the conventional reactive divided wall distillation column.

Keywords: methyl acetate, reactive dividing wall column, simulation, heat integration

1. Introduction

Distillation Technique is a chief process division extensively used in chemical manufacturing, and the growth of distillation column strategy has involved more and more consideration in the latest ages [1, 2]. Reactive distillation (RD) is a mixture of synthetic reaction and partition simultaneously. Catalytic distillation (CD) is a Reactive distillation process in which chemical reactions happen in a solid catalyst. The blend of the split process with catalytic reactions in a catalytic distillation column has many benefits, for example, improved conversion for stability and expected improvement of item selectivity because of the removal of the yields over in situ partings. In accumulation, the produced heat in the reaction might practice for distillation. Thus, the investment and operative expenses can be reduced [3, 4]. The reactive distillation process has been a part of importance most recent 20 years. The mixture of reaction and separation in a single unit is a substitute to traditional distillation, which incorporates reaction, and division in the number of units consequently expands the investment cost of the plant. The three significant useful areas of the reactive distillation column are:

1. Distillation column comprises a reactive unit, which prompts the transformation of reactants into items

2. It works on the partition in the section by changing the part volatilities

3. Intensifications the selectivity of the item [5].

To feat the likelihood of reactive distillation, procedures have been established for initial process design. Two major methods happen for the group of substitutes for a given reaction-parting problem: mathematical optimization and graphically based conceptual design methods. Mathematical optimization methods are generally very powerful for generating and evaluating design alternatives [6]. Reactive distillation technology is an encouraging process that can rise reaction change, overcome energy feeding, and recover selectivity and investment yield [7]. In previous years, Reactive distillation was widely inspected due to the projecting benefits, and excessive successes have been gained in positions of dynamic control and development strategy [8–12]. The results of the simulation proved that this novel technology is economical on the process charges and easily controls the purity of the product with the only use of a temperature control loop, which shows the potentials of the heat-integrated reactive distillation methodology. To complete additional energy savings, scientists have focused on the project of DWC to superior distillation structures, for example, reactive divided wall distillation, extractive distillation, or azeotropic distillation [10, 13, 14]. Reactive dividing wall column (RDWC) has newly involved countless importance since it has the rewards of together RD and DWC. A technique for the theoretical strategy of the RDWC created on the smallest vapor stream process planned the rate-based modeling method for RDWC [15]. Therefore, it is necessary to study the Heat integrated reactive distillation performances of reaction systems with different characteristics.

ASPEN PLUS simulation provides the benefits in covering steady-state to dynamic simulation for safety analysis and control process. The physical properties methods are required during the Aspen model, to calculate enthalpy, density viscosity, heat capacity, etc. ASPEN PLUS simulator has been used for physical chemistry, chemical thermodynamics, mass and energy balances, chemical reaction engineering, unit operations, and process design and control. It uses an inbuilt numerical model equation to stabilized the process performance. The perfect showing of thermodynamic properties is mainly significant in the parting of non-ideal mixtures and ASPEN PLUS has big information of retreated factors. Methanol (MeOH) and acetic acid (HAc) are essential raw materials in polyvinyl alcohol plants, and they could produce from Methyl Acetate (MeAc) hydrolysis process. Therefore, this process is considering for heat integration purposes.

1.1 Dividing wall column (DWC)

The petrochemical and chemical divisions are the major manufacturing power clients, representing generally 10% of overall global energy interest and 7% of worldwide greenhouse gases (GHG) outflows. In the chemical process industry, roughly distillation processes utilize 40% of absolute energy [16]. In the distillation procedure, high temperature is utilized, for example, an isolating means. Heat is provided to the lower section of the reboiler to vanish a fluid saturation at a more temperature and it decreases at less temperature while melting in the condenser at the upper section of the distillation column. Hence, the situation is extremely unproductive in the utilization of power. In the 1970s and 1980s, the start of oil emergencies, the power costs turned into the central point in column rate and made a resolve to discover to decrease the energy requirements of distillation. Subsequently, in the new distillation process, the essential objective is process strategies in distillation systems is that how to cut the power utilization. Different strategies have been used to utilized to make the process of distillation more energy effective and extra economical like divided wall columns (DWC), heat integrated distillation columns (HIDiC), and thermally coupled distillation columns (Petlyuk column).

