CSTR Design for the Production of 100,000 tons per year of Cumene from the Catalytic Alkylation of Propylene and Benzene

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Abstract

The research showed that 100,000 tons / year of cumene is produced from catalytic alkylation of benzene and propylene at 95% fractional conversion of the feed concentration in an adiabatic continuous stirred tank reactor (CSTR). The study employed the conservation principle of material and energy balance to develop the design of a Continuous Stirred Tank Reactor (CSTR) and models for temperature effects under steady-state process conditions. The models were simulated using MATLAB to determine the optimal CSTR size specifications, including volume, height, diameter, space time, space velocity, heat produced, and heat produced per unit volume. The results were 52.296 m^3, 6.343 m, 3.217 m, 8.038 s, 0.124 s^{-1}, 0.694 J/s, and 0.013 J/s·m^3, respectively, at a fractional conversion of 0.95 and an operating temperature of 481.1 K. The relationship between fractional conversion and operating temperature was illustrated through profiles, which aligned with the reactor performance model trends. The height and diameter of the CSTR stirrer design was 5.843m and 2.217m with allowance of 0.5m and 1m dependent on the CSTR height and diameter respectively. The yearly production cost of the reactor dependent on its optimum volume in Dollar and Naira are $5,422.080 and ₦8,946,432 as at 11th of January, 2025. This article has shown that the CSTR design is crucial for sustainability and production of cumene in order to meet the global demand of the economic and viable product.

Keywords: *Cumene, Propylene, Benzene, CSTR, Design, MATLAB Simulation*

1. Introduction

Cumene, also known as isopropyl benzene, is a volatile and colorless liquid at room temperature and aromatic hydrocarbon with molecular formula C_9H_{12} and characterized with high antiknock value. It can be produced industrially from the catalytic alkylation of propylene and benzene in a chemist reactor [1]. Cumene is a petrochemical product that has a wide range of industrial application such as its utilization as a feedstock in the manufacturing of phenol and acetone, solvents in production of paints, costings and ink, [2]. In polymer industries, cumene derivatives are cuscial in the production of polystyrene, rubber and elastoners [3]. Certain cumene derivatives can be used in pharmaceutical industries in the production of analgestics, anti-inflammatory agents and antiseptics.

This research aims to investigate the detailed design considerations for implementing a continuous stirred tank reactor (CSTR) specifically for producing 100,000 tons of cumene annually, focusing on the economic viability of this petrochemical product. It will delve into chemical kinetics and reactor design, including the application of mass and energy conservation principles in developing reactor design models. These models are crucial for determining functional parameters or sizing the reactor, which is fundamental to the production of nearly all industrial chemicals [4][5][6][7][8][9][10][11] The chemical reactor is a vessel or system in chemical process where raw materials undergo chemical transformation into desired products through controlled chemical reactions [12]. In the context of this research, the CSTR which is characterized with steady state operation involving in and out flow of reactants and products, uniform mixing of reactant species using the stirrer / agitator is thoroughly examine [13].

Significant research has been conducted on the production of cumene, with a few notable studies cited here. [14] mentioned that cumene is industrially produced through the alkylation reaction of benzene and propylene, using zeolite as a catalyst. The researcher utilized the Badger cumene technology licensor in the development of the simulation flow sheet configuration using HYSYS as the simulation software. During the process, the reactant feed benzene is usually in excess and referred to as the excess reactant while propylene is the limiting reactant. The cumene production plant consists of two dedicated adiabatic fixed-bed reactors. In these reactors, both the alkylation reaction for cumene production and the removal of unwanted products like p-diisopropyl benzene are achieved through the integration of transalkylation. The process was optimized by performing a sensitivity analysis to determine the optimal operating conditions, including temperature, pressure, molar ratio, as well as the diameter and height of the reactors. The research highlighted the advantages of using a zeolite catalyst [13] over the Friedel-Crafts alkylation of benzene with propylene [5] or sulfuric acid as a catalyst. The latter can cause corrosion issues and lead to complicated neutralization and recycling steps. The use of zeolite catalyst for alkylation reaction have demonstrated better performance characteristics compared to alternative use of solid phosphoric acid supported on alumina which also possess corrosion problems [15]. This cumene can also be synthesized from transalkylation process using modified beta zeolite catalyst [16; 17]. Cumene is a crucial component of crude oil, used as a feedstock in process industries for producing phenol, acetone, and hydroperoxide. It can be produced industrially through the catalytic alkylation of benzene and propylene [18]. The researchers developed design models for basic cumene plant units using the principles of material and energy balance. These models were based on a HYSYS simulation flowsheet that utilized characterized natural gas composition and plant data for cumene production from the Utorogu Gas Field.

