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STUDY ON DYNAMICS OF CONTINUOUS STIRRED TANK REACTOR USING MULTI INPUT- MULTI OUTPUT SYSTEM

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ABSTRACT

A continuous stirredtank reactor is a measure unit operation in industrial engineering. An experimental and modeling investigation was conducted to study the dynamics ofsaponificationreaction using the flow rate of cooling water and Ethel acetate as forced function and the concentration of sodium acetate and temperature as response variables.The system identification was conducted and the results showed that the multi input multi output system can be represented by the following matrix

$$\begin{matrix} C_D \\ T \end{matrix} = \begin{bmatrix} \frac{0.022e^{-0.33s}}{15S+1} & \frac{5e^{-0.33s}}{21S+1} \\ \frac{0.0056e^{-6s}}{21S+1} & \frac{5.9e^{-0.33s}}{21S+1} \end{bmatrix} \begin{matrix} F \\ F_c \end{matrix}$$

The study showed a good agreement between the linearized model and the experimental results.

KEYWORDS: CSTR, Sodium acetate, Dynamics system.

INTRODUCTION

Chemical reactors are unquestionably the most vital parts of many chemical, biochemical, polymer, and petroleum processes because they transform raw materials into valuable chemicals. A vast variety of useful and essential products are generated via reactions that convert reactants into products. Much of modern society is based on the safe, economic, and consistent operation of chemical reactors [1].Chemical reactors are very important unit operation in industrial practice. The reactor is generally assembled with a jacket or coil in order to maintain the reaction temperature properly [2]. Alkaline hydrolysis of ethyl acetate which is the goal of our study is an irreversible and second order reaction, industrial product of the reaction is sodium acetate and ethanol [3]. Alkaline Hydrolysis frequently is called saponification because it is the type of reaction used in the preparation of soaps the products also used in food additive, pharmaceutical, biofuel …etc [4],. HirooTsujikawa et al. studied the reaction rate of the alkaline hydrolysis of ethyl acetate by means of a continuous measurement of the electric conductivity change [5]. IhsanUllah et al. studied optimization of saponification reaction in a continuous stirred tank reactor the aim of the study is to maximize the conversion of Saponification reaction in a mixed flow reactor using statistical experimental design [6]. Afzal Ahmad et al. studied comparative study of alkaline hydrolysis of ethyl acetate a statistical design of experiments was utilized to enhance conversion in both batch and plug flow reactors [3].ChonthidaNaummaneerat studied kinetics of The alkaline hydrolysis of ethyl acetate In CSTR using simultaneous temperature scanning and composition modulation technique [7]. The mathematical model is describes relations between state variables in the mathematical way, it's come from material and heat balances inside the reactor. To ensure the successful operation of a continuous stirred tank reactor, it is very necessary to understand the dynamic characteristic. Realistic process model can predict the dynamic behaviors of plant. If there is any fault in the plant, the process engineer may realize it through the discrepancy between the model predictions and plant output, and then the necessary corrective measures can be taken accordingly [8]. The design and operation of continuous stirred tank chemical reactors (CSTR's) significantly impacts the economic viability of many chemical manufacturing processes. CSTR's present challenging operational problems due to complex open-loop nonlinear dynamic behavior such as input and output multiplicities, ignition/extinction behavior, parametric sensitivity, and nonlinear oscillations. [9].The aim of this work is to study the dynamic behavior of CSTR using material and energy balance and compare it with experimental work.

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FORMULATION OF MATHEMATICAL MODEL OF THE REACTION SYSTEM

The dynamic behavior of the continuous stirred tank reactor can be modeled by a set of nonlinear equations based on the mass and energy balances for the reactor and heating system. The reactions inside the reactor can be described by following reaction:-

Ethyl acetate (A) + Sodium hydroxide (B)→ sodium acetate (D) + ethanol (E)
Design equation for reactant A for the CSTR is obtained by writing the mass balance for reactant A over the entire volume of the reaction mixture V as follows:

