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Economic Analysis for Energy Efficient Reactive Distillation

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Abstract: Complex chemical reactions and downstream processing can be performed in reactive distillation column to overcome with equilibrium limitations and to make it an economical process. An existing reactive distillation unit is costly to modify due its complex configuration and existing limitations of structure, space area, etc. Modifying an existing plant is a tedious task and more complex than a new process. Thus, to modify the existing operating conditions and input design variables it is necessary to verify by applying the same in real plant condition. This is done using revamping based on rigorous simulation and optimization in Aspen Plus process simulator. The main form of energy generator used in a distillation column is reboiler which directly affects the utilities such as cooling water, electricity and steam. Therefore, optimizing this reboiler duty to reduce energy losses is done using optimization model analysis tool of Aspen Plus. This reduction of energy demands diminishes the operating cost as per the reduction in utility cost. Now this reduction in operating cost is evaluated corresponding to the optimized reflux ratio and number of plates as obtained using sensitivity analysis tool of Aspen Plus.

Keywords: Economic analysis, Methyl acetate, Optimization, Reactive distillation

I. INTRODUCTION

Methyl acetate is a carboxylate ester with the formula CH_3COOCH_3. It is a flammable liquid and found its major use as a solvent. Methyl acetate is produced industrially by liquid phase reaction of acetic acid and methanol in presence of an acid catalyst. In homogeneous phase reaction sulfuric acid is treated as a catalyst but for a heterogeneous reaction most of the ion exchange resin such as Amberlyst 15 is used as a catalyst in solid form [1].Apart from esterification there are many other processes by which methyl acetate can be produced[2-4]. Reactive Distillation (RD) is a combination of reaction and distillation in a single vessel owing to which it enjoys several specific advantages over conventional sequential approach of reaction followed by distillation or other separation techniques[5]. Selectivity can be improved by continuous removal of product from reaction mixture, which is the major advantage of reactive distillation technology The most cited example of reactive distillation in industry is for the production of methyl acetate at Eastman Company [6].The economic benefit of reactive distillation includes: (i) lower capital investment (ii) lower capital cost (iii) lower energy cost and higher product yield[7]. As per the literature various commercial process simulators are used to simulate reactive distillation for production of different products during last decades. Steady state simulation of reactive distillation column using aspen plus is done for various cases[8]. Optimization using sensitivity analysis tool of Aspen plus was a major concern in recent years as it validates the result of optimization [9].

In recent years many research works have been done for energy loss prevention of a distillation as well as for reactive distillation column. CO_2 emission is a major disadvantage for those cases in which high energy losses occurred. The CO_2 emissions from burning the fuel in the furnace is calculated by the equation developed in (Delaby and Smith, (1995) [10].In this paper, two designs of heat-integrated reactive distillation for the hydrolysis of methyl acetate were studied. The first one employs internal heat-integrated reactive distillation column (r-HIDIC) and the other utilizes feed-split reactive distillation column (r-FS). The savings in energy consumption and total annual costs are focused on the reactive column only [11]. Bodo Linnhoff’s discussed that good integration between distillation and overall process can result in column operating at zero utility cost. Retrofits suggest modifications for existing distillation columns to reduce the costs of operations by increasing the efficiency in energy utilization[12]. The materials, unit operations and processes involved are identified; therefore, the retrofit design is preferable than the grass-roots design for oil refineries (Pejpichestakul, 2013)[13]. Many researchers worked on revamping crude distillation units by sequential approaches, or in simultaneous approaches with targets of Pinch Analysis (Gadallaa et al., 2003)[14]. Standard objectives of this work are revamping to increase the product purity, reducing the energy demands, utilizing more efficiently the input design variables and thus the overall economic optimization of reactive distillation column. All these objectives preferably be fulfilled without modifying much the physical constraints of the unit, such as column actual diameter, pump around and side columns locations, in fact is done using various operating conditions of the distillation column, including number of plates, feed flow rates, reflux ratio and reboiler. The optimization results will be set of optimum input design variables and optimum cost corresponding to highest product purity.

