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Plug Flow Reactor (PFR) 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

In a bid to meet the ever-growing global demand for cumene based on its wide range of industrial applications and economic importance, the research considered the design of a plug-flow reactor (PFR) for the production of 100,000 tons of cumene per year from the catalytic alkylation of propylene and benzene. The PFR design models were developed by performing the mass and energy balance over the reactor at steady-state operation. The steady-state PFR performance models were simulated using the MATLAB R2023a version at an initial feed and operating temperature of 481.10 K and 483 K with varying fractional conversions from 0 to 0.95 at 0.05 intervals. At a maximum fractional conversion of 0.95, the PFR design specification for volume, height, diameter, space time, space velocity, quantity of heat generated, and quantity of heat generated per unit volume of the reactor was 19.7707 m3, 4.6523 m, 2.3261 m, 3.8766 s, 0.2580 s-1, 1.8035 J/s, and 0.03448 J/sm3, respectively. The profile behavior of the PFR functional parameters at changes in fractional conversion is in agreement with the trend for PFR operation at steady-state conditions, as shown in Figures 2–10. The evaluation of the PFR yearly production dependent on the reactor volume stood at $2,049.838. The article has shown that PFR is a suitable reaction medium for the catalytic alkylation process for optimum production of cumene and sustainability.

Keywords: Propylene; benzene; cumene; design; Plug flow reactor; simulation

1. Introduction

Cumene at room temperature is a volatile, colorless, and non-corrosive aromatic liquid (Scotti et al., 2017). It is insoluble in water but soluble in alcohol and other organic solvents and can occur naturally from crude oil refining processes. It is essential in the formulation of high-octane gasoline (Nikfar & Behboudi, 2014). Cumene is economically viable and can be utilized as a starting material in the production of phenol, acetone, paints, inks, coating materials, and corrosion inhibitors (Hilma, 2022).

Industrially, cumene is produced from the catalytic alkylation of propylene and benzene occurring in a chemical reactor (Roberts, 2006). Certain derivatives of cumene can be used in the production of polystyrene, rubber, elastomers, analgesics, anti-inflammatory agents, anticeptics, fats, and resins (Mahmondianet et al., 2021; Gelareh & Zahra, 2024). This research is necessitated by the diverse applications of cumene and focuses on the design of a plug-flow reactor (PFR) for the production of 100,000 tons per year of cumene from the catalytic alkylation of propylene and benzene in a bid to meet the global and ever-growing demand for cumene and sustainability. The reactor design requires good knowledge, experience, and applications of chemical engineering aspects such as chemical reaction engineering, reaction kinetics, thermodynamics, transport phenomena, heat, and mass transfer, as well as the application of the principle of mass and energy balance in the development of the reactor design and temperature effect models of the alkylation process (Wordu & Wosu, 2019; Wosu et al., 2023; Wosu & Ezeh, 2024; Ojong et al., 2024; Wosu et al., 2024a; Wosu et al., 2024b).

Researchers have conducted considerable work on the application and production of cumene, with significant studies cited as follows: Ojong et al. (2024) researched the design and simulation of a 30,000-ton per year cumene plant from a natural gas field, describing cumene as an essential component of crude oil that serves as a starting material in the manufacture of phenol, acetone, and hydroperoxide. They applied the principles of mass and energy balance and utilized plant data from the Utorogu gas field to develop the process flow sheet for cumene production, concluding that the plant is feasible, economical, and should be built in Nigeria. Several researchers have shown that cumene can be produced from the alkylation of propylene and benzene using catalysts like Friedel-Crafts, sulfuric acid, or solid phosphoric acid supported on alumina. However, these methods pose corrosion problems, complicated neutralization and recycling steps associated with acid catalysts, safety hazards, and sustainability issues (Cowley et al., 2006). Currently, the use of zeolite as a catalyst has proven to be the most suitable technology for catalytic alkylation of propylene and benzene, often applied in process industries (Hilman, 2022; Cowley et al., 2006; Yogesh et al., 2012; Robert, 2006) because it is safe, cheap, and free of corrosion-related issues. The zeolite catalyst is modified to beta zeolite technology and utilized for cumene production from the transalkylation reaction of 1,4-diisopropylbenzene (DIPB) and benzene (Thakur et al., 2016).

Past and recent reviews have highlighted the industrial applications and economic importance of cumene production. The uniqueness of this research article, distinguishing it from past studies, lies in its development of PFR design or performance models from the first principles of mass and energy balance. These models were simulated using MATLAB R2023a at initial feed and operating temperatures of 481.10 K and 483 K with varying fractional conversions within the range of XA $\geq$0 $\leq$0.95. The research also presents profiles showing the effect of fractional conversion

and temperature on the PFR design parameters such as volume, height, diameter, space-time, space velocity, quantity of heat generated, and the quantity of heat generated per unit volume of the reactor. Additionally, it examines the production cost of 100,000 tons per year of cumene as a function of the reactor volume at optimum conversion to ensure continuous production and sustainability to meet the world's ever-growing demand for cumene.