MassA entering the CSTR per unit time = Mass A leaving the CSTR per unit time + Mass A accumulated within the CSTR per unit time + Mass A disappearing by the reaction within the CSTR per unit time
The material balance equation of CSTR:

$$\frac{dC_A}{dt} = FC_{Ao} - FC_A - K_o {C_A}^2 e^{-\frac{E}{RT}} \qquad (1)$$

Linearization

$$\frac{dC_A}{dt} = FC_{Ao} - FC_A - K_o\left[e^{-\frac{E}{RT_s}}{C_{A_s}}^2 + 2e^{-\frac{E}{RT_s}}C_{A_s}(C_A - C_{A_s}) - \frac{E}{{RT_s}^2}e^{-\frac{E}{RT_s}}{C_{A_s}}^2(T - T_s)\right] \qquad (2)$$

At steady state

$$0 = F_s C_{Ao_s} - F_s C_{A_s} - K_o {C_{A_s}}^2 e^{-\frac{E}{RT_s}} \qquad (3)$$

Rearrange (2) and (3)

$$\frac{dC_A}{dt} = FC_{Ao} - F_s C_A - 2K_o e^{-\frac{E}{RT_s}}C_{A_s}C_A - F\,C_{A_s} + K_o\frac{E}{{RT_s}^2}{C_{A_s}}^2 e^{-\frac{E}{RT_s}}\,T \qquad (4)$$

Rearrange

$$\frac{dC_A}{dt} = F(C_{Ao} - C_{A_s}) - C_A(F_s + 2K_o e^{-\frac{E}{RT_s}}C_{A_s}) + K_o\frac{E}{{RT_s}^2}{C_{A_s}}^2 e^{-\frac{E}{RT_s}}\,T \qquad (5)$$

$$\frac{dC_A}{dt} = F(C_{Ao} - C_{As}) - a\,C_A + bT \qquad (6)$$

Where: $a = F_s + 2K_o e^{-\frac{E}{RT_s}} e^{-\frac{E}{RT_s}} C_{As}, b = \frac{E}{RT_s}K_o e^{-\frac{E}{RT_s}}C_{As}^2$

The energy balance equation of continuous stirred tank reactor becomes:

$$\rho C_p \frac{d}{dt}(VT) = \rho C_p(FT_i - FT) - \Delta H_r V K_o e^{-\frac{E}{RT}}{C_A}^2 - \rho C_p F_c(T_{co} - T_{ci}) \qquad (7)$$

Divide by ρC_p

$$\frac{d}{dt}(VT) = (FT_i - FT) - \frac{\Delta H_r V K_o}{\rho C_p}e^{-\frac{E}{RT}}{C_A}^2 - F_c(T_{co} - T_{ci}) \qquad (8)$$

At Volume =1 Liter

$$\frac{d}{dt}(T) = FT_i - FT - \lambda e^{-\frac{E}{RT}}{C_A}^2 - F_c(T_{co} - T_{ci}) \qquad (9)$$

Where $\lambda = \frac{\Delta H_r K_o}{\rho C_p}$

Linearization

$$FT = F_s T_s - F_s(T - T_s) - T_s(F - F_s) \qquad (10)$$

$$e^{-\frac{E}{RT}}{C_A}^2 = e^{-\frac{E}{RT}}{C_{A_s}}^2 - \frac{E}{{RT_s}^2}e^{-\frac{E}{RT}}{C_{A_s}}^2(T - T_s) + 2e^{-\frac{E}{RT}}C_{A_s}(C_A - C_{A_s}) \qquad (11)$$

Equation (10) and (11) in (9)

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$$\frac{dT}{dt} = FT_i - F_sT_s - F_s(T - T_s) - T_s(F - F_s) - \lambda \left[e^{-\frac{E}{RT}} C_A{}^2 - \frac{E}{RT_s{}^2} e^{-\frac{E}{RT}} C_A{}^2 (T - T_s) + 2e^{-\frac{E}{RT}} C_{A_s}(C_A - C_{A_s}) \right] C_A{}^2 - F_c(T_{co} - T_{ci}) \quad (12)$$

At steady state:

$$\frac{dT_s}{dt} = 0 = F_sT_{i_s} - F_sT_s - \lambda\, e^{-\frac{E}{RT_s}} C_{A_s}{}^2 - F_{c_s}(T_{co_s} - T_{ci_s}) \quad (13)$$

Subtract (13) in (12)

$$\frac{dT}{dt} = FT_i - F_s\,T - T_sF + \lambda \frac{E}{RT_s{}^2} e^{-\frac{E}{RT}} C_{A_s}{}^2 T - 2\lambda\, e^{-\frac{E}{RT}} C_{A_s} C_A - F_c(T_{co} - T_{ci}) \quad (14)$$