II. METHODOLOGY

2.1. Simulation using Aspen plus

In this work simulation of methyl acetate esterification in a reactive distillation column is carried out using Aspen plus process simulator. The reactive distillation column is represented using RadFrac module and NRTL property method is used to estimate the property of the system. The column specifications are given in table1.

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Table 1: Column Configuration in Aspen Plus

COLUMN SPECIFICATIONS	
No. of plates	10
Rectifying Section	1-3
Reactive Section	3-6
Stripping Section	6-10
Reboiler	Jacketed
Condenser	Total vertical
Non-reactive zone packing	Katapak-S
Reactive zone packing	Amberlyst-15
Property Method	NRTL

After simulation, the revamping of input design variables is performed to get an optimized value of these variables corresponding to the highest product purity. Using the process condition as described above the highest product purity obtained was 90%. In our research work the input design variables which are considered for revamping are reflux ratio, number of plates and reboiler duty. The optimized values of these input variables as obtained using revamping are validated using optimization model analysis tool of Aspen plus.

2.2. Sensitivity analysis

The sensitivity model analysis tool of Aspen plus simulator is used to get an optimized value of a process variable within the range provided by the user. In our work the optimized value of input design variables as obtained from revamping and optimization model analysis tool are further validated using sensitivity analysis and it is found that highest product purity correspond to the same values of reflux ratio, number of plates and reboiler duty as obtained using both the three methods.

2.3. Economic analysis

Total operating cost includes the operating parameters like flow rate, reboiler duty, reflux ratio etc. needed to produce a product. Here we have taken reflux ratio as the basis for evaluation of optimized total operating cost. Total capital cost includes onetime investment such as land, building, equipment etc. Total number of plates in the reactive distillation column is a crucial parameter which is to be optimized as this directly affects the reflux ratio which is again a contributing factor for the operating cost. Thus the challenge of this paper is to find the optimized value of design variables to get highest product purity with an optimized cost. Thus optimization of overall cost which includes total operating cost, total capital cost and total utility cost of reactive distillation column is carried using economic analysis tool in Aspen plus.

2.4. Reducing energy losses using utility cost optimization

The main source of energy provided to a reactive distillation column is in the form of heat energy supplied by the reboiler at the bottom. To provide this heat energy three major utilities are involved which is electricity, cooling water at the top of the column to cool down the vapor to get the product in liquid form and steam which may be used in the form of jacketed heating medium. Therefore, we can say that reducing the utility cost is directly related to the prevention of energy losses. Thus, to optimize utility cost corresponding to higher product purity, reboiler duty may be taken as basis.

Figure 1: Pilot scale experimental setup

2.5. Application of simulation result in pilot scale reactive distillation column

The simulations results obtained from Aspen plus are applied to a real pilot reactive distillation column under the same optimized operating condition as used in Aspen plus. The product purity from the experiment is determined and is found to be 93% which is approximately like that obtained from simulation. Figure 1 shows the pilot plant experimental setup. The reactive distillation used is a packed column but is represented in the form of segment. The non-reactive section comprises of stripping and rectifying section and is filled with Katapak-S packing. The rectifying section starts from segment 1-3, reactive zone extends from segment 3-6 and stripping section extends from 6-9. The reboiler is considered as the 10th stage. The reactive zone is filled with a solid ion exchange catalyst (Amberlyst 15) to enhance the rate of reaction.

III. RESULTS AND DISCUSSION

3.1. Simulation of methyl acetate esterification in a reactive distillation column

Esterification of methyl acetate was considered as case study for two feed and two product system. Methanol and acetic acid are the two feed considered and methyl acetate, water are top and bottom product respectively. RadFrac module using NRTL property method corresponding to the provided operating condition and column specification which is shown in table II provides the highest product purity of 90%.

Table 2: Operating and Feed Condition in for Simulation

FEED CONDITIONS	
Feed flow rate	• Methanol=0.02l/min • Acetic acid=0.02l/min
Reboiler duty	1.5 KW
Reflux Ratio	5

The simulation diagram is shown in figure 1 and the

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results are plotted in figure 2.

