

**COMPARISON OF CALCIUM STEARATE PRODUCTION FROM
DIFFERENT TYPES OF REACTOR****DOLLAH¹, E. E, & UKPAKA², C. P**Department of Chemical/Petrochemical Engineering, Rivers State University, Nkpolu, Port Harcourt
NigeriaEmail: meetsomuchdollah1@gmail.com**ABSTRACT**

The Comparison on the design of Batch Reactor, Continuous Stirred Tank Reactor and Plug Flow Reactors was carried out to examine the rate of mathematical models developed for the production of Calcium Stearate. Design models were also developed from the conservation principles of mass and energy on the reactors to obtain functional parameters. The non-isothermal energy balance models were developed for the reactors taken into consideration voidage on the Stoichiometry of the reaction that gave Calcium Stearate. The design models for both isothermal and non-isothermal reactors developed were resolved numerically using 4th order Runge-Kutta algorithm. Various results were obtained on the basis of different molar feed rates, $M = 1.5, 2, 2.5$ and 3 with functional parameters of the reactors. The models result shows that at fractional conversion of 0.9 and molar feed rate of 2 mol/s gave maximum yields: $VPFR = 31.8m^3$, $VBR =$

$21.25m^3$ and $VCSTR = 6.14m^3$. The results indicate that CSTR is a better Performed Reactor at molar feed rate of

2 and gave economical and profitable yield for the production of Calcium Stearate than the other reactors. Also the heat

generated per unit volume gave $q_{BR} = 0.09W/m^3$, $q_{CSTR} = 0.01KW/m^3$ and $q_{PFR} = 0.35KW/m^3$. The costs of the reactors are respectively \$1041; \$1041; \$1013; and \$959 for CSTR, PER and BR.

Keywords: Performance evaluation, Reactors, Calcium Stearate, Voidage, Non-isothermal and Functional parameters.

INTRODUCTION

According to Lee, et al., (2009), Calcium Stearate as an aromatic hydrocarbon is among the most important raw materials in the chemical industry and is obtained exclusively from fossil resources. Calcium stearate is a detergent/soap derived from fatty-acids (lipids) which is a conjugate weak acid and alkali (strong base), so its aqueous solution is Alkaline. One major route of calcium stearate production is by the neutralization reaction of stearic acid and calcium hydroxide. Although, stearic acid, one of the raw materials for the production of calcium stearate is majorly obtained from petrochemical industries, it is also found naturally in fruits like palms, plums, pineapples, lemon and several other natural foods. Hence, when stearic acid from their natural fluids and food and species are used in calcium stearate production, it implies that it has a naturally containing ingredient. Thus calcium stearate is produced from stearic acid extracted from fruits and species commonly found in palm fruits, fruit juice products and fermented foods such as wines etc. (Nora et al, 2001).

Different literatures cited on the production of calcium stearate and performance are stated as thus: Haftom, et al, (2017) researched on performance evaluation of absorber reactors for solar fuels production written by where experimental work was carried on stainless steel, copper, ceramic and glass reactors as absorber materials of parabolic dish, aperture diameter 1.8m, coated with Al pet as reflective materials.

Hyang-Bok, et al, (2008) carried out research on Production of calcium-stearate by lipase using Hydrogenated Beef tallow. Their work employ suitable lipase at optimum reaction conditions of Ca(OH)_2 and Hydrogenated beef tallow at 95% of beef tallow in 2.5hrs and commercial lipase SDL451. Firstly fatty acid was initially produced by lipase and conversion into calcium-stearate. Theirwork also confirms that chemical production of calcium-stearate can be replaced by enzymatic reaction, thereby creating a cleaner process.

Wilcox, (2016) worked on Performance evaluation of reactor types for sodium benzoate production. Though, the work is already in the completion stage was reviewed to ascertain the present research study.

Table 1: Physical Properties of Calcium Stearate:

Parameter	Values
Melting point	147-149°C
Density	1.08g/cm ³
Solubility	Soluble in hot pyridine, slightly soluble in oil, but insoluble in alcohol and ether
Form	power
Colour	white

Chemical Properties

Calcium stearate also called calcium octadecanoic acid is light white crystalline powder with chemical formula: $[\text{C}_{17}\text{H}_{35}\text{COO}]_2\text{Ca}$; and molecular weight 607.00, decomposes by heat, insoluble in H_2O , cold ethanol and di-ethyl ether, soluble in hot Benzene, toluene and turpentine, slightly soluble in hot ethanol and di ethyl ether. It reacts with strong acid to be decomposed into stearic acid and corresponding calcium salt.

Dilute soap is made by the reaction of melt stearic acid NaOH , reacting with CaCl_2 , and Calcium stearate in obtained.

About 1.2 g a sample is accurately weighted, added 0.1mol/L , HCL boiled 10min, or until the fatty layer is clear. If necessary adding H_2O to maintain the original volume. Cooled and filtered, the filtrate and flask was washed thoroughly with H_2O until last washing liquor no longer acidic to litmus. Filtrate is treated with NaOH solution and it is neutral to litmus. Stirred with magnesium stirrer about 30ml 0.05ml/L NaEDTA is added via a 50ml burette, addition Ethane Di-Amine Tetra Acetate (EDTA) is added.

The work is aimed to investigate the performance of Batch, Continuous Stirred Tank Reactor and Plug Flow Reactors in the production of Calcium Stearate. To achieve the study aim, the logical steps stated are taken: Develop reactors models using materials balance principles, Obtain reactors parameters from the models developed such as volume, space times, space velocity and yield, Simulation of the reactors parameters numerically, evaluation of the functional dimension and parameters of the reactors and Comparison of the performances of the reactors functional parameters.

OBJECTIVES

The main objective of the study is to identify the challenges in the implementation of the newly adopted Philippine Health Agenda 2016-2022 in terms of health care delivery system in the Municipality of Jose Abad Santos, Davao Occidental. Specifically, this provided a description of the practiced health care system; examined different approaches to the Local Government Unit, financing and delivery of health services and the role of the main actors in health systems; described the institutional framework, process, content and implementation of health and health care policies; and highlighted challenges and areas that require more in-depth analysis.

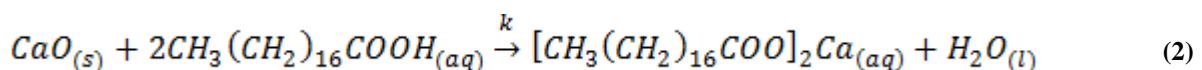
METHODOLOGY

The Materials involved are reactors (equipment), material balance, literature values/data and thermodynamic data. The design models development will apply material balance principles considering the modifications/assumptions for derivation.

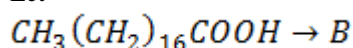
The performance equations are developed for Batch, Continuous Stirred Tank Reactor and Plug flow Reactor (Tubular Reactor) with the general material balance stated below:

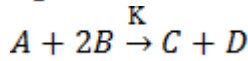
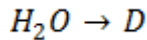
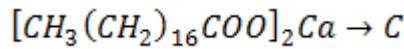
$$\left(\begin{array}{c} \text{Rate of accumulation} \\ \text{of materials within} \\ \text{the reactor} \end{array} \right) = \left(\begin{array}{c} \text{Rate of inflow of} \\ \text{materials into} \\ \text{the reactor} \end{array} \right) - \left(\begin{array}{c} \text{Rate of outflow of} \\ \text{materials from} \\ \text{the reactor} \end{array} \right) - \left(\begin{array}{c} \text{Rate of depletion of} \\ \text{materials due to} \\ \text{Biochemical reaction} \\ \text{within the reactor} \end{array} \right) \quad (1)$$

The rate expression for the production of calcium stearate from calcium oxide and stearic acid is written as:



Let $\text{CaO} \rightarrow A$





$$r_c = K C_A C_B^2 \quad (3)$$

Interms of fractional conversion; α_A

$$C_A = C_{A0}(1 - \alpha_A) \quad (4)$$

$$C_B = C_{A0}^2(M - \alpha_A)^2 \quad (5)$$

$$\text{Where } k = k_o \exp\left(\frac{-E_i}{RT}\right) \quad (6)$$

Combining equations (4) to (6) into (3) yields

$$(r_c) = k_o \exp\left(\frac{-E_i}{RT}\right) C_{A0}^3 (1 - \alpha_A)(M - \alpha_A)^2 \quad (7)$$

Since the process is adiabatically, Temperature does not change and the rate expression is independent of temperature.

Hence let $k_o \exp\left(\frac{-E_i}{RT}\right) C_{A0}^3$ be constant say μ

$$(r_c) = \mu(1 - \alpha_A)(M - \alpha_A)^2 \quad (8)$$

Where $\mu = k_o \exp\left(\frac{-E_i}{RT}\right) C_{A0}^3$

k_o = pre - exponential factor

E_i = Activation energy of species i kJ/kmol

R = Gas constant; kJ/kmol.k

R = Absolute temperature; k

$$M = C_{B0} / C_{A0}$$

C_{B0} = initial concentration of species, B .

C_{A0} = Initial concentration of species, A all in mol/m^3

2.2 Batch Reactor Design Model Development

Analyzing equation (1) mathematical for a Batch Reactor and Stating some of the Assumptions give: That the reactor is stationary and does not move, material are changed once, processed and removed before another charging takes place.

$$\left(\begin{array}{c} \text{Rate of inflow of materials} \\ \text{into the reactor} \end{array} \right) = \left(\begin{array}{c} \text{Rate of outflow of materials} \\ \text{from the reactor} \end{array} \right) = 0$$

Equation (1) becomes:

$$\left[\begin{array}{c} \text{Rate of Accumulation of} \\ \text{materials within the Batch Reactor} \end{array} \right] = \left[\begin{array}{c} \text{Rate of depletion of materials} \\ \text{within the Batch Reactor due to chemical} \\ \text{reaction} \end{array} \right] \quad (9)$$

Analyzing equation (9) mathematically gives:

$$\frac{dN_i}{dt} = -(-r_i)V_{BR}$$

$$\Rightarrow -(-r_i)V_{BR} = \frac{dN_i}{dt} \quad (10)$$

In terms of production

$$(r_c)V_{BR} = \frac{dN_c}{dt}$$

$$V_{BR} dt = \frac{dN_c}{(r_c)} \quad (11)$$

But in terms of fractional conversion gives:

$$V_{BR} \int_0^t dt = \int \frac{dN_c}{(r_c)} \quad (12)$$

$$N_c = N_{A,0}(-\alpha_A)M \quad (13)$$

$$dN_c = d\{N_{A,0}[1 - \alpha_A]\}$$

$$dN_c = -N_{A,0} d\alpha_A \quad (14)$$

Into equation (12) by substituting equation (14) yields

$$V_{BR}t = -N_{A,0} \int_0^{\alpha_A} \frac{d\alpha_A}{k_o \exp\left(\frac{-E_i}{RT}\right) C_{A,0}^3 (1-\alpha_A)(M-\alpha_A)^2} \quad (15)$$

