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Design of a CSTR for the Production of 1,000,000 tons Per Year of Ethyl Acetate from Esterification Reaction of Acetic Acid and Ethyl Alcohol

Wosu[1], Chimene Omeke; Okoro[2] Mabel Chigozie
[1, 2]Department of Chemical Engineering, Federal University Otuoke, Bayelsa, Nigeria.
Corresponding Author: wosuco@fuotuoke.edu.ng

Abstract— *The economic importance and industrial applications of ethyl acetate in the production of solvents, printing inks, flavors, plasticizers, rubbers, enamels, car care chemicals, synthetic fruits and pharmaceuticals is the intrinsic urge that necessitated the design of a continuous stirred tank reactor (CSTR) for the production of ethyl acetate via esterification of acetic acid and ethyl alcohol. The design models were developed by incorporating the reaction kinetic scheme for the esterification into the first principle of mass and energy balance of the process at steady state operation. The steady state models were simulated at feed and operating temperature of 299.8k and 343.15K with varying fractional conversion of the reactant species feed rate within range* $X_A \geq 0.05 \leq 0.95$. *At maximum conversion of 95%, the optimum value of the reactor parameters such as its volume, height, diameter, space time, space velocity, quantity of heat generated and the quantity of heat generated per unit volume of the reactor were* $80.880m^3$, *7.441m, 3.720m, 15.859sec., 0.063sec.*$^{-1}$, *12821.58j/s and* $158.526j/sm^3$*respectively. The yearly production cost of the reactor dependent on its maximum volume for a life span of 20 years with no salvage value was obtained as $7,453.68. The effects of the operating temperature and fractional conversion as well as the relationship between the reactor functional parameters were presented in profiles and the trends were in agreement with CSTR process behavior during production at steady state operation.*

Keywords— *Ethyl Acetate, Acetic acid, Ethyl Alcohol, CSTR, Design, MATLAB Simulation.*

I. INTRODUCTION

Ethyl acetate is one of the simplest carboxylate esters and a colorless liquid with a sweet, fruity and pleasant smell. It is an important organic compound and chemical intermediate utilized in large number of industrial processes such as manufacture of solvents, printing inks, flavors, plasticizers, rubber, enamels, car care chemicals, synthetic fruits and pharmaceuticals (Nagamalleswara, 2015; Karan, 2017). The petrochemical product can be produced industrially in an exothermic, reversible and highly selective reaction of acetic acid and ethyl alcohol in the presence of an acid catalyst (Calvar *et al*., 2007; Evelien *et al*., 2014). This reaction between acetic acid and ethyl alcohol is called esterification reaction and occurs in chemical reactors like the continuous stirred tank reactor (Tang *et al*., 2016), plug flow reactors (Ni & Meunier, 2007), fixed bed reactors (Son *et al*., 2011), microwave reactors (Umrigar *et al*., 2022; Baraka *et al*., 2023) and membrane reactors (Ghahremani *et al*., 2021). However, in this research, the design of a continuous stirred tank reactor, also known as mixed flow reactor is considered based on the physiochemical properties of the reactant species which determines the reaction phase (liquid phase esterification). The choice of the reaction system that operates in the safest and most efficient manner can be the key to the economic success or failure of the production process. The reactor design usually involves sizing of the reactor (Wordu & Wosu, 2019; Oba *et al*., 2024; Wosu & Uhuwangho, 2024; Wosu, 2024a; Wosu, 2024b; Wosu, 2024c; Wosu, 2024d). Economic importance of ethyl acetate in areas of food and industrial applications have necessitated several research on its production, applications and thus;

(Ikhazuangbe & Oni, 2015). Researched on hydrolysis of ethyl acetate using sodium hydroxide as a catalyst and the result of the experiment showed that the rate of reaction is a function of concentration of the reactant species while the rate constant is time dependent. (Abdulaziz *et al*., 2023). Performed a comparative analysis of flow reactors performance in traditional esterification reaction in a CSTR and PFR using ethanol-rich feed. The Aspen plus software was utilized as the simulation tool for sensitivity analysis.