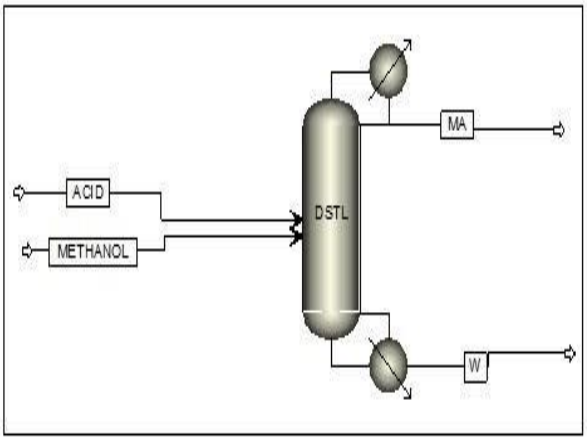

Figure 2: Schematic diagram of reactive distillation column in Aspen plus

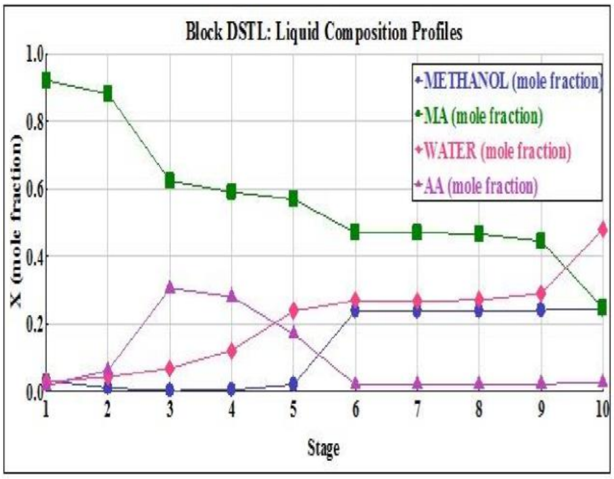

Figure 3: Composition profile in packed reactive distillation column in Aspen Plus

3.2. Revamping of input design variable and optimization in Aspen plus

Revamping of input variable is done to study the changes in product composition corresponding to the change in combination of input design variables. The input variables considered here are reflux ratio, number of plates and reboiler duty. The various conditions used and the results obtained are shown in table 3.

Table 3: Revamping Conditions and Product Purity

REVAMPING CONDITIONS AND RESULTS			
Reflux ratio	**Reboiler duty(KW)**	**No. of plates**	**Product purity (%)**
3	2	10	58
4	2.5	10	77
5	1.5	10	90
6	3	8	85
10	1	6	83
12	2	4	66
13	4	14	59

From the above table we can infer that at the reflux ratio of 5, reboiler duty of 1.5KW and number of plates 10 we are getting highest product purity of 90%.

The resultant graphs are show in figures below.