Partializing and integrating the left hand side of equation (15) gives:

$$V_{BR} = \frac{N_{A,0}}{\mu, t} \left[\frac{1}{(M-\alpha_A)^2} \left\{ \ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right\} + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \right] \quad (16)$$

$$D = \left(\frac{2N_{A,0}}{\pi \mu t} \left\{ \left[\frac{1}{(M-\alpha_A)^2} \left\{ \ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right\} + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \right] \right\} \right)^{1/3} \quad (17)$$

The heat generated per unit area is given by:

$$q_B = \frac{(-\Delta H)F_{A,0}\alpha_A}{V_{BR}}$$

$$q_B = \frac{(M-\alpha_A)^2 (-\Delta H)F_{A,0}\alpha_A \mu t}{N_{A,0} \left\{ \left[\ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right] + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \right\}} \quad (18)$$

2.3 Design Models Development for Continuous Stirred Tank Reactor (CSTR)

The material balance equation, for equation (1) is used to develop the performance equations for a Continuous Stirred Tank Reactor.

v_0

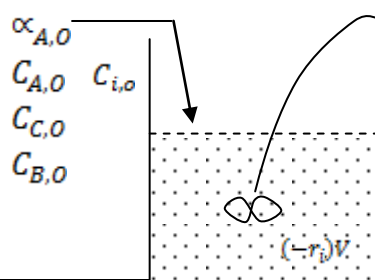


Figure 1: Diagram of CSTR Showing Material Balances

The steady state material balance of the CSTR is given by:

$$V_{CSTR} = \frac{v_0 C_c}{\mu(1-\alpha_A)(M-\alpha_A)^2} \quad (19)$$

2.3.1 The Functional Parameters of the CSTR

The space time of the continuous stirred tank reactor and the design models

$$\tau_{CSTR} = \frac{F_{AO} \alpha_A}{\mu(1-\alpha_A)(M-\alpha_A)^2 v_0} = \frac{C_{AO} \alpha_A}{\mu(1-\alpha_A)(M-\alpha_A)^2} \quad (20)$$

The space velocity of the CSTR model is given by:

$$S_{v,CSTR} = \frac{\mu(1-\alpha_A)(M-\alpha_A)^2}{C_{AO} \alpha_A} \quad (21)$$

$$L_{CTR} = \frac{C_{AO} \alpha_A}{\pi D^2 \mu(1-\alpha_A)(M-\alpha_A)^2} \quad (22)$$

$$q_{CSTR} = (-\Delta H_c) \mu(1-\alpha_A)(M-\alpha_A)^2 \quad (23)$$

2.4 Non-isothermal Energy Balance for CSTR at steady state;

$$\left(\frac{1-\varepsilon}{1+\varepsilon} \right) V_R (-r_i) = V_0 (C_i - C_{i,o})$$

$$\frac{1}{3} V_R (+r_i) = V_0 (C_i - C_{i0}) \quad (24)$$

$$\tau = \frac{3 \alpha_A \exp \left[\frac{E_i}{RT} \right]}{k_0 C_{A0}^2 (1-\alpha_A) (M-\alpha_A)^2} \quad (25)$$

$$T = T_0 + \tau \frac{(\Delta H_R)}{\rho C_p} (r_i)$$

$$T = T_0 + \tau \frac{(\Delta H_R)}{\rho C_p} k_0 \exp \left[\frac{-E_i}{RT} \right] C_{A0}^3 (1-\alpha_A) (M-\alpha_A)^2$$

$$T = T_0 + 3 C_{AO} \frac{(\Delta H_R)}{\rho C_p} \alpha_A \quad (26)$$

2.5 Design Model Development for Plug Flow Reactor (PFR).

The material / mass balance equation (3.1) is used to generate the models for the performance of PFR as follows:

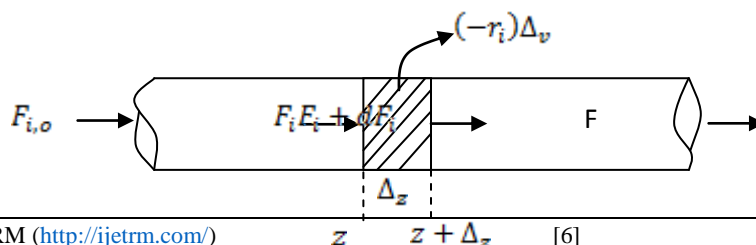


Figure 2: Schematic Diagram Showing the Differential Element of PFR.

$$V_{PFR} = -F_{AO} \int_0^{\alpha_{AF}} \frac{d\alpha_A}{\mu(1-\alpha_A)(M-\alpha_A)^2} \quad (27)$$

$$V_{PFR} = \frac{F_{AO}}{\mu} \left[\frac{1}{(M-\alpha_A)^2} \left\{ \ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right\} + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \right] \quad (28)$$

2.5.1 Functional Parameters of Plug Flow Reactor Design Models

The space time, space velocity, length, diameter, heat generated per unit volume and pressure drop of the plug flow reactor design models is stated below:

$$\tau_p = \frac{C_{A,0}}{\mu} \left[\frac{1}{(M-\alpha_A)^2} \left\{ \ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right\} + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \right] \quad (29)$$

$$S_{VP} = \frac{\mu}{C_{A,0} \left[\frac{1}{(M-\alpha_A)^2} \left\{ \ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right\} + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \right]} \quad (30)$$

$$L_{PFR} = \left\{ \left[\frac{4F_{AO}}{\pi(0.4)^2\mu} \right] \left[\frac{1}{(M-\alpha_A)^2} \left\{ \ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right\} + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \right] \right\}^{1/3} \quad (31)$$

$$q_p = \mu(M-\alpha_A)^2(-\Delta H_r) \alpha_A \left\{ \ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right\} + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \quad (32)$$

$$\Delta P = 0.16 \left\{ \frac{\left\{ \left[\frac{4F_{AO}}{\pi(0.4)^2\mu} \right] \left[\frac{1}{(M-\alpha_A)^2} \left\{ \ln \left[\frac{(M-\alpha_A)}{M(1-\alpha_A)} \right] \right\} + \frac{1}{(M-1)} \left(\frac{1}{M} - \frac{1}{M-\alpha_A} \right) \right] \right\}^{1/3} \rho^{0.84} \mu^{0.16} u^{1.84}}{D^{1.16}} \right\} \quad (33)$$

2.6 Non isothermal Energy balance

The steady state energy balance is given as:

$$\begin{aligned} & \left[\begin{array}{l} \text{Rate of inflow of energy into the} \\ \text{differential volume of reactor} \end{array} \right] \\ &= \left[\begin{array}{l} \text{Rate of outflow of energy from} \\ \text{the differential volume of reactor} \end{array} \right] - \\ & \left[\begin{array}{l} \text{Rate of depletion of energy within the} \\ \text{differential volume of reactor} \end{array} \right] \\ &+ \left[\begin{array}{l} \text{Rate of energy added into the} \\ \text{differential volume of reactor} \end{array} \right] \quad (34) \end{aligned}$$

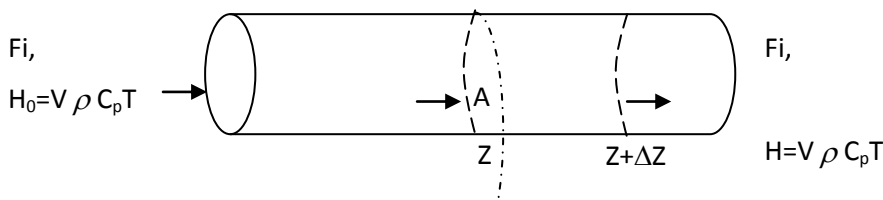


Figure 3: Plug Flow Reactor Sketch Showing the Material Balance taking place in Differential Control Volume
Mathematical analysis of equation (3.4) at steady state adiabatic condition gives the following equations:

$$\frac{dT}{dZ} = \frac{1}{u\rho C_p} (\Delta H_R)(-r_i)\tau \quad (35)$$

2.7 Cost of Reactors

Considering jacketed, agitated Reactors (CSTR, BR & PFR), the estimated cost according to (Sinnott, *et al*, 2009) is given by:

$$Ce = a + b(V)^n \quad (3.6)$$

Where:

A=\$177, b=\$93.3, n=0.8 and V= volume of reactors in m³

2.8 Simulation Parameters

The inputs parameters used to perform the calculations or simulation data and hence for evaluation of the reactors functional parameters and dimensions are presented in Table 3.1. The simulation was implemented with MATLAB computer program, (Ode 45 Runge- Kuttanumerical method) to facilitate the processing output data of the reactors. Models developed for Batch, Continuous Stirred-Tank and Plug Flow reactors.

Table 2: Summary of Input Parameters

Parameters	Value	Reference
Initial concentration, $C_{AO}(\text{mol m}^{-3})$	0.293	Perry etal, 2004
Volumetric flow rate, $v_o(\text{m}^3/\text{s})$	3.125	Assumed
Heat of Reactor, $\Delta H_r(\text{KJ/mol})$	310.5	Perry etal, 2004
Density, $\rho, (\text{kg/m}^3)$	1635	Perry etal, 2004
Mean viscosity, $\mu(\text{N}_s/\text{m}^2)$	1.6782×10^{-5}	Perry etal., 2004
Molar flow rate, $F_{AO}, (\text{mol/s})$	0.915625	Calculated
Activation Energy, $\epsilon_a, (\text{kJ/mol})$	86082.5	Perry <i>et al</i> , 2004
Pre-exponential factor, $k_o(\text{m}^6/\text{mol}^2.\text{s})$	800000.72	Perry <i>et al</i> , 2004

RESULTS AND DISCUSSION

The Comparison of Batch Reactor, Plug Flow Reactor and ContinuoSus Stirred Tank Reactorat various operating variables, for the production of calcium have been investigated and presented in this chapter. The size and heat generated per reactor volume for the reactors were analyzed and also compared. For Flow Reactors,like the Continuous Stirred Tank Reactor, and the Plug Flow Reactors functioned parameters (such as space time,

space velocity) were equally compared and analyzed also, the pressure drop as the characteristics associated only with plug flow reactor was evaluated against the fractional conversion.

3.1 Batch reactor functional parameters

The results obtained from the simulation process using MATLAB and graphs plotted using M.S excel in figure 4.1 to 4.5 analyzed and discusses the extent of conversion of stearic acid and stake line to give product (calcium state). The Batch Reactor volume, length, heat generated per unit volume and holding time was also investigated at varying molar feed ratios with increasing fractional conversion to 90%.