2. Materials and Methods

2.1 Materials

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

2.2 Methods

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

2.2.1 Development of the Reaction Kinetic Models

The reaction kinetic scheme for the catalytic alkylation of propylene and benzene is given by Equation 1.

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

The second-order liquid-phase alkylation reaction can be expressed symbolically by Equation 2.

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

The rate law of the alkylation process, dependent on the kinetic parameters, is given by Equation 3.

$$-rA = k_o C_{Ao}{}^2 e^{-E/RT}(1 - x_A)(m - x_A)$$

2.2.2 Development of the PFR Design/Sizing Model

Consider the schematic representation of a plug flow reactor with mass and heat effects shown in Figure 1.

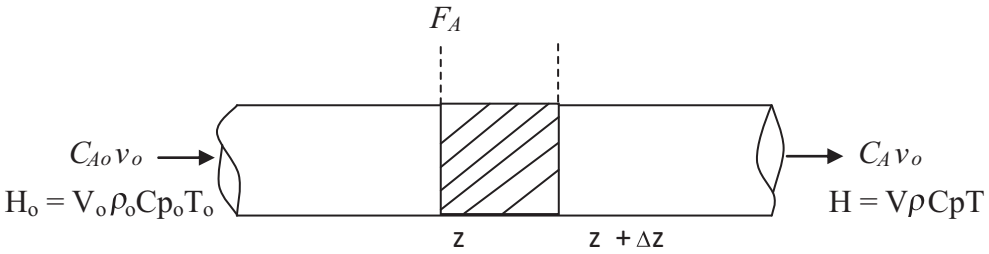

Figure 1: PFR Schematic with Mass and Heat Effect

The design model of the reactor volume, height, diameter, space time, space velocity, quantity of heat generated, and quantity of heat generated per unit volume of the PFR, as well as the PFR temperature effect model, can be developed by applying the conservation principle of mass and energy (Equation 4).

principle of mass and energy (Equation 4).

$$\left[\begin{array}{c}\text{Rate of Accumulation of } \textit{Mass/Energy} \text{ Within the Volume}\end{array}\right] = \left[\begin{array}{c}\text{Rate of input of } \textit{Mass/Energy} \text{ into the Volume}\end{array}\right] - \left[\begin{array}{c}\text{Rate of Outflow of } \textit{Mass/Energy} \text{ from the Volume}\end{array}\right] - \left[\begin{array}{c}\text{Rate of depletion of } \textit{Mass/Energy} \text{ due to chemical reaction}\end{array}\right] \quad (4)$$

The terms in Equation 4 can be defined for mass balance at steady state (Equations 5-8) as follows:

$$\left[\begin{array}{c}\text{Rate of Accumulation of Material with the Volume}\end{array}\right] = 0 \quad (5)$$

$$\left[\begin{array}{c}\text{Rate of input of feed io the Volume}\end{array}\right] = F_A \quad (6)$$

$$\left[\begin{array}{c}\text{Rate of output of feed from the Volume}\end{array}\right] = F_A + dF \quad (7)$$

$$\left[\begin{array}{c}\text{Rate of depletion of feed due to chemical reaction}\end{array}\right] = (-r_A)V_R \quad (8)$$

Combining Equations 5 to 8 into Equation 4 yields

$$0 = F_A - (F_A + dF_A) - (-r_A)V_R$$

$$0 = F_A - F_A + dF_A - (-r_A)V_R$$

$$dF_A + (-r_A)V_R = 0 \quad (9)$$

But $F_A = F_{Ao}(1 - x_A)$ (10)

$$dF_A = F_{Ao}\, dx_A$$

$$-F_{Ao}\, dx_A = -(-r_A)V_R$$

$$F_{Ao}\, dx_A = (-r_A)dV_R$$

By Rearranging

$$\int_0^V \frac{dV_R}{F_{Ao}} = \int_0^{x_A} \frac{dx_A}{-r_A}$$

$$\frac{V_R}{F_{Ao}} = \int_0^{x_A} \frac{dx_A}{-r_A}$$

$$V_R = F_{Ao} \int_0^{x_A} \frac{dx_A}{-r_A} \quad (11)$$

Substituting Equation 3 into Equation 11 yields Equation 12.

$$V_R = F_{Ao} \int_0^{x_A} \frac{dx_A}{k_o C_{Ao}^2 e^{-E/RT}(1 - x_A)(m - x_A)} \quad (12)$$

But $F_A = C_{Ao} v_o$ (13)

Equation 12 will therefore transform to

$$V_R = v_o \int_0^{x_A} \frac{dx_A}{k_o C_{Ao}^2 e^{-E/RT}(1 - x_A)(m - x_A)} \quad (14)$$

Where VR is the volume of the PFR in (m3). Since the reactor is cylindrical, the volume of a cylindrical reactor is given by Equation 15.

$$V_R = \pi R^2 H_R \quad (15)$$

where R is the radius of reactor (m), H_R is the height of the reactor (m) and p is constant. Considering the fact that the radius of a cylindrical reactor is half of its diameter (Equation 16).

$$R = \frac{D_R}{2} \quad (16)$$

where DR is the diameter of the reactor (m).