Hilmioglu (2022). Stated that the use of sulfo succinic acid catalyst technology during ethyl acetate production from esterification reaction in a batch reactor is more economically viable compared to the processes that obeys Le Chaterlier principle involving the use of excess reactants which shifts the esterification reaction forward. The sulfo succinic technology involves acid conversion during the process which is determined by titration. As the hydrogels capture more water, the reaction favors the formation of the target product. Traditionally, ethyl acetate is produced via esterification reaction of acetic acid and ethanol. This reaction occurs in the presence of a homogeneous catalyst usually sulfuric acid (Ding *et al*., 2012; Nurhayati *et al*., 2017). Recently, research has shown that ethyl acetate can be utilized as an alternative fuel (Green premium) for cars and electric generators (Heuser, *et al*., 2019). This article focused on the design of the reacting media (CSTR) for esterification process to enhance sustainability and effective utilization of the petrochemical industrially and domestically.

II. MATERIALS AND METHODS

2.1 Materials

The materials utilized in the research are computer set, data obtained from journals, textbooks and the simulation tool used is MATLAB.

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2.2 Methods

The methodology adopted in this research is quantitative and the data used were obtained from thermodynamic properties of the reactant species and products, literature data, and calculated/derived data and the following procedures were sequentially adopted;

2.2.1 Development of the Reaction Kinetic Models

The Kinetic model of the esterification reaction is obtained from the reaction chemistry of the process in equation (1)

$$\text{Acetic acid + Ethyl alcohol} \xrightarrow{k_1} \text{Ethyl acetate + Water} \quad (1)$$

Equation (1) can be expressed molecularly as;

$$CH_3COOH + CH_3OH \xrightarrow{K_1} CH_3COOCH_3 + H_2O \quad (2)$$

Symbolically, equation (2) can be expressed as;

$$A + B \xrightarrow{k_1} C + D \quad (3)$$

where A represents acetic acid, B is ethyl alcohol, C is ethyl acetate, D is water and k_1 represents kinetic rate constant which is an indication that the reaction process is temperature dependent and the process condition is exothermal. The depleting rate of the reactant species is related to the rate constant, fractional conversion, initial concentration of the limiting reactant, temperature, activation energy as shown in equation (4)

$$-r_i = k_o e^{-E/RT} C_{io}(1 - x_i) \quad (4)$$

2.2.2 Development of CSTR Design/Sizing Models

Consider the schematic representation of a continuous stirred tank reactor with feed stream, product stream and heat effect.

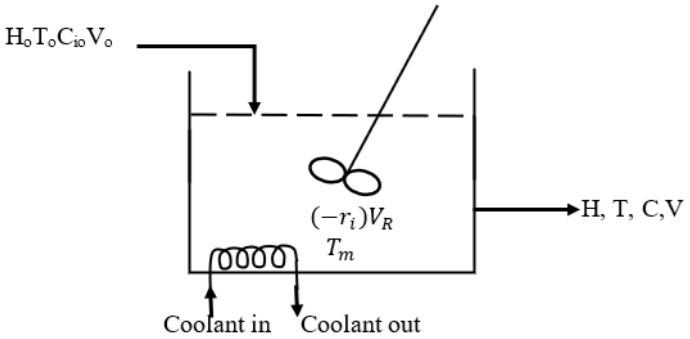

Figure 1:CSTR with Feed Stream, Product Stream and Heat Effect

The mass and energy balance model for the CSTR design is developed using the following assumptions.

i. The feed assumes a uniform composition throughout the reactor
ii. The reacting mixture is well stirred
iii. The composition of the exit stream is the same as that within the reactor
iv. Shaft work by the impeller or stirrer is negligible
v. Constant density
vi. The temperature within the reactor is kept at a constant value by the heat exchange medium

The design models of the CSTR in terms of its volume, height, diameter, space time and space velocity can be obtained by applying the principle of material balance stated as follows

$$\begin{bmatrix}\text{Rate of accumulation of material within the volume}\end{bmatrix} = \begin{bmatrix}\text{Rate of input of feed into the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of outflow of feed from the voume}\end{bmatrix} - \begin{bmatrix}\text{Rate of depletion of feed due to chemical reaction}\end{bmatrix} \quad (5)$$

The terms in equation (5) can be defined, substituted and simplified at steady state operation to yield the following CSTR functional parameters thus;

$$V_R = \frac{F_{io}x_i}{k_o e^{-E/RTC_{io}(1-x_i)}} \quad (6)$$

$$H_R = \left[\frac{16F_{io}x_i}{\pi K_o e^{-E/RTC_{io}(1-x_i)}}\right]^{\frac{1}{3}} \quad (7)$$

$$D_R = \frac{\left[\frac{16F_{io}x_i}{\pi K_o e^{-E/RTC_{io}(1-x_i)}}\right]^{\frac{1}{3}}}{2} \quad (8)$$