Table 3: Performance of Batch Reactor, PFR and CONTINOUS STIRRED TANK Reactor Parameters at 90% Conversion of Calcium Hydroxide

PARAMETERS	BATCH REACTOR	CONTINOUS STIRRED TANK REACTOR	PFR
Conversion	0.9	0.9	0.9
Diameter (m)	1.50	1.85	1.25
Volume (m ³)	14.25	16.15	15.50
Length (m)	4.83	3.78	3.49
Space Time (s)	N.A	8.85	4.58
Space Velocity (s ⁻¹)	N.A	0.035	0.09
Heat Gen. per volume (KW/m ³)	0.4	0.01	0.09
Holding time (s)	6.8	N.A	N.A
Pressure Drop (Pa)	N.A	N.A	3.73E-08

Table 4: Cost of Reactors per annum [Sinnott, *et al*, 2009]

Reactor	Cost (\$)	Cost (N)
CSTR	1041	374,760.00
PFR	1013	364,680.00
BR	959	345,240.00

In terms of cost, Continuous Stirred Tank Reactor is the most cost reactor due to high volume, since the cost estimate is a function of volume as shown in equation 3.92 above, then for the volume of reactors respectively 16.16m³, 15.50m³ and 14.25m³ for CSTR, PFR & BR, the cost estimate shows the trend in table 4.

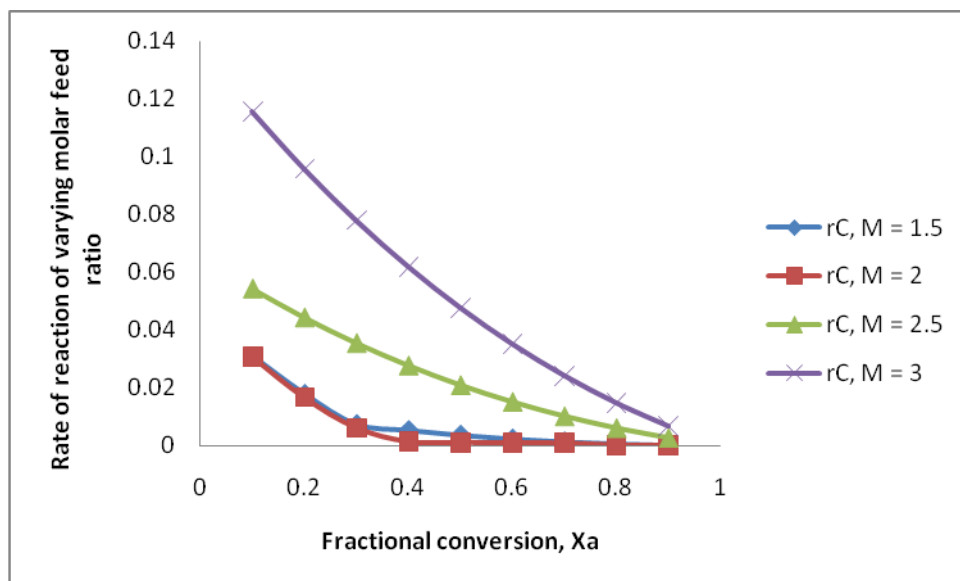


Figure 4 Rate of Reaction of Varying Molar Feed Ratio versus Fractional Conversion

Figure 4 is the rate of reaction at different molar feed ratio: $M=1.5, 2, 2.5$ and 3 varying with fractional conversion. The graph predicts that at $M=1.5, 2$ and 2.5 , then there is decrease in rate as conversion increases to 1 . At lower X_A , higher rates and at higher X_A , lower rate. Again, at $M=3$, rate of reaction is highest initially and lowest finally.

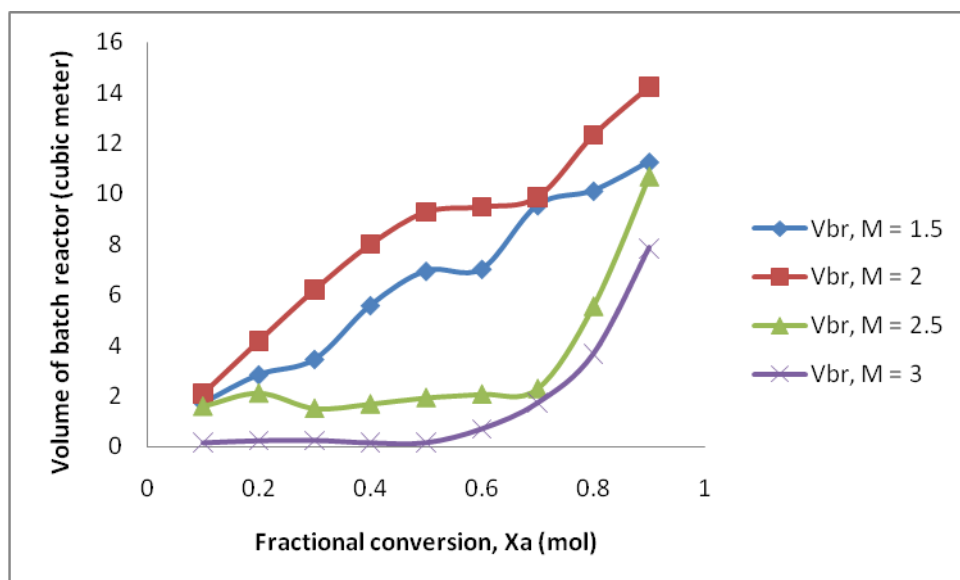


Figure 5 Volume of Batch Reactor with Varying Molar Feed Ratio versus Fractional Conversion

Figure 5 depicts the volume of product in the batch reactor present at varying molar feed ratio with fractional conversion.

The molar feed ratio (ration of stearic acid to calcium hydroxide (slake lime) was varied.

From 1.5 to 3.0 at intervals of 0.5, the result presented in figure 5 showed that increasing the molar feed ratio, M results in decrease of volume of the batch reactor at every CaOH to stearate product with corresponding values at 90% conversion of CaOH as: the volume of bath reactors are 11.26m^3 , 14.25m^3 , 10.69m^3 and 7.86m^3 respectively. From the graph and result, it can be said that molar feed of 1.5 and 2.0 is good enough for better yield of calcium stearate produced in a batch reactor.

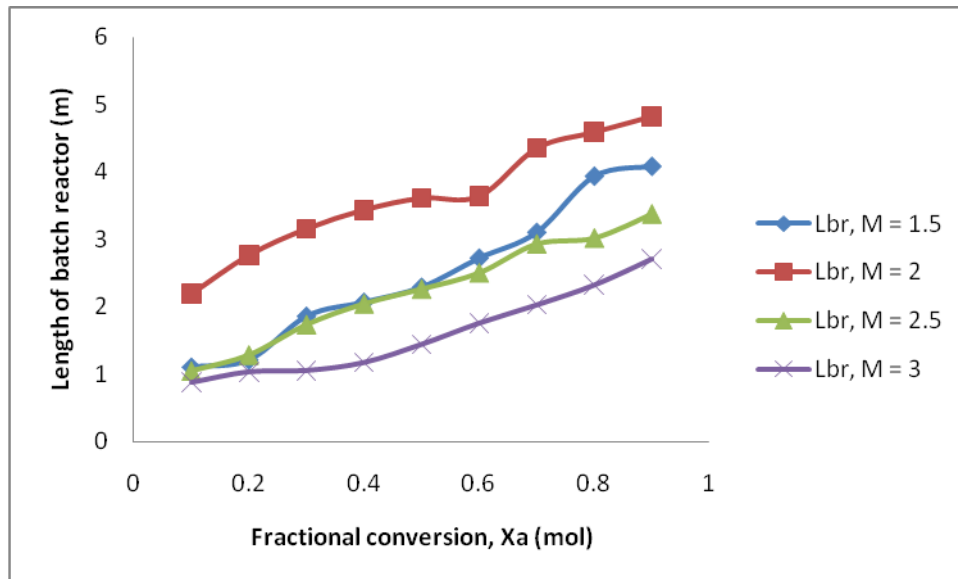


Figure 6 Length of Batch Reactor with Varying Molar Feed Ratio against Fractional Conversion

The length of the batch reactor was evaluated at different molar feed ratios. Figure 6 shows that increasing the molar feed, reduces the volume and hence the length of the batch reactor. At conversion of 90%, the length of batch at different molar feed are respectively 4.09m, 4.83m, 3.38m and 2.71m of 1.5, 2.0, 2.5 and 3 respectively.

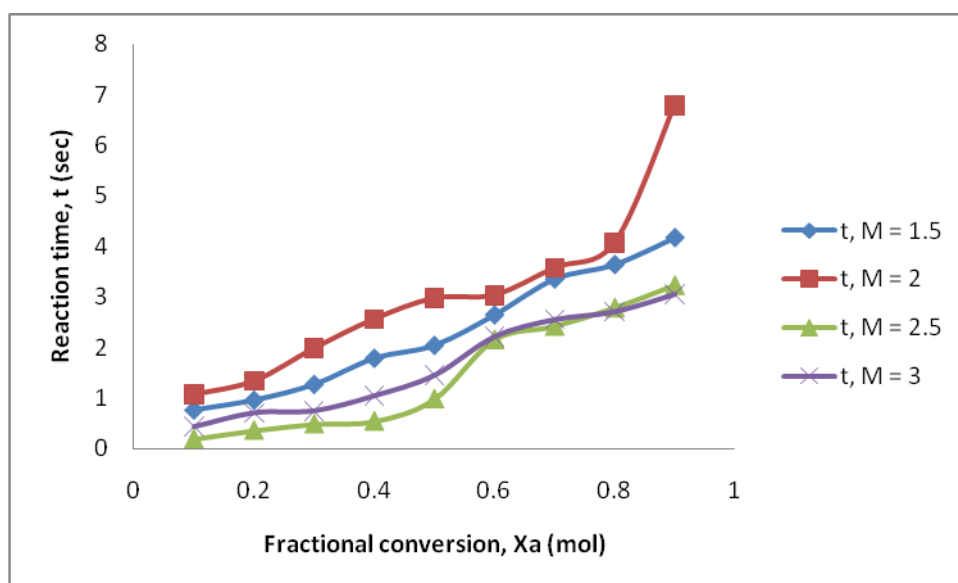


Figure 7 Influence of Reaction Time with Varying Molar Feed Ratio versus Fractional Conversion

The influence of reaction time was investigated at different molar feed ratio with X_A . Figure 7 depicts increase of reaction time (t) with fractional conversion. But increasingly molar feed ratio, decreases the holding time or reaction time) and hence reduces the yield of stearate. Preferably, $M=1.5$ and 2 may be considered for good yield of stearate for in batch.