Substituting Equation 16 into Equation 15 yields Equation 17.

$$V_R = \pi\left(\frac{D_R}{2}\right)^2 H_R \quad (17)$$

For a PFR, height to diameter ratio is given by Equation 18 (Perry et al., 2008).

$$\frac{H_R}{D_R} = 2.5$$

$$D_R = \frac{H_R}{2.5} \quad (18)$$

Substituting Equations 18 and 17 yields Equation 19.

$$V_R = \frac{\pi\left(\frac{H_R}{2.5}\right)^2 H_R}{4}$$

$$V_R = \frac{\pi H_R^3}{2.5}$$

$$H_R = \left(\frac{2.5V_R}{\pi}\right)^{\frac{1}{3}} \quad (19)$$

Substituting Equation 14 into 19 yields Equation 20

$$H_R = \left[\frac{2.5V_o}{\pi} \int_0^{x_A} \frac{dx_A}{k_o C_{Ao}\, e^{-E/RT}(1 - x_A)(m - x_A)}\right]^{\frac{1}{3}} \quad (20)$$

The diameter of the reactor (DR) can be determined by substituting Equation 20 into Equation 18 yields Equation 21.

$$D_R = \frac{\left[\frac{2.5V_o}{\pi}\int_0^{x_A}\frac{dx_A}{k_o C_{Ao} e^{-E/RT}(1 - x_A)(m - x_A)}\right]^{\frac{1}{3}}}{2.5} \quad (21)$$

The space velocity of the PFR is defined as the ratio of reactor volume to the volumetric flow rate (Equation 22).

$$\tau_{PFR} = \frac{V_R}{V_o} \quad (22)$$

Substituting Equation 14 into 22 yields Equation 23.

$$\tau_{PFR} = \int_0^{x_A}\frac{dx_A}{k_o C_{Ao} e^{-E/RT}(1 - x_A)(m - x_A)} \quad (23)$$

The (S_v) space velocity is defined as the reciprocal of space time (Equation 24).

$$S_V = \frac{1}{\tau_{PFR}} \quad (24)$$

Substituting Equation 23 into Equation 24 yields Equation 25.

$$S_V = \frac{1}{\int_0^{x_A}\frac{dx_A}{k_o C_{Ao} e^{-E/RT}(1 - x_A)(m - x_A)}} \quad (25)$$

The quantity of heat generated (Q) during the alkylation process is mathematically given by Equation 26 while the quantity of heat generated per unit volume of the reactor (q) can be obtained by dividing the quantity of heat generated by the volume of the reactor (VR) (Equation 27).

$$Q = \Delta H_R F_{Ao} x_A \quad (26)$$

$$\frac{Q}{V_R} = \frac{\Delta H_R F_{Ao} x_A}{V_R} \quad (27)$$

$$q = \frac{\Delta H_R F_{Ao} x_A}{} \quad (28)$$

where q is the quality of heat generated per unit volume of the reactor.

For the isothermal process, the energy balance can be made on the PFR in Figure 1 by defining the terms in equation (4), substituting the defined terms and simplifying the model at steady state process condition to yield the temperature effect model thus;

$$\frac{dT}{dZ} = \frac{1}{u\rho C_p}(\Delta H_R)(-r_i) \quad (29)$$

The models in equation (26) to (29) holds for the isothermal process since the reference temperature Tref is assumed as zero during the catalytic alkylation process in the PFR (Lenenspiel, 1999)

The capital cost for yearly production of cumene as a function of the PFR volume at maximum fractional conversion is given by (John, 2007)

$$\text{Cost} = \$200{,}000\left(\frac{V_{PFR}}{1000}\right)^{0.6} \quad (30)$$

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

2.2.3 Data for Evaluation

The data for evaluation in this research are the properties and thermodynamic data, calculated or derived data, and data obtained from the literature as presented in Tables 1 and 2.

Table 1: Properties and 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	483 K	Operating temperature	Hilman, 2022
k_0	6.510 x 10^3 s^{-1}	Frequency factor	Hilman, 2022
k_i	4.124 x 10^{-3} s^{-1}	Rate constant	Hilman, 2022
$-r_A$	1.305 x 10^{-5} mol/m^3 s	Reaction rate	Hilman, 2022
E	52564 kJ/kmol	Activation energy	Hilman, 2022

Results and Discussion

The results of the PFR design or size specification obtained from the MATLAB R2023a software simulation is presented in Table 3.