$$\tau_{CSTR} = \frac{x_i}{K_o e^{-E/RT(1-x_i)}} \quad (9)$$

$$S_V = \frac{K_o e^{-E/RT(1-x_i)}}{x_i} \quad (10)$$

$$Q = \Delta H_R F_{io} x_i \quad (11)$$

$$q = \frac{\Delta H_R F_{io} x_i}{V_R} \quad (12)$$

The energy balance equation of the CSTR in Figure 1 the exothermic esterification process can be obtained by applying the principles of conservation of energy given as;

$$\begin{bmatrix}\text{Rate of accumulation of heat within the volume}\end{bmatrix} = \begin{bmatrix}\text{Rate of Input of heat to the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of Output of heat from the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of depletion of heat due to chemical reaction}\end{bmatrix} - \begin{bmatrix}\text{Rate of heat removal to the surrounding}\end{bmatrix} + \begin{bmatrix}\text{Shaft work done by the shirrer}\end{bmatrix} \quad (13)$$

The terms in equation (13) can be defined, substituted and simplified at steady state to give the temperature effect model of the reactor thus;

$$T = \frac{\tau\Delta H_R r_i v_o + UA_c T_c + \rho v_o c_p T_o}{\rho v_o c_p + UA_c} \quad (14)$$

The capital cost of the CSTR is given by (John, 2007)

$$\text{Cost} = \$200{,}000 \left(\frac{V_{CSTR}}{1000}\right)^{0.6} \quad (15)$$

where V_{CSTR} is the volume of CSTR in m^3. The above model is for a life of 20years with no salvage values.

Data for Evaluation

The data for evaluation in this research are the properties/thermodynamic data and data obtained from literatures as presented in table 1 and 2 respectively.

Table 3 is a tabular representation of the CSTR design for production of 1,000,000 tons per year of ethyl acetate from esterification of acetic acid and ethyl alcohol. The results of CSTR functional parameters such as its volume, height,

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diameter, space time, space velocity, quantity of heat generated as well as the quantity of heat generated per unit volume of the reactor were obtained from mass and energy balance models simulated using MATLAB at various fractional conversion and operating temperature during the process.

TABLE 1. Properties/ Thermodynamic Data

Data/Parameter	Values	Description
ρ_A	1050Kg/m^3	Density of acetic acid
ρ_B	789Kg/m^3	Density of ethyl alcohol
ρ_C	902Kg/m^3	Density of ethyl acetate
ρ_D	997Kg/m^3	Density of water
P_o	101325Kg/m^3	Initial pressure
R	8314Nmmol^{-1}K^{-1}	Gas constant

At initial and operating temperature of 299.83K and 343.15K respectively and fractional conversion of 0.95, the CSTR optimum volume, height, diameter, space time, space velocity, quantity of heat generated and the quantity of heat generated per unit volume of the reactor are 80.880m^3, 7.441m, 3.720m, 15.895seconds, 0.063sec^{-1}, 12821.580j/s and 158.526j/sm^3 respectively.

TABLE 2. Data Obtained from Literature

Data	Values	Description	References
T	343.15K	Operating temperature of the reactor	Nagamalleswara *et al*., 2015
r_i	5.28×10^7mol/m^3	Reaction rate	Nagamalleswara et al, 2015
E	59.403kJ/mol	Activation energy	Nagamalleswara et al, 2015

III. Results and Discussion

3.1 Design Results

The results of the continuous stirred tank reactor (CSTR) design or size specification is presented in table 3 below.

TABLE 3. MATLAB Simulation Results Showing Fractional Conversion, Temperature, Reactor Volume, Height, Diameter, Space time, Space Velocity, Quantity of Heat Generated and Quantity of Heat Generated Per Unit Volume of the Reactor.

X_A	T(K)	V_R(m^3)	H_R(m)	D_R(m)	τ (s)	S_V(s^{-1})	Q(J/s)	q(J/m^{3}s)
0.05	299.83	0.012	0.392	0.196	0.002	432.503	674.820	57227.770
0.15	299.83	0.044	0.608	0.304	0.009	115.414	2024.460	45813.920
0.25	299.83	0.095	0.784	0.392	0.019	53.913	3374.100	35668.280
0.35	299.83	0.176	0.965	0.482	0.035	28.925	4723.740	26790.840
0.45	299.83	0.317	1.173	0.583	0.062	16.107	6073.380	19181.610
0.55	299.83	0.578	1.433	0.717	0.113	8.822	7423.020	12840.580
0.65	299.83	1.129	1.792	0.896	0.221	4.516	8772.660	7767.758
0.75	299.83	2.554	2.352	1.176	0.501	1.997	10122.300	3963.142
0.85	299.83	8.041	3.447	1.723	1.577	0.634	11471.940	1428.731
0.95	299.83	80.880	80.880	7.441	15.859	0.063	12821.580	158.526

3.2 Results of the CSTR MATLAB Simulation

The effect or relationship of fractional conversion and operating temperature on the CSTR functional parameters are presented in the profiles below.

