Review Article

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A review:control of reactive divided wall distillation column

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Abstract
The objective of this review paper is to survey of future and present status in the field of control of a reactive distillation column and reactive divided wall column. Different studies show that designing, operation and process of RD column is highly complex task due to process nonlinearity and complex interactions between the vapour – liquid equilibrium and chemical reactions. Different types of control techniques have been studied in reactive distillation, a simple proportional integral (PI) controller, proportional–integral–derivative controller(PID) controller, model predictive controller (MPC) such as dynamic matrix control (DMC), quadratic dynamic matrix control (QDMC) and mixed integer dynamic optimization (MIDO). The design of controllers and controller performance is important in industries to optimize energy conservation, cost effectiveness and performance of process operation. The main objective of control is to maintain the product purity.

Keywords
Reactive distillation column, Reactive divided wall distillation column, Conventional control, Dynamic matrix control, and cost effectiveness.

1.Introduction
Distillation the widely used separation technique in chemical industries but the problems in convention separation techniques are high energy requirements, large carbon footprint and high investment costs, operating and maintenance cost. Reactive distillation is combination of reaction and separation process in single column reactions that cannot be completed without separation of one product, are called equilibrium limited reactions. Such reactions are called 'equilibrium limited' reactions such as esterification, ester hydrolysis and trans-esterification; these reactions can be accomplished in reactive distillation column. This offers distinct advantages over the conventional sequential approach. In distillation the principal objective, is separation which is normally measured by the product purity. The modelling of RD column is difficult task due to reaction and separation in the same column. The process of RD was first patented in 1920 and was commercialized on 1980s since Eastman Company owned and run a commercial process for the production of methyl acetate.

To make distillation column as energy efficient system, fully thermally coupled distillation column (or petlyuk column) or dividing wall column (DWC)that integrates the two columns of a Petlyuk system into one column shell) is used.

These systems can reduce energy consumption by 30-50% over conventional distillation sequences for the separation of some mixtures. DWCs can be applied to azeotropic, extractive, and reactive distillations, which lead to azeotropic dividing wall columns (ADWC) [1], extractive dividing wall columns (EDWC) [2] and reactive dividing wall columns (RDWC) [3].

Reactive distillation column and dividing wall column both are good examples of process intensification. If reactive distillation and DWC are further integrated, a reactive divided wall distillation column (RDWDC) will be generated. RDWDC has a highly integrated configuration that consists of one condenser, one reboiler, reactive zones, a pre-fractionator and the main column together in a single-shell distillation setup. The literature study reveals that a variety of controllers are used for distillation columns. Generic Model Control (GMC) control algorithm comprises the nonlinear state-space model of the process within the control algorithm.

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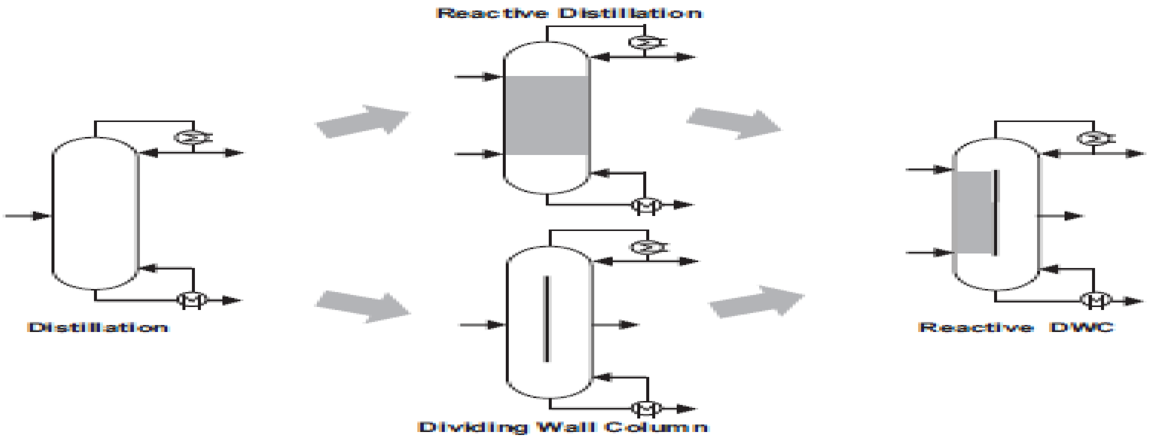

