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Simulation & Control Studies of Dual Reactive Distillation for Fatty Acid Esters

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Abstract: ***Present study aims at carrying out steady state & dynamic simulation of a dual Reactive Distillation(RD) using aspen plus. Aspen dynamics simulation is a useful tool for finding required control structure to the process. Controller interaction and response of the system for various disturbances in Lauric acid feed (temperature, molar flow rate). Studying the performance subjected to changes in feed is known as regulatory performance. In the present study exothermic irreversible reaction of lauric acid and 2-ethyl-hexanol, lauric acid and methanol along with separation is carried out in a reactive distillation column to form methyl laurate and 2-ethylhexanyl laurate. The dynamic response of the process studied for three different control structure those are default control structure, single point control structure and two point temperature control structure. The response studied for various disturbances in Lauric acid feed and result were reported. The response of the process has been found to be faster in the case of two point control structure when compared to default and single point control structure.***
Keywords: Reactive Distillation, Fatty acid esters, simulation, biodiesel, Process Control

I. INTRODUCTION

Reactive distillation, also called catalytic distillation, can be considered as reaction and distillation combined into one new unit operation. Distillation itself is here considered in the wide sense, i.e. the separation by use of vapor–liquid composition difference. So it includes distillation columns, flashers, strippers and condensers. The reactions in reactive distillation considered include heterogeneous catalytic reactions, homogeneous catalytic reactions, and thermal (non-catalyst) reactions. In nearly all cases reactions take place in the liquid phase, but reactions taking place in the gas phase and locating the catalyst in the vapour phase of the column is conceivable [1].

Reactive distillation technique is advantageous in case of reversible reactions, because for such reactions, generally the reactant conversion is less due to equilibrium limitations. But if these reactions are carried out in RD, then conversion can be increased far beyond expectations by shifting the equilibrium towards the product side due to the continuous removal of reaction products from the reactive zone. The suitability of RD for a particular reaction depends on various factors such as volatility of reactants and products along with the feasible reaction and distillation temperature. Hence, the use of RD for every reaction may not be feasible [2].

Important advantages of reactive distillation which includes lower capital & operating cost, improved conversion of reactant, increased yield, improved selectivity & Heat integration benefits [3].Generally, reactive distillation can be used with a wide variety of reactions including, esterification, etherification, hydrolysis, isomerization and trans-esterification [4].

It has been reported that the synthesis of high purity fatty esters is feasible by reactive distillation (RD) using solid catalyst for esterification of the dodecanoic acid with 2-ethylhexanol and methanol. It is ensured that selective water removal that shifts the chemical equilibrium to completion, and preserves the catalyst activity [5].

In this paper process system for dual reactive distillation described with steady state simulation followed with the dynamic simulation for different control structure.

II. PREACTIVE DISTILLATION PROCESS

Dual reactive distillation was reported as a novel approach based on dual esterification of fatty acid with light and heavy alcohols, namely methanol (CH_4O) and 2-ethylhexanol ($C_8H_{18}O$) in single column. Lauric acid reacts with methanol to form Methyl Ester ($C_{13}H_{26}O_2$) and 2-ethylhexanol reacts with lauric acid ($C_{12}H_{24}O_2$) to form Ethyl Ester ($C_{20}H_{40}O_2$) by using solid catalyst sulphated zirconia.

The following irreversible reactions are considered for simulation of the column:

$$C_8H_{18}O + C_{12}H_{24}O_2 \rightarrow C_{20}H_{40}O_2 + H_2O \ldots (1)$$

$$CH_4O + C_{12}H_{24}O_2 \rightarrow C_{13}H_{26}O_2 + H_2O \ldots . (2)$$

The process is strongly non ideal due to presence of light & heavy alcohol and water in the system.

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III.PROCESS SIMULATION

Fig. 1 represents the process flow sheet of the reactive distillation column. The column contains basically three sections, top section is rectifying section, middle section is reaction zone and bottom section is stripping section. Top & bottom sections are filled with suitable packing i.e. BX packing & reaction zone are filled with the catalytic packing with the sulphated zirconia as a catalyst.

