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Comparative design of flow reactors for synthesis of cumene by catalytic alkylation of propylene and benzene

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ABSTRACT

This research is driven by the need to ensure effective, economic and sustainable processes for cumene production from the catalytic alkylation of propylene and benzene in flow reactors. The flow reactors are the continuous stirred tank reactor (CSTR) and the plug flow reactor (PFR) where the alkylation reactions occur. The reactors were designed by exploring the conservation principle of mass and energy over the reactors. The performance model of the reactors was simulated using MATLAB R2023a version at the same initial feed temperature and operating temperature of 481.1k and 483k respectively with fractional conversion changes within the range of 0≤ XA≤ 0.95 at an interval of 0.05. The comparative analysis of the flow reactor design was based on the target product yield (cumene yield) and the energy efficiency of the process. The cumene yield is dependent on the reactor volume while the energy efficiency of the process depends on the quantity of heat generated per unit volume of the reactor. At the maximum fractional conversion of 0.95, the volume of the CSTR and the PFR design were 52.296m3 and 19.771m3 respectively with a percentage difference of 22.6% while the quantity of heat generated per unit volume of the CSTR and PFR were 0.013j/sm3 and 0.035j/sm3 respectively with a percentage difference of 22.9%. The above comparative design analysis in this article showed that in terms of cumene yield, the CSTR displayed better performance characteristics as indicated by the reactor volume while in terms of energy efficiency, the PFR showed better performance characteristics as indicated by the quantity of heat generated per unit volume of the reactors.

INTRODUCTION

The production of cumene in process industries is of high significant importance because of its wide range of applications as a feed material in the production of high-octane gasoline, phenol, acetone, paints, coating materials, inks, polymer materials, pharmaceutical products and solvents (Nikfar and Behboudi, 2014; Hilman, 2022; Mahmondian *et al*, 2021; Galereh and Zahra, 2024). Commercially, cumene is produced via catalytic alkylation of propylene and benzene occurring in flow reactors (Roberts, 2006; Scotti *et al*, 2017). The design of flow reactors (CSTR and PFR) has emerged as innovative tools revolutionizing the rapid evolution of the world of chemical synthesis and manufacturing, driven by the need for more efficient and sustainable processes. In this article, we will explore the conservation principle of mass and energy in the development of flow reactor models for the production of 100,000 tons per year of cumene from the catalytic alkylation of propylene and benzene.

The conservation principle of mass and energy serves as the basis for all chemical engineering equipment design (Wosu *et al*, 2023; Wosu and Ezeh, 2024; Wordu and Wosu, 2019; Wosu *et al*, 2024; Oba *et al*., 2024; Wosu, 2024a). The performance analysis of the CSTR and PFR was

based on the target product yield (cumene yield) and energy efficiency of the process. The choice of flow reactors (CSTR and PFR) design is considered since they are most suitable for gas phase, liquid phase and slurry reactions which are solely dependent on the nature of the reactant species for the economic success of the plant.

The MATLAB R2023a was utilized as the simulation tool of the flow reactors' performance or design models for size specification of the reactors in terms of volume, height, diameter, space-time, space velocity, the quantity of heat generated and the quantity of heat generated per unit volume of the reactor.

Ojong *et al* (2024) designed a process plant for the yearly production of 30,000 tons of cumene using data obtained from the Utorogu gas field which was simulated using HYSYS. The researchers highlighted the importance of cumene in the production of phenol, acetone and hydroperoxide. Catalysts such as Friedel-craft, sulphuric acid, and solid phosphoric acid supported by alumina can be applied during the alkylation of propylene and benzene for cumene production (Cowley *et al*, 2006; Luyben, 2010).

However, problems such as corrosion, safety hazards, complications and sustainability issues associated with the above catalysts have resulted in the use of zeolite catalysts as their replacement by modern researchers (Yogesh *et al*, 2012). The zeolite catalyst is cheap, safe, possesses no corrosion challenges and can be modified to beta zeolite technology in trans-alkylation processes for cumene production (Thakur *et al*, 2016). One way of ensuring the effectiveness and sustainability of cumene production is by performing a comparative analysis in terms of product yield and energy efficiency of flow reactor designs for the alkylation process which is the main focus of this research.

MATERIALS AND METHODS

Materials

The materials used in this research are computer sets, data obtained from relevant works of literature, textbooks and the simulation tool used is MATLAB R2023a.