Convert to S-domain (Laplace transform)

$$ST = F\,(T_i - T) - T\left[F_s - \lambda \frac{E}{RT_s{}^2} e^{-\frac{E}{RT}} C_{A_s}{}^2\right] - 2\,\lambda\, e^{-\frac{E}{RT}} C_{A_s} C_A - F_c(T_{co} - T_{ci}) \quad (15)$$

$$ST = F\,(T_i - T) - d\,T - EC_A - F_c(T_{co} - T_{ci}) \quad (16)$$

Where: $d = F_s - \lambda \frac{E}{RT_s{}^2} e^{-\frac{E}{RT}} C_{A_s}{}^2, E = 2\,\lambda\, e^{-\frac{E}{RT}} C_{A_s}$

Rearrange

$$(S + d)T = F\,(T_i - T) - EC_A - F_c(T_{co} - T_{ci})E = 2\,\lambda\, e^{-\frac{E}{RT}} C_{A_s} \quad (17)$$

$$T = \frac{(T_i - T)}{(s + d)} F - \frac{E}{(s + d)} C_A - \frac{(T_{co} - T_{ci})}{(s + d)} F_c \quad (18)$$

Put (18) in (6)

$$\frac{dC_A}{dt} = F(C_{Ao} - C_A) - a\,C_A + b\left[\frac{(T_i - T)}{(S + d)} F - \frac{E}{(S + d)} C_A - \frac{(T_{co} - T_{ci})}{(S + d)} F_c\right] (19)$$

Multiply by (S + d)

$$S(S + d)C_A = (C_{Ao} - C_A)(S + d)F - a\,(S + d)C_A + b(T_i - T)F - Eb\,C_A + (T_{co} - T_{ci})F_c \quad (20)$$

$$[S(S + d) + a\,(S + d) + Eb]C_A = (C_{Ao} - C_A)(S + d)F + b(Ti - T)F + (T_{co} - T_{ci})F_c (21)$$

$$C_A = \frac{(C_{Ao} - C_A)(S + d) + b(Ti - T)}{[S(S + d) + a\,(S + d) + Eb]} F + \frac{(T_{co} - T_{ci})F_c}{[S(S + d) + a\,(S + d) + Eb]} F_c \quad (22)$$

At 50% step change and use the physical properties

$$C_A = \frac{0.022(S + 3.2) + (0.00057 \times 3)}{S(S + 3.2) + 0.4(S + 3.2) - 0.004} \times \frac{0.5}{S}$$

$$= \frac{0.11S + 0.036}{S(S + 3.2) + 0.4(S + 3.2) - 0.004}$$

$$= \frac{A}{S} + \frac{B}{S + 0.4} + \frac{C}{S + 3.2}$$

So, Equation will be

$$\boldsymbol{C_A = 0.0281 - 0.0278\, e^{-0.4\,t} - 0.00024\, e^{-3.2\,t}} \quad (23)$$

EXPERIMENTAL WORK

In this work sodium hydroxide (NaOH) and ethyl acetate (EtAc) were used as reactants. The experimental work was carried out in reaction system as shown in figure 1, supplied by Brodit (Germany) .The reaction system consists of 2L Borosilicate glass reactor supplied with stainless steel water heating coil, stainless steel mechanical stirrer of two blades, two transparent tanks A and B for feed and two peristaltic pumps. The details of device of reaction system are shown in table 1. First of all a steady stat reaction was conducted. The reactor was filled with 0.5 L of 0.1M ethyl acetate and0.5 L of 0.1M sodium hydroxide (1 L operation volume).The feed flow rates for each tanks into the CSTR are adjusted to be 20 ml/min using peristaltic pumps. The conductivity and temperature of the reaction medium in the