Most literatures in the past and recent past have shown the importance of cumene in industrial application as well as the advantage of using the zeolite technology as a catalyst for effective alkylation process. This research delves into the design of a CSTR for the production of 100,000 tons of cumene per year, exploring its technical feasibility, economic viability and sustainability.

2 Materials and Methods

2.1 Materials

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

2.2 Methods

The methodology adopted in this research is quantitative and the data used are obtained from thermodynamic properties of the reactant species and products, literature data, plant data and calculated/derived data. The procedures or steps adopted in this work are;

i. Development of the rate law or reaction kinetic models
ii. Development of design and temperature balance models
iii. Consideration CSTR stirrer design
iv. Reactor production cost determination.

2.2.1 Development of the Rate Law or Reaction Kinetic Models

Cumene is produced from the catalytic alkylation of propylene and benzene and the reaction kinetic scheme is given as;

$$C_3H_6 + C_6H_6 \xrightarrow{k_1} C_9H_{12} \quad (1)$$

The second order liquid phase alkylation reaction can be expressed symbolically as

$$A + B \xrightarrow{k_1} C \quad (2)$$

where A and B are the reactant species (Propylene and benzene), C represents the target product (cumene) and k_1 is the kinetic rate constant which is an indication that the reaction process is temperature dependent and the process condition is non-isothermal

The rate law of the liquid-phase alkylation reaction can be expressed as a function of feed rate depletion and kinetic parameters given as;

$$-r_A = k_o C_{Ao}{}^2 e^{-E/RT}(1 - x_A)(m - x_A) \quad (3)$$

Where $-r_A$ is the depleting rate of the limiting reactant, k_o is the Arrhenius constant also called pre-exponential constant for cumene production, E is the activation energy in kJ/Kmol of the feed reactants, T is the reacting temperature of the process in kelvin and R is the gas constant in J/molK, C_{AO} is the initial concentration of the limiting reactant specie in mol/m^3, X_A is the fractional conversion of specie A and m is the ratio of excess reactant and limiting reactant.

2.2.2 Development of CSTR Design/Sizing Models

Consider the schematic representation of a continuous stirred tank reactor with mass and heat effect.

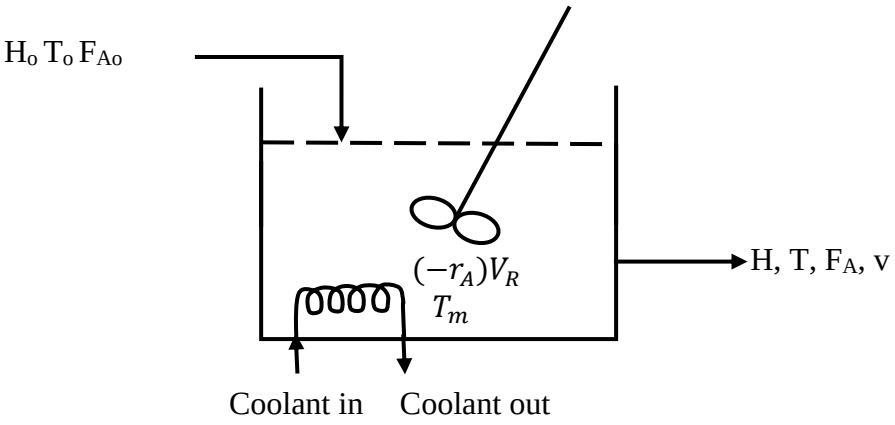

Figure 1: CSTR with Mass and Heat Effect for Cumene Production

The CSTR mass and energy balance model is developed using the following assumptions;