In **Figure 1**, Wright's patent the divided wall column (DWC) in 1949. DWC can save both energy requirements and economic expenses related to conventional distillations. The energy utilization decreases about 20–30% associate with another conventional distillation column [17, 18].

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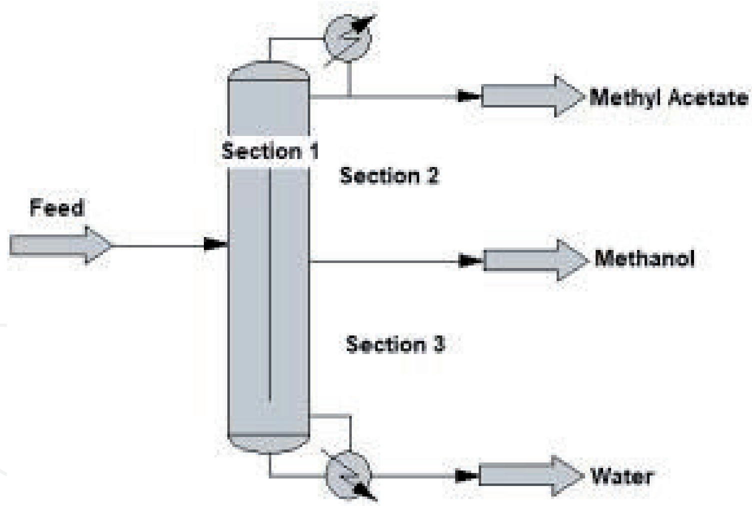

Figure 1.
Divided wall column.

The Divided wall column contains more than two distinctive split process units into single and more than one vertical section in the middle area. Dividing walls also differentiate a single column into two sections: a pre-fractionator area and the main column. It also used the condenser and reboiler at the top and bottom respectively [19].

Advantages and disadvantages of divided wall columns

1. Lower capital investment

2. Reduced energy requirements

3. High purity for all products

4. Less construction volume

A divided wall column might be offered the potential for decreasing both economic and energy prices, the dividing wall columns have main disadvantages. They are:

1. Higher columns dues to the increased number of theoretical stages.

2. Due to the higher number of theoretical stages, the increase in pressure drops.

3. Operating pressure is available only once.

1.2 Reactive distillation column (RDC)

Many numerical problems arise in the modeling, design, and optimization of the RDC, which results in simpler and intensified processes with fewer recycle streams, and decreasing waste handling reflects lower investments and operating costs. RDC offers an advanced reaction rate and selectivity; stops the performance of azeotrope, less energy intake, and solvent treatment. Despite all these benefits, the RDC has partial commercial applications; it is because of the control performance and the complexity in the operation of the RDC. For modeling, we have supposed that it operates in adiabatic conditions with the liquid phase. There is no vapor hold-up

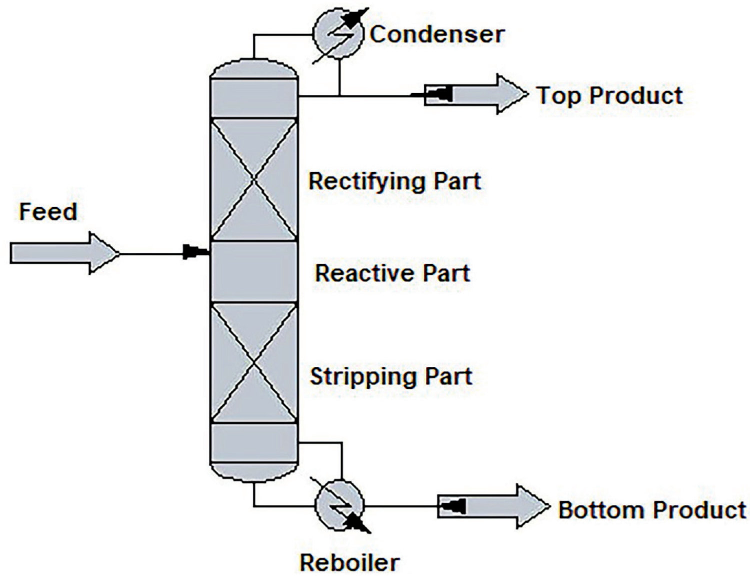

Figure 2.
Reactive distillation column.