Figure 1 Path from conventional setup to reactive dividing-wall column (R-DWC)

Figure 1 illustrates the evolution of dividing wall column and reactive DWC from the conventional distillation column. The energy efficiency of the DWC may be improved by allowing heat transfer through the wall[4].A more practical approach is suggested by Serra et al. [5] . They proposed a feedback control system by using a linearized model to keep the liquid in the tank and reboiler an optimal level by using two PI control.

A more advanced approach for a DWC is the MPC strategy reported by Adrian et al. [6] . In this study three temperatures were controlled by manipulating reflux ratio, liquid split, and side product flow rate. A control structure is proposed [7]. In this case study they proposed a control structure using PID controllers. They concluded that the composition of the heavy component at the top of the prefractionator is an implicit and practical way to minimize energy consumption in the presence of feed disturbances. This specific composition was controlled by the liquid split variable (R_L).

using dividing-wall columns can save up to 30% in the capital invested and up to 40% in the energy costs[8]. Particularly for close boiling-species (Perry's Handbook, 2008). The books by Doherty and Malone[9], Sundmacher and Kienle [10],Luyben & Yu[11] , Stichlmair and Fair [12]give updated summaries of modelling, simulation and control of reactive distillation.

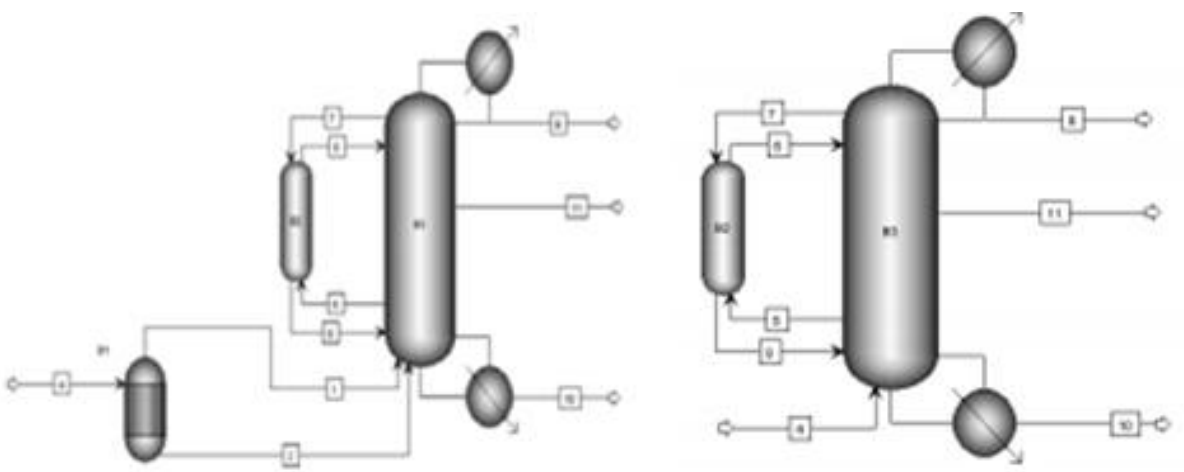

Figure 2 Reactor plus column and reactive dividing wall distillation column

Wang et al. [13] investigate the design and control strategies of a reactive distillation process with partially thermal coupling for the production of methanol and n-butyl acetate by trans- esterification reaction of methyl acetate and n-butanol. Adams and Seider [14] introduced a semi-continuous process that alternates between reactive extraction and reactive distillation in a single packed column. They have shown a different control scheme with different tuning parameters, which triggers for the various process functionalities. Wang et.al. [15] investigated the control strategies of the reactive distillation with thermally coupled extractive distillation process for the production of dimethyl carbonate (DMC) and ethylene glycol. Dynamic simulation results shows that designed temperature control strategy can maintain reactant in the RDC and product purities at their desired set point values under feed flow rate and feed composition disturbances. *Figure 2* illustrates the evolution of reactive divided wall column by combining the reactive distillation column and simple distillation column into a single column.