Table 3: Model Results of the CSTR Design

X_A	T(K)	$V_R (m)^3$	$H_R (m)$	$D_R (m)$	(s)	$S_V (S)^{-1}$	Q(J/s)	$q(J/sm)^3$
0.05	481.10	0.055	0.653	0.327	0.011	93.123	0.095	12.450
0.15	481.10	0.184	0.978	0.489	0.036	27.773	0.285	9.967
0.25	481.10	0.347	1.209	0.604	0.068	14.704	0.475	7.760
0.35	481.10	0.560	1.418	0.709	0.110	9.102	0.665	5.828
0.45	481.10	0.851	1.631	0.815	0.167	5.990	0.854	4.173
0.55	481.10	1.272	1.864	0.932	0.249	4.010	1.044	2.793
0.65	481.10	1.932	2.143	1.072	0.379	2.639	1.234	1.690
0.75	481.10	3.121	2.515	1.257	0.612	1.634	1.424	0.862
0.85	481.10	5.897	3.108	1.554	1.156	0.865	1.614	0.310
0.95	481.10	19.771	4.652	2.326	3.877	0.258	1.803	0.034

Table 3 shows the design results of different parameters in terms of fractional conversion, temperature of reactor (K), volume of reactor (m^3), height of reactor (m), diameter of reactor (m), residence time (s), space velocity (1/s), quantity of heat generated (J/s), and quantity of heat generated per unit volume of reactor (J/sm^3). From Table 3, it can be observed that the value of fractional conversion ranges from 0 to 0.95 at intervals of 0.05. The temperature of the reactor remained constant because it was operated isothermally at 481.10 K. The volume of the reactor is seen to be increasing with fractional conversions of reactants due to the fact that as more reactants are consumed to form products, the volume continues to rise. The volume of the reactor is directly proportional to the diameter and height of the reactor, so as the volume increases, the diameter and height also increase. The residence of the reactor, defined as the time taken to process one mole of feed inside the reactor, is seen to be increasing with fractional conversion because the volume of the reactor is directly proportional to the residence time. On the other hand, the space velocity of the reactor, which is the inverse of residence time, is decreasing with fractional conversion of the reactor. The reason for this decrease is because the volume of the reactor is inversely proportional to the space velocity of the reactor, and if volume is increasing, then we expect the space velocity of the reactor to decrease, as depicted in Table 3. The quantity of heat generated, also known as the heat load, is increasing with fractional conversion because when the energy barrier known as activation energy has been overcome, product formation proceeds; hence, this requires energy to break the activation energy, so it is expected to increase with fractional conversion. Lastly, the quantity of heat generated per unit volume of reactor is seen to be decreasing with fractional conversion.

3.1 Effect of Fractional Conversion on Process Parameters

The effect of fractional conversion on process parameters such as volume of reactor, temperature of reactor, diameter, height, residence time, space velocity, quantity of heat generated, quantity of heat generated, and quantity of heat generated per unit volume of reactor is presented in Figures 2 to 9.

3.1.1 Effect of Fractional Conversion on Volume of Reactor

The effect of fractional conversion on volume of reactor is presented in Figure 2.

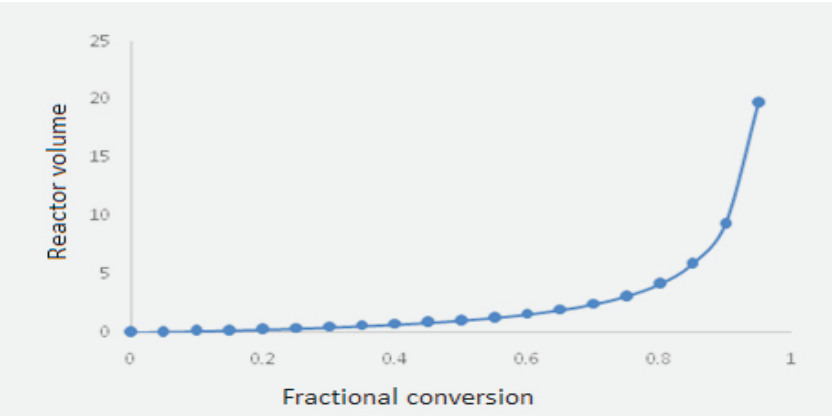

Figure 2: Volume of Reactor and Fractional Conversion

Figure 2 shows the effect of varying fractional conversion on the volume of the reactor. The fractional conversion of the reactor was varied from 0 to 0.95 at intervals of 0.05, and this caused a corresponding increase in the volume of the reactor from 0 m3 to 19.77 m3. This indicates that as more reactants are converted into products, the reactor needs to accommodate a larger volume of reaction mixture to maintain the desired conditions. The relationship between fractional conversion and reactor volume could be influenced by factors such as reaction kinetics, desired

product yield, and the need to maintain optimal conditions for the reaction to proceed efficiently. For example, as the reaction progresses and more reactant is consumed, the reactant concentration decreases, which might require a larger reactor volume to achieve the same level of conversion.

3.1.2 Effect of Fractional Conversion on Height of Reactor

The effect of fractional conversion on height of reactor is presented in Figure 3.