in any stage of the distillation column (DC). No hydrodynamic effects have been considered escaping the modeling difficulties [20]. **Figure 2** is an actual sketch of the reactive distillation column.

1.3 Reactive dividing wall distillation column (RDWC)

A reactive dividing-wall column (RDWC) incorporates a reactor and a separator in a single distillation column. The multiple products, non-reacting components, or excessive reagents can be isolated in such a column, that reactive systems have. Because of the strong corporation among control loops, control engineers have a provoking position to control RDWC. Up until now, the investigation of reactive distillation in one divided wall column is scant, particularly for the control. The reason for this work is to consolidate the advantages of reactive distillation with DWC to deliver MeAc and afterward examine the design and control of an RDWC with an exceptional focus on the foundation of control structures. Initially, a subjective connection between the process flow sheet and phase equilibria is set up, and then an RDWC flow sheet is set up.

The reactive distillation column (RDC) and dividing wall column (DWC) both are genuine instances of process heat intensification. Uncertainty reactive distillation and DWC have combined, a reactive divided wall column (RDWC) has been produced. RDWC has an extremely integrated arrangement that contains one condenser, one reboiler, reactive zones, a pre-fractionator, and the main column together in a single distillation setup. The synthesis of Methyl Acetate has been chosen as a test reaction for heat integration purposes.

The synthesis of Methyl Acetate and its reverse reaction are given below.

$$\text{Methanol} + \text{Acetic Acid} \leftrightarrow \text{Methyl Acetate} + \text{Water} \qquad (1)$$

In reactive distillation, it is likely to get more conversion by continuously removing the products from the reaction section. Products have been removed from the lower part of a reactive distillation column and isolated into the distillation column. By joining the reactive distillation column and separation column into the single column, which turns into the reactive divided wall column with side product methanol stream, also the residence period of methanol with acetic acid and water in the sump has come to a minimum level.

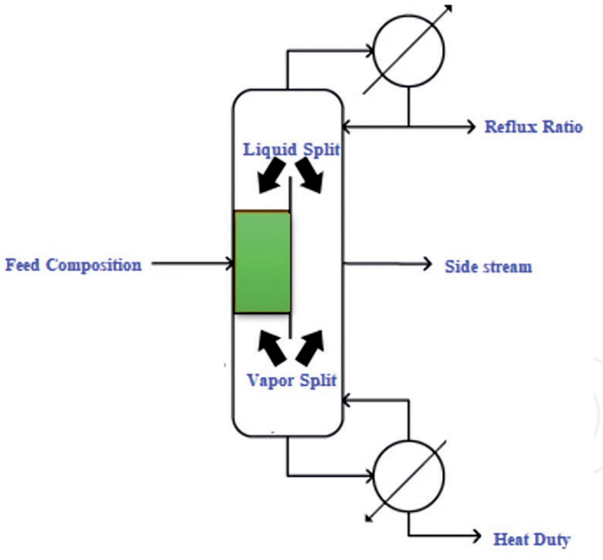

Figure 3.
Reactive dividing wall column.

It has achieved greater attention in the chemical industry for the separation process and saves both energy and capital cost. The RDWC technology has not been confined up to ternary separation only but it can also carry out azeotropic separations. The feasibility of the RDWC in the industry depends upon the thermodynamic properties, the composition of the stream that has separated, and the product requirements. **Figure 3** shows the actual pictorial diagram of the RDWC. Although, **Figure 4** shows the simulation sheet of the two-column reactive divided wall distillation column.

