



SIMULATION STUDIES FOR HEURISTIC OPTIMIZATION OF HEAT INTEGRATED REACTIVE DISTILLATION PROCESS FOR ISOAMYL ACETATE (IAAc) SYNTHESIS

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Abstract: In any separation process one of the most important targets is to achieve cost optimization through managing the energy utilization for the degree of separation being the constraint. Reactive Distillation is one such process which combines reaction and separation in one single process unit to reduce the cost of process, and heat integration in such process can add one more dimension of optimizing energy demand. The present work is to simulate and analyze the heat integration aspect of Reactive distillation process for the production of Isoamyl Acetate (IAAc). Rigorous heuristic optimization is done using DWSIM simulation software, to arrive at process and design specifications which give minimum energy demand without compromising the product purity (96% pure).

Index Terms - Reactive distillation, heat integration, simulation, optimization, IAAc(Isoamyl acetate), Isoamyl alcohol, Acetic acid

I. INTRODUCTION

Isoamyl Acetate is widely used in chemical industries as a solvent for some varnishes, used to test the effectiveness of respirators or gas masks. Isoamyl Acetate is an esterification process of Isoamyl alcohol and Acetic acid. Isoamyl acetate is produced industrially by two methods: Reaction and Separation & Reactive Distillation Process. Reactive Distillation is one such process which combines reaction and separation in one single process unit to reduce the cost of process [1]. Process intensification presents one of the most important trends in the current chemical engineering and process technology. Reactive Distillation (RD), one of the best-known examples of process intensification [5].

II. PROCESS DESCRIPTION

Isoamyl Acetate is an esterification process of Isoamyl alcohol and Acetic acid. It is produced by conventional process i.e. Reaction and separation process in different units, which requires more heat duty hence overall cost for the process. Hence, Reactive distillation process is used to minimize the heat duty and cost. The heat duty can be further minimized by utilizing heat being wasted from outgoing streams i.e. Heat Integration Process. Heat duty is a function of number of stages, feed stages, reflux ratio, capacity of column, product composition. The current work analyses this possibility along with utilizing waste heat going out with outlet stream by heat integration method to reduce the overall cost of the process. The analysis is done by the simulation of process flow sheet in DWSIM by changing various parameters.

2.1 Heat-Integration Process:

Heat integration is done by recycling of streams, reboiler flashing, avoiding condenser etc. The outlet temperature of product stream 1 is about 180°C. The dependency of heat duty on temperatures of various streams is examined and it is decided to choose stream 1 for heat integration. Avoiding condenser, the condenser heat duty is minimized to zero. The flow sheet of Heat integration process is shown in figure 1.

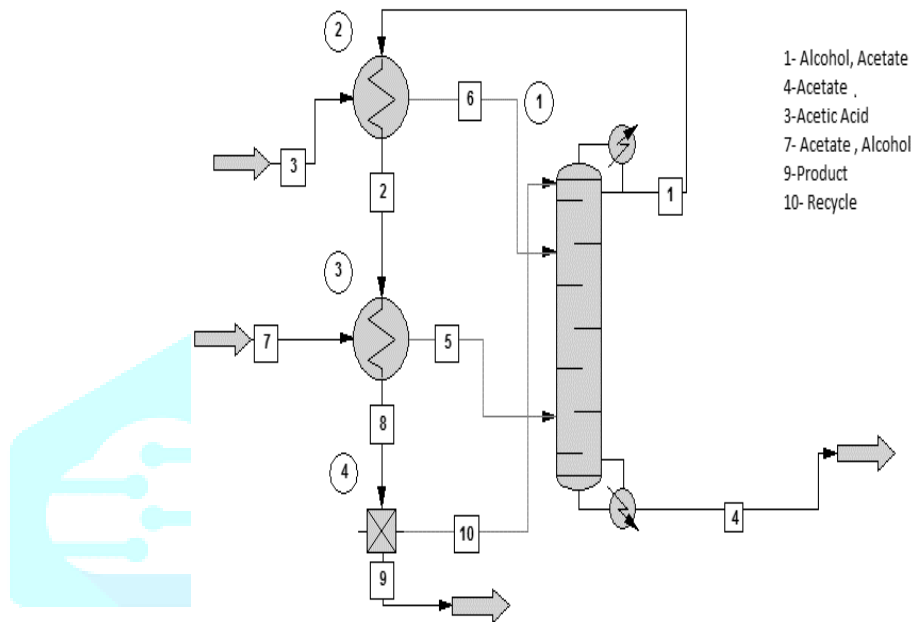


Figure 1 Process Flow Diagram

III. RESULTS & DISCUSSION

3.1 Reactive Distillation Process:

The analysis of simulation of synthesis of IAAC by reactive distillation is done by changing various parameters such as number of stages; feed stages, reflux ratio, capacity of column, product composition and the optimum results for heat duty is obtained. The current process work will minimize the heat duty and hence overall cost.

3.2 Heat-Integration Process:

The condenser duty in minimized to zero avoiding condenser use and recycling of product stream will further reduce the total heat duty for the process. The same procedure will be followed as followed in RD simulation process. The number of stages, feed stages and recycle stages are varied consecutively and total heat duty is noticed for each variation keeping product composition constant.

3.2.1 Total number of Stages:

The total number of stages is varied consecutively keeping product composition constant and the change in total heat duty is noticed. The optimum result obtained is shown in table 1.