A control structure of DWC is shown in *Figure 3* in which MPC controller is applied to control the compositions of three products (benzene, toluene, and o-xylene) by controlling the corresponding temperatures of respective tray.

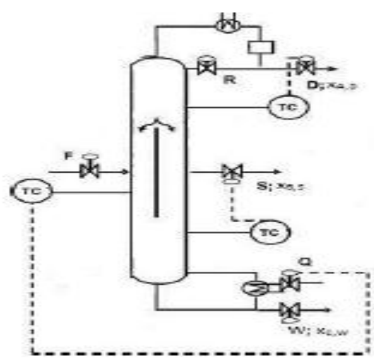

Figure 3 Control structures of divided wall column[16] (2011)

2.Control methodologies

2.1Control of TAME (2-methoxy 2-methylbutane) RD System

Tert-Amyl Methyl Ether (TAME) is an oxygenated additive for green gasoline. It is used to enhance octane number; it also improves the combustion of gasoline and reduces the CO and HC emission.

TAME is produced by the reaction of methanol (MeOH) and the isoamylenes 2-methyl-1-butene (2M1B) and 2-methyl-2-butene (2M2B). There are three simultaneous equilibrium reactions in the formation and splitting of TAME: the two etherification reactions and the isomerization between the isoamylenes:

2M1B +MeOH ↔TAME (1)

2M2B +MeOH ↔TAME (2)

2M1B ↔2M2B (3)

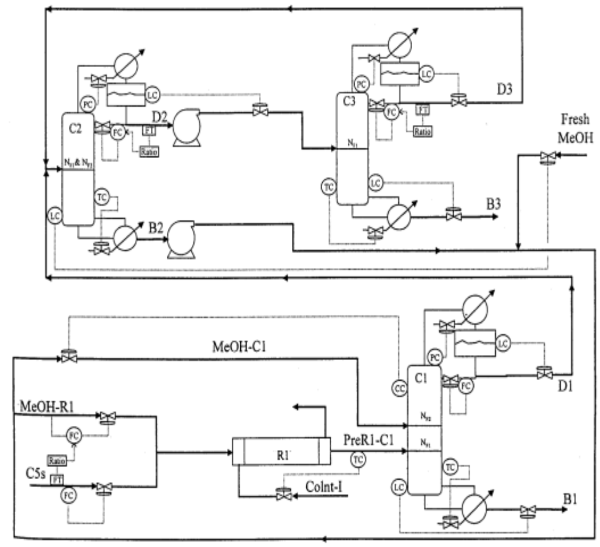

Figure 4 Control structure proposed by Al-Arfaz and Luyben (2004)

The control structure proposed by Al-Arfaz and Luyben [17] as shown in *Figure 4* was studied the plant wide control of TAME reactive distillation column.

The feeds to the reactor are subcooled methanol and subcooled C5s. In the TAME system the methanol feed to the reactive column is used to control an internal methanol composition. The C5s feed is used as the production handle. Although both fixed reflux ratio and fixed reflux strategies were found to work. Fixed reflux was selected because it is desirable to take the azeotrope in the distillate to the recovery units and not to recycle it back to the reactive column.

2.2Control of MTBE system

Methyl tert-butyl ether (MTBE) is a commonly used antiknock compound added to gasoline to increase its octane number. It has been probably the most studied reacting system in reactive distillation.

Huang et al. [18] studied a reactive distillation column that decomposes methyl tertiary butyl ether (MTBE) into isobutylene (IBUT) and methanol (MEOH) using direct composition control.

MTBE↔isobutene(IB)+methanol(MeOH) (4)

Barlett [19] studied the control of a methyl tert-butyl ether (MTBE) reactive distillation column. They discussed the several schemes using conventional PI controllers. The PI control systems were tuned in a sequential manner. For each control loop, a relay-feedback test was performed to obtain the ultimate gain and ultimate frequency. *Figure 5* shows the control configuration of MTBE decomposition in which purities of top and bottom products are controlled.