Profile of CSTR Volume (V_R) and Fractional Conversion (X_A)

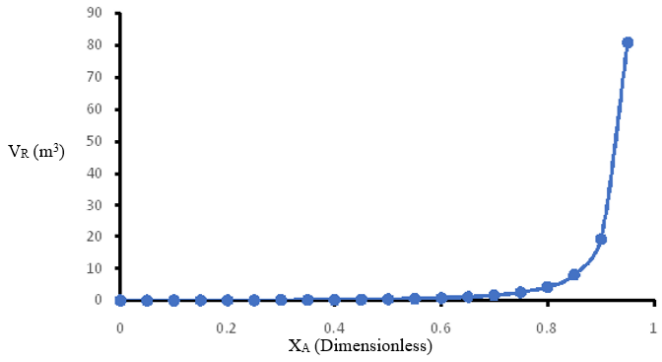

Figure 2: Graph of CSTR Volume (V_R) and Fractional Conversion (X_A)

Figure 2 is a graphical representation of the effect of fractional conversion of reactant species (acetic acid and ethyl alcohol) and target product (ethyl acetate) on the reactor volume during esterification reaction in a CSTR. From the plot, the volume of the reactor increases exponentially as the fractional conversion increases. This signifies more yield of the target product (ethyl acetate) as more reactants are converted during the reaction. At fractional conversion of 0.05, 0.55 and 0.95, the volume of the reactor was 0.012m^3, 0.578m^3 and 80.880m^3 respectively. This shows that the reactor volume for yearly optimum production of ethyl acetate is at maximum fractional conversion of 0.95.

Profile of CSTR Height (H_R) and Fractional Conversion (X_A)

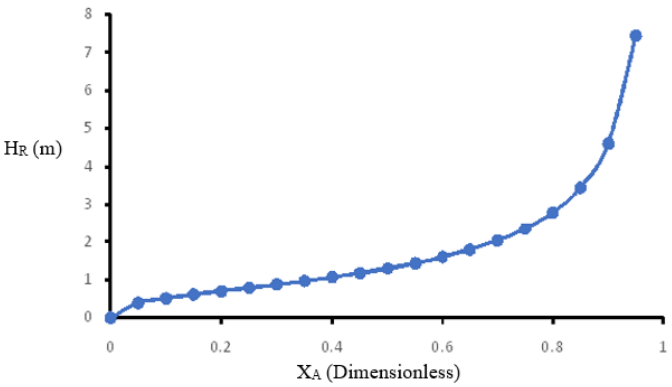

Figure 3: Graph of CSTR Height (H_R) and Fractional Conversion (X_A)

Figure 3 shows that the reactor height increase exponentially as the fractional conversion increases during the production of ethyl acetate from esterification reaction of acetic acid and ethyl alcohol. This simply shows that the more the reactants or feed are converted, the more the height or level of the liquid in the tank will increase and thus, an increase in production of the target product will be achieved. At fractional

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conversion of 0.05, 0.55, and 0.95, the height of the liquid in the tank rises to 0.392m, 1.433m and 7.441m respectively.

Profile of CSTR Diameter (D_R) and Fractional Conversion (X_A)

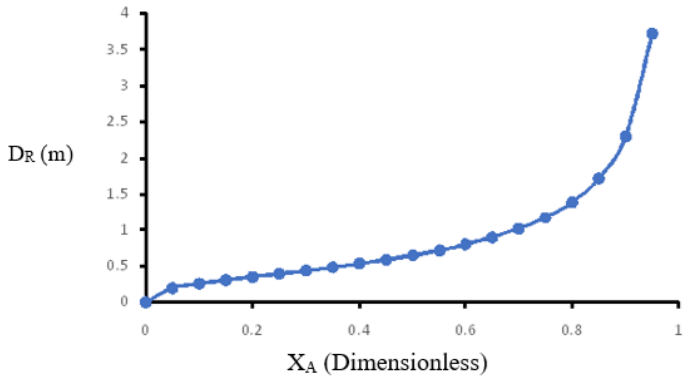

Figure 4: Graph of Diameter (D_R) and Fractional Conversion (X_A)

Figure 4 shows that an increase in fractional conversion during esterification reaction of acetic acid and ethyl alcohol for production of ethyl acetate will result to an exponential increase in the CSTR diameter. This signifies that more yield of the target product (ethyl acetate) will be recovered during the process. A fractional conversion of 0.05, 0.55 and 0.95, the reactor diameter was 0.196m, 0.717m and 3.720m respectively.