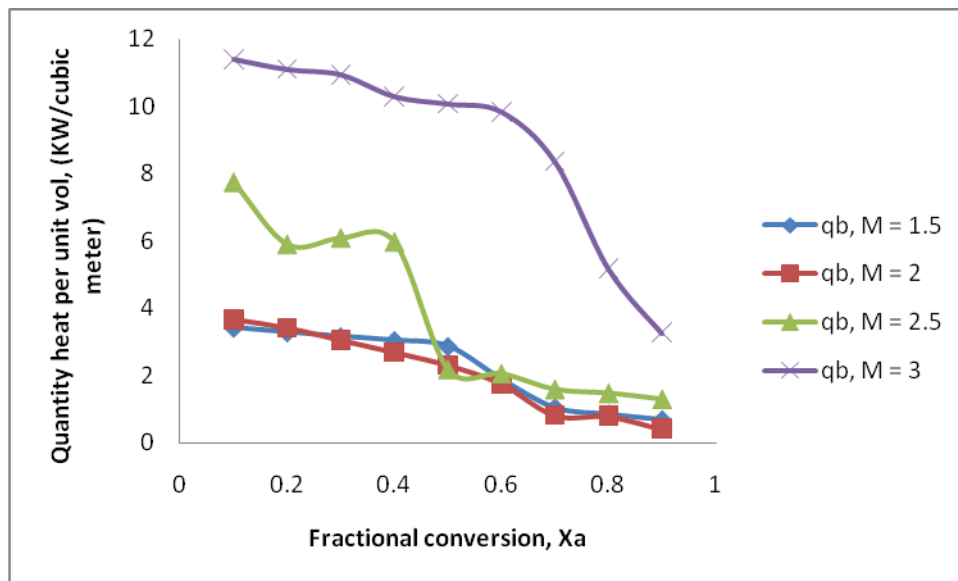


Figure 8 Heat Generated Per Unit Volume Varying with Molar Feed Ratio against Fractional Conversion

The heat generated per batch volume evaluate ratio is shown in Figure 8 at higher molar feed ratios, heat generated per unit volume for batch increase, but at lower feed ratios, lower heat generated per unit volume for batch increases, but at lower generated per unit volume. At 90% conversion, the q for $m=1.5$, 2, 2.5 and 3.0 are respectively 0.68KW/m^3 ; 0.40KW/m^3 ; 1.3kw/m^3 , and 3.256kw/m^3 .

3.2 Continuous Stirred Tank Functional Parameters

The results obtained from the simulation of the Continuous Stirred Tank Reactor models developed are discussed and presented in figure 9-15. The Continuous Stirred Tank Reactor functional parameters (space time, space velocity, length, temperature) were investigated at different molar feed ratio ($M=1.5$, 2, 2.5 and 3) of stearic acid and slake time at 90% conversion.

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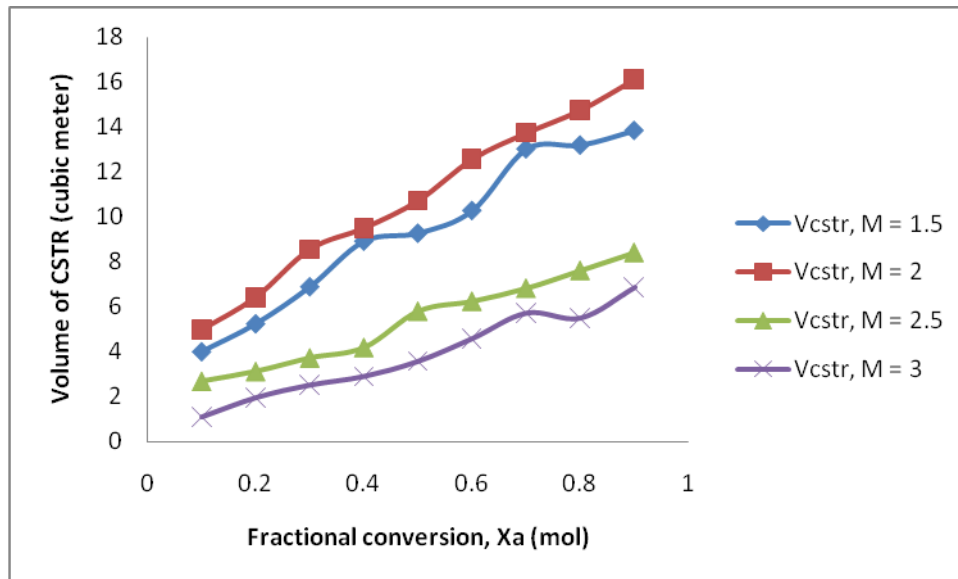


Figure 9 Volume of Continuous Stirred Tank Reactor of Varying Molar Feed Ratio against Fractional Conversion

Figure 9 shows the volume of Continuous Stirred Tank Reactor against degree of fractional conversional varying molar feed ratio at ambient temperature of 25°C . The volume of Continuous Stirred Tank Reactor increases as fractional conversion, but decreases as molar feed ratios increases. Hence at $M=1.5$ and 2 , a reasonable volume of the reactor is obtained. Thus at conversion of 90% ; the respectively volume is: 13.86m^3 , 16.15m^3 , 8.43m^3 and 6.90m^3 for molar feed ratio of 1.5 , 2.0 , 2.5 , and 3.0 respectively.

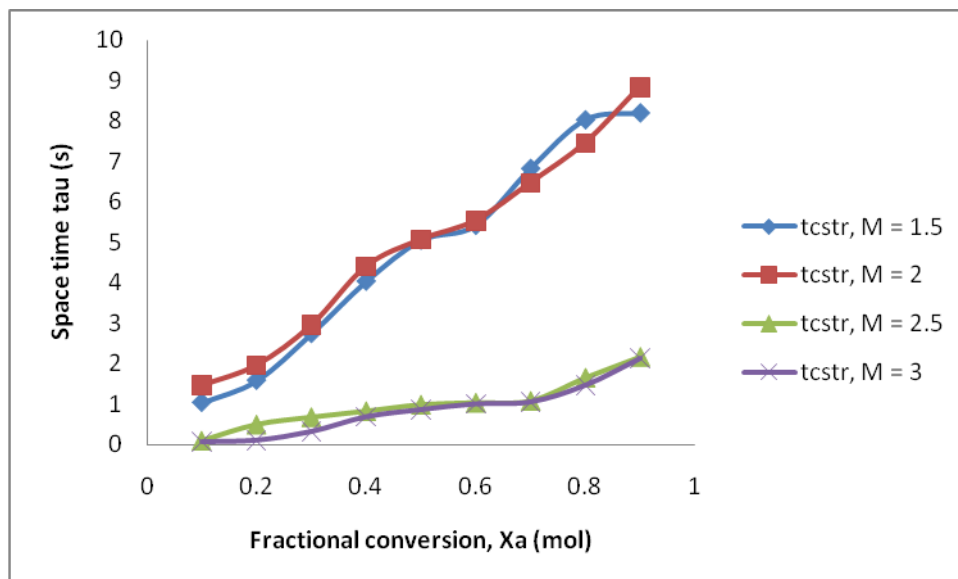


Figure 10 Space Time Varying with Molar Feed Ratio against Fractional Conversion

Figure 10 depicts Continuous Stirred Tank Reactor space time against fractional conversion at varying molar feed ratios. At ambient temperature, 25°C , the space time increases from 0.02sec to 8.85sec highest for the 4 different molar feed ratios. Importantly, $M=1.5$ and 2 have good space time values of 8.19secs and 8.85secs respectively, indicating that enough amount of stearate will be produced at such molar feed ratios of 1.5 and 2. As molar feed ratios increases, the volume reduces and off course, reduces the space values.

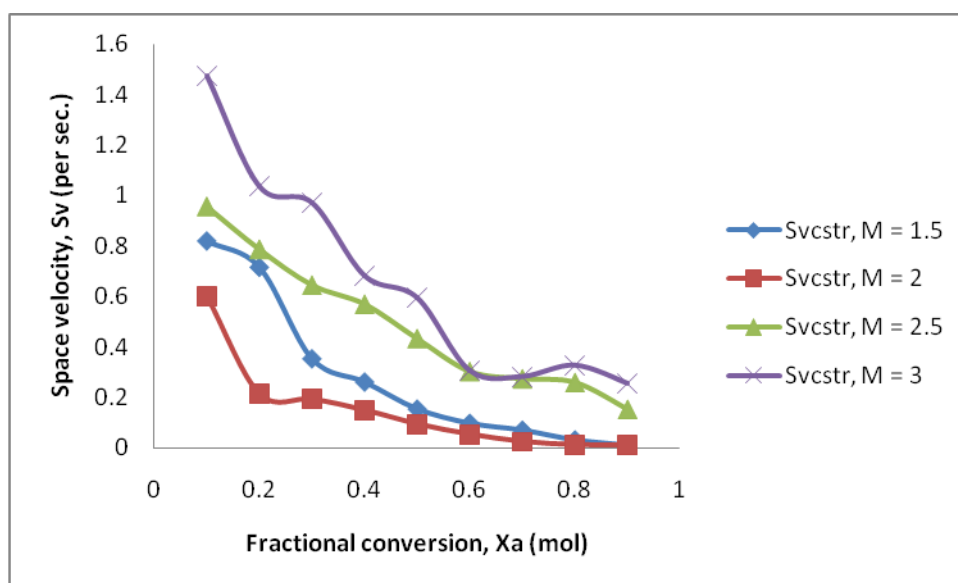


Figure 11 Space Velocities with Varying Molar Feed Ratio against Fractional Conversion

Space velocity is one of the functional parameter of Continuous Stirred Tank Reactor and it decreases as fractional conversion decreases and becomes least at lower molar feed ratios of 1.5 and 2 respectively given values of 0.01s^{-1} and 0.01s^{-1} at 90% conversion and higher at molar feed ratios of 2.5, 3 of 0.015s^{-1} and 0.026s^{-1} respectively. This is depicted in Figure 11.

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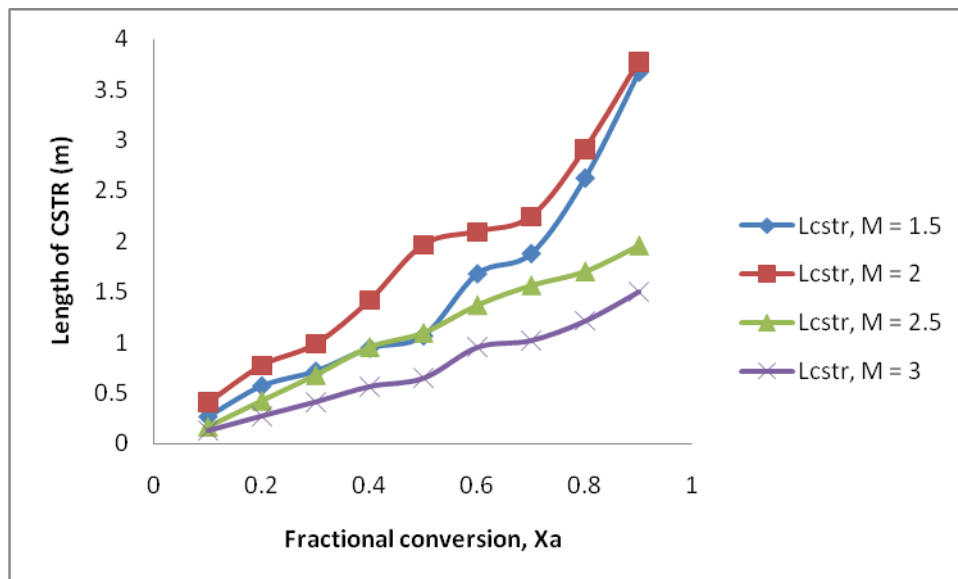


Figure 12 Length of Continuous Stirred Tank Reactor Varying with Molar Feed Ratio against Fractional Conversion

Figure 12 shows the length of Continuous Stirred Tank Reactor against Fractional Conversion at varying molar feed ratios. Increase in length as fractional conversion increases and decreases in length as molar feed ratio increases as shown above. Molar feed ratio of 1.5 and 2 give a value of 3.67m and 3.78m respectively at 90% conversion and 1.96m and 1.50m respectively are values gotten at 2.5 and 3 molar feed ratios. Hence larger volume gives larger length and vice versa.