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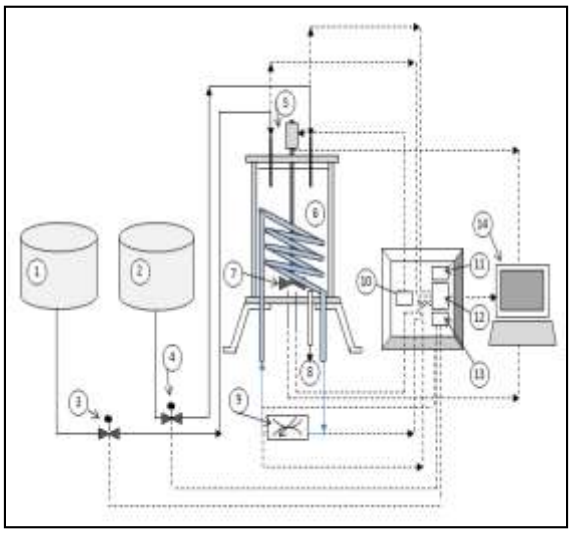
CSTR were measured every 2 minutes until reach to steady state. The flow rates of inlet and outlet liquids, conductivity and pH for the liquids in the reactor were recordedusing data logger. After reachingthesteady state, a 50% step change on the flow rate of ethyl acetate (A) was introduced.The conductivity and temperature were measured everytwo minutes till reaching to a new steady state. The same procedure was done using 50% step change on the hot water.

The conductivity obtained throughout the experiment is converted into concentration data using calibration curve.



No.	device
1	Tank A
2	Tank B
3	peristaltic pump of Tank A
4	peristaltic pump of Tank b
5	Electrical motor
6	Reactor
7	Two Blades
8	Outlet Flow
9	Heater
10	The digital regulator of the mixer
11	Power Switch
12	Temperature controller system
13	Flow rate controller system
14	Computer

Figure 1 Schematic diagram of laboratory CSTR reactor system

RESULTS AND DISCUSSION

The dynamic of the system was studied experimentally using step change in the manipulated variables Ethel acetate flow rate and water coil flow rate (F and Face) and examine the transient response of sodium acetate and reaction temperature.Figures2 and 3show the response on sodium acetate and temperature of the reaction respectively for 50% step change in Ethel acetate flow rate, while figures 4 and 5 show the effect of manipulated variable water in coil on sodium acetate and temperature of the reaction respectively. Layben [10] stated that probably 80% of chemical process can be represented by first order plus dead time (FOPDT). The main difference between over damped or critical damped for second order system forced by step change and first order system is that the second order system hasan S shape with a maximum slope at inflection point. The first order response has their maximum slope initially [16].

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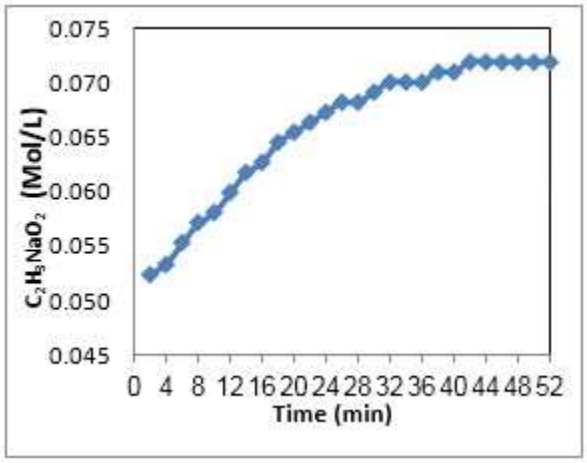

Figure 2 response of the concentration using 50 % step change of feed ethyl acetate.

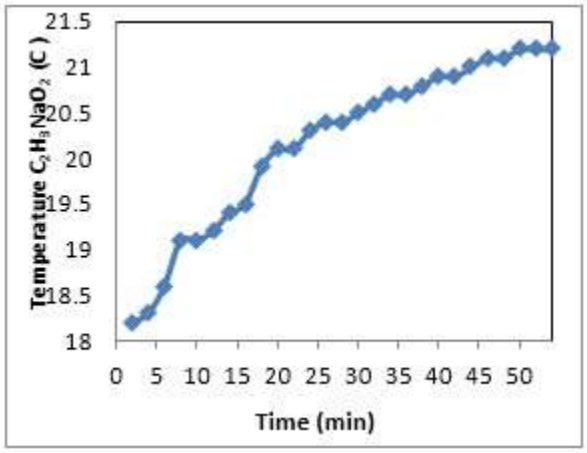

Figure 3 response of reactor temperature using 50 % step change of feed Ethyl Acetate.