Profile of CSTR Space Time (τ) and Fractional Conversion (X_A)

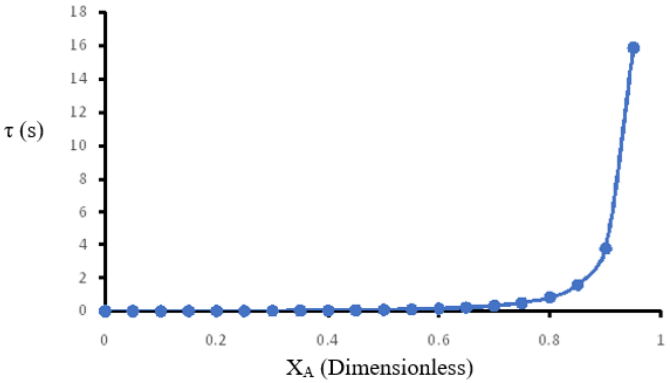

Figure 5: Graph of CSTR Space Time (τ) and Fractional Conversion (X_A)

Figure 5 shows that there is a gradual or slow exponential increase in space time between fractional conversion of 0.05 to 0.6 during ethyl acetate production from esterification reaction in a CSTR. Higher fractional conversion above 0.7 displayed a rapid exponential increase of the space time. This simply means that the more time an element of feed spends in the reactor will increase the conversion rate as well as the yield of the target product. At fractional conversion of 0.05, 0.55 and 0.95, the space time required are 0.002seconds, 0.113seconds and 15.859seconds respectively.

Profile of CSTR Space Velocity (S_V) and Fractional Conversion (X_A)

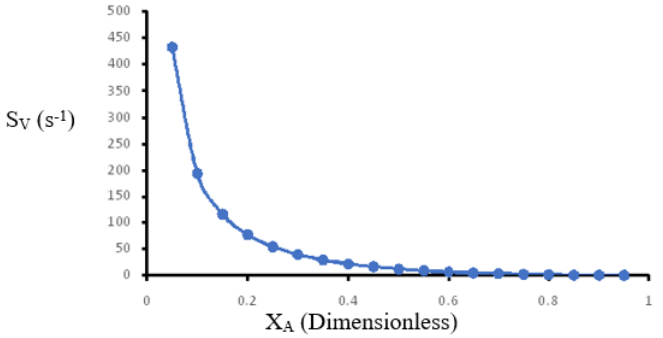

Figure 6: Graph of CSTR Space Velocity (S_V) and Fractional Conversion (X_A)

Figure 6 shows the relationship between space velocity (reciprocal of space time) and fractional conversion during the production of ethyl acetate from esterification reaction of acetic acid and ethyl alcohol. From the profile, there is an inverse exponential decrease of the space velocity as the fractional conversion increases. This profile behavior is in compliance with the mathematical relationship between the space velocity and space time. At fractional conversion of 0.05, 0.55 and 0.95, the space velocity was432.503sec^{-1}, 8.822sec^{-1} and 0.063sec^{-1} respectively. This simply means that are higher fractional conversion above 0.95, the space velocity value tends towards negative infinity (-ve ∞).

Profile of CSTR Quantity of Heat Generated (Q) and Fractional Conversion (X_A)

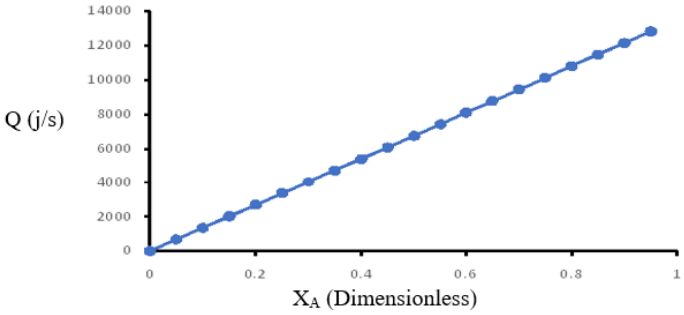

Figure 7: Graph of CSTR Quantity of Heat Generated (Q) and Fractional Conversion (X_A)

Figure 7 depitch a linear increase relationship between the quantity of heat generated and fractional conversion during ethyl acetate production from esterification of acetic acid and ethyl alcohol in a CSTR. From the plot, as the quantity of heat increases, more of the reactants or content of reactor are processed and converted for high yield of the target product. At fractional conversion of 0.05, 0.55 and 0.95, the quantity of heat increases to 678.820j/s, 7423.020j/s and 12821.550j/s respectively.

