International Journal of Advanced Technology in Engineering and Science
Vol. No.5, Issue No. 04, April 2017
www.ijates.com
ijates
ISSN 2348 - 7550

MODELLING AND SIMULATION OF SAPONIFICATION REACTION IN DIFFERENT TYPE OF REACTOR

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ABSTRACT

This work presents the kinetic modelling and simulation of saponification of ethyl acetate in the presence of Sodium hydroxide in a plug flow reactor, Continues stirred tank reactor using Aspen Plus simulation Software. The continuous flow stirred-tank reactor (CSTR), also known as vat- or back mix reactor, is a common ideal reactor type in chemical engineering. A CSTR often refers to a model used to estimate the key unit operation variables when using a continuous agitated-tank reactor to reach a specified output. Plug flow reactors are widely used in the industry due to the non-mixing property. The use of plug flow reactors becomes significant when there is a need for continuous large scale reaction or fast reaction. Plug flow reactors have a high volumetric unit conversion as the occurrence for side reactions is minimum.

Keywords: Modelling, Simulation. Plug flow reactor, continuous flow stirred-tank reactor.

I. INTRODUCTION

Tubular reactor, the feed enters at one end of a cylindrical tube and the product stream leaves at the other end. The long tube and the lack of stirring prevent complete mixing of the fluid in the tube. Hence the properties of the flowing stream will vary from one point to another, namely in both radial and axial directions. In the ideal tubular reactor, which is called the “plug flow” reactor, specific assumptions are made about the extent of mixing: no mixing in the axial direction, i.e., the direction of flow complete mixing in the radial direction uniform velocity profile across the radius. The absence of longitudinal mixing is what defines this type of reactor[1]. The validity of the assumptions will depend on the geometry of the reactor and the flow conditions. Deviations, which are frequent but not always important, are of two kinds:

1. Mixing in longitudinal direction due to vortices and turbulence
2. Incomplete mixing in radial direction in laminar flow conditions

Continuous stirred tank reactors (are used very commonly in industrial processes. For this type of reactor, mixing is complete, so that the temperature and the composition of the reaction Mixture are uniform in all parts of the vessel and are the same as those in the exit stream [2].

Three stages of the continuous operation of a CSTR can be modeled.

1.From beginning to overflow

2.From overflow to steady state

3.Steady state operation

II. RELATED DESIGN

Design of Plug flow reactor:

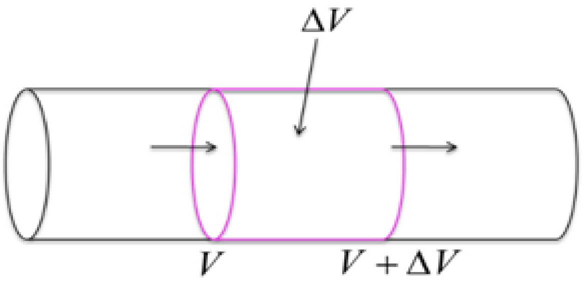


Figure 2.1 Plug Flow Reactor

For a time element Δt and a volume element ΔV at steady state, the mass balance for species 'i' is given by ,

$$v\, C_A \Big|_v \Delta t - v\, C_A \Big|_{v+\Delta v} \Delta t - r_A \Delta V \Delta t = 0 \quad 1$$

....……………………………….(1)

where

v: total volumetric flow rate

CA : concentration of reactant A

rA : rate of disappearance of reactant A

Dividing Eq 1 by ΔV and Δt results in Eq.2

$$\frac{v\, C_A|_V - v\, C_A|_{V+\Delta V}}{\Delta V} = -\frac{r_A}{v}$$

…………………………………………………….(2)

and taking limit as ΔV →0 gives

$$\frac{dC_A}{dV} = \frac{r_A}{v}$$

………………………………………………………………………….(3)

At the entrance:

V = 0

CA= C

A0 (inlet concentration of reactant A)

At the exit:

V = VR (total reactor volume)

CA= CA (exit conversion)

$$\int_0^{V_R} \frac{dV}{v} = \int_{C_{AO}}^{C_A} \frac{dC_A}{r_A} \quad \text{...}(4)$$

$$-r_A = kC_AC_B \quad \text{...}(5)$$

$$C_A = C_{A0}(1-X);\;\; C_B = C_{A0}\,(\theta_B - X) \quad \text{...}(6)$$

Combining equations 4, 5 & 6 the following expression is obtained

$$\int_0^{V_R} \frac{dV}{v} = -\int_{C_{AO}}^{C_A} \frac{dC_A}{kC_AC_B}$$

$$\int_0^{V_R} \frac{dV}{v} = -\int_{C_{AO}}^{C_A} \frac{dC_A}{kC_{A0}{}^2(1-X)(\theta_B - X)}$$