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

The CSTR functional parameters such as its volume (V_R), height (H_R) diameter (D_R) space time (τ) and space velocity (S_V) can be obtained by applying the principle of mass balance stated as follows

$$\begin{bmatrix}\text{Rate of accumulation of material within the volume}\end{bmatrix} = \begin{bmatrix}\text{Rate of input of feed into the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of outflow of feed from the voume}\end{bmatrix} - \begin{bmatrix}\text{Rate of depletion of feed due to chemical reaction}\end{bmatrix} \quad (4)$$

Mathematically, the terms in equation (4) can be stated, substituted and resolved at steady state operation to give the CSTR design models as follows;

$$V_R = \frac{F_{Ao}x_a}{k_o C_{Ao}{}^2 e^{-E/RT}(1-x_A)(m-x_A)} \quad (5)$$

$$H_R = \left[\frac{16F_{Ao}x_A}{\pi k_o {C_{Ao}}^2 e^{-E/RT}(1-x_A)(m-x_A)}\right]^{\frac{1}{3}} \quad (6)$$

$$D_R = \frac{\left[\frac{16F_{Ao}x_A}{\pi k_o {C_{Ao}}^2 e^{-E/RT}(1-x_A)(m-x_A)}\right]^{\frac{1}{3}}}{2} \quad (7)$$

$$\tau_{CSTR} = \frac{x_A}{k_o {C_{Ao}}^2 e^{-E/RT}(1-x_A)(m-x_A)} \quad (8)$$

$$S_V = \frac{k_o {C_{Ao}}^2 e^{-E/RT}(1-x_A)(m-x_A)}{x_A} \quad (9)$$

where F_{Ao} is equivalent to the product of initial volumetric flow rate v_o and initial concentration of specie C_{Ao}.

The quantity of heat generated and quantity of heat produced per unit volume of the CSTR are expressed mathematically as;

$$Q = \Delta H_R F_{Ao} x_A \quad (10)$$

$$q = \frac{\Delta H_R F_{Ao} x_A}{V_R} \quad (11)$$

where q is the quantity of heat generated per unit volume of the reactor

The energy balance model of the reactor can be obtained by applying the principles of conservation of energy as follows;

$$\begin{bmatrix}\text{Rate of accumulation of heat within the volume}\end{bmatrix} = \begin{bmatrix}\text{Rate of Input of heat to the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of Output of heat from the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of depletion of heat due to chemical reaction}\end{bmatrix} - \begin{bmatrix}\text{Rate of heat removal to the surrounding}\end{bmatrix} + \begin{bmatrix}\text{Shaft work done by the shirrer}\end{bmatrix} \quad (12)$$

Mathematically, the terms in equation (12) can be stated, substituted and resolved at steady state condition to give the temperature effect model in equation (13)

$$T = \frac{\tau \Delta H_R r_A v_o + UA_c T_c + \rho v_o c_p T_o}{\rho v_o C_p + UA_c} \quad (13)$$

2.2.3 Stirrer Design Model Development

Usually, a clearance (C) is allowed between the stirrer blade and the reactor height (H_R)

The length of the stirrer (L_{st}) can be expressed mathematically as given by [8]

$$L_{st} = H_R - C \quad (14)$$

The diameter of the stirrer (D_{st}) can be obtained from the equation

$$D_{st} = D_R - 2C \quad (15)$$

2.2.4 Costing of the CSTR

The capital cost of a continuous flow stirred tank reactor is given by [19]

$$\text{Cost} = \$200{,}000 \left(\frac{V_{CSTR}}{1000}\right)^{0.6} \quad (16)$$

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

2.2.6 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 were computed and simulated using MATLAB.