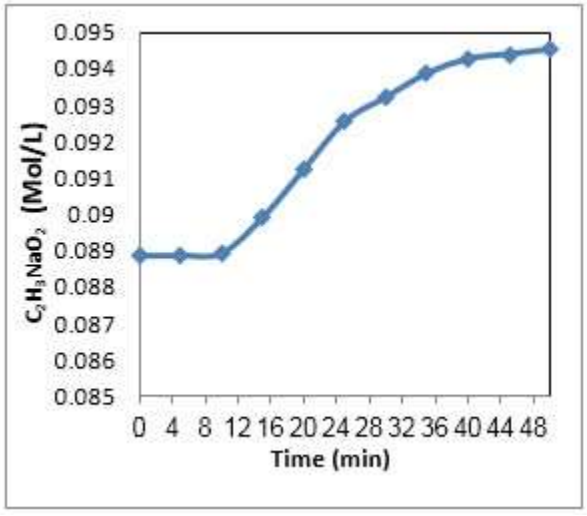

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Figure 4 response of the process concentration using 50 % step change of water in coil.

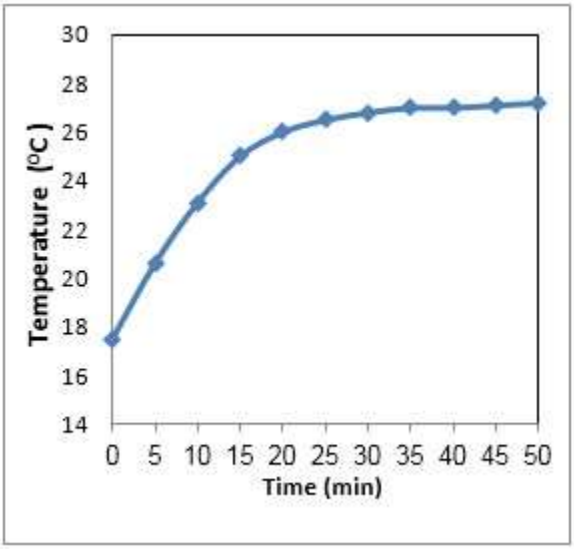

Figure 5 response of the process concentration using 50 % step change of water in coil.

From these figure it is clear that the transfer functions can be represented by first order plus dead time:

$$G_{11} = \frac{C_D}{F} = \frac{0.022e^{-0.33s}}{15S+1}$$

$$G_{12} = \frac{C_D}{F_C} = \frac{5\,e^{-0.33s}}{21S+1}$$

$$G_{21} = \frac{T}{F} = \frac{0.0056e^{-6s}}{21S+1}$$

$$G_{22} = \frac{T}{F_c} = \frac{5.9e^{-0.33s}}{21S+1}$$

In matrix form:

$$\begin{matrix} C_D \\ T \end{matrix} = \begin{bmatrix} \frac{0.022e^{-0.33s}}{15S+1} & \frac{5e^{-0.33s}}{21S+1} \\ \frac{0.0056e^{-6s}}{21S+1} & \frac{5.9e^{-0.33s}}{21S+1} \end{bmatrix} \begin{matrix} F \\ F_c \end{matrix}$$

Block diagram of matrix is shown in Figure (6).

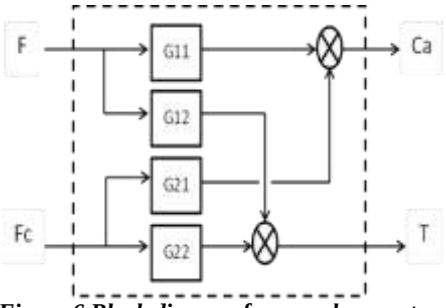

Figure 6 Block diagram for open loop system

Figures 7 and 8 shows a comparison between the experimental work and mathematical modeling using equation 23.A high agreement between theoretical and experimental results was obtained especially at steady state. The deviation

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between a theoretical and experimental can be attributed to uncertainty in the experimental measurements considering a constant of physical properties of reactants and products with temperature variation and imperfect mixing system.