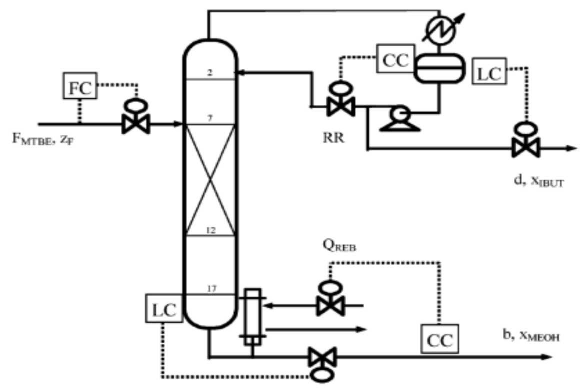

Figure 5 Control schemes for the MTBE decomposition reactive distillation column

2.3Control of ethyl acetate RD system

In this study a Mixed-Integer Dynamic Optimization (MIDO) model and solution strategy is used to study the interactions between process design and process control of an ethyl acetate reactive distillation system Al-arfaj&Luyben [20] compared the control of an ideal reactive distillation column with that of a similar real chemical system, the production of methyl acetate.

A number of control structures were evaluated for both systems. Gruner et al.[21] proposed a non-linear control scheme for an industrial reactive distillation column operated investigated model gain scheduling for an ETBE reactive distillation column [22]. The methodology employed in this work relies on a systematic mixed-integer dynamic optimization (MIDO) framework exploring simultaneously the interactions between process and control system design [23]. The main problems encountered in achieving high purity products in ethyl acetate reactive distillation are the temperature profile in the column, separation difficulties due to azeotrope formation and same K values of water, ethyl acetate, and ethanol. To overcome this problem two strategies are used in the first strategy, column design is optimized by keeping control scheme fixed. The column design includes number of trays and feed location, column diameter, exchanger areas, controller tuning parameters. In the second strategy control structure selection is decided shown in *Figure 6*.

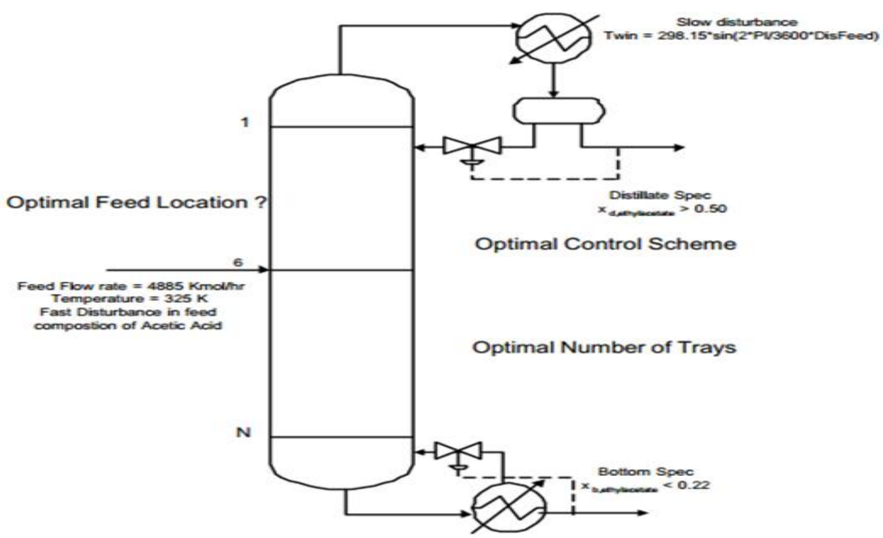

Figure 6 Ethyl acetate column structure

This work considers an advanced MIDO framework for studying the interaction between process design, process control and operability in a reactive distillation system. In fixed control scheme two PI controllers were used to control the distillate ethyl acetate composition and bottom ethyl acetate composition. Only P controllers were used to control the level. Economic advantages of the order of 3.7% are obtained with dynamic performance, production specifications and operational restrictions despite the presence of rapidly varying disturbances.

2.4Control of ethylene glycol RD system

Ethylene glycol is produced from ethylene, via the intermediate ethylene oxide. Ethylene oxide reacts with water to produce ethylene glycol according to the chemical equation

$$C_2H_4O + H_2O \rightarrow HOCH_2CH_2OH \qquad (5)$$

A consecutive reaction also takes place in which ethylene oxide reacts with ethylene glycol to form di-ethylene glycol.