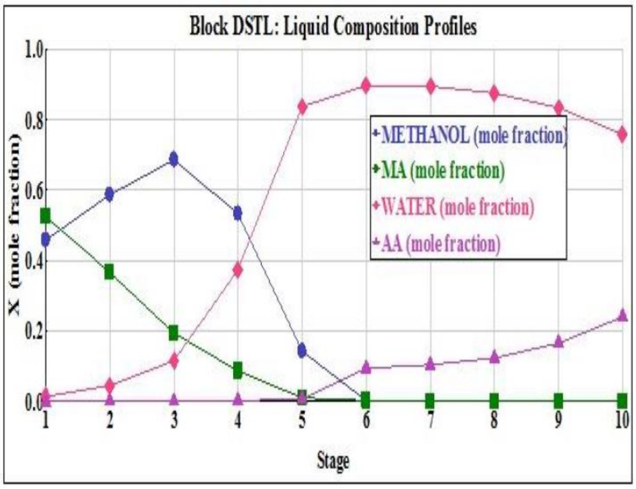

Figure 4: Composition Graphs from Aspen plus corresponding to RR=3, RD=2, NP=10

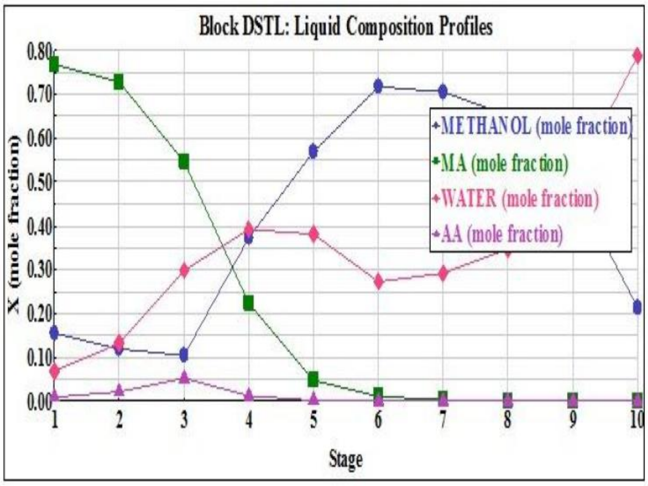

Figure 5: Composition Graphs from Aspen plus corresponding to RR=4, RD=2.5, NP=10

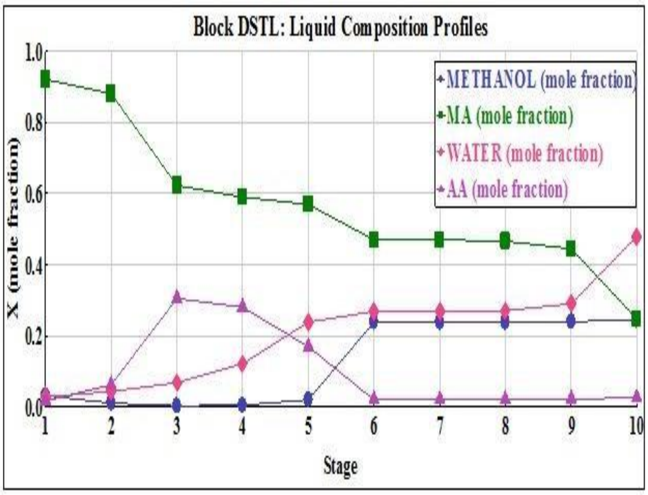

Figure 6: Composition Graphs from Aspen plus corresponding to RR=5, RD=1.5, NP=10