Methods

The procedures adopted in this research are;

i. Development of the reaction kinetic models
ii. Development of design and energy balance models
iii. Consideration of flow reactors comparative analysis

Development of the Reaction Kinetic Models

Cumene is produced from the catalytic alkylation of propylene and benzene and the reaction kinetic scheme is given by Ojong *et al*, 2024 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;

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

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

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

Development of the CSTR and PFR Design/Sizing Models

The conservation principle of the mass and energy balance can be applied to the CSTR and PFR schematics in Figures 1 and 2 in the development of the flow reactor design or performance models. Consider the schematic representation of a continuous stirred tank reactor with mass and heat effect in Figure 1

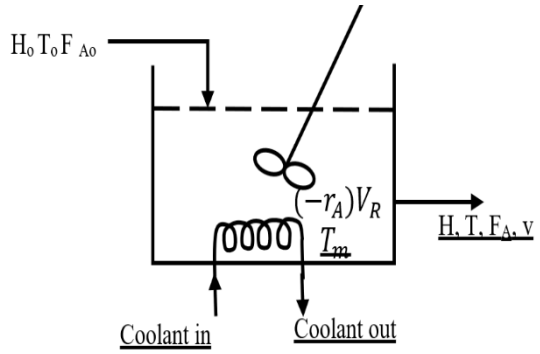


Figure 1: CSTR with Mass and Heat Effect for Cumene Production

In the CSTR, the following assumptions can be made;

i. The reacting mixture is well stirred and the feed assumes a uniform composition throughout 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 flow reactor 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

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

The terms in equation (4) can be defined mathematically and simplified at steady-state operation to give the CSTR design models as follows;

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

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

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

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

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

Generally, the quantity of heat generated and quantity of heat generated per unit volume of reactors are expressed mathematically as;

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

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

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

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

For the CSTR, terms in equation (12) are defined mathematically and simplified at steady state conditions to give the temperature effect model in equation (13)

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

Consider the schematic representation of a plug flow reactor with mass and heat effect.

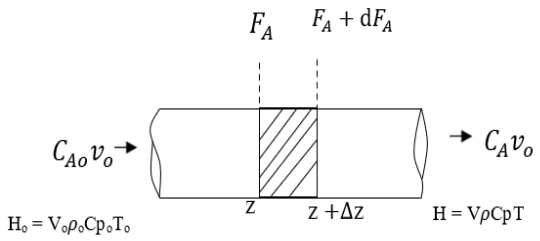


Figure 2: PFR Schematic with Mass and Heat Effect

The design and temperature effect model of the PFR is developed by the application of the conservation principles of mass and energy in equations (4) and (12) respectively. The terms in equation (4) can be defined, substituted and simplified at steady state to yield the PFR performance model for volume, height, diameter, space-time, space velocity, the quantity of heat generated as well as the quantity of heat generated per unit volume of the reactor thus;

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

$$H_{R(PFR)} = \left[\frac{25v_o}{\pi}\int_0^{x_A} \frac{dx_A}{k_o C_{Ao} e^{-E/RT(1-x_A)(m-x_A)}}\right]^{\frac{1}{3}} \quad (15)$$

$$D_{R(PFR)} = \frac{\left[\frac{25v_o}{\pi}\int_0^{x_A} \frac{dx_A}{k_o C_{Ao} e^{-E/RT(1-x_A)(m-x_A)}}\right]^{\frac{1}{3}}}{25} \quad (16)$$

$$\tau_{PFR} = \int_0^{x_A} \frac{dx_A}{k_o C_{Ao} e^{-E/RT(1-x_A)(m-x_A)}} \quad (17)$$

$$S_V = \frac{1}{\int_0^{x_A} \frac{dx_A}{k_o C_{Ao} e^{-E/RT(1-x_A)(m-x_A)}}} \quad (18)$$

The temperature effect model of the PFR in Figure 2 was developed from the conservation principle of energy balance in equation (12).

The terms in equation (12) can be defined, substituted and simplified to yield the temperature effect model thus;

$$\frac{dT}{dZ} = \frac{1}{u\rho C_p}(\Delta H_R)(-r_i) \quad (19)$$

Data for Evaluation

The data for evaluation in this research are the properties/thermodynamic data and data obtained from literature as presented in Tables 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	Hilman, 2022
k_o	$6.510 \times 10^3 s^{-1}$	Frequency factor	Hilman, 2022
k_i	$4.124 \times 10^{-3} s^{-1}$	Rate constant	Hilman, 2022
$-r_A$	1.305×10^{-5} mol/m^3/s	Reaction rate	Hilman, 2022
E	52564KJ/Kmol	Activation energy	Hilman, 2022

Solution Techniques

The design models of the flow reactors were solved numerically using the Runge Kutta Algorithm built in the MATLAB Code.

RESULTS AND DISCUSSION

The results of the comparative design of flow reactors for cumene production from the catalytic alkylation of propylene and benzene are presented in Table 3 and Figures 3 to 10. Table 4 is the comparative analysis of CSTR and PFR design for the production of cumene from the catalytic alkylation of propylene and benzene at the same

initial feed temperature and operating temperature condition.

Table 3: Calculate Design Data

Data/ Parameter	Values	Description
M_A