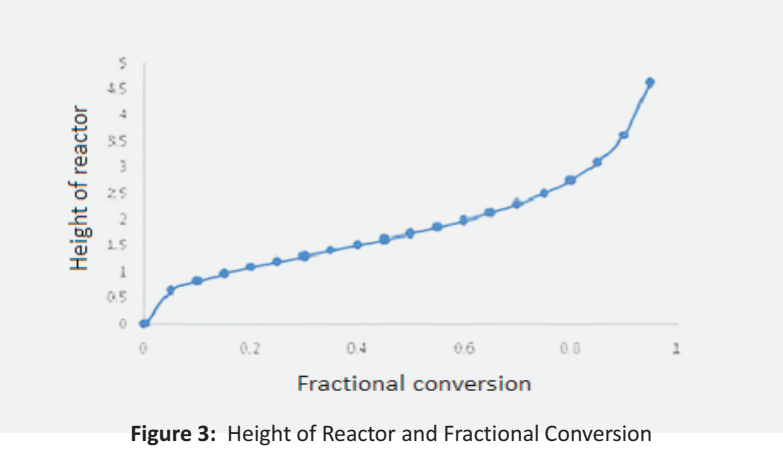

Figure 3: Height of Reactor and Fractional Conversion

As revealed in Figure 3 the fractional conversion of the reactor was varied from 0 to 0.95 at intervals of 0.05, and this caused a corresponding increase in the height of the reactor from 0 m to 4.65 m. This suggests that as more reactant is converted into products, a greater height of the reactor is required to accommodate the reaction mixture. The relationship between fractional conversion and reactor height could be influenced by factors such as reaction kinetics, mass transfer limitations, and the need to maintain optimal conditions for the reaction to proceed efficiently. As the reaction progresses and more reactant is consumed, the reactant concentration decreases, which might require a greater height of the reactor to achieve the same level of conversion.

3.1.3 Effect of Fractional Conversion on Diameter of Reactor

Figure 4 shows the effect of varying fractional conversion on the diameter of the reactor.

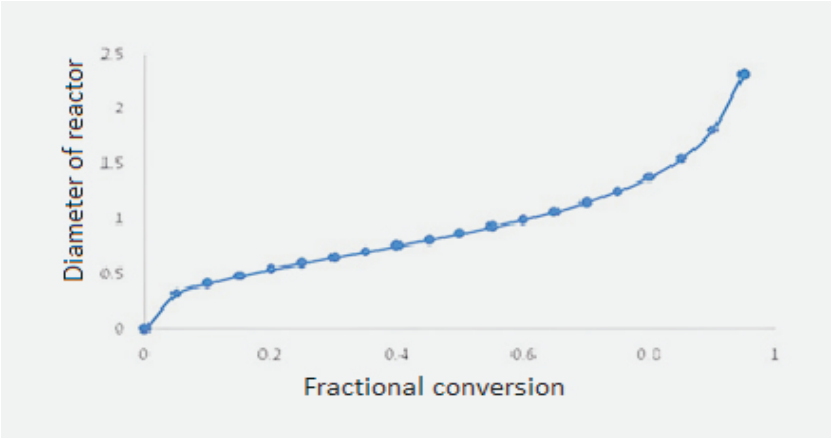

Figure4: Diameter of Reactor and Fractional Conversion

As shown in Figure 4, fractional conversion of the reactor was varied from 0 to 0.95 at intervals of 0.05 and this caused a corresponding increase in the height of the reactor from 0 m to 2.32 m. This suggests that the diameter of the reactor does not significantly change with increasing conversion in the plotted range. The lack of significant variation in reactor diameter with increasing conversion could indicate that the reaction system does not require adjustments in reactor diameter to accommodate changes in conversion. Alternatively, it may suggest that other factors, such as reactor height or volume, play a more significant role in accommodating the reaction mixture as conversion progresses.

3.1.4 Effect of Fractional Conversion on Residence Time of Reactor

Figure 5 shows the effect of varying fractional conversion on the diameter of the reactor.