1.4 Heat integration of reactive dividing wall column

The main approach to improve the energy efficiency of the distillation system is by providing heat integration technology [21]; vapor recompression (VRC) and internally heat-integrated distillation column (HIDiC) [22] are two popular techniques for the same. The energy demands and expenses are expanding due to joined hazards, global warming, and the improved requirement upon lubricant introduced from electorally insecure quantities of the sphere have caused in the importance of the thermodynamic efficiency of recent engineering progress for

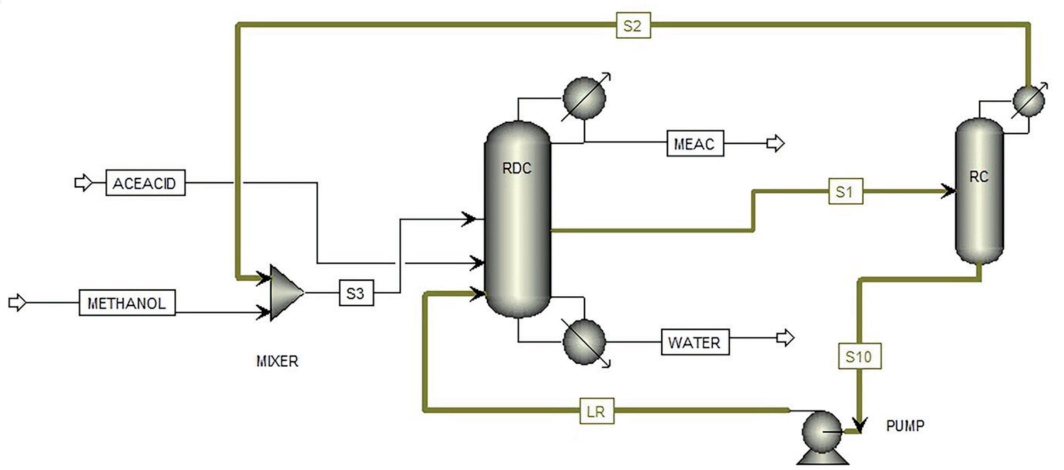

Figure 4.
Flowsheet of RDWC.

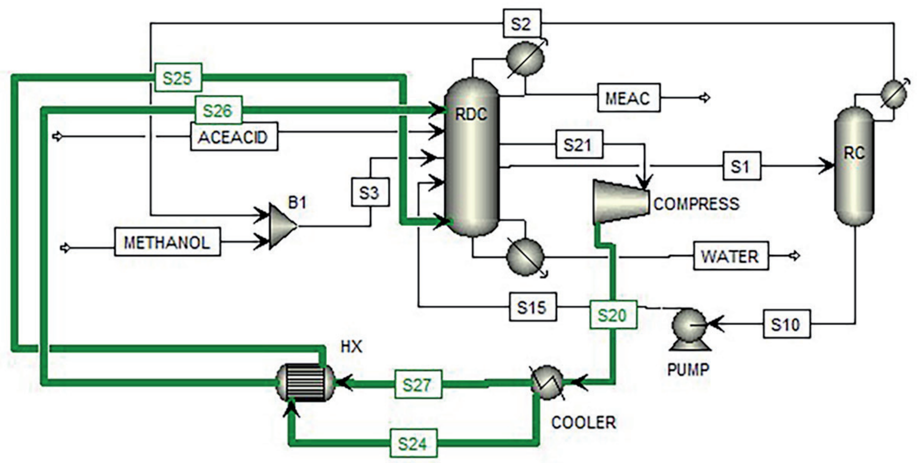

Figure 5.
Flowsheet of heat integrated reactive dividing wall column.