Table 1: Properties/Thermodynamic Data

Data/Parameter	Values	Description
ρ_A	613.9Kg/m^3	Density of propylene
ρ_B	876Kg/m^3	Density of benzene
ρ_C	862Kg/m^3	Density of cumene
R	8314Nmmol^{-1}K^{-1}	Gas Constant

Table 2: Data Obtained from Literature

Data	Values	Description	References
T	483K	Operating temperature	[2]
k_o	$6.510 \times 10^3 s^{-1}$	Frequency factor	[2]
k_i	$4.124 \times 10^{-3} s^{-1}$	Rate constant	[2]
$-r_A$	1.305×10^{-5} mol/m^3/s	Reaction rate	[2]
E	52564KJ/Kmol	Activation energy	[2]

3 Results and Discussion

The CSTR design results are presented in the tables and profiles 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 Produced per unit Volume of the CSTR is Presented.

X_A	T(K)	$V_R(m^3)$	$H_R(m)$	$D_R(m)$	τ (s)	$S_V(s^{-1})$	Q(J/s)	$q(J/m^3s)$
0.00	481.1	0.000	0.000	0.000	0.000	Inf	0.000	NaN
0.05	481.1	0.008	0.339	0.169	0.001	853.310	0.037	4.788
0.10	481.1	0.017	0.442	0.221	0.003	382.920	0.073	4.298
0.15	481.1	0.029	0.526	0.263	0.004	227.710	0.110	3.833
0.20	481.1	0.043	0.603	0.301	0.007	151.280	0.146	3.396
0.25	481.1	0.061	0.678	0.339	0.009	106.370	0.183	2.984
0.30	481.1	0.084	0.754	0.377	0.013	77.215	0.219	2.560
0.35	481.1	0.114	0.834	0.417	0.017	57.067	0.256	2.242
0.40	481.1	0.153	0.920	0.460	0.024	42.547	0.292	1.910
0.45	481.1	0.205	1.014	0.507	0.032	31.779	0.329	1.605
0.50	481.1	0.275	1.119	0.560	0.042	23.637	0.365	1.326
0.55	481.1	0.374	1.239	0.620	0.058	17.406	0.402	1.074
0.60	481.1	0.516	1.380	0.690	0.079	12.607	0.438	0.849
0.65	481.1	0.730	1.549	0.775	0.112	8.909	0.475	0.650
0.70	481.1	1.070	1.760	0.880	0.165	6.078	0.511	0.478
0.75	481.1	1.652	2.034	1.017	0.254	3.940	0.547	0.332
0.80	481.1	2.752	2.411	1.206	0.423	2.364	0.584	0.212
0.85	481.1	5.199	2.981	1.490	0.880	1.251	0.621	0.119
0.90	481.1	12.386	3.981	1.990	1.904	0.525	0.657	0.053
0.95	481.1	52.296	6.343	3.217	8.038	0.124	0.694	0.013

Table 3 presents the design results and size specifications for the CSTR at different levels of fractional conversion and operating temperatures. The data indicate that as fractional conversion increases, the CSTR's volume, height, diameter, space time, and the quantity of heat required also increase. Conversely, other parameters such as space velocity and the quantity of heat produced per unit volume decrease with higher fractional conversion. At a fractional conversion of 95%, the optimal values for the reactor's functional parameters—volume, height, diameter, space time, space velocity, amount of heat produced, and amount of heat produced per unit volume—are 52.296 m^3, 6.364 m, 3.217 m, 8.038 sec, 0.124 sec^{-1}, 0.694 J/s, and 0.013 J/m^3s, respectively. This outcome illustrates that the CSTR sizing is dependent on its operating parameters, including temperature, fractional conversion, feed rate, and reactant concentration.

Variation of Reactor Volume (V_R) with Fractional Conversion (X_A)

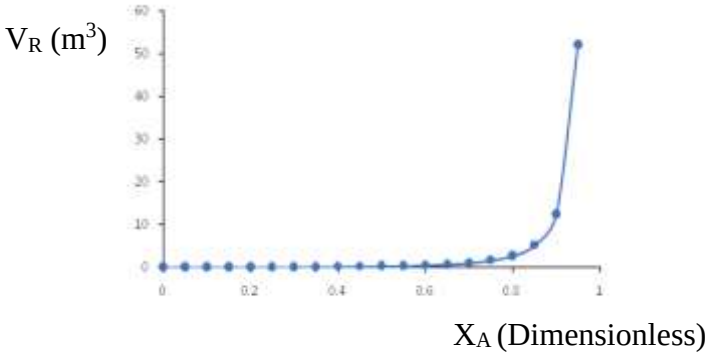

Figure 2: Profile of Reactor Volume (V_R) with Fractional Conversion (X_A)