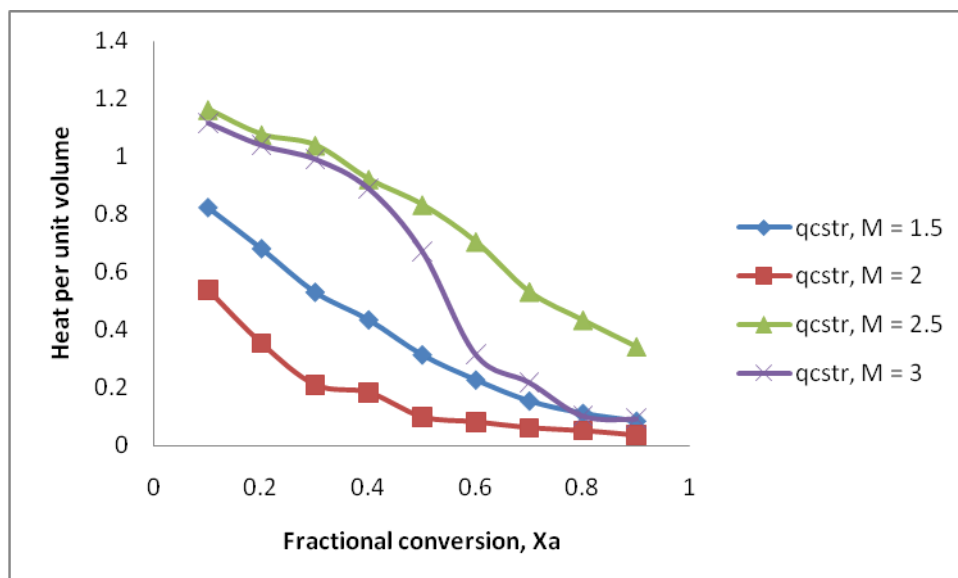


Figure 13 Heat Per Unit Volume With Varying Molar Feed Ratio versus Fractional Conversion

Figure 13 depicts the profile of heat generated per unit volume (q) of Continuous Stirred Tank Reactor with X_A at varying molar feed ratios.

Least values of q at $M=1.5$ and 2 and high values of q at $M=2.5$ and 3 . The heat generated per unit volume of Continuous Stirred Tank Reactor decreases as X_A increases such that at 0.9 conversion, q is respectively 0.08KW/m^3 ; 0.035KW/m^3 , 0.34KW/m^3 , and 0.09KW/m^3 for 1.5 , 2 , 2.5 and 3.0 molar feed ratio.

This is happening at $T=298\text{K}$ (25°C)

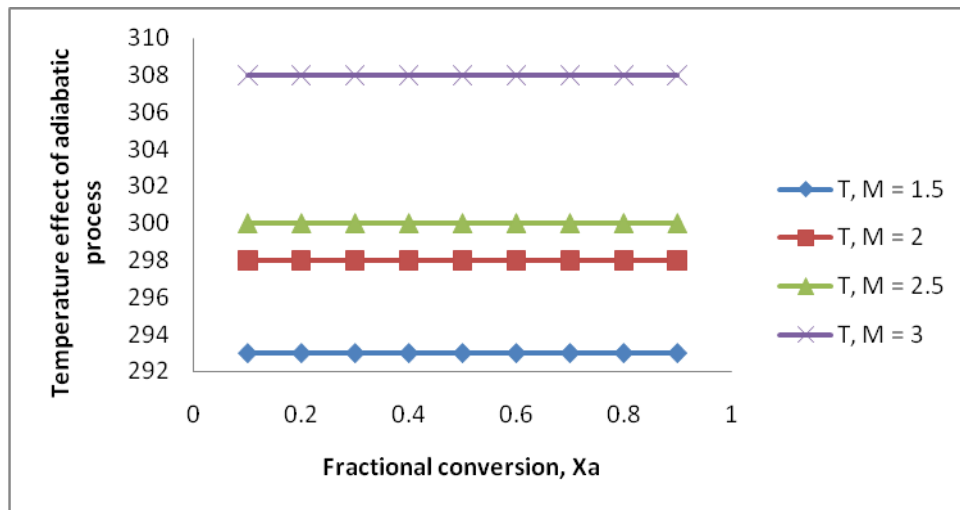


Figure 14 Adiabatic Temperature Effects with Varying Molar Feed Ratio versus Fractional Conversion

Figure 14 depicts non-isothermal adiabatic temperature profile of Continuous Stirred Tank Reactor with Fractional Conversion at varying molar feed ratios. There is increase in temperature at increasing X_A . Temperature increases too with increases molar feed ratio. The aim is to conserved heat and spent less for the production process but at higher molar feed ratios, temperature increases and cannot be conserved, hence at lower molar feed ratios provided better reduction of heat and minimize cost. At $M=1.5$ and 2.0 , the temperature values at 0.9 conversion are respectively 293.00K , and 298.00K while at $M=2.5$ and 3.0 , the temperature values are 300K and 308K .

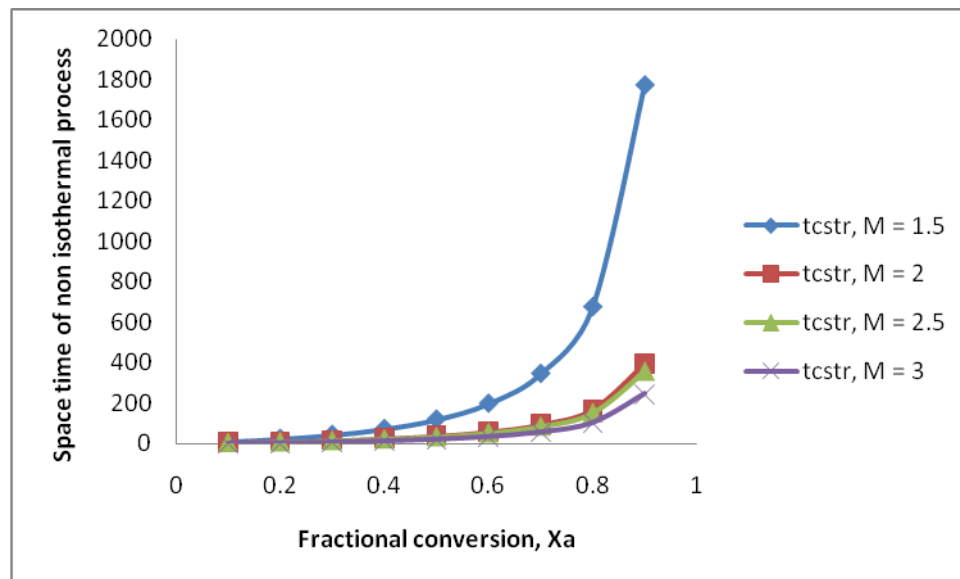


Figure 15 Space Time of Continuous Stirred Tank Reactor with Varying Molar Feed ratio against Fractional Conversion

Figure 15 shows the profile of non-isothermal space time of Continuous Stirred Tank Reactor with fractional conversion at varying molar feed ratios.

Equally, at $M=1.5$ and 2 , the space time increases to higher values at increase X_A and at changing temperature given respectively values of 1775secs , and 398.50secs . While at higher M -values, say 2.5 and 3.0 , lower t Continuous Stirred Tank Reactor are obtained every 896secs and 246.53secs respectively higher to Continuous Stirred Tank Reactor values gives rise to high volume produced and thus better output of stearate.

3.3 Plug Flow Reactor Functional Parameters

The results obtained from the MATLAB simulation provided a template for the discussion and analysis of the plug flow reactor's functional parameters, pressure drop and non-isothermal temperature variations with fractional conversion and at different molar feed ratios.

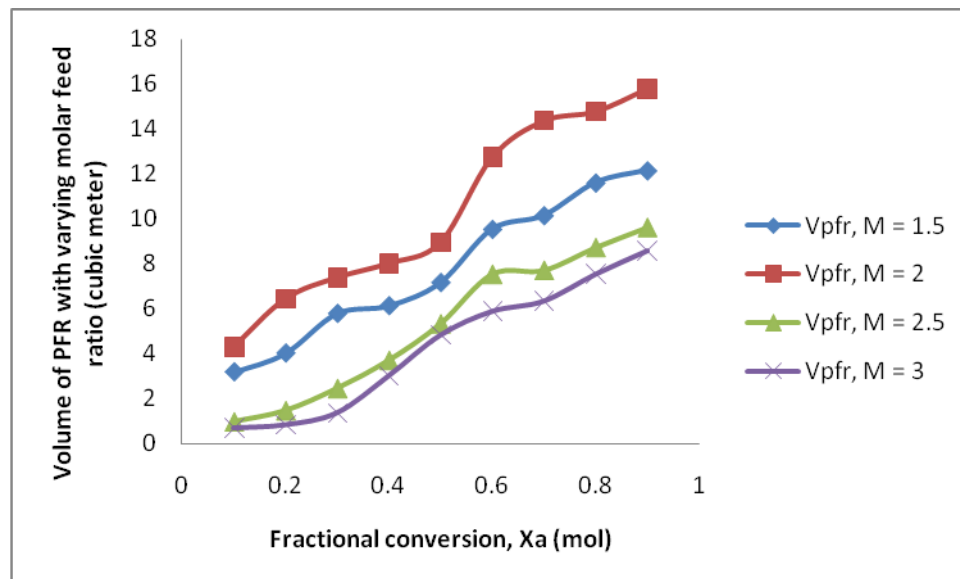
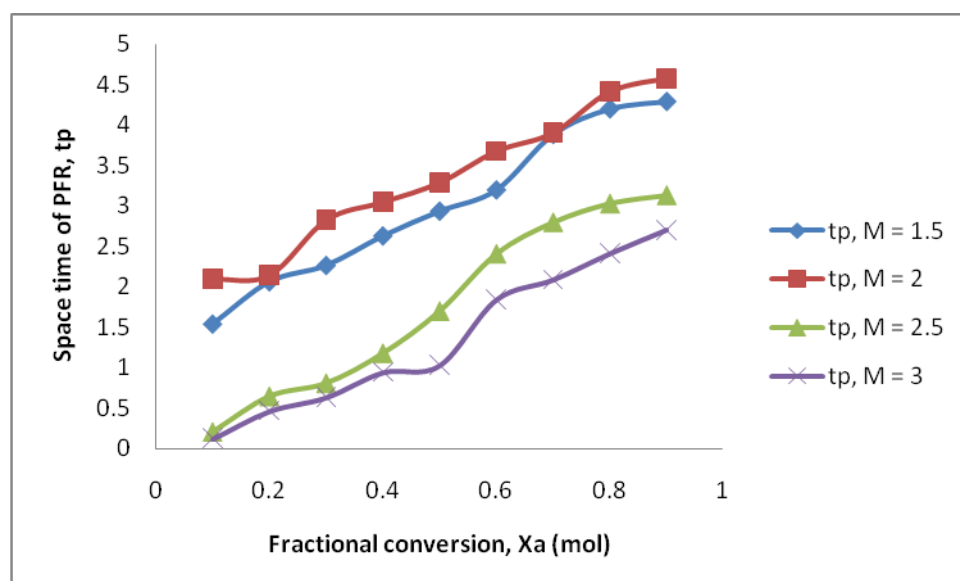


Figure 16 Volume of PFR with Varying Molar Feed Ratio versus Fractional Conversion

Figure 16 shows volume of PFR against degree of conversion at varying molar feed ratios. Increase of values of reactor at higher value of X_A . Again, the volume is highest at $M=2$ and good for the process given respectively.