improving. Expanding power efficiency in compound routes not individual offers cost-effective profits and turns into the decreasing radiations resultant from the development activity. The distillation technology is maybe the important significant and extensively used removable technique in the world today about 95% of all liquid split in the synthetic production industry used. Regardless of its evident significance, in general, most of the thermodynamic efficiency of a conventional distillation is about 5–20% [23]. The concept of process intensification has presented to the distillation development in 1970 for further development of energy efficiency [24]. Nevertheless, the energy efficiency of RDWC is not constantly high since the entire heat can only be added to the bottom reboiler at the maximum temperature and impassive from the top condenser at the final temperature. The heat integration technology such as VRC the exciting energy intake has been reduced [25, 26]. The conventional VRC and side VRC techniques are combined into one RDWC; to deliver the intensified heat integrated technique of VRC that are associated with the RWDC structure. Into intensified heat integrated structures, the unoriginal VRC has further divided between the top and bottom of the RDWC to improve overheat vapor through the heat flow as greatly as possible, into more temperature, compressed fluid from the downward reboiler has recycled into the adjacent fluid to vaporize in a transitional reboiler (IR) [27]. The fundamental thought of heat integration technology is that the high-temperature route streams that exchanged heat with cold route streams, which affect in financial use of assets. Subsequently, numerous sorts of exploration on heat-integrated distillation column (HIDiC) has been done in the past few years to research its achievability and reasonableness in certifiable applications as shown in **Figure 5**. Distillation columns such as the Petlyuk column, divided-wall column, heat pump assisted column, adiabatic distillation column, ideal HIDiC (i- HIDiC), and many more this investigation has led to the formation of different technology. The HIDiC structure has until not accepted by many industries then later small scale trials are accepted by the New Energy and Industrial Technology Development Organization (NEDO), Japan; a combined organization between NEDO and TERI (The Energy & Resources Institute), India undertakings more projects in the field of process intensification technology at a conference at New Delhi in January 2017 [28]. This tends to an original thought of process integration by joining reactive dividing wall column and ethics of heat integrated distillation column i.e. R-HIDiC that accepted the synthesis of methyl acetate with significantly lesser energy consumption. The mixture of methyl acetate employing a reactive dividing wall column system is the most effective and main application of process intensification [29]. Nevertheless, the greatly needed attention to decrement the energy feeding and intensification the efficiency of the current reactive dividing wall column has considered in this research.

2. Methodology

2.1 Column configuration

The method used for the simulation is the UNIQAC method, RadFrac model is used for the design of RDWC and Hi-RDWC in ASPEN simulation. The UNIFAC method is used for the estimate of activity coefficients calculated on the idea that a fluid mixture might be measured as a result of the structural elements after which the particles are produced slightly than a result of the particles themselves. The RadFrac model is the chief partition block option in Aspen Plus. The block option can execute sizing, simulation, rating of the tray, and packed columns. The ideal requirement, completed in the Format form, needs full conditions of column structure, feed, product, and any side streams. The feed material was methanol and acetic acid. The detailed operating parameters are shown in **Table 1.**

2.2 Intensified heat integration configurations

The standard VRC assisted RDWC configuration (VRC-RDWC) presented in **Figure 6**, the overhead vapor has compacted to a surpassing temperature to turns into vapor the lowermost fluid, and formerly converts the saturated condensed fluid into the reboiler, and the condensed fluid must be low to the topmost pressure through the throttle valve (TV) that returning at the RDWC at the upper section. Now this method, in the isentropic compressor the less amount of saturated vapor was condensed and less amount of saturated fluid will flash into the throttle valve, so a heater was essential to preheat the overhead vapor and the flew vapor condensed totally by the use of cooler. While the compression ratio (CR) is

Sr. no	Parameters	Value (unit)
1	Feed-Methanol	100 mol/hr
2	Feed-Acetic Acid	80 mol/hr
3	Pressure	1.013 bar
4	Reflux Ratio (RDC)	6.7
5	Distillate Rate (RDC)	80 mol/hr
6	Side Rate (RC)	20 mol/hr
7	Bottom Rate (RC)	80 mol/hr
8	Feed Tray location (a) Methanol	10
9	Feed Tray location (b) Acetic Acid	2
10	Number of Stages	36
11	Number of Stages RDC	25
12	Number of Stages RC	11

Table 1.
Operating parameters.