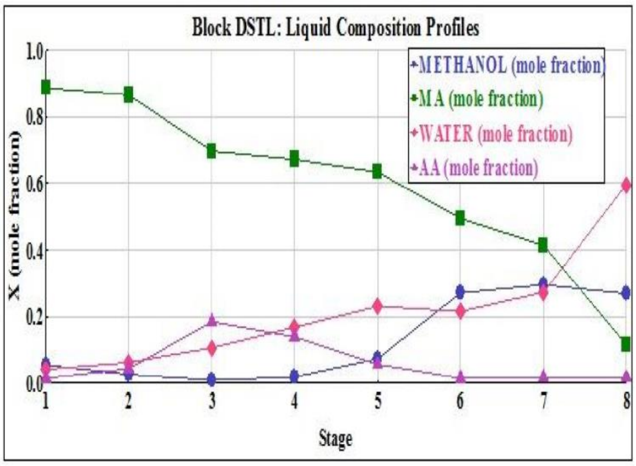

Figure 7: Composition Graphs from Aspen plus corresponding to RR=6, RD=3, NP=8

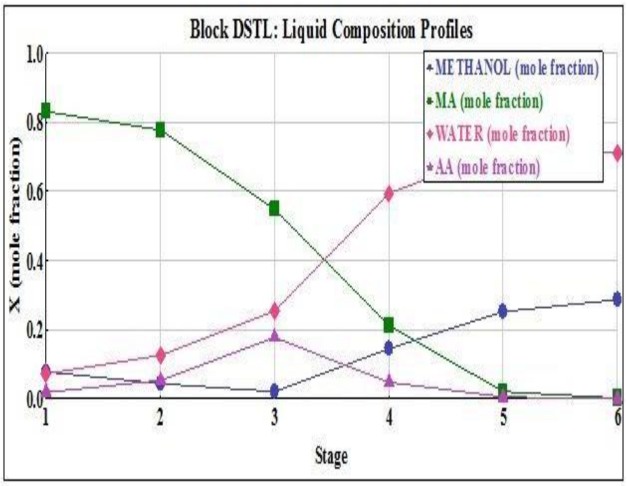

Figure 8: Composition Graphs from Aspen plus corresponding to RR=10, RD=1, NP=6

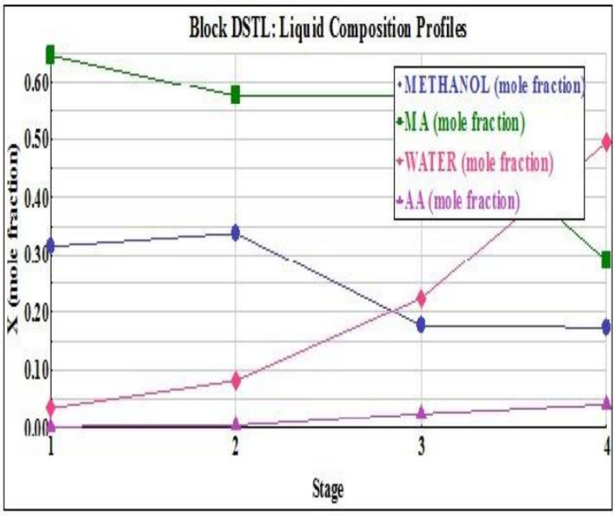

Figure 9: Composition Graphs from Aspen plus corresponding to RR=12, RD=2, NP=4

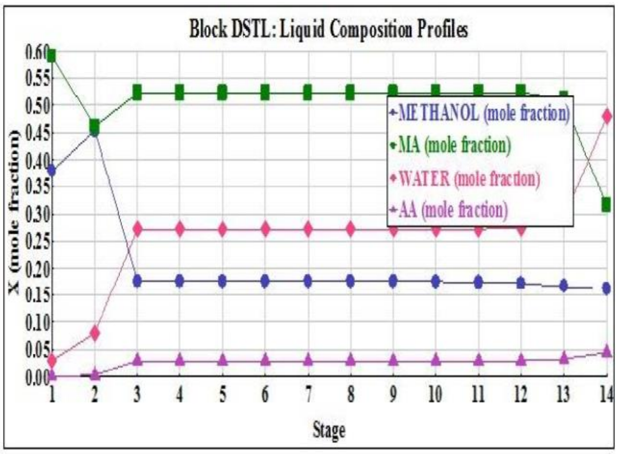

Figure 10: Composition Graphs from Aspen plus corresponding to RR=13, RD=2, NP=14

Now to validate the revamping results optimization model analysis tool is used in Aspen plus whose results are shown in table 4.

Table 4: Optimization Results from Aspen Plus

MANIPULATED VARIABLE			MEASURED VARIABLE
Reflux ratio	**Reboiler duty (KW)**	**No. of plates**	**Product purity (%)**
5	1.5	10	90

Thus, our revamping results are validated using optimization model analysis tool in Aspen plus.

3.3. Sensitivity analysis in Aspen plus

To validate the revamping and optimization result sensitivity analysis in Aspen plus is done. In this tool the lower and the upper limit of the manipulated variable is provided by the user and the corresponding measured variable is calculated by the simulator. The ranges for reflux ratio, reboiler duty and the number of plate are given and the product purity is calculated whose results are same as obtained from revamping and optimization. The results are plotted in figures below.

3.4 Economic analysis

Economic analysis tool of Aspen plus calculates the total operating cost, total utility cost and total capital cost automatically using the input conditions provided by the user. Revamping of input variable is done in this case to obtain those values of this cost corresponding to highest product purity. The revamping conditions and results are same as in table IV and results are plotted in figures below.