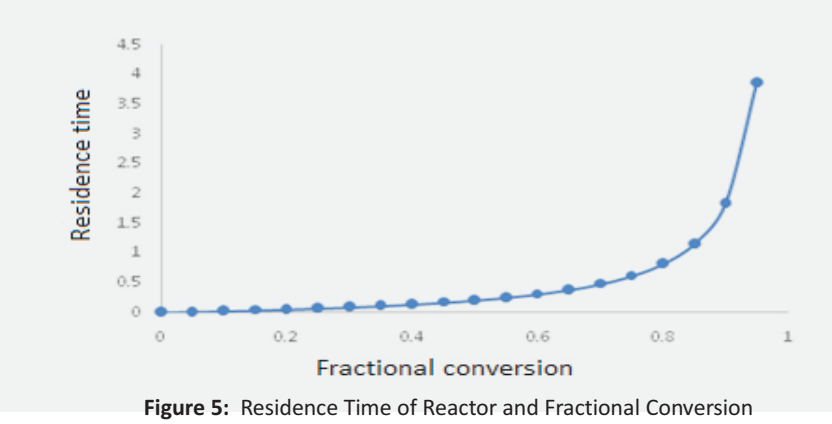

Figure 5: Residence Time of Reactor and Fractional Conversion

As shown in Figure 5, fractional conversion of the reactor was varied from 0 to 0.95 at intervals of 0.05 and this caused a corresponding increase in the residence time of the reactor from 0 seconds to 3.87 seconds. This suggests that as more reactant is converted into products, less time is required for the reaction to achieve the desired conversion level. The relationship between fractional conversion and reactor residence time reflects the kinetics of the reaction and the efficiency of the reactor design. As the reaction progresses and more reactant are consumed, the reaction rate might increase, requiring less time for the reactants to achieve the same level of conversion.

3.1.5 Effect of Fractional Conversion on Space Velocity of Reactor

Space Velocity represents the flow rate of reactants through the reactor per unit volume of the catalyst. It is measured in reciprocal seconds (1/s) and indicates how quickly the reactants are being processed. The space velocity is calculated as the ratio of the volumetric flow rate of the reactants to the volume of the catalyst in the reactor. Figure 6 shows the effect of varying fractional conversion on the space velocity of the reactor.

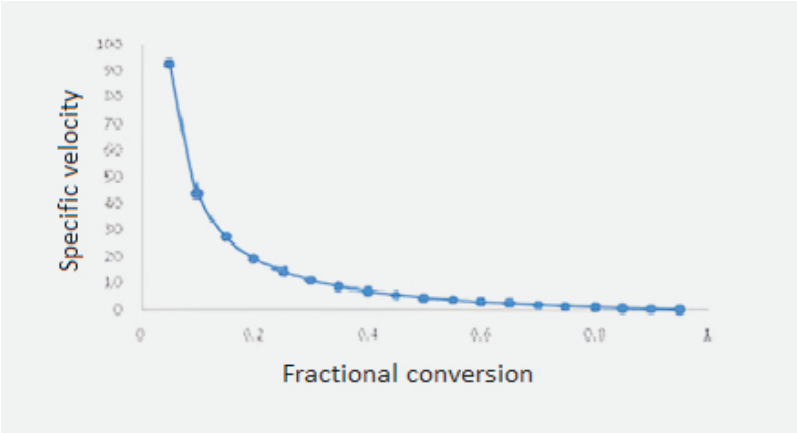

Figure 6: Space Velocity of Reactor and Fractional Conversion

As revealed in Figure 6, fractional conversion of the reactor was varied from 0 to 0.95 at intervals of 0.05 and this caused a corresponding increase in the residence time of the reactor from 93.122 per second to 0.258 per second. This suggests that as more reactant is converted into products, the rate at which reactants flow through the reactor per unit volume of catalyst decreases. The relationship between fractional conversion and space velocity reflects the dynamics of the reaction and the performance of the reactor. As the reaction progresses and more reactant is consumed, the reactant concentration decreases, leading to a decrease in the rate at which reactants flow through the reactor to achieve the same level of conversion.

3.1.6 Effect of Fractional Conversion on Quantity of Heat of Reactor

The quantity of heat (Q) represents the rate of heat generation or consumption in the reaction system. It is measured in Joules per second (J/s) and indicates the amount of heat either released or absorbed by the reaction per unit time. Figure 7 shows the effect of varying fractional conversion on the quantity of heat generated in the reactor.

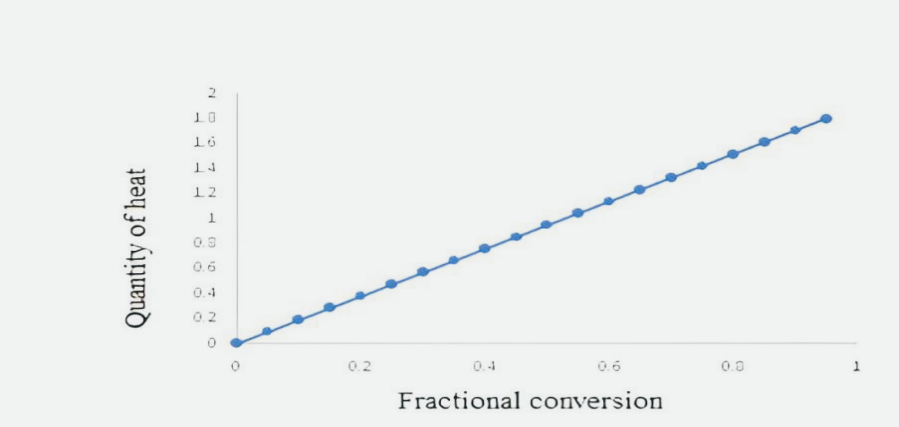

Figure 7: Quantity of heat of reactor and fractional conversion

As shown in Figure 7, the fractional conversion of the reactor was varied from 0 to 0.95 at intervals of 0.05, and this caused a corresponding increase in the quantity of heat in the reactor from 0 to 1.80 kilojoules per second. This suggests that as more reactants are converted into products, less heat is generated or consumed by the reaction per unit time. The relationship between fractional conversion and the quantity of heat reflects the thermodynamics of the reaction and the energy balance within the reactor. As the reaction progresses and more reactants are consumed, the rate of heat generation or consumption may decrease due to changes in reactant concentrations, reaction kinetics, and heat transfer effects.