Figure 2 presents the variation or change between the CSTR volume and the fractional conversion from the profile, during the production of cumene from the catalytic, alkylation of propylene and benzene, the volume of the reactor was exponentially increased with an increase in fractional conversion. This showed that as the reactant feed continue to react, more of the target product (cumene) are formed during the process. At fractional conversion of 0.05, 0.5 and 0.95, the volume of the reactor are 0.008m^3, 0.275m^3 and 42.296m^3 respectively.

Variation of Reactor Height (H_R) with Fractional Conversion (X_A)

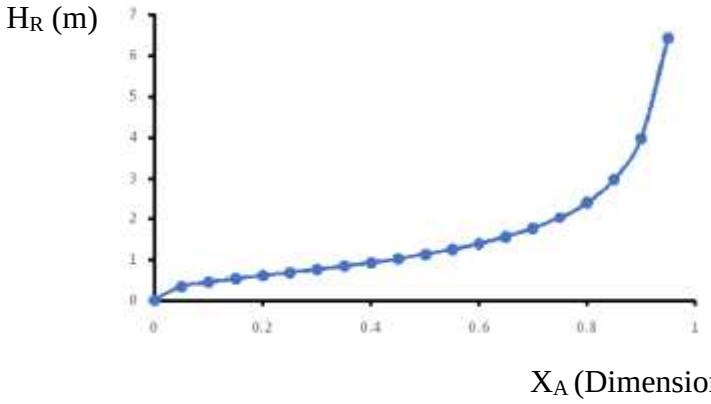

Figure 3: Profile of Reactor Height (H_R) with Fractional Conversion (X_A)

Figure 3 represents the relationship between the reactor height and fractional conversion of reactant feed (propylene and benzene) for cumene production in a CSTR. According to the plot, the reactor height experienced an exponential increase as the amount of conversion increases. The significant of this is that the volume of the target product (cumene) increases at higher fractional conversion. At fractional conversion of 0.05, 0.5 and 0.95, the reactor height are given as 0.339m, 1.119m and 6.343m respectively.

Variation of Reactor Diameter (D_R) with Fractional Conversion (X_A)

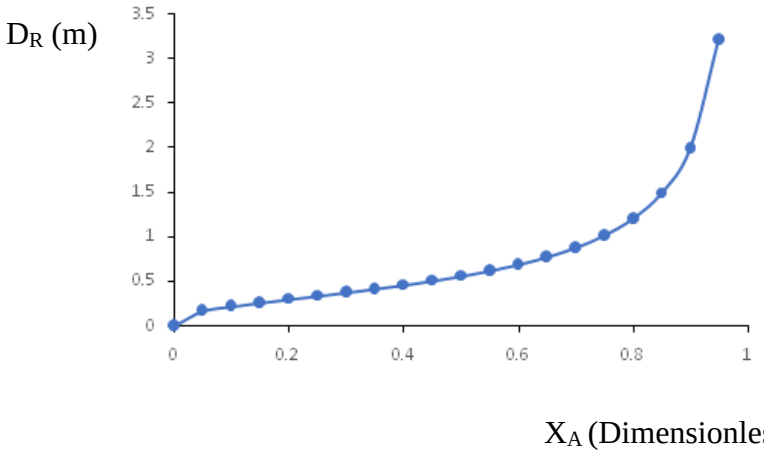

Figure 4: Profile of Reactor Diameter (D_R) with Fractional Conversion (X_A)

Figure 4 represents the relationship between the diameter and fractional conversion during the alkylation of propylene and benzene for cumene production. Just like the rector volume and height, the diameter of the reactor also experienced an exponential rise as the amount of reactant conversion increases. The significant of this is that the quantity of the target product produced is a function of the reactor design or specification and fractional conversion. At fractional conversion of 0.05, 0.5 and 0.95 the diameter of the reactor stood at 0.169m, 0.560m and 3.217m respectively.