Kumar and Daoutidis [24] studied the control of an ethylene glycol reactive distillation column and concluded that an advanced nonlinear inverse-based controller is needed Monroy-Loperens [25] also studied the control of ethylene glycol reactive distillation column. They controlled the ethylene glycol composition in the product by manipulating the reboiler boil-up ratio. They used a modelling error compensation approach to demonstrate that a PI configuration with anti-reset windup (ARW) is able to control the ethylene glycol reactive distillation column. Similarly, Al-Arfaz [26]in their study demonstrated that ethylene glycol reactive distillation columns can be controlled effectively by a simple PI control scheme. For controlling product quality composition analyzer is used which is very expensive so temperature measurement is preferred over composition measurement. In the stripping section of ethylene glycol reactive column, there is a large temperature change as the water is separated from the ethylene glycol. so the temperature on tray 3 from the bottom is controlled by manipulating reboiler heat input.

The PI control scheme demonstrated by [20] is shown in *Figure 7* the concentration of ethylene oxide throughout the column is very small, and conversion of ethylene oxide is essentially 100%. Therefore, production rate can be controlled by controlling the fresh feed of ethylene oxide. By manipulating condenser heat duty pressure of column is controlled.

Reflux drum level is controlled by manipulating the fresh water feed and the column base level is controlled by manipulating bottoms product flow. The temperature control loop has a first-order lag with a time constant of 0.5 min and a dead time of 4 min, which give very conservative estimates of performance. The temperature loop is tuned using the relay-feedback test and Tyreus-Luyben settings.

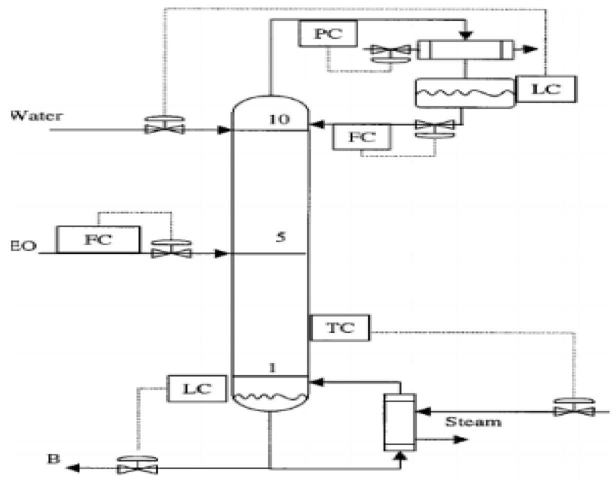

Figure 7 Control structure of ethylene glycol

2.5Control of methyl acetate hydrolysis

The synthesis of Methyl Acetate and the reverse reaction, the hydrolysis of Methyl Acetate are popular test systems for studies of Reactive Distillation. The equilibrium of the reaction of Methyl Acetate with Water to Acetic Acid and Methanol lies on the side of the products.

Methyl Acetate+ Water ↔Methanol + Acetic Acid

Using Reactive Distillation it is possible to increase conversion by continuously removing the products from the reaction zone. As shown in *Figure 8*, Products are withdrawn from the bottom of reactive distillation column and separated out in further distillation column.

By combining the Reactive Distillation Column and separation column in a single column which is Reactive Divided Wall Column with Methanol as a side product stream, the residence time of Methanol together with Acetic Acid and water in the sump is reduced to a minimum.

Kumar and Kaistha studied the effect of internal heat integration by catalyst redistribution on the controllability of an ideal and a methyl acetate reactive distillation (RD) column[27].They also evaluated the two-temperature control structure for a methyl acetate reactive distillation (RD) column on the basis of ratio control scheme [28]. Volker et al. [29] studied the heterogeneously catalyzed esterification of methanol and acetic acid to methyl acetate in a semi batch process in a reactive distillation column. Al-Arfaz [20]explore three control structures applied to both the methyl acetate and the ideal systems shown in *Figure 9*.