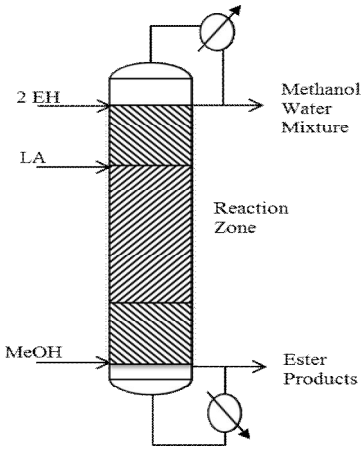


Fig.3.1 Reactive Distillation flow sheet

Kinetic Parameters for esterification of Lauric acid with 2-ethyl hexanol & methanol are available in the previous work [6]. Since reverse reaction is negligible hence simple kinetic expression is used in the simulation is

$$r = kC_AC_B \text{ .....(3)}$$

The kinetic constants are

$k_1 = 1.2 \times 10^5 \exp(-55000/RT)$ for esterification of lauric acid with methanol & $k_2 = 6 \times 10^4 \exp(-55000/RT)$ for esterification of lauric acid with 2ethylhexanol where activation energy is expressed in KJ/kmol & reaction rate in kmol/(m^3 h).

Aspen Plus has been used for model development & simulation of reactive distillation of esterification process [5]. The purpose of this simulation is to carry out dynamic simulation of system & study three different control structures i) default control structure ii) single point control structure & iii) two point control structure subjected to disturbances in feed temperature and feed flow rate.

In Aspen Plus simulator RD column simulated using rigorous RADFRAC unit [7]. The physical properties considered for simulation is UNIQUAC to estimate missing parameters in Aspen database [8]. Design parameters used in the simulation are shown in Table 1.

TABLE I PACKED COLUMN SPECIFICATIONS [9]

PARAMETER	VALUE
Lauric acid feed (kmol/hr)	100 (3.5 bar, 150 ^oC)
Methanol feed (kmol/hr)	130 (4 bar, 150 ^oC)
2 ethyl hexanol feed (kmol/hr)	20 (3.5 bar, 100 ^oC)
Number of Theoretical Stages	25
Reactive Stages	20
Reflux Flow Rate (Set) (Kg/h)	2500
Column Diameter (m)	1.2
HETP (m)	0.5
Reboiler Duty (Set) (KW)	1750
Condenser Duty (KW)	−1492

The key element is temperature in Reactive Distillation (RD). It can be changed by removing or adding heat by maintaining the Reboiler steam flow rate so that dynamic disturbances can be safely handled without RD runways. When the steady state simulation is exported to dynamic state, it is required to specify Reboiler sump and condenser collector geometry (length and diameter). Also specify holdup on each stage along with column diameter and HETP.

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When the steady state simulation is exported to dynamic simulation default control structure will be generated in Aspen dynamics. The default control structure generated has only two level controllers and one pressure controller. The process response for these controllers has been studied. The control structure has been modified to eliminate some of the drawbacks resulting from the use of default structure.

IV. RESULTS AND DISCUSSION

The dynamic simulation of reactive distillation column has been studied with three different control structures and the response of the system is presented in results and discussion. The default control structure and the two additional control structures used in the present study are shown in the following figures Fig 4.1, 4.2 and 4.3