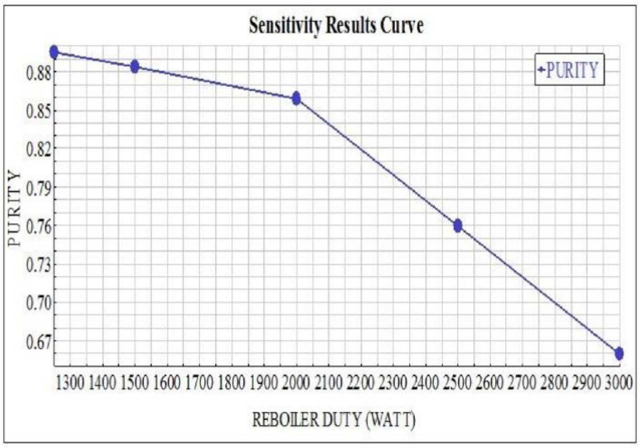

Figure 11: Sensitivity result for the variation of purity with reboiler duty

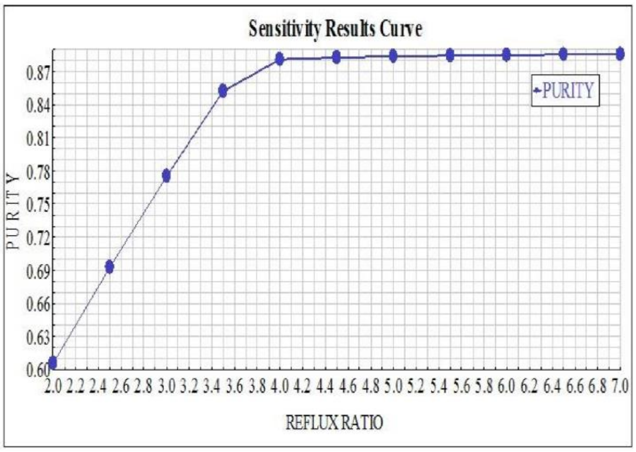

Figure 12: Sensitivity result for the variation of purity with reflux ratio

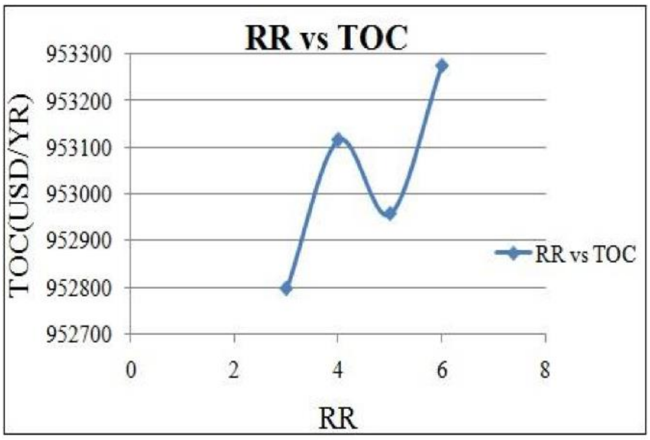

Figure 13: Variation of TOC with RR

From figure 14 we observe that as the value of reflux ratio increases the total operating cost also increases but it shows a minimum at reflux ratio of 5 after which on further increasing the reflux ratio the operating cost again start rising. Thus we can say that the reflux ratio of 5 is the optimized value corresponding to the lowest operating cost and highest product purity.