$M=1.5$, $V_{PFR} = 12.15\text{m}^3$; $M=2$; $V_{PFR} = 15.50\text{m}^3$,

$M=2.5$, $V_{PFR} = 9.62\text{m}^3$ and $M=3$; $V_{PFR} = 8.00\text{m}^3$.



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Figure 17 Space time of PFR with Varying Molar Feed Ratio against Fractional Conversion

Figure 17 depicts PFR space time against degree of conversion at varying feed ratio. The time increases as increasing X_A and at lower $M=1.5$ and 2.0 , while though it increases but not compared to those with 1.5 and 2 .

Values of space time at 0.9 conversions and at varying molar feed ratios are respectively 4.28secs , 4.58secs , 3.14secs and 2.71secs .

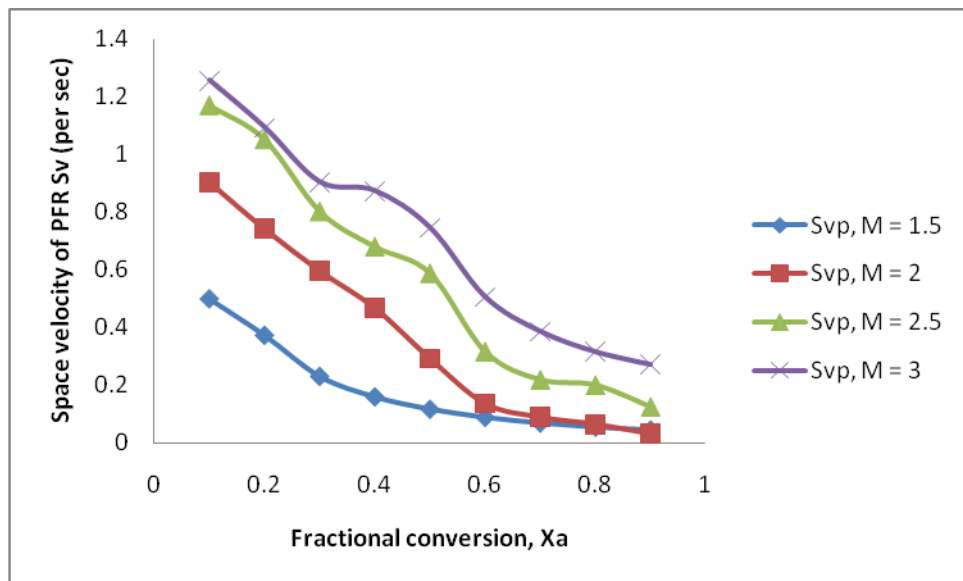


Figure 18 Space velocity of PFR with Varying Molar Feed Ratio against Fractional Conversion

Figure 18 depicts PFR space velocity against X_A at varying molar feed ratios. Space velocity decreases as X_A decreases but higher spaces velocity values are obtained $M=2.5$ and 3.0 while lower values of space velocity occurs at $M=1.5$ and 2 . Hence molar feed ratio of 2 is recommended for better yield.

At 0.9 conversions, space velocities are: 0.045 per sec ; 0.032s^{-1} , 0.123s^{-1} and 0.27s^{-1} at $M=1.5$, 2 , 2.5 and 3.0 respectively.

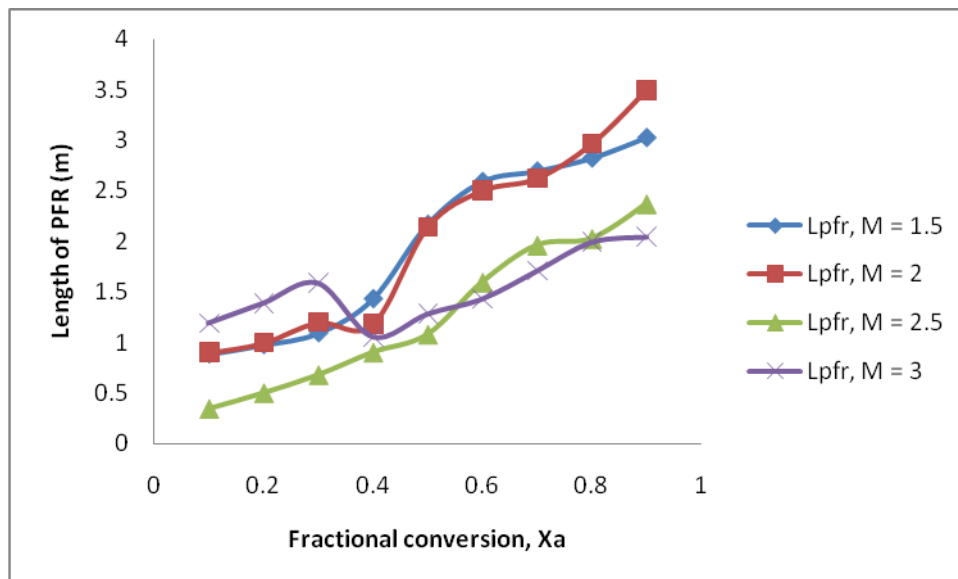


Figure 19 Length of PFR Varying with Molar Feed Ratio against Fractional Conversion

Figure 19 showed the length of PFR against X_A , at varying m -values. The length increases at X_A increases but higher values of it are at $M=2.5$ and 3 . At higher values of Length of PFR, volume is high and production is good. At 0.9 conversions, length of PFR gives respective values: 3.03m , 3.49m , 2.37m and 2.05m .

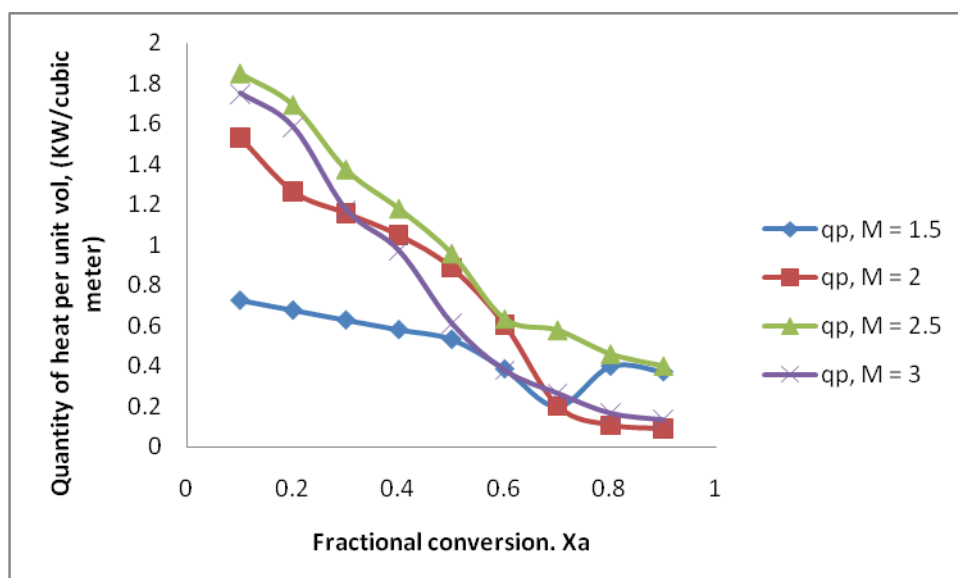


Figure 20 Quantity Heat Per Unit Volume Varying with Molar Feed Ratio against Fractional Conversion

Figure 20 indicates the quantity of heat generated per unit volume of PFR with X_A at varying molar feed ratios ($m=1.5, 2.0, 2.5, 3.0$).

Generally, the heat generated per unit volume reduces at increasing X_A . The values at 0.9 conversions gave: 0.37KW/m^3 , 0.09KW/m^3 ; 0.40KW/m^3 and 0.13KW/m^3

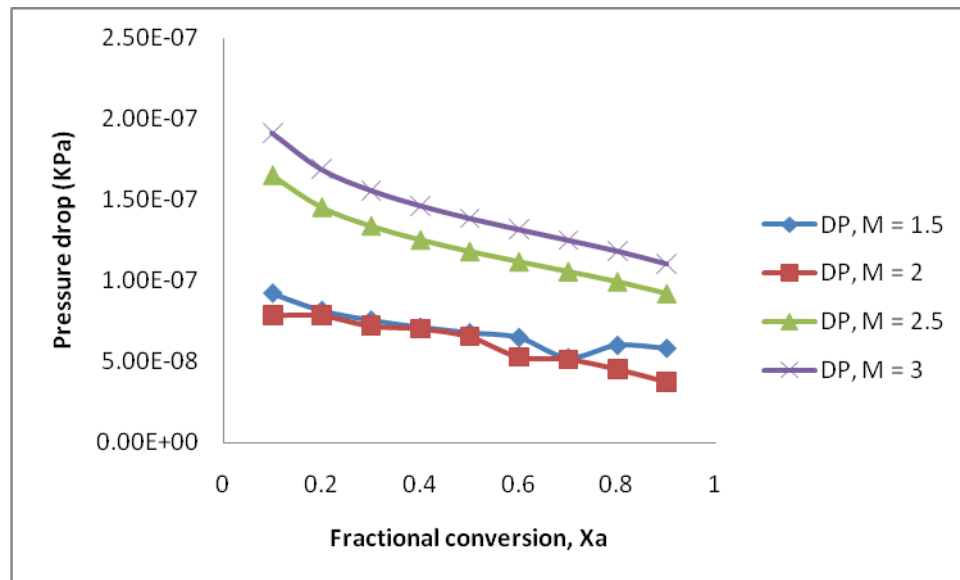


Figure 21 Pressure Drop with Varying Molar Feed Ratio versus Fractional Conversion

Figure 21 indicates profile of pressure drop against X_A , at varying M -values (1.5, 2, 2.5 and 3)

Pressure reduces at lower $M=1.5$ as conversion increases and increase at higher values of M and at increases X_A though there is general decrease of pressure drop at increases X_A given respective values of $5.85\text{E-}08$, $3.73\text{E-}08$, $9.19\text{E-}08$ and $1.11\text{E-}07$ for $M=1.5, 2.0, 2.5$ and 3.0 .