Profile of Quantity of Heat Generated per Unit Volume of CSTR (q) and Fractional Conversion (X_A)

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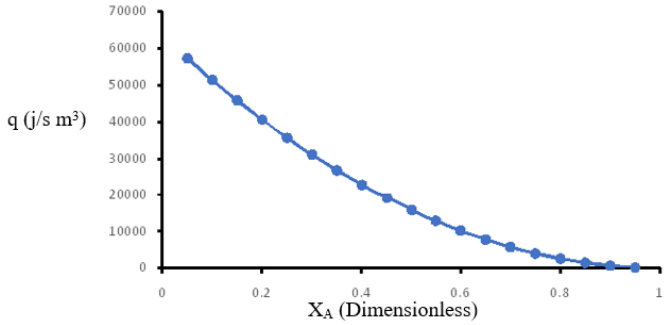

Figure 8: Graph of Quantity of Heat Generated per Unit Volume of CSTR (Q) and Fractional Conversion (X_A)

Figure 8 shows that there is an exponential decrease in the quantity of heat generated per unit volume of the CSTR as the fractional conversion increases during the production of ethyl acetate from esterification of acetic acid and ethyl alcohol. This is in compliance with the mathematical relationship between quantity of heat generated and the quantity of heat generated per unit volume of the reactor. At a fractional conversion of 0.05, 0.55 and 0.95, the quantity of heat generated per unit volume of the reactor decreases to 57227.770j/sm^3, 12840.580j/sm^3 and 158.526j/sm^3 respectively. This means that less heat will be generated per unit volume of the reactor for high yield of ethyl acetate.

Profile of Feed Temperature (T) and Fractional Conversion (X_A)

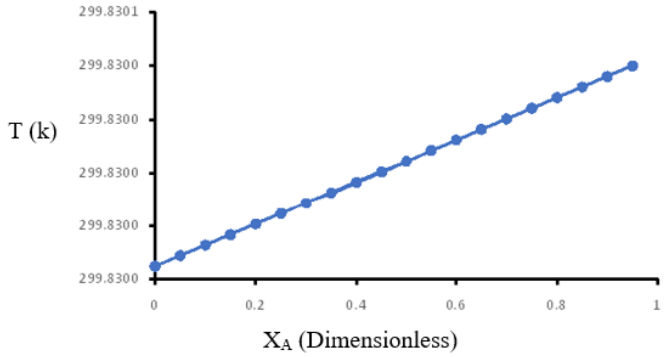

Figure 9: Graph of Feed Temperature (T) and Fractional Conversion (X_A)

Figure 9 shows the relationship between the CSTR operating temperature and fractional conversion. According to the profile, at a feed and operating temperature of 299.83K and 343.15K, the reactor operates optimally with increase in fractional conversion. Here, no swing or fluctuation of temperature occurs and the system is said to be a steady state of operation for the production of ethyl acetate from esterification of acetic acid and ethyl alcohol. At fractional conversion of 0.95, high yield of the target product is achieved.

IV. Conclusion

The research considered the design of CSTR for the production of 1,000,000tons per year of ethyl acetate from esterification of acetic acid and ethyl alcohol. The research was necessitated based on the economic viability of ethyl acetate in domestic and industrial applications. The research procedure involved the development of the rate law or reaction kinetic scheme of the esterification process from the elementary or hypothetical reaction of the esterification process, the application of the conservation law of mass and energy balance in the development of the reactor design models and temperature (energy) balance model of the process for determination of the reactor size or design parameters such as volume, height, diameter, space time and space velocity, quantity of heat generated as well as the quantity of heat generated per unit volume of the reactor, the design or specification of the CSTR stirrer in terms of its height and diameter and the cost analysis of ethyl acetate production in CSTR as a function of the reactor volume. The CSTR models developed were simulated using MATLAB and the results showed that ethyl acetate is produced in a continuous stirred tank reactor and the reactor design is keep for sustainability of the economic product.

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