CONTINUOUS FLOW STIRRED-TANK REACTOR

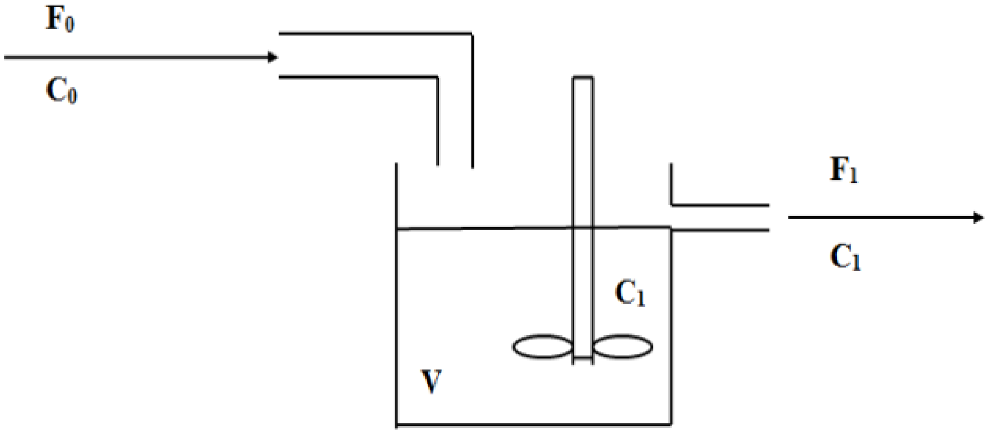


Figure 2.2 Continuous Flow Stirred-Tank Reactor

One stage:

This stage is semi batch. There is no output because the reactor contents do not yet reach the overflow level. With assuming that the saponification reaction of ethyl acetate with sodium hydroxide is second order overall, a material balance on either NaOH or ethyl acetate (both reactants are at the same concentration and flow rate).

rate of accumulation = rate of input -rate of consumption

$$\frac{d(VC)}{dt} = vC_0 - VkC^2 \qquad \textbf{Or} \qquad V\frac{dC}{dt} + C\frac{dV}{dt} = vC_0 - VkC^2$$

where

C = concentration

C0 = initial concentration

M= volumetric flow rate

k = reaction rate constant

t = time, (min)

V =volume of reactor

But ‘V’ is a function of time, and since the system is of constant density and flow rate, a total mass balance gives

$$\frac{dV}{dt} = v \qquad \text{or} \qquad V = vt$$

$$\frac{dC}{dt} = \frac{C_0}{t} - \frac{C}{t} - kC^2$$

Stage Two

The second stage is continuous but not yet steady. The concentration is changing with time but the volume of the reactants is constant.

rate of accumulation = rate of input - rate of output - rate of consumption

$$V\frac{dC}{dt} = vC_0 - vC - VkC^2$$

$$\frac{dC}{dt} = \frac{C_0}{\tau} - \frac{C}{\tau} - kC^2$$

$$\tau = V/v, \text{(min)}$$

Stage Three

rate of input = rate of output + rate of consumption

$$vC_0 = vC_s + VkC_s{}^2$$

$$k\tau C_s{}^2 + C_s - C_0 = 0$$

The calculation of the specific rate constant k can be

$$k = \frac{(v_{A+}v_B)}{V}\frac{(C_{A0} - C_A)}{C_A{}^2},$$

For a reactant A in a reactor operating at steady state, the volume (V) may be assumed constant and the steady state concentration of NaOH in the reactor (CA) may be used to calculate the specific rate constant (k) [3, 4].`

III.EXPERIMENTAL WORK:

$$\begin{array}{ccccccccc} NaOH & + & CH_3COOC_2H_5 & \rightarrow & CH_3COONa & + & C_2H_3OH \\ \\ \textit{Sodium Hydroxide} & + & \textit{Ethyl Acetate} & \rightarrow & \textit{Sodium Acetate} & + & \textit{Ethyl Alcohol} \\ (A) & & (B) & & (C) & & (D) \end{array}$$

PLUG FLOW REACTOR:

1. Prepare 100 ml of 0.05 M NaOH solution in a 1000 ml beaker, record conductivity data.
2. Add 100 ml distilled water to the beaker to dilute the NaOH solution, make sure it is perfectly mixed, and record conductivity data. Repeat this step six more times to prepare a calibration curve.
3. Prepare 5 L of 0.05 M ethyl acetate and 0.05 M NaOH solutions. Pour these solutions into the feed tanks.
4. Adjust a constant flow rate by setting the pump speeds of both reactants.
5. Record the conductivity when steady state is reached