3.1.7 Effect of Fractional Conversion on Quantity of Heat per unit Volume of Reactor

Quantity of Heat per Unit Volume (q) represents the rate of heat generation or consumption per unit volume of the reactor. It is measured in Joules per second per cubic meter (J/s/m^3) and indicates the amount of heat either released or absorbed by the reaction per unit volume of the reactor per unit time. Figure 8 shows the effect of varying fractional conversion on the quantity of heat generated per unit volume of the reactor.

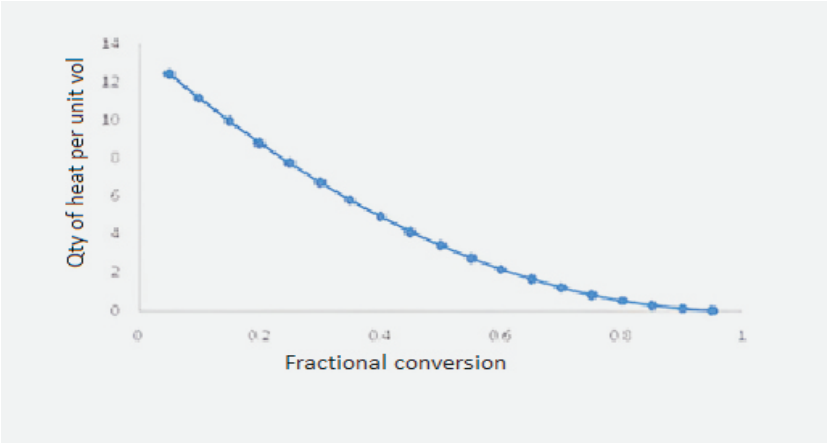

Figure 8: Quantity of heat per unit volume of the reactor and fractional conversion

As shown in Figure 8, the fractional conversion of the reactor was varied from 0 to 0.95 at intervals of 0.05, and this caused a corresponding increase in the quantity of heat per unit volume of the reactor from 12.45 kJ/m^{3}s to 0.35 kJ/m^{3}s. This suggests that as more reactants are converted into products, less heat is generated or consumed per unit volume of the reactor per unit time. The relationship between fractional conversion and quantity of heat per unit volume reflects the thermodynamics and kinetics of the reaction, as well as the heat transfer characteristics within the reactor. As the reaction progresses and more reactant is consumed, the rate of heat generation or consumption per unit volume may decrease due to changes in reactant concentrations, reaction kinetics, and heat transfer effects.

4.2.8 Effect of Fractional Conversion on Temperature of Reactor

Reactor temperature represents the temperature of the reactor in Kelvin (K). It indicates the thermal energy present in the reactor and can significantly influence the reaction kinetics and equilibrium of the reaction. Figure 9 shows the relationship between fractional conversion variation from 0 to 0.95 at an interval of 0.05 and the process temperature during the alkylation process for cumene production.

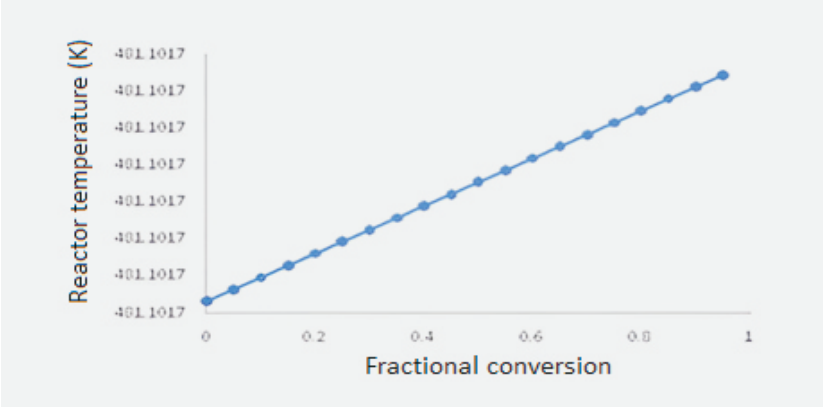

Figure 9: Temperature of reactor and fractional conversion

As shown in Figure 9, the process temperature of 481.10 k remained constant as the reaction proceeded, even with changes in fractional conversion. This played a key role in the optimum operation of the reactor during the process and clearly showed that the alkylation process is favored or promoted at the standard process temperature within the specific range of operation. On the other hand, a process temperature above or below the standard range for operation, as in the case of non-isothermal, will result in the loss of materials or the low quality of the target or product of interest without the configuration of a temperature controller in the reactor.