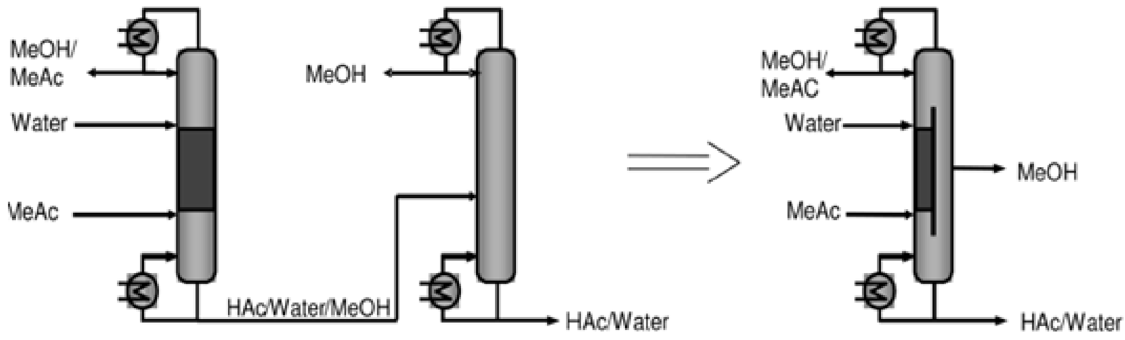

Figure 8 Principle of combining the reactive distillation column with the following separation column to form the reactive divided wall column (RDWC)

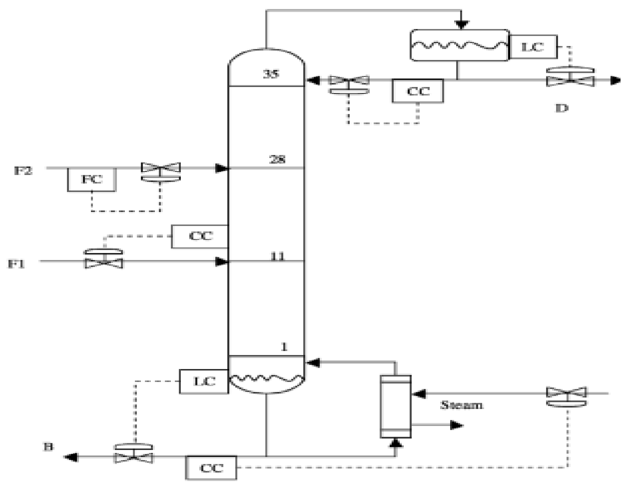

Figure 9 Control structure of methyl acetate

2.6Dimethyl ether synthesis in a reactive dividing-wall column

Dimethyl ether (DME) is of great industrial interest due to its use as clean fuel for diesel engines or in combustion cells, as a precursor to other organic compounds, as well as a green aerosol propellant that can effectively replace chloro-fluoro-carbons. DME is synthesized in a catalytic fixed-bed reactor by dehydration of methanol which is produced from syngas, and followed by a direct sequence of two distillation columns.

$$CO_2 + 3H_2 = CH_3OH + H_2O \quad (1)$$
$$CO + H_2O = CO_2 + H_2 \quad (2)$$
$$2CH_3OH = CH_3OCH_3 + H_2O \quad (3)$$

The key problem of this conventional process is the high investment costs for several units that require a large overall plant footprint, as well as the high energy requirements. To solve these problems, reactive dividing-wall column (R-DWC) is used for the DME synthesis that integrates reactive distillation (RD) unit with the DWC technology in a single column. The double integrated system allows the production of high-purity DME in only one unit, with minimal footprint and significantly lower costs.

In this study a fair comparison between the conventional DME process and the optimally designed process alternatives based on RD and R-DWC, has been done as shown in *Figure 10*. All processes are optimized in terms of minimal energy requirements, using the state of the art sequential quadratic programming (SQP) method implemented in Aspen Plus. The results clearly demonstrate that the R-DWC process has superior performances as compared to the conventional or RD process: significant energy savings of 12–58%, up to 60% reduced CO_2 emissions, as well as up to 30% lower capital investment costs.