Continuous flow stirred-tank reactor:

1. Prepare 100 ml of 0.05 M NaOH solution in a 1000 ml beaker, record conductivity data.
2. Add 25 ml distilled water to the beaker to dilute the NaOH solution, make sure it is perfectly mixed, and record conductivity data. Repeat this step three more times (add 40, 80 and 250 ml distilled water) to prepare a calibration curve.
3. Make up 4 liter batches of 0.05 M sodium hydroxide and 0.05 M ethyl acetate.
4. Remove the lids of the reagent vessels and carefully fill the reagents. Refit the lids.
5. Set the pump speeds of both reactants to give 50 ml/min flow rate.
6. Set the agitator speed controller to 7.0.
7. Switch on the feed pumps and agitator motor. Start the stopwatch.
8. Collect conductivity data each minute for 45 minutes

IV. RESULIT:

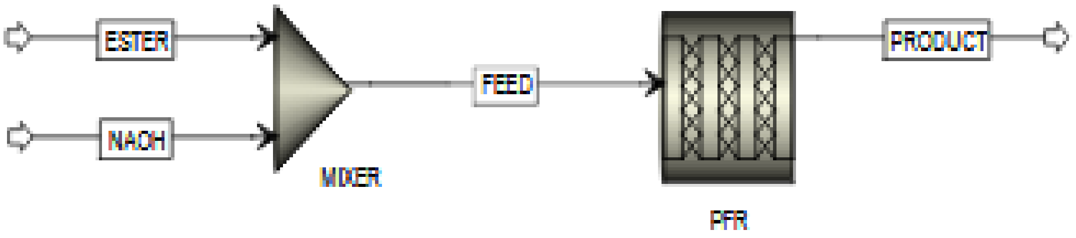
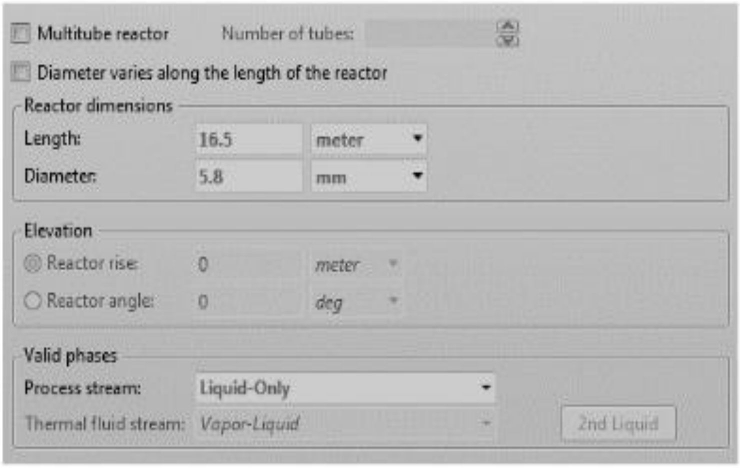
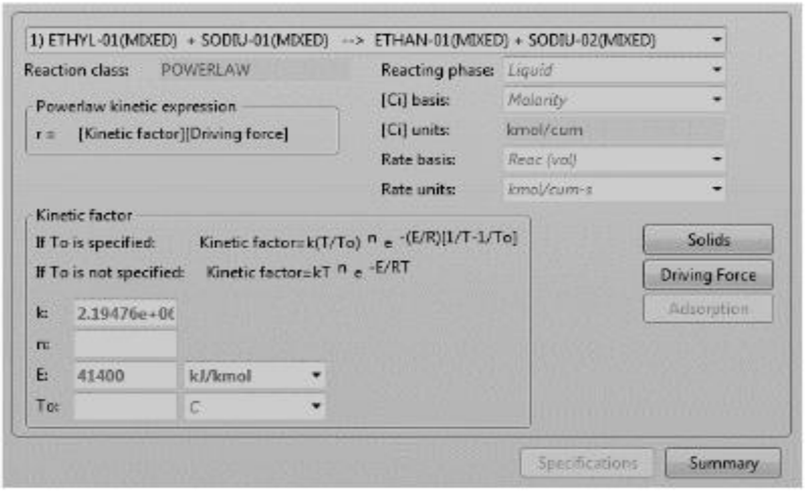