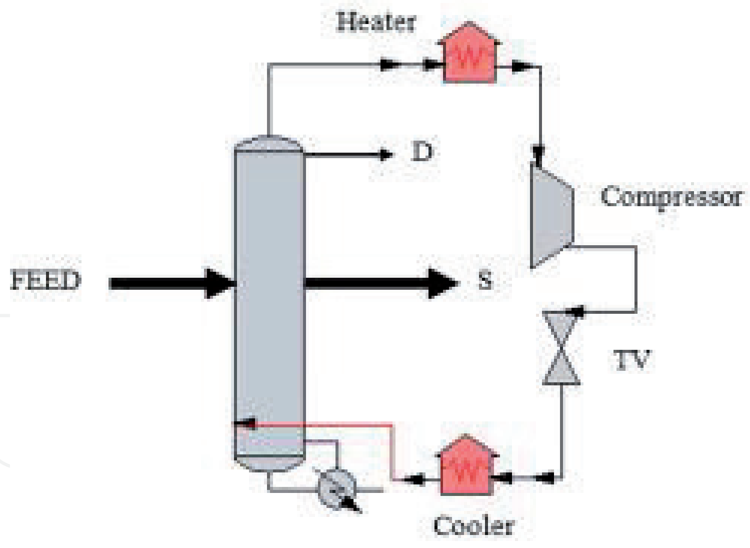

Figure 6.
Schematic diagram of vapor recompression RDWC (VRC-RDWC).

insignificant, the heater and cooler have been discounted due to the heat duties, then below large CR, these heat duties will convert huge and straight shrink the power effectiveness of VRC knowingly. The unused heat created by the VRC has recovered by intensifying the process of the heat integration technique between the VRC and RDWC (**Figure 5**).

3. Results and discussion

3.1 Temperature and composition profile

The temperature difference between the overhead and the bottom product is high i.e. 98°C. Therefore, the compression ratio (CR) has been regulated to meet the heat transfer needed in VRC-RDWC structures as shown in **Figure 5**. The total number of stages used in both columns including i.e. RDC and Rectifying column (RC)) are 36. The composition profile of the RDC column is shown in **Figure 7.** As per the physical phenomena that the excess amount of reactant and products should be at the output side. Although, the full consumption of the limiting reactant. The graph shows a similar response as per the process phenomena. The temperature of the column continuously increases with the increase in the number of the stages as

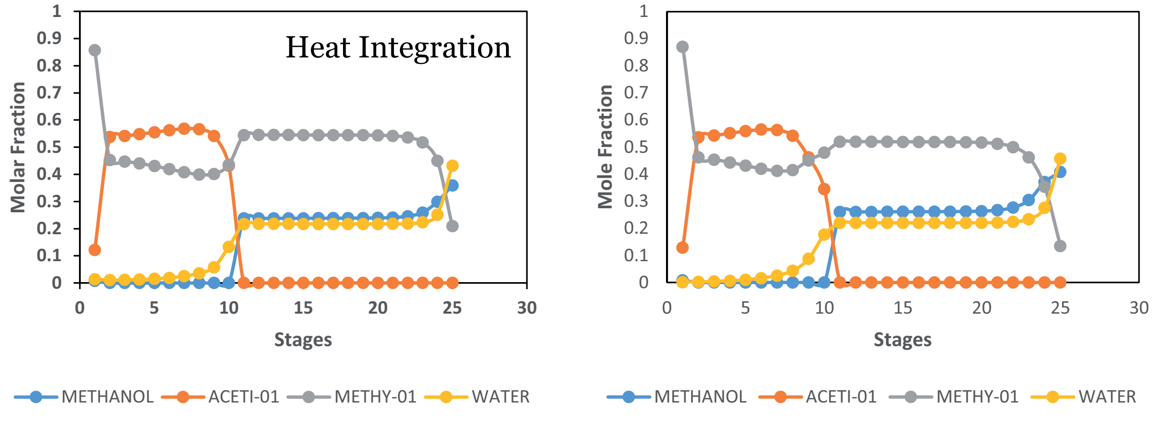

Figure 7.
Composition profile of RDC column (heat integration and without heat integration).