3.Reactive DWC process

The reactive dividing-wall column is a highly integrated setup that consists of only one column shell, one reboiler and one condenser. Due to the absence of an off-shelf DWC unit in Aspen Plus, two coupled RADFRAC units were used as the thermodynamically equivalent of the R-DWC. The main condition in integrating two distillation columns is that similar operating conditions should be applied. The Aspen Plus model for the RDC + DC sequence is used as the starting point for the R-DWC simulation, providing initial estimates for the number of trays, feed tray locations, liquid and vapour split and size of the reactive zone.

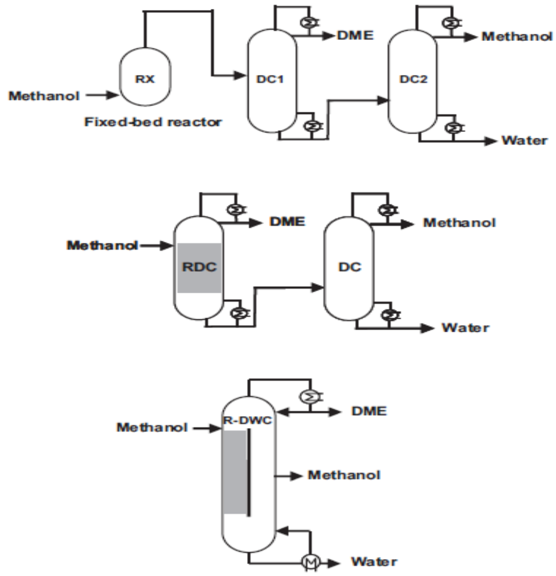

Figure 10 Simplified DME production processes alternatives: conventional process (top), reactive distillation (mid) and reactive dividing-wall column (bottom)

The objective of the optimization is to minimize the total reboiler duty required, as follows:

Min (Q)= f(N_T, N_F, N_R, N_{RZ}, N_S, N_{SS}, N_{DWS}, SFR, RR, V, r_v, r_l)

The design problem is a complex optimization problem with both continuous (SFR, RR, V, r_v, r_l) and discrete (N_T, N_F, N_S, N_{SS}, N_{DWS}) decision variables.

where N_T is the total number of stages, N_F is the feed stage, N_R is the number of reactive stages, N_{RZ}, is the location of the reactive zone, N_{DWS} is the number of dividing-wall stages, N_{DWC} is the location of the dividing-wall, NSS is the stage of the side-product withdrawal, RR is the reflux ratio, V is the boilup rate, FSS is the flow rate of the side stream product, r_L and r_V are the liquid and vapor split ratio, respectively.

The state of the art sequential quadratic programming (SQP) method implemented in Aspen Plus is a very effective tool in finding the optimal process design in terms of minimum energy requirement, constraint by the required purities for DME and water, and using several discrete and continuous optimization variables: total number of stages, feed stage, number of reactive stages, location and length of the dividing-wall, location of the side-stream, reflux ratio, boilup rate, liquid and vapor split ratio.

4.Conclusion

In this paper, control structures for different chemical systems, i.e., MTBE, TAME, ethyl acetate, methyl acetate, Di methyl ether etc. have been discussed. There are several types of controllers which have been studied in the reactive distillation literature, ranging from simple proportional-integral (PI) controllers to advanced model predictive controllers (MPC), such as dynamic matrix control (DMC), The proportional-integral-derivative (PID) controller has gained widespread use in many process control applications due to its simplicity in structure, robustness in operation, and easy comprehension of its principle but PID algorithm was not effective in controlling the highly interactive system concurrently at a large number of constraints so the application of advanced control techniques such as advanced adaptive control, pattern based predictive control, stochastic optimization algorithms and model predictive control have been propounded in the RD control literature. Reactive divided wall distillation column (RDWDC) is a novel concept to reduce capital cost and make system more energy efficient because it consists one condenser and one reboiler thus it reduces energy requirement and by consisting reactive zones, pre-fractionator and main column into a single column, reduces the capital cost . These systems are useful for such type of reactions where intermediate boiling product is formed.

Acknowledgment

None.

Conflicts of interest

The authors have no conflicts of interest to declare.

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