Variation of Space Time (τ) with Fractional Conversion (X_A)

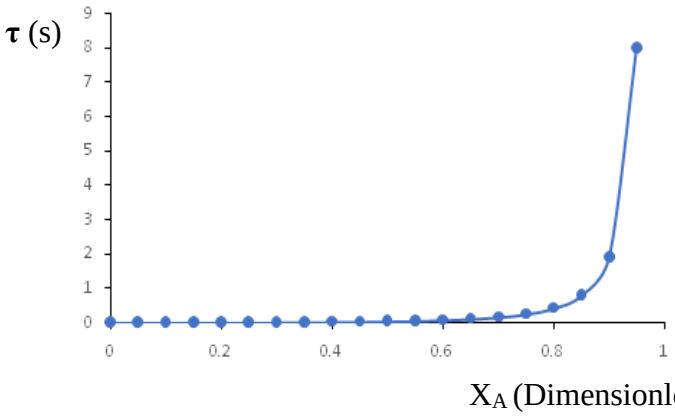

Figure 5: Profile of Space Time (τ) with Conversion (X_A)

Figure 5 is a graphical effect of fractional conversion on the space time during the production of cumene from catalytic alkylation of propylene and benzene in a CSTR. According to the plot, a slow exponential increase in space time was observed at fractional conversion between the initial

to 0.65. This increase became rapid or more significant at fractional conversion above 0.8. This is an indication that more time is required to process higher amount of feed introduced in the reactor. At fractional conversion of 0.05, 0.5 and 0.95, the space time recorded were 0.001 seconds, 0.042 seconds and 8.038 seconds respectively.

Variation of Space Velocity (S_V) with Fractional Conversion (X_A)

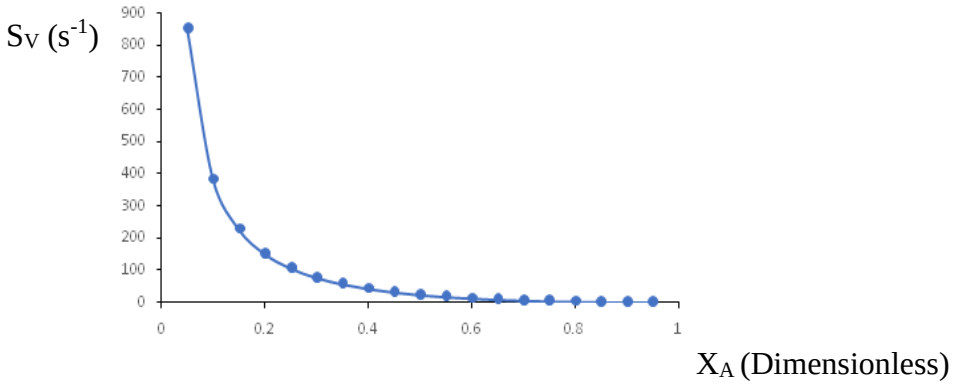

Figure 6: Profile of Space Velocity (S_V) with Fractional Conversion (X_A)

Figure 6 shows a plot of space velocity and fractional conversion during catalytic alkylation of propylene and benzene for cumene production. According to the profile, the space velocity experienced an exponential decrease with increasing fractional conversion. This is in agreement with the mathematical variation between the time quantities. At a fractional conversion amount of 0.05, 0.5 and 0.95, the space velocity of $853.310s^{-1}$, $23.6375s^{-1}$ and $0.124s^{-1}$ were obtained and at higher fractional conversion above 0.95, the space velocity decreases and tends towards negative infinity (-∞).