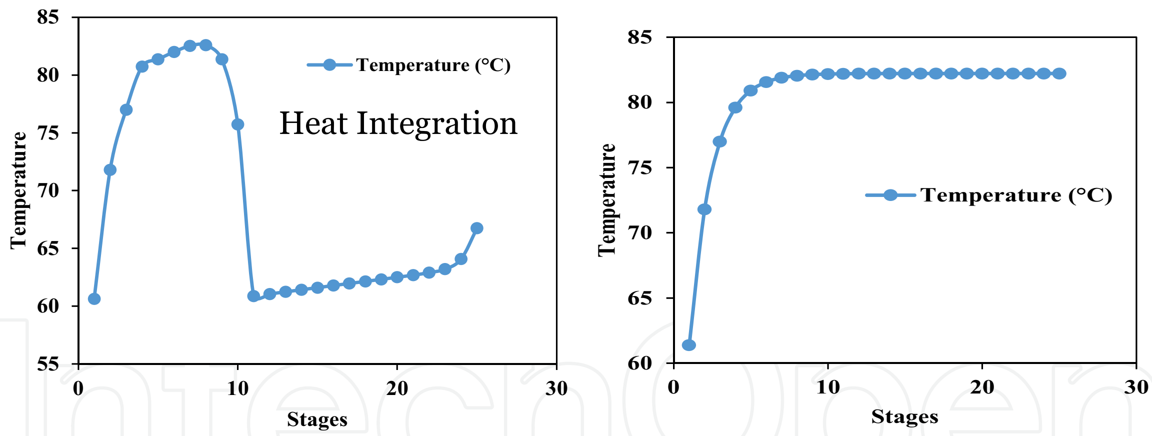

Figure 8.
Temperature profile of RDC column (heat integration and without heat integration).

Results	RDWC (2 column)	Hi-RDWC (2 column)	Energy saving (%) (2 column)
Condenser duty (kW)	−1.386	−1.358	**0.020**
Cooler duty (kW)	0	0.0936	0
Reboiler duty (kW)	0.6667	0.5718	**14.23**
Heater duty (kW)	0	0	0
Compressor duty (kW)	0	2.302e-05	0

Table 2.
Results of heat integrated RDWC (2 column).

shown in **Figure 8.** The maximum has risen the temperature is 85°C but with the implementation of the heat integration technique, the temperature is decreasing at about 65°C. There are no changes in composition profile by the use of heat integration technique as shown in **Figure 7.**

3.2 Heat integration of two column RDWC

To analyze the heat recovery in two columns design, a rigorous simulation has performed for the heat integrated simulation flowsheet. The Aspen simulation flowsheet of the RDWC is shown in **Figure 4.** Therefore, an enormous amount of condensed fluid flashed in the throttle valve (TV) from the compression ratio. The cooler with a heat duty of 0.020 kW condenses the flashed liquid. The reboiler duty of RDWC is 0.6667 kW after the Heat Integration of RDWC the reboiler duty was decreased by 0.5718 kW. However, the energy-saving of the intensified configuration technology is significant in comparison to the conventional column. The heat-integrated data of the divided wall distillation column is given in **Table 2.**

4. Conclusion

In this book chapter, Aspen Plus software is used to simulate the process of producing methyl acetate. The new technology used in this research was reactive dividing wall distillation technology. The position of methanol and acetic acid feed stream is set to be on the Reactive Distillation column (RDC) at 10 and 2 respectively. It is concluded that after the VRC-RDWC heat integration technique the reboiler duty is reduced from 0.6667 to 0.5718 kW and the condenser duty is reduced from −1.386 to −1.358 kW in the case of two-column configuration Therefore, it is observed after the integration the heat load on the reboiler is reduced up to 14.23% and condenser duty is to reduce up to 0.020% in case of two-column configuration. Results also showed that all products compositions could be kept at desired purity against feed disorder.

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Conflict of interest

There is no interest of conflict. The used data is properly cited and acknowledged here.

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