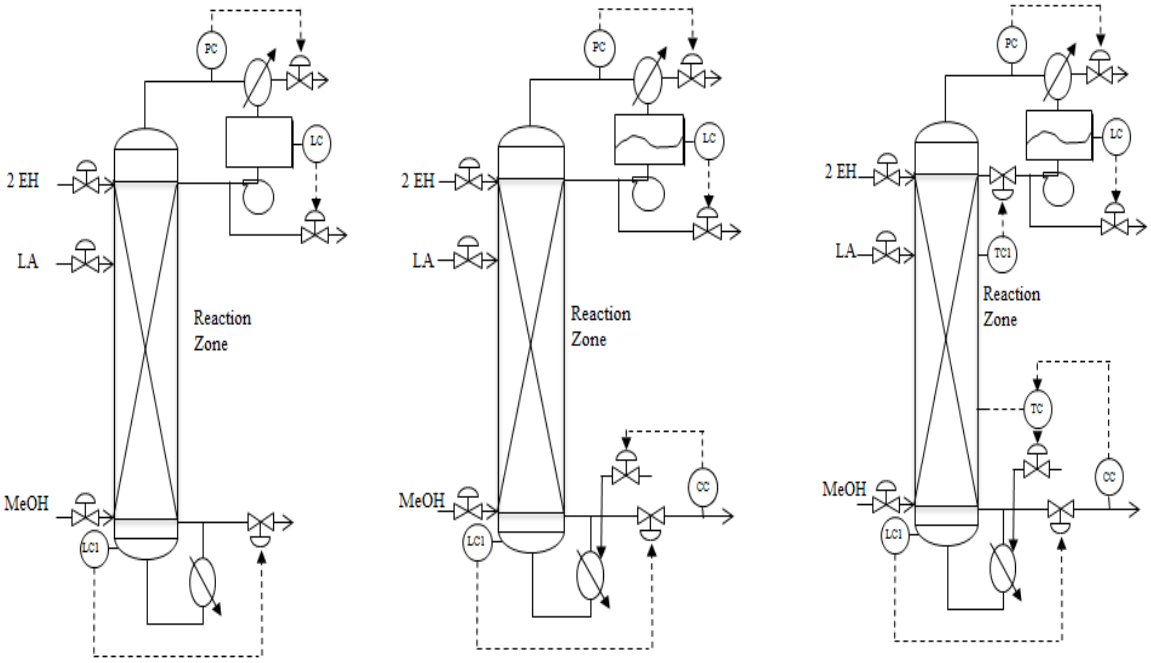


Fig.4.1 Default Control Structure Fig.4.2 Single Point Control Structure Fig.4.3 Double Point Control Structure

A simple two product distillation column has five degrees of freedom. These correspond to the following quantities: distillate flow rate, bottom rate, Reboiler duty, reflux rate, condenser duty. The column pressure, Reboiler sump level, reflux accumulator level must all stabilized for column to operate in steady state. Process response of the system has been studied under three different control structures, subjected to disturbances in feed temperature and feed flow rate.

Feed Temperature & Flow of Lauric Acid as Disturbance (+ 10 %)

The change in feed temperature of lauric acid has been changed from 423.5 K to 465 K. The system performance has been observed for all the three control structures. 4.4, Fig. 4.5 and Fig. 4.6 explain the performance for default control structure, single point control structure and two point temperature control respectively for product mass fraction.

A. Performance Based on Mass Fraction

Due to change in temperature of lauric acid feed the conversion of methyl flow rate decreases as 2-ethyl haxanyl laurate increases which disturb the system and change in desired value of product fraction which control by manipulating reboiler heat duty and bottom reflux rate. In above control best control action done by two point control only

B. Performance Based on Product Mole Rate

The change in feed flow rate of lauric acid has been changed from 100 to 110 kmol/hr. The systems performance is shown in Fig. 4.7, Fig. 4.8 and Fig. 4.9 for default control structure, single point control structure and two point temperature control structure respectively.

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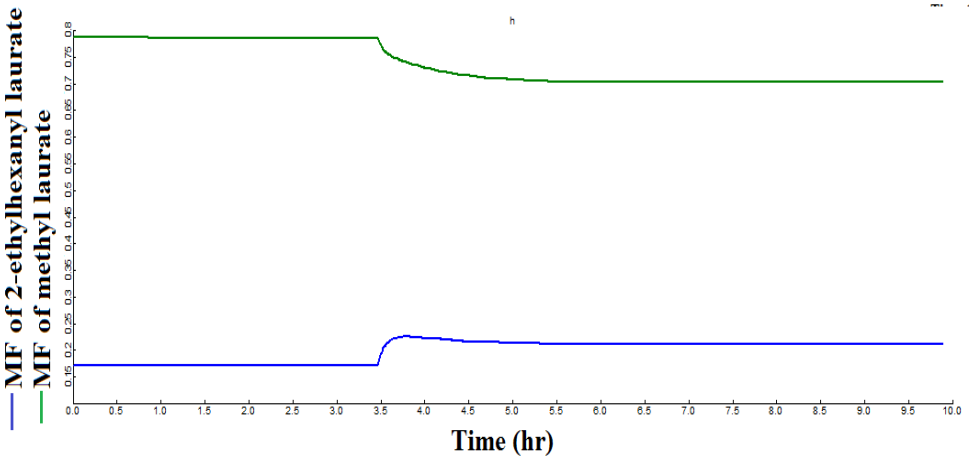