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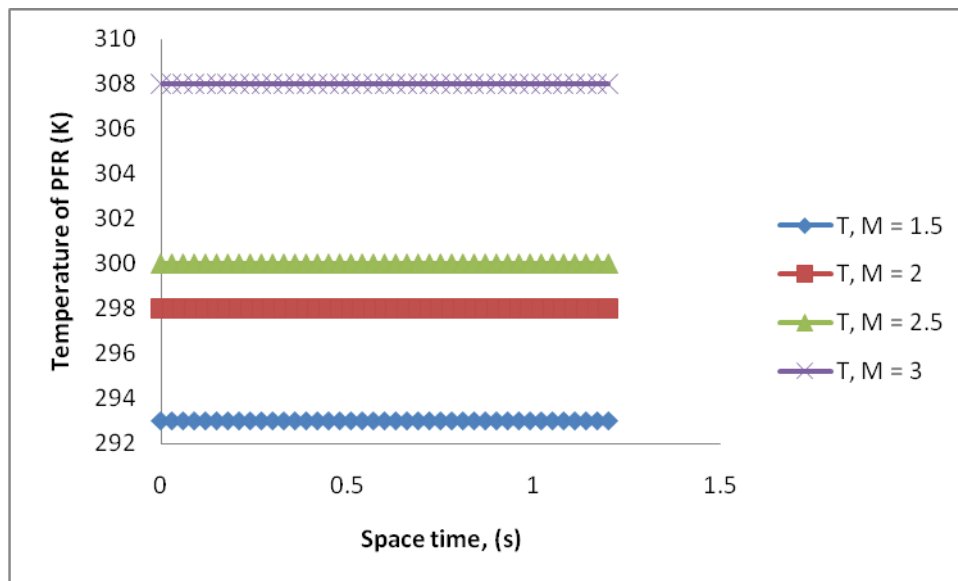


Figure 22 Adiabatic Temperature Effect of PFR with Varying Molar Feed Ratio versus Space Time

Figure 22 Is The Adiabatic Temperature effects of Plug Flow Reactor at varying molar feed ratios with space time there is increase in temperature values as space time varies and change of M-values (1.5, 2.0, 2.5 and 3.0).

Higher molar feed ratios gave higher temperature as compared to lower molar feed-ratio. Recommendation should be M=1.5 and 2 should give better results.

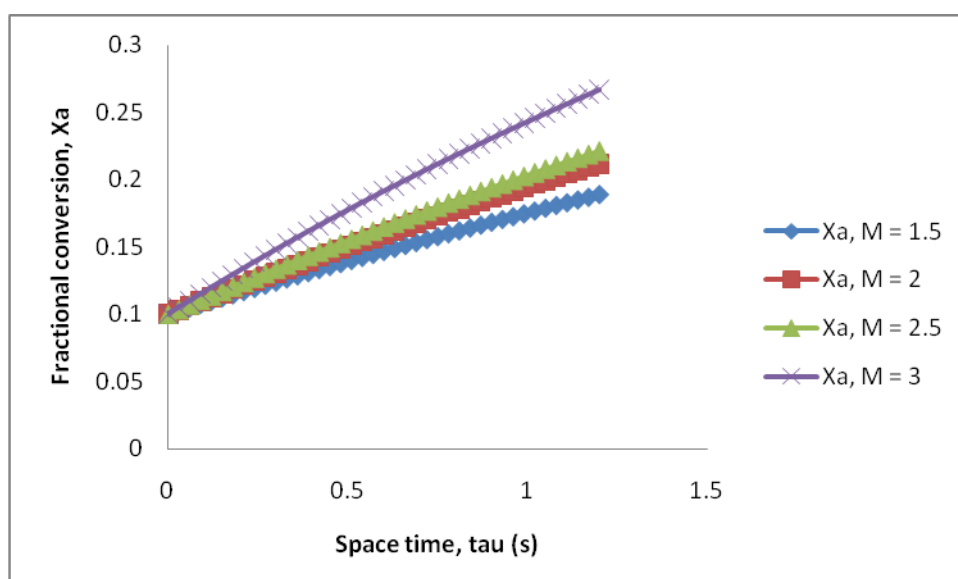


Figure 23 Fractional Conversion of PFR with Varying Molar Feed Ratio versus Space Time

Figure 23 Shows Plot of Fractional Conversion X_A Space Time with varying Molar Feed ratios.

Fractional Conversion increases at increase Space Time with $M=1.5$ and 2 given lower values of X_A with respect to τ while, higher molar feed ratios, 2.5 and 3, gave, higher X_A -values.

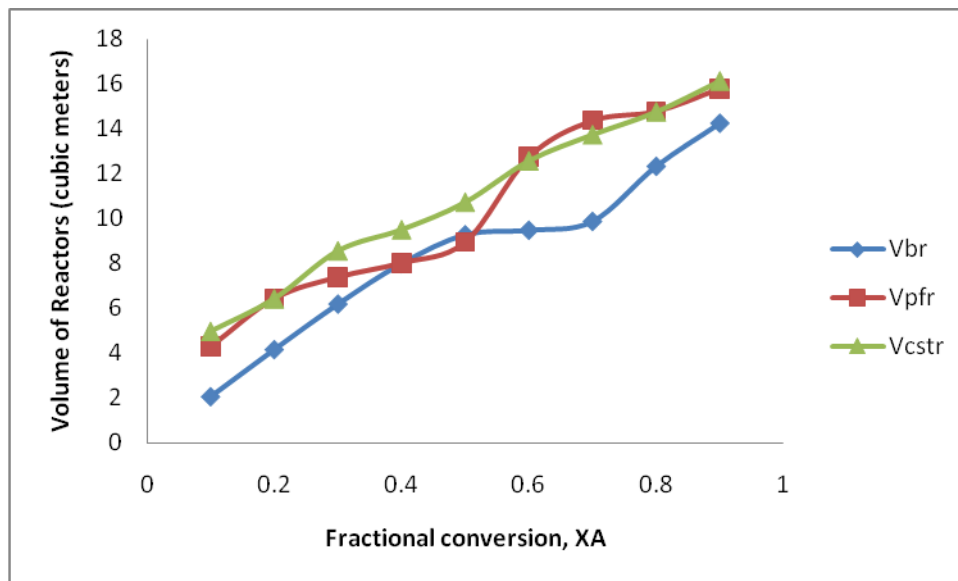
**Figure 24 Volume of Reactors (Batch, PFR & CSTR) versus Fractional Conversion**

Figure 24 Depicts The Plots of Volume of the Three Reactors (BR, CSTR and PFR) against Fractional Conversion, X_A . The plots indicate that the volume of the plug flow reactor is the best performed reactor compared to the other reactors at same conditions of fractional conversion and other condition being constant.

That is for instance, at fractional conversion,

$$X_A = 0.90, V_{PFR} = 15.5m^3, V_{CSTR} = 16.15m^3 \text{ and } V_{BR} = 14.25m^3.$$

This is shown in table 3.

$$\text{Hence: } V_{CSTR} > V_{PFR} > V_{BR}$$

Thus the optimum yield of the product (calcium stearate) occurs at **90%** and takes place in a continuous stirred tank reactor as completely shown in Figure 4. The volume of the reactors increases as fractional conversion (X_A) increases, but the reactor with the maximum volume is CSTR reactor at same conditions for the three reactors.

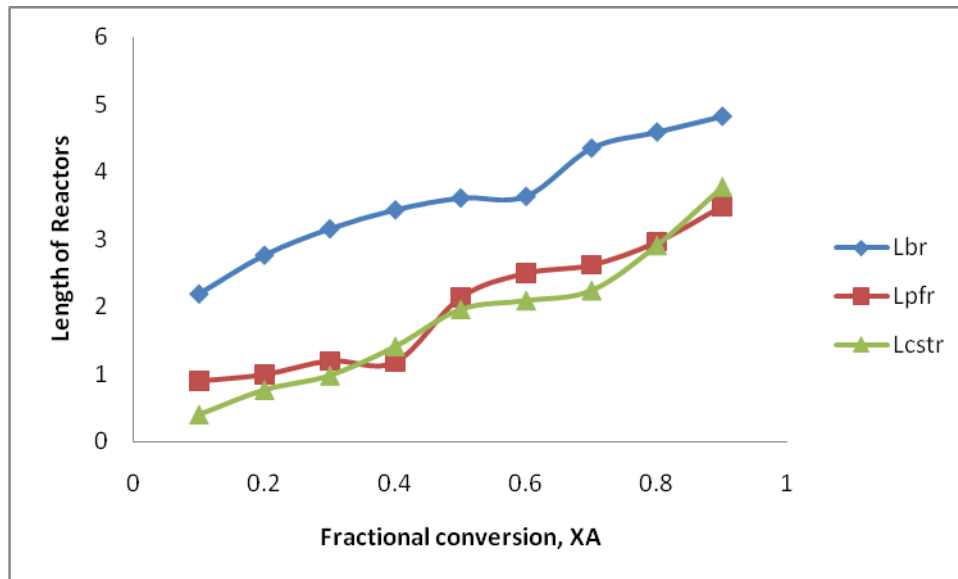


Figure 25: Length of Reactors (Batch, PFR & CSTR) against Fractional Conversion

Figure 25, Depicts the Variation Profiles of Length of Reactors (for BR, CSTR and PFR) with fractional conversion. From the plots, there is progressive increase in length of the Reactors as fractional conversion increases from $\alpha_A = 0$ to $\alpha_A = 0.90$. this can also show that the increase in length of Plug Flow reactor is greater than CSTR and Batch. The maximum length is $4.88m$ and occurs for plug flow reactor. Comparatively, the table 4.6 and 4.9, are the best fractional conversion for maximum yield $X_A = 0.90$, $L_{PFR} = 3.49m$, $L_{CSTR} = 3.78m$ and $L_{BR} = 4.83m$.

In the same vain, since volume of the reactor is mathematically expressed as:

$V_R = \frac{\pi D^2}{4} LR = f(D)$ i.e the length of the reactor is a function of diameter. Keeping all others parameter constant, the volume of the reactor is directly proportional to the square of the Diameter. And the length of the reactor is directly proportional to the diameter of the reactor depending on the constant of proportionality, k .