Figure 4.1 Aspen Flow Sheet



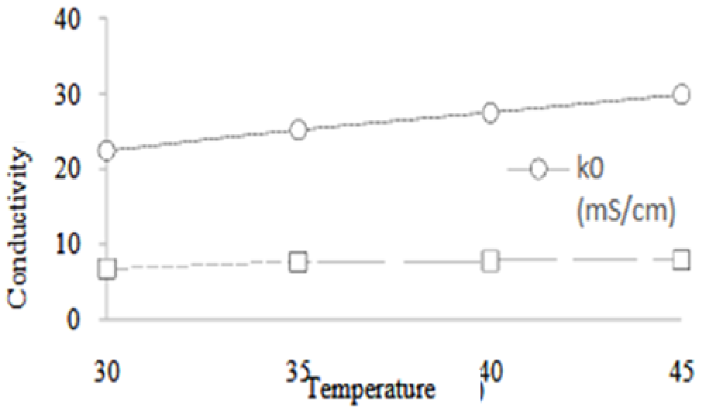
☐ Multitube reactor Number of tubes:
☐ Diameter varies along the length of the reactor
Reactor dimensions
Length: 16.5 meter
Diameter: 5.8 mm
Elevation
● Reactor rise: 0 meter
○ Reactor angle: 0 deg
Valid phases
Process stream: Liquid-Only
Thermal fluid stream: Vapor-Liquid

Figure 4.2 PFR Configuration

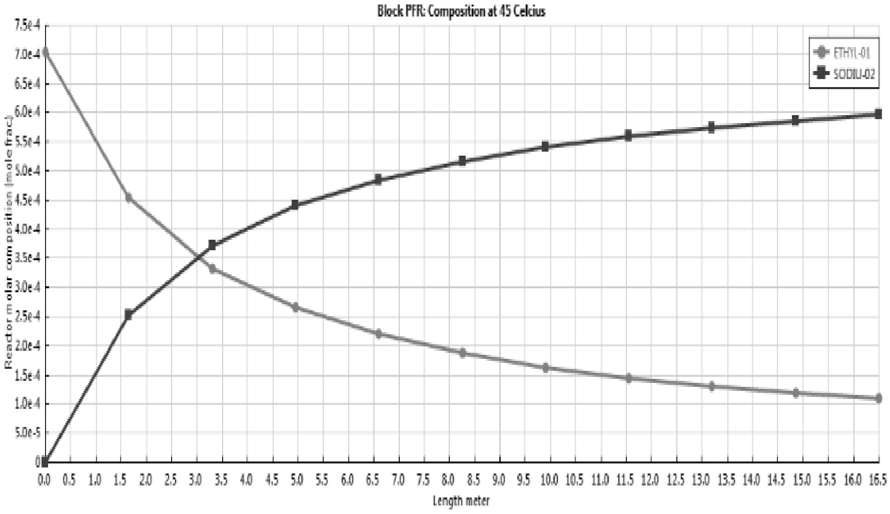


1) ETHYL-01(MIXED) + SODIU-01(MIXED) --> ETHAN-01(MIXED) + SODIU-02(MIXED)
Reaction class: POWERLAW
Reacting phase: Liquid
[Ci] basis: Molarity
[Ci] units: kmol/cum
Rate basis: Reac (vol)
Rate units: kmol/cum-s
Powerlaw kinetic expression
r = [Kinetic factor][Driving force]
Kinetic factor
If To is specified: Kinetic factor=k(T/To) ^{n} e $^{-(E/R)[1/T-1/To]}$
If To is not specified: Kinetic factor=kT ^{n} e $^{-E/RT}$
k: 2.19476e+0(
n:
E: 41400 kJ/kmol
To: C