Fig 4.4 Regulatory response of product in bottom for Default Control Structure

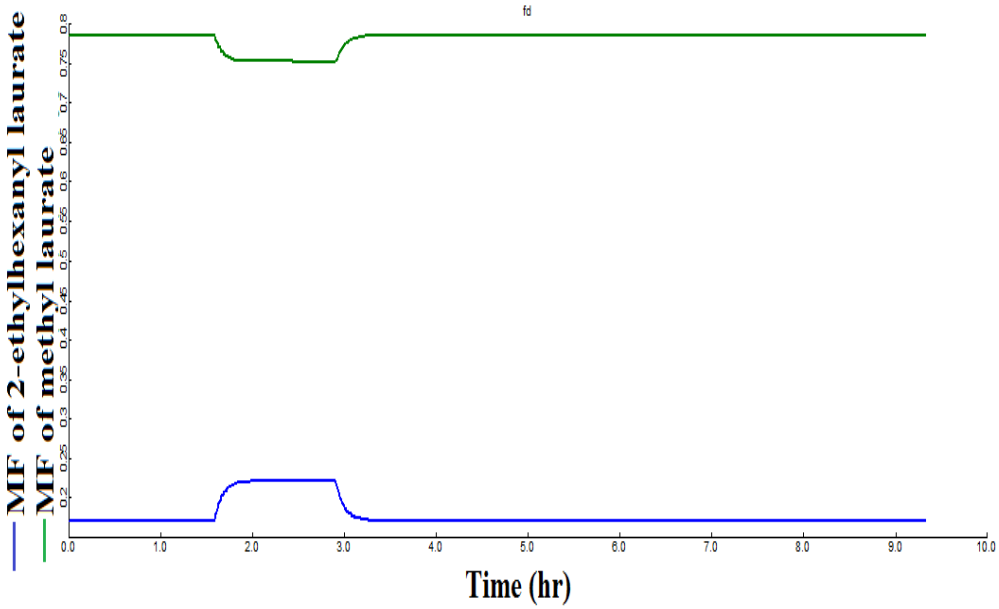


Fig 4.5 Regulatory response of product in bottom for Single Point Control Structure

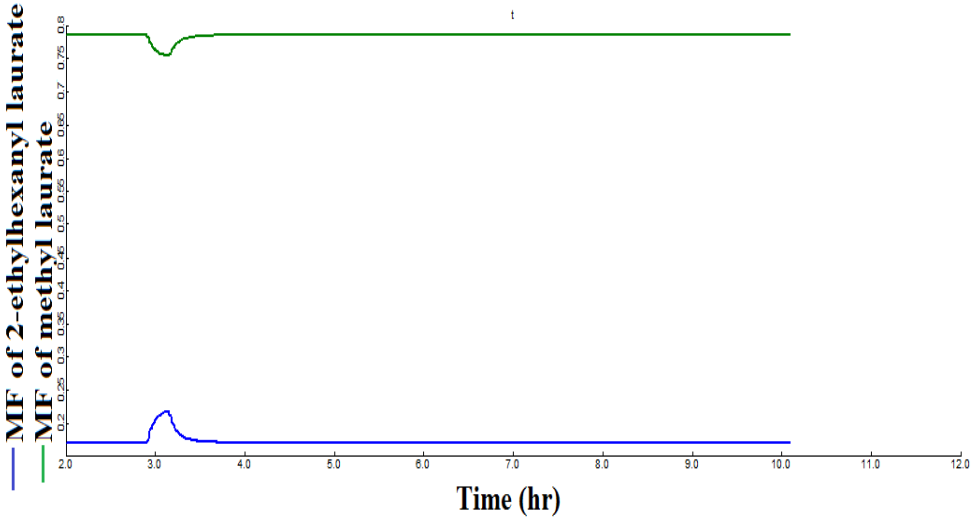


Fig 4.6 Regulatory response of product in bottom for Two Point Temp Control Structure

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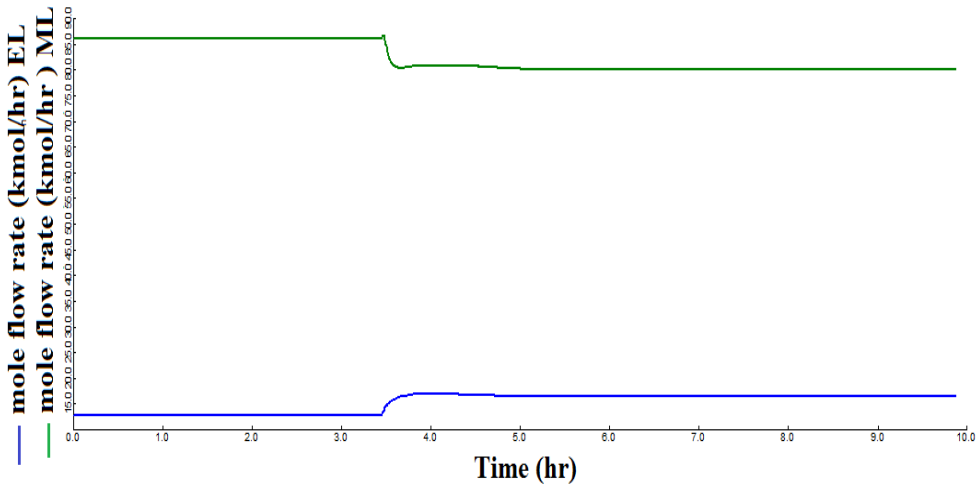