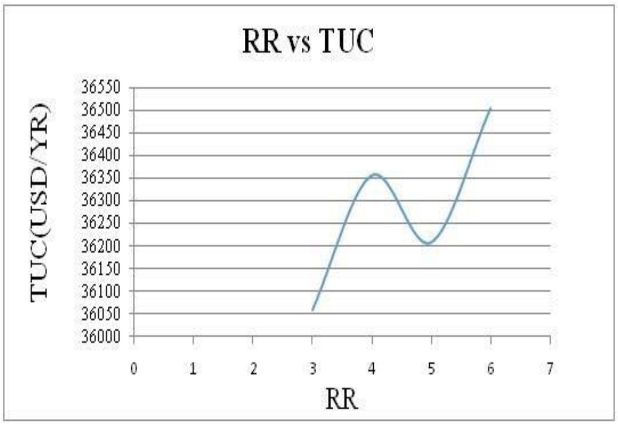

Figure 14: Variation of TUC with RR

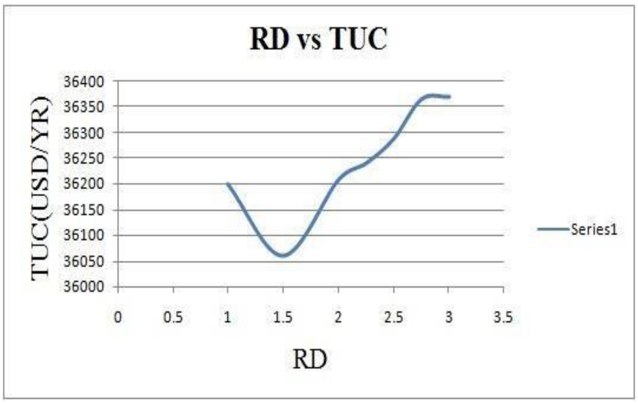

Figure 15: Variation of TUC with RD

The utility cost includes electricity, steam and cooling water cost. As reflux ratio increases more of the reboiler heat is consumed to vaporize the incoming liquid which results in energy loss. Also more of the steam for heating purpose will be wasted. Because of the higher reboiler duty as the more volatile component reaches the condenser with higher rate thus more of the cooling water will be required which again results in a loss of energy. From the economic analysis tool of Aspen plus this statement is validated and is observed in figure 15 and figure 16 that with increasing the reflux ratio TUC increases but achieve a minimum at RR=5; increasing the reboiler duty increases the TUC but at RD=1.5 the TUC reduces which on further increase in RD start rising. Thus we can say that a reflux ratio of 5 and reboiler duty of 1.5 KW are the optimized values corresponding to lowest TUC.

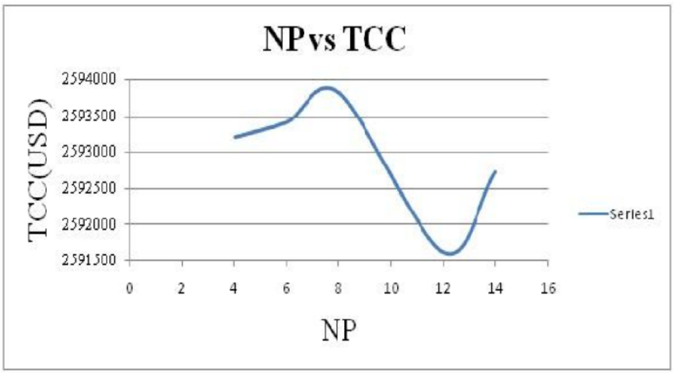

Figure 16: Variation of TCC with NP

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Total capital cost is a onetime investment cost which includes land, auxiliaries, equipment and accessories cost. This cost cannot be modified once the system is being installed. Now for reactive distillation column number of plates is a parameter which is defined prior to its installation. Once the column is installed number of plates cannot be changed practically. Thus in our work we have varied number of plates to observe its effect on total capital cost whose result is plotted in figure 16 which shows that NP=12 the TCC is achieving a minimum , however the simulation results shows that at NP=12 the product purity reduces to 60% which is a major drawback. However, at NP=10 the product purity reaches its maximum i.e. 90% and TCC also remains in the minimum cost domain. Thus NP=10 is the optimized value corresponding to highest product purity and minimum TCC.

III. CONCLUSION

Optimization of reactive distillation column with respect to product purity and the overall cost is a challenging but crucial task which must be considered as it directly relates to the energy consumption. Simulation of methyl acetate esterification is carried out in a reactive distillation column using Aspen plus. Optimization of input design variables using conventional revamping, optimization and sensitivity analysis tool of Aspen plus are done to obtain the optimized input condition corresponding to highest product purity. Along with the prioritization of product purity the overall cost and energy saving is considered in this paper. Economic analysis tool along with conventional revamping is done and the result of model analysis tool and economic analysis tool are combined to obtain the overall optimized condition which is RR=5, RD=1.5KW and NP=10 corresponding to the product purity of 90%.

NOMENCLATURE

NP number of plates
RD reboiler duty, KW
RR reflux ratio
TCC total capital cost, USD
TOC total operating cost, USD/YR
TUC total utility cost, USD/YR
USD united states dollar
KW kilowatts
YR year

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