Thus, it can be concluded that as the volume increases, the length of the reactor also increases and vice versa as fractional conversion.

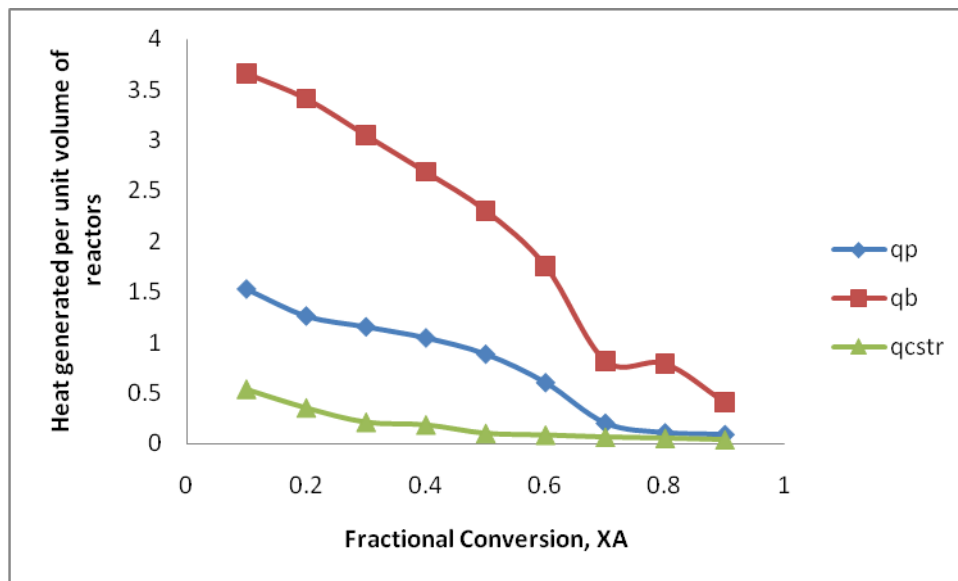


Figure 26: Heat Generated Per Unit Volume of Reactors (Batch, PFR & CSTR) against Fractional Conversion

Figure 26, Indicates Profile plots of rate of heat generated per unit volume of (kw/m^3) with fractional conversion, (X_A) as shown. The rate of heat generated per unit volume of the reactors is inversely proportional to the fractional conversion.

Hence, at higher fractional conversion, say, $X_A = 0.9$, q (heat generated) is very small or decreases and among the Reactors, the one with the least value of q (heat generated) is Plug Flow Reactor. This is because of the large volume produced at the same conditions with Batch Reactors. Hence the smaller the value of q (heat generated) the best performed a reactor is.

Hence, $q_{BR} \ll q_{PFR} \ll q_{CSTR}$ for optimum yield of the product this occurs when

$$X_A = 0.90, q_{PFR} = 0.09 \text{ KW}/M^3 \gg q_{CSTR} = 0.01 \text{ KW}/M^3 \ll q_{BR} = 0.40 \text{ KW}/M^3$$

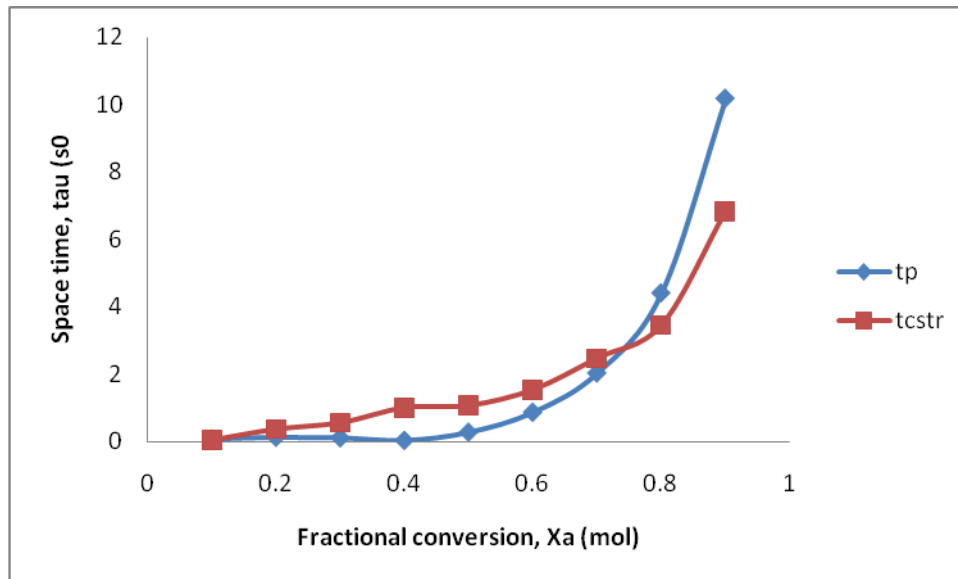


Figure 27: Space Times (PFR&CSTR) versus Fractional Conversion

Figure 27 shows the profile plots of the Space Time of the three reactors (BR, CSTR and PFR) with fractional conversion. However, for Batch reactor, it is not seen as space time but holding time and compared with the space time of Continuous Stirred Tank Reactor and PFR. It is the least time that is increasing as the fractional conversion increases.

Hence among all the time in the plot, Space Time for PFR have the maximum increase as compared to the Space Time of Continuous Stirred Tank Reactor and Holding Time of Batch reactor.

The space time, $\tau = V_R/v_0$ (Ratio of the volume of reactor to volumetric flow rate) also, Holding Time is similar too; i.e. $t = V_R/v_0$. This tells us that as volumetric flow rate is constant, the space time or holding time is directly proportional to the volume of the reactor, $\tau/t \propto V_R$. Thus increasing the reactor volume, increases the τ/t (ie space time or holding) and vice versa. Since the Plug Flow Reactor is the best performed reactor to Continuous Stirred Tank Reactor and Batch Reactors, $\tau_{PFR} > \tau_{CSTR} > t_{BR}$

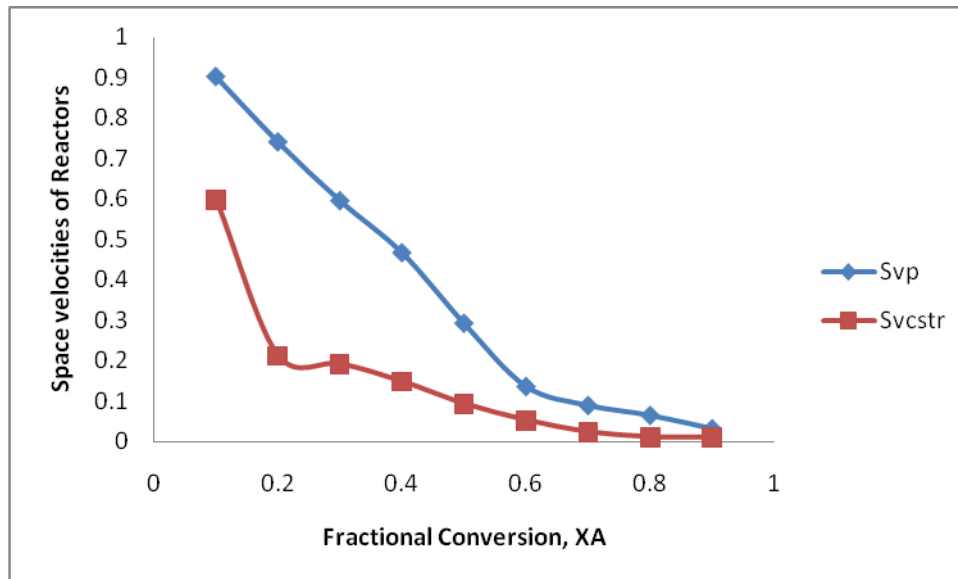


Figure 28: Space velocities (PFR&Continuous Stirred Tank Reactor) against Fractional Conversion

Figure 28 shows the variation plots of Space Velocity of the reactors with Fractional Conversion. As shown, only Continuous Stirred Tank Reactor and PFR are compared; as Batch reactors do not have this functional parameter.

From the plots, Space Velocity of the Reactors is inversely proportional to the Fractional Conversion. For Continuous Stirred Tank Reactor, a very high increase of space velocity S_v , occurs at lower fractional conversion and vice versa.

In terms of optimum performance as expected the Space Velocity should be low. This is agreed by the values obtained for Plug Flow Reactor i.e. higher volume of plug flow reactor at higher fractional conversion; say $\alpha_A = 0.90$, lower value of space velocity, since

$$S_v \propto 1/V_R$$

Thus, increasing the volume of the reactor reduces the space velocity.

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CONCLUSION

The design of the different types of reactors (Batch, Continuous Stirred Tank Reactor and Plug Flow Reactor) was carried out. The design was aimed at comparing the best type of reactor in terms of production rate and profit maximization at given conditions of the reactors types.

The fundamental basic principles of material and energy balances was carried out from the types of reactors to developed the volume of the reactors and functional parameters of the reactors for the production of calcium stearate from stearic acid and the base. The kinetic model was studied and developed from the stoichiometric of the chemical reaction process.

The non-isothermal energy balance models were developed taking into account the voidage for the reactor. The steady state adiabatic energy models developed were resolved numerically using 4th order Runge-Kutta algorithm and various plots shown in Figures 4 to 28 obtained.

Figures 24-26 and Tables 3 - 4 actually explain the aim of this research work which agrees with the research objectives.

NOMENCLATURE

		UNITS
L_{BR}	Length of a Batch Reactor	m
V_O	Volumetric Flow Rate	m ³ /s
F_{AO}	Molar Flow Rate	mol/s
ΔH_R	Heat of Reaction for Reactant	KJ/mol
L_{PFR}	Length of a Plug Flow Reactor	m
τ_p	Space Time for Plug Flow Reactor	s
L_{CSTR}	Length of a CSTR	m
τ	Space Time	s
\bar{t}	Holding Time	s
ΔP	Pressure Drop	KPa
M	Molar Feed Ratio	-
q	Heat Generated per Unit Volume	KW/m ³
α_A	Fractional Conversion	-
S_V	Space Velocity	s ⁻¹
H_2O	Water	-
NH ₃	Ammonia	-
NaHCO ₃	Sodium Bicarbonate, (baking soda)	-
CaCO ₃	Calcium Carbonate	-
CaCl ₂	Calcium Chloride	-
$[CH_3(CH_2)_{16}COO]_2Ca$	Calcium Stearate	-
$(CH_3(CH_2)_{16}COOH)$	Stearic Acid	-
CaO	Calcium Oxide	-
$NaOH$	Sodium Hydroxide (caustic soda)	-
C_{AO}	Initial Concentration of A	mol/m ³
C_{BO}	Initial Concentration of B	mol/m ³

Abbreviation	Meaning
BR	Batch Reactor
CSTR	Continuous Stirred Tank Reactor
PFR	Plug Flow Reactor
EDTA	Ethane Diamine Tetra Acetate

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