Variation of Quantity of Heat Generated (Q) with Fractional Conversion (X_A)

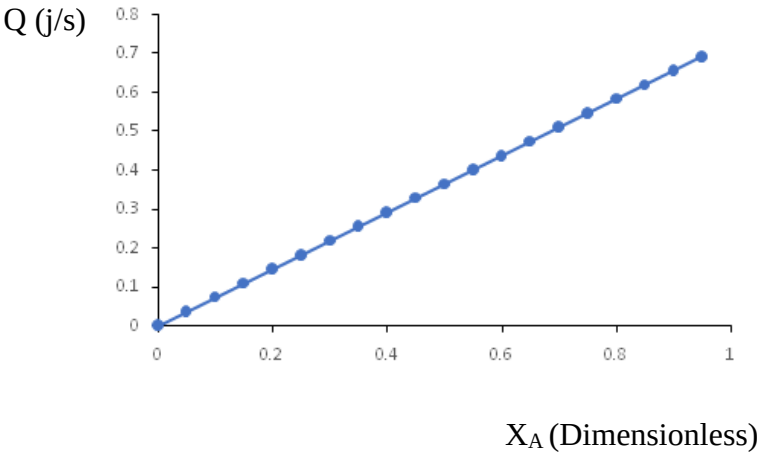

Figure 7: Profile of Quantity of Heat Generated (Q) with Fractional Conversion (X_A)

Figure 7 is a graphical variation between the amount of heat produced and reactant species conversion during the production of cumene from catalytic alkylation of propylene and benzene. According to the profile, the amount of heat generated increases linearly with a rise or increase in fractional conversion during the process. At fractional conversion of 0.05, 0.5 and 0.95. the corresponding linear increase in quantity of heat generated are 0.037j/s, 0.365j/s and 0.694j/s respectively. At higher fractional conversion above 0.95, the quantity of heat generated increases and tends towards positive infinity.

Variation of Amount of Heat Produced per unit Volume of the CSTR (q) with Fractional Conversion (X_A)

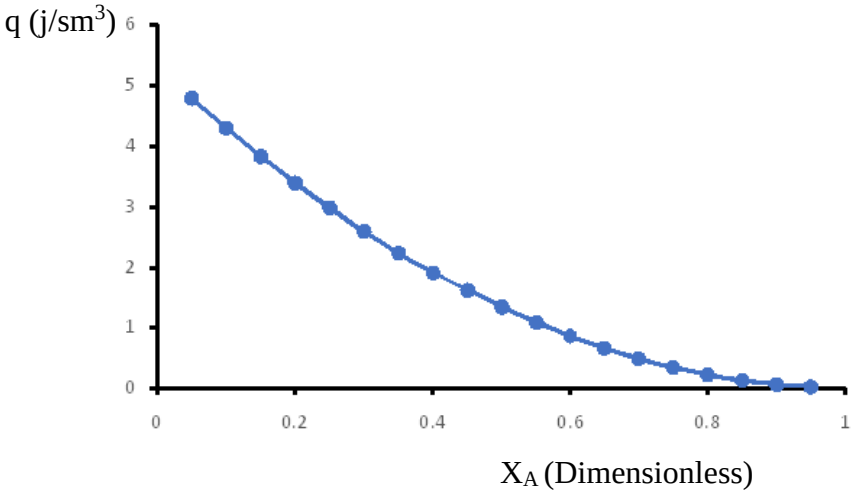

Figure 8: Graph showing the Amount of Heat Generated per unit Volume of the CSTR (q) with Fractional Conversion (X_A)

Figure 8 is a profile that represents the relationship between the amount of heat produced per unit volume of the CSTR and fractional conversion during the catalytic alkylation of propylene and benzene for cumene production. According to the profile, there is an exponential decrease in the amount of heat produced per unit volume of the CSTR as the fractional conversion of the feed (reactants) increases. At conversion of 0.05, 0.5 and 0.95, the amount of heat produced per unit volume of the CSTR decreases to 4.788j/sm^3, 1.326j/sm^3 and 0.013j/sm^3. Also, at higher fractional conversion above 0.95, the amount of heat generation per unit volume of the CSTR tends towards negative infinity (-∞) which is an indication of heat loss if the process continues beyond the optimum conversion or space time.