4. Conclusion

This work considered the design of a continuous stirred tank reactor for the production of 100,000 tons per year of cumene. The design equations were formulated to compute process parameters such as the volume, temperature, residence time, space velocity, quantity of heat generated, and quantity of heat generated per unit volume of reactor by varying the fractional conversion of the reactor from 0 to 0.95 at intervals of 0.05. After the formulation of the model equations, they were then solved through the application of MATLAB R2023a software to compute the desired design parameters of the reactor. Finally, the effect of varying fractional conversion on volume, temperature, residence time, space velocity, quantity of heat generated, and quantity of heat generated per unit volume of reactor were studied, after which the effect of varying the volume of reactor on residence time and temperature of reactor was also carried out.

Nomenclature

Symbol	Definition	Unit
ΔH_R	Charge in enthalpy of reactants	J/mol
A	Propylene	-
B	Benzene	-
C	Cumene	-
C_i	Initial concentration of species	mol/m^3
D_R	Diameter of the reactor	M
E	Activation Energy	J/mol
F_A	Initial molar flow rate	mol/S
H_i	Enthalpy of species	J/mol
H_R	Heightof 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
τ	Space time	Seconds

References

Cowley, M., de Klerk, A., Nel, R.J.J. & Rademan, J. D. (2006). Alkylation of benzene with 1-pentene over solid phosphoric acid. *Industrial Engineering & Chemistry Research*. 45(22), 7399-7408

Gelareh, A. & Zahra, B. (2024). Cumene. Encyclopedia of Toxicology, 4th Edition, 337 – 343.

Hilman, A. H. (2022). Process simulation & sensitivity analysis of cumene production from an integrated alkylation and transalkylation reaction. *Journal of Chemical Process.* 7(2). 64 – 78

John, B. B. (2007). Reactor Design and Reactor Kinetics Engineering. 5thEdition,Butter-Worth-Heinemann.

Levenspiel, O. (1999). Chemical Reaction Engineering. 3rd Edition, John Wiley & Son's Inc U.S.A.

Mahmondian, F., Moghaddam, A. H. &davach, S. M. (2021). Genetic-based multi-objective optimization of alkylation process by a hybrid model of statistical and artificial intelligence approaches. *The Canadian Journal of Chemical Engineering*. 1-13.

Nikfar, S. &Behbondi, A. F. (2014). Cumene. Encyclopedia of Toxicology, 1082 – 1085.

Ojong E. O., Wosu, C. O., Aguma, E & Pascal, A. U. (2024). Design and simulation of 30,000 tons per year of cumene plant from natural gas field. *International Union of Pure andApplied Chemistry*. https://doi.org/10.1515/pac2023-1135. 1-11

Roberts, J. S. (2006). Cumene production. *Encyclopedia of Chemical Processing*. 603 – 616.

Scotti, F., Fabricators, N., Sephacci, P. & Manca D. (2017). A MOO approach towards sustainable process design: integrating the three pillars of sustainability, in comp. Aided chem. Eng. Els., A. Espuna, M. Graells, L. Puigjaneo (Eds) 40, 637-642, *Elsevier*, Oostende, Netherland.

Thakur, R., Barman, S. & Kumar, R. G. (2016). Synthesis of cumene by transalkylation over modified beta zeolite: A kinetic study. *Brazelian journal of chemical Engineering*. 33(4). 957-967.

Wordu, A. A. &Wosu, C. O. (2019). CSTR design for propylene glycol chemical production. *Internal Journal of Latest Technology in Engineering Management & Applied Science* 8(2), 18-30.

Wosu, C. O. & Ezeh, E. M. (2024). Design and optimization of glycol- based natural gas dehydration plant. *International Journal of Recent EngineeringScience*. https://doi.org/10.14445/23497157/IJRES. 11(1). 22-29

Wosu, C. O., Akpa, J. G., Wordu, A. A., Ehirim, E. & Ezeh, E. M. (2024a). Design modification and comparative analysis of glycol-based natural gas dehydration plant. *Applied Research*. https://doi.org/10.1002/appl.202300093. 1-14

Wosu, C. O., Ezeh, E. M.&Owu, F. U. (2024b). Design and mechanical analysis of a continuous stirred tank reactor (CSTR) for the optimum operation and production of propylene glycol from propylene oxide hydrolysis. *Sustainable Chemical Engineering*. https://doi.org/10.37256/sce.5220244713. 5(2), 367-383

Wosu, C.O., Ezeh, E. M. & Uku, E. P. (2023). Design and performance analysis of an industrial triethylene glycol recovery regenerator of a dehydration process. *International Journal of Recent Engineering Science*. https://doi.org/10.14445/23497157/IJRES. 10(5). 39-48

Yogesh, K. C., Chumbhale, V. R. &Answar, A. S. (2012). Alkylation of benzene to cumene over mor zeolite catalysts. Revue Roumaine de Chimie