Fig 4.7 Regulatory response of product in bottom for Default Control Structure

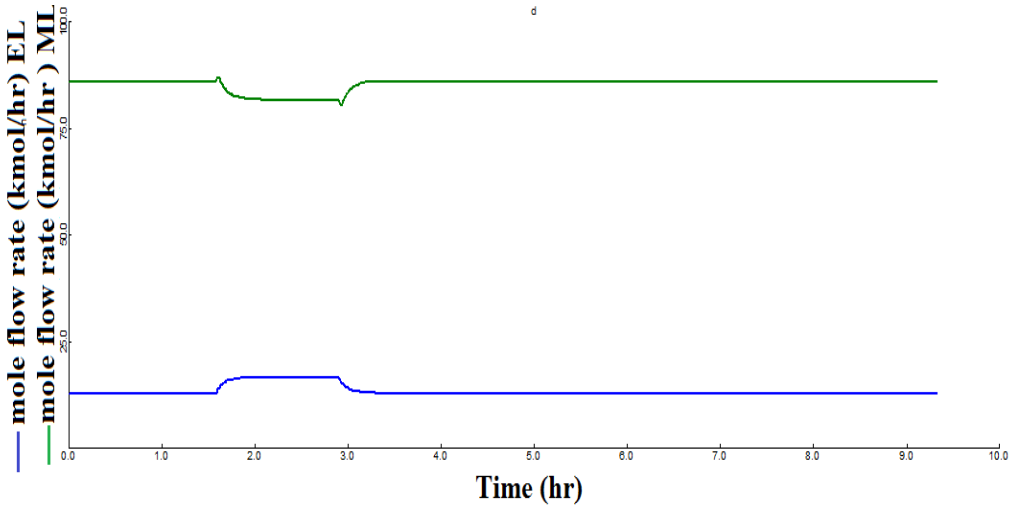


Fig 4.8 Regulatory response of product in bottom for Single Point Control Structure

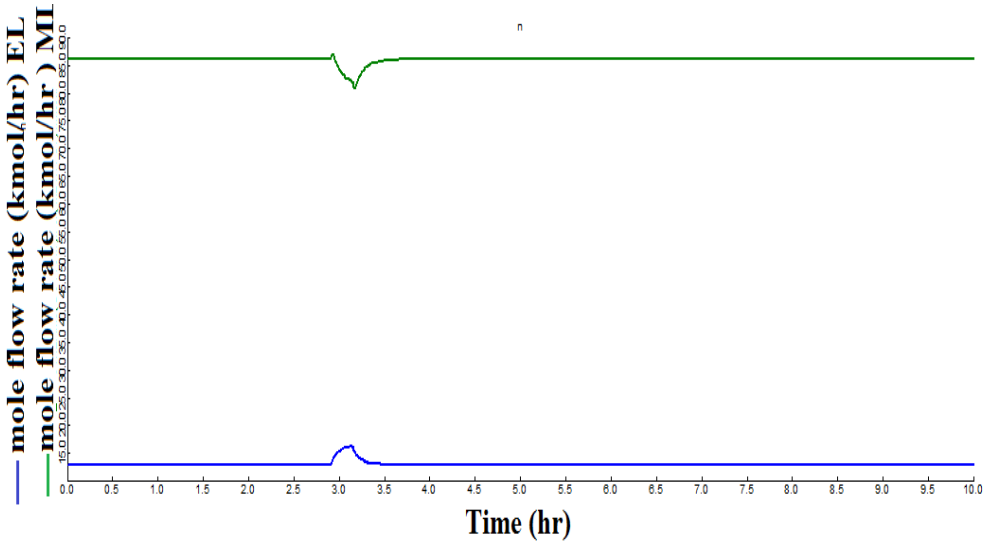


Fig 4.9 Regulatory response of product in bottom for Two Point Temp Control Structure