Variation of Temperature (T) with Fractional Conversion (X_A)

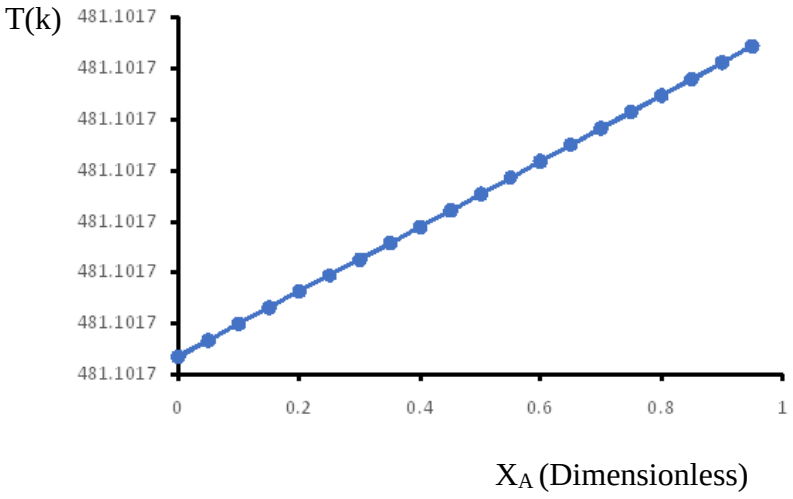

Figure 9: Profile of Temperature (T) with Conversion (X_A)

Figure 9 is a plot of the process operating temperature and fractional conversion. According to the profile, the operating temperature of 481.1k remains constant even at varying fractional conversion during the cumene production process from alkylation of propylene and benzene. At operating temperature below or above the limit of specification for cumene production will result to poor performance of the reactor or low productivity of the process.

CSTR Stirrer Design

Table 4: Design of the CSTR Stirrer Height and Diameter

Stirrer Parameter	Value (unit)
Height	5.843m
Diameter	2.217m

Table 4 shows the design specification of the height and diameter of the CSTR stirrer obtained from the CSTR height and diameter of 6.343m and 3.217m respectively at 0.9 fractional conversion. The result shows that the CSTR stirrer height is the difference between the reactor height and 0.5 clearance or allowance while the stirrer diameter is the difference between the reactor diameter and twice 0.5 clearance or allowance.[11]

Conclusion

The design of a Continuous Stirred-Tank Reactor (CSTR) for producing 100,000 tons per year of cumene from the catalytic alkylation of propylene and benzene was carried out, highlighting the economic significance of this petrochemical product in both domestic and industrial applications, which contributes to national development. To achieve optimal and efficient cumene production,

the research focused on several key aspects, including developing the rate law or reaction kinetic scheme for the alkylation process, applying fundamental principles of material and energy conservation to design the CSTR, and modeling the temperature effects of the process. Additionally, the economic evaluation considered the reactor's cost as a function of its volume. The research concluded that the CSTR is an appropriate reaction medium for the alkylation process, providing high yields of cumene production and ensuring sustainability.

Nomenclature

Symbol	Definition	Unit
ΔH_R	Charge in enthalpy of reactants	J/mol
A	Propylene	-
B	Benzene	-
C	Cumeme	-
C_i	Initial concentration of species	mol/m^3
C_P	Species heat capacity	J/mol
D_R	Diameter of the reactor	M
E	Activation Energy	J/mol
F_{Ao}	Initial molar flow rate	mol/S
H_i	Enthalpy of species	J/mol
H_R	Height of the Reactor	M
K_o	Pre-exponential factor	S^{-1}
Q	Quantity of Heat generated	J/S
Q	Quantity of heat generated per reactor volume	J/Sm^3
R	Gas constant	$Nmmol^{-1}k^{-1}$
r_A	Reaction rate of species	$mol/m^3/s$
S_V	Space velocity	Sec^{-1}
T	Operating Temperature	Kelvin
T_c	Temperature of coolant	K
T_o	Initial or fed temperature	K
UAc	Heat transfer coefficient	Kg/m^2SK
V_i	Fractional conversion	Dimensionless
V_o	Volumetric flow rate	m^3/S
V_R	Volume of the Reactor	m^3
ρ_i	Density of species	Kg/m^3
τ	Space time	Seconds

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