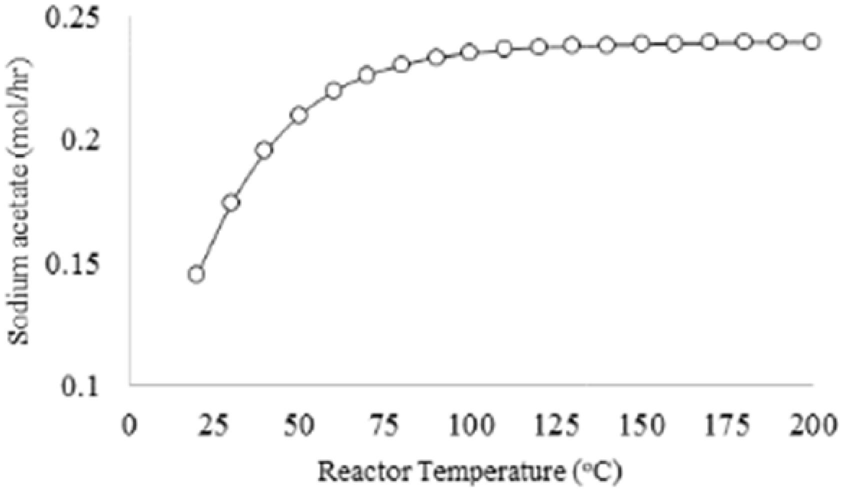
Figure 4.3 PFR Reaction Kinetic data



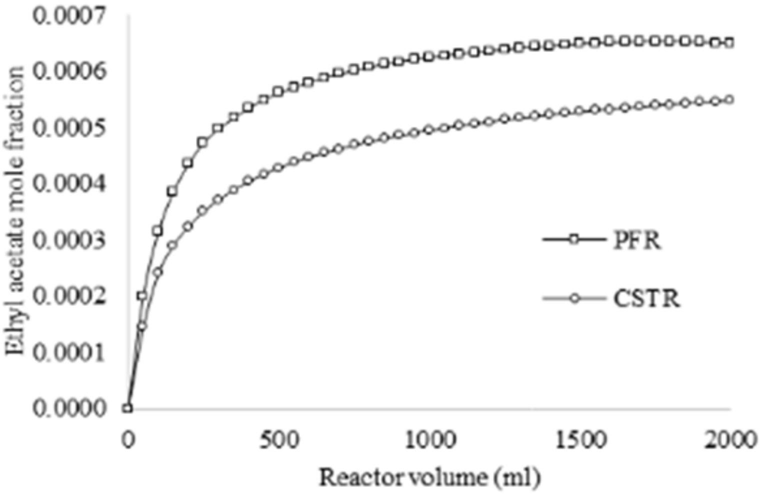
Graph 4.1 Conductivity Vs. Temperature



Graph No 4.2 Ethyl acetate mole fraction vs PFR at 45 ^{0}C



Graph No 4.3 Ethyl Variation of sodium acetate flow rate with reactor temperature



Graph No 4.4 Ethyl acetate mole fraction vs reactor volume

1.Effect of Reactant Flow Rates on the Reaction

A sensitivity analysis was done in Aspen Plus model to investigate the effect of reactant flow rates towards the reaction. The mole fractions of sodium acetate vary for different flow rates of NaOH and ethyl acetate. It shows that in each case the highest mole fraction of sodium acetate can be achieved when equal flow rates of NaOH and ethyl acetate are pumped to the plug flow reactor. According to the stoichiometry of [7] it is clear that equal amounts of reactants are needed to obtain the highest yield. When the flow rate of ethyl acetate exceeds the flow rate of NaOH as there is no more NaOH left in the reawith ethyl acetate, the excess ethyl acetate remains in the Variation of ethyl acetate mole fraction with acetate and NaOH flow rates.

2. Effect of Reactant Flow Rates on the Reaction

A sensitivity analysis was done in Aspen Plus model to investigate the effect of reactant flow rates towards the how the mole fractions of sodium acetate vary for different flow rates of NaOH and ethyl acetate. It shows that in each case the highest mole fraction of sodium acetate can be achieved when equal flow rates of NaOH and flow reactor. According [6] it is clear that equal amounts of reactants are needed to obtain the highest yield.

3. Volume Comparison of CSTR and PFR

Volume required for a PFR is relatively less when compared to the volume required for a Continuous Stirred Tank Reactor (CSTR) to achieve the same conversion for a reaction while maintaining [4]. This theory is well applied for the saponification reaction of ethyl acetate with sodium hydroxide. During this study it has also proven with using Aspen simulation that the volume of CSTR to achieve the same conversion that of a PFR .Therefore, it is economically feasible to use a PFR to carry out this saponification reaction in industrial scale even when producing with large quantities.

V. CONCLUSION

Aspen Plus model proved that the rate of reaction increases as the reactor temperature and the length of the plug flow reactor increase.These results improve the understanding of reaction kinetics with reference to the saponification reaction and would be very useful in the design of plug flow reactors. The model was validated by the experimental results obtained from EDIBON Plug Flow Reactor module. The experimental results showed a good fit to the Aspen Plus model.

In this work, a simulation model was deceleration of saponification of ethyl acetate in the presence of sodium hydroxide inside a plug flow reactor using Aspen Plus. The highest yield of the reaction was obtained at a reactor temperature.

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ACKNOWLEDGMENTS

This research was supported by Dr. D. Y. Patil Institute of Engineering, Management &Research, Akurdi, and Pune.We are thankful to our Principal Dr. Mrs .A. V. Patil. for provided expertise that greatly assisted the research. We have to express our appreciation to the Mr. Bhushan Zare for sharing their pearls of wisdom with us during the course of this research.