Table 1 Total number of stages

Sr. No.	Total Stage	Feed Stage 1	Feed Stage 2	Feed Ratio	Recycle Feed Stage	Composition	Total Heat Duty (MJ/hr.)
1.	30	13	14	3:2	1	0.96	26230

Heat duty v/s total stage

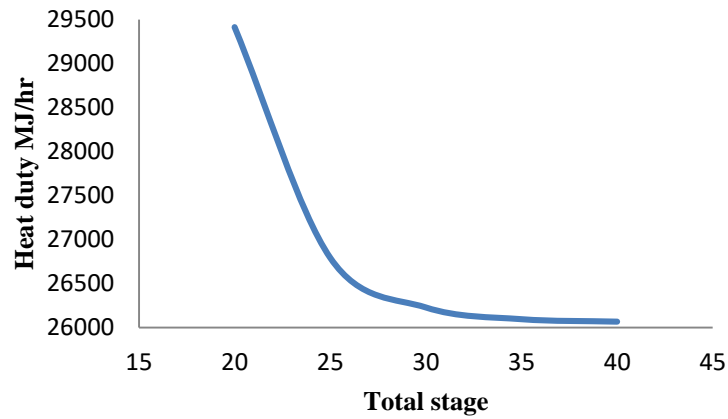


Figure 2 Heat duty v/s total stage

3.2.2 Feed Stage:

The feed stages of the streams are varied consecutively keeping product composition constant, total heat duty is noticed. The optimum result obtained from iterations is as per table 2.

Table 2 Feed Stages

Sr. No.	Total Stage	Feed Stage 1	Feed Stage 2	Feed Ratio	Recycle Stage	Feed	Composition	Total Heat Duty (MJ/hr.)
1.	30	5	9	3:2	1		0.96	25982

Heat duty v/s feed stage

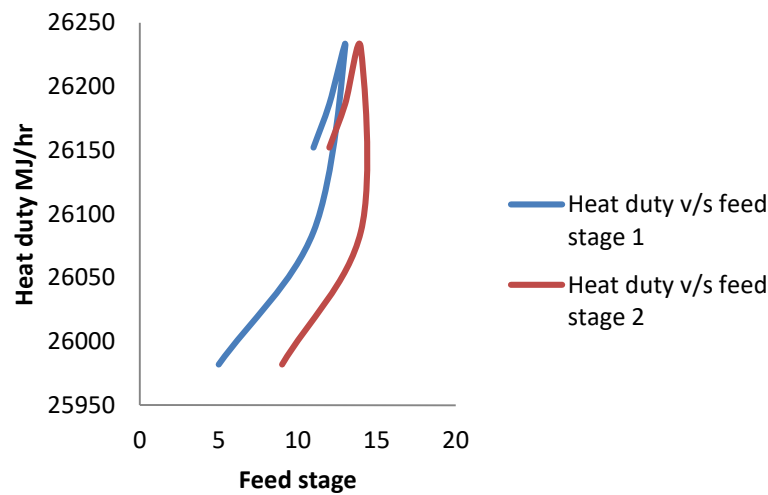


Figure 3 Heat duty v/s feed stage

3.2.3 Recycle Ratio:

The feed ratio i.e. ratio of flow rates of recycle stream going back to column and product that coming out is varied consecutively and total heat duty variation for each change is noticed. The optimum result obtained is shown in table 3.

Table 3 Recycle ratio

Sr. No.	Total Stage	Feed Stage 1	Feed Stage 2	Feed Ratio	Recycle Feed Stage	Composition	Total Heat Duty (MJ/hr.)
1.	30	5	9	1:1	1	0.96	25191

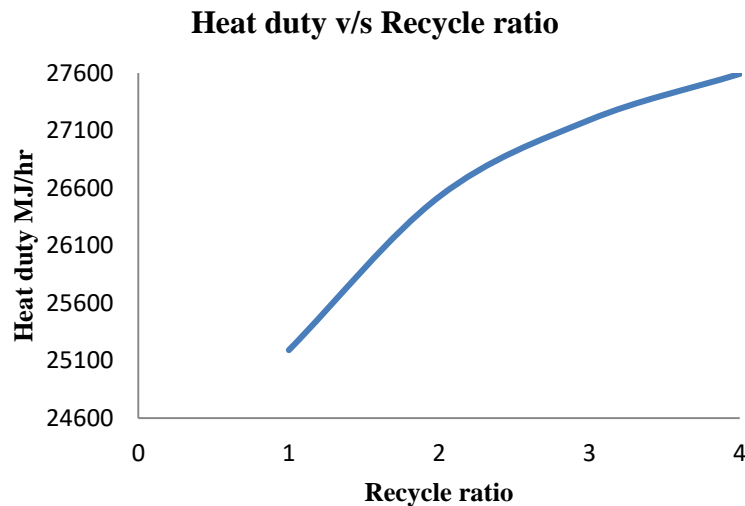


Figure 4 Heat duty v/s Recycle ratio

IV. RESULT AND DISCUSSION

The comparison of results of RD process and Heat Integrated RD process is shown in table 4. From obtained result, it can be concluded that in Isoamyl acetate production, the total heat duty can be reduced to as low as one-third by heat integration technique.

Table 4 Comparison of both the processes

Sr. No.	Parameters	RD Process	HI RD Process
1.	Total stage	25	30
2.	Feed stage 1	11	5
3.	Feed stage 2	12	9
4.	Reflux ratio	2	-
5.	Composition	0.96	0.96
6.	Recycle ratio	-	1:1
7.	Heat duty	65162	25191

V. CONCLUSION

The simulation of heat integrated reactive distillation using DWSIM is effective process than conventional methods for obtaining optimum configuration for IAAC synthesis. Use of simulation software like DWSIM facilitates rigorous simulation to generate solution/results, which can be good basis for experimental validation. It can also be seen that in future, there is a scope for analyzing the possibility of reboiler flashing or using the heat carried by the bottoms stream.

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