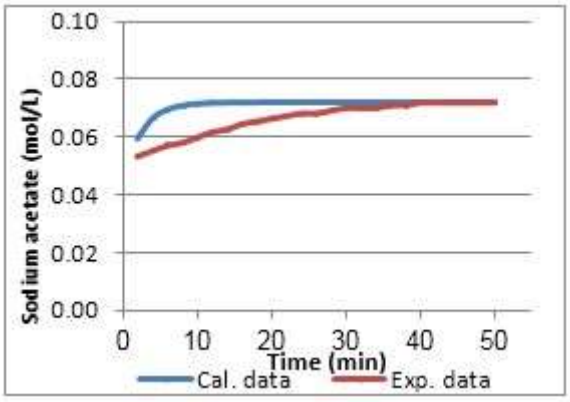

Figure 7 Response of product concentration using 50%step change in Ethyl acetate.

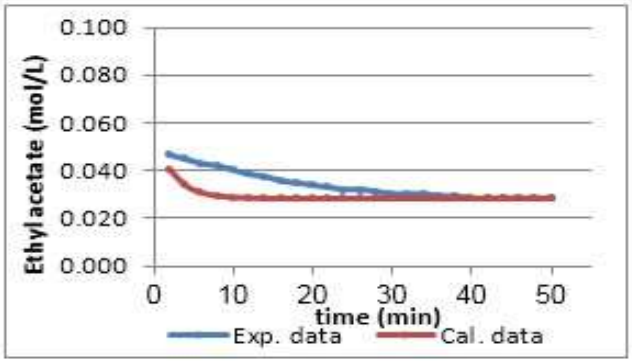

Figure 8 Response of reactant concentration using 50%step change in Ethyl acetate.

CONCLUSION

The present experimental work showed that the dynamic behavior of CSTR can be represented by first order plus dead time (FOPDT).The mathematical model, showed that the transfer function represented by second order. It is worthy to say that FOPDT using first pade approximation is identical to the second order system. The comparison between the experimental work and mathematical modeling gives high agreement.

ACKNOWLEDGEMENTS

CA: concentration of Ethyl acetate in the reactor (goml/L)
CAo: concentration of A in the reactor (gmol/L)
CD: concentration of Sodium acetate in the reactor (gmol/L)
Fi: volumetric flow rate in the inlet stream (L/min)
F: volumetric flow rate in the outlet stream (L/min)
Fs: volumetric flow rate at steady state (L/min)
Fc: volumetric flow rate of the heating water (L/min)
Ko: reaction rate constant (min-1)
E: activation energy (kJ/kmol)
R: gas constant (J/mol K)
T: temperature of the reactor (K)
Ti: temperature in the inlet stream (K)
TCO: temperature of the outlet heating coil of water (K)

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ρ : density of mixture on reactant (g/L)
CP: heat capacity (J/mol.K)
Δ Hr: heat of reaction (J/mol)
TCi: temperature of the inlet heating coil of water (K)
Ts: temperature of the reactor at steady state (K)

REFERENCES

1. William L. Luyben, Chemical Reactor Design and Control, P (xiii), 2007.
2. Amiya K. jana,Chemical Process Modelling& Computer Simulation,2nd Edition, P (43) , 2005.
3. Afzal Ahmad, Muhammad Imran Ahmad , Muhammad Younas, Hayat Khan, Mansoorul Hassan Shah, Comparative Study of Alkaline Hydrolysis of Ethyl Acetate Using Design of Experiments, Volume 32, Page 33-4, 2013.
4. Philip E. Slade, Handbook of Fiber Finish Technology, Nylon Technical Center, Pensacola, Florida, CRC Press, P(56), 1997
5. HirooTsujikawa And Hakuai Inoue, The Reaction Rate of Aalkaline Hydrolysis of Ethyl Acetate, Bull. Chem. Soc., 1966.
6. IhsanUllah and Muhammad Imran Ahmad, Optimization of Saponification Reaction in a Continuous Stirred Tank Reactor, UET, Peshawar, Pakistan ,2010
7. ChonthidaNaummaneerat, Kinetics Study of the Alkaline Hydrolysis of Ethyl Acetate in CSTR Using Simultaneous Temperature Scanning and Composition Modulation Technique, Chemical Engineering, Department of Chemical Engineering , 2009
8. Modeling and Simulation Study of the CSTR for Complex Reaction by Using Polymath, P(79),2012
9. Louis P. Russo and B. Wayne Bequette ,CSTR Performance Limitations due to Cooling Jacket Dynamics Department of Chemical Engineering, Rensselaer Polytechnic Institute , USA,1992
10. Michael L. Luyben" Essentials ofProcessControl",Department of Chemical Engineering Lehigh University, 1997.