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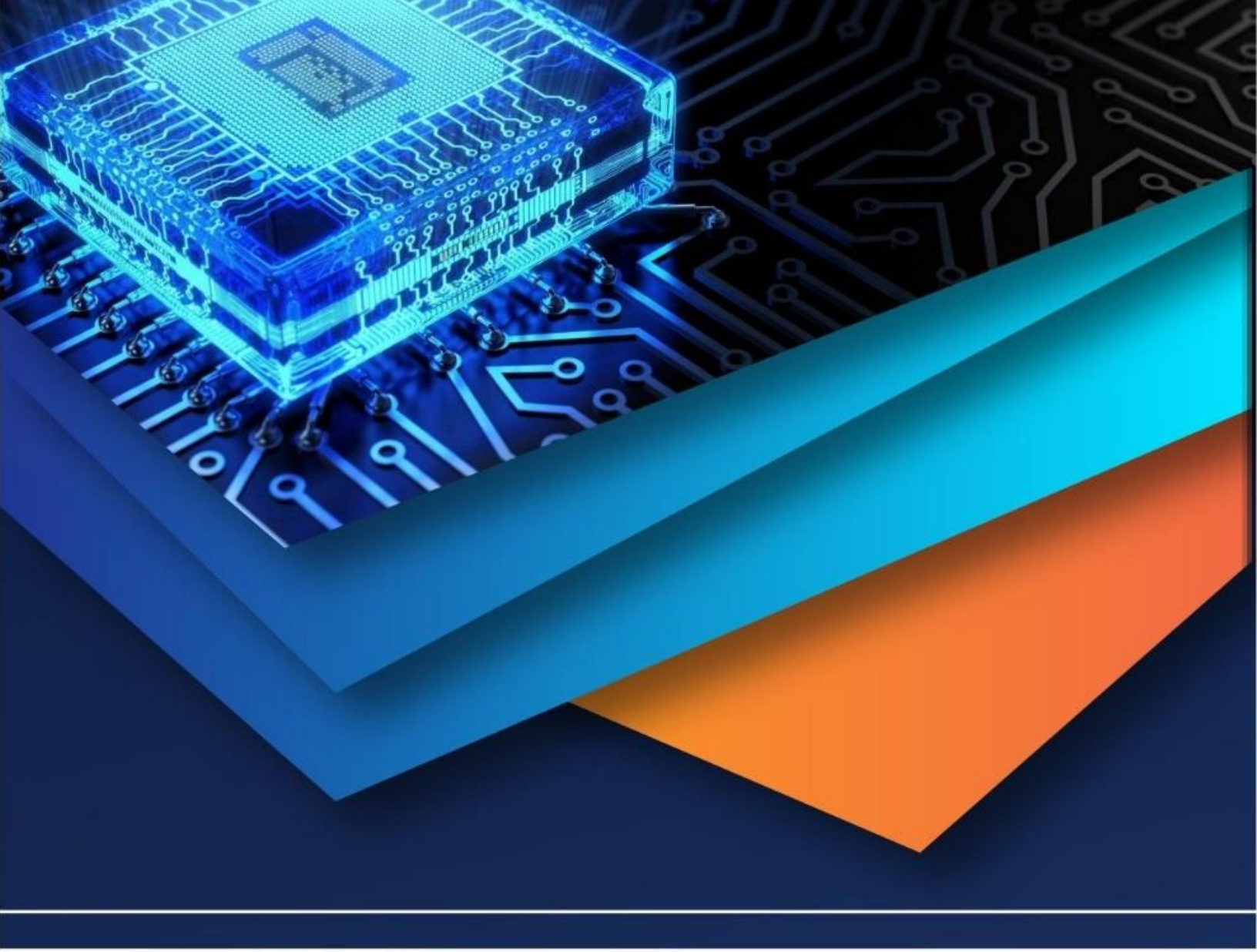
V. CONCLUSION

In this study, the effects of feed temperature & flow of lauric acid as a disturbance on the control structure studied for default control, single point control & two point control structure. There is no control action in case of default control structure. The response for single point control structure is sluggish. The response of two point control is quicker compared to that of single point control. The two point temperature control structure is found to be suitable for controlling the disturbances in feed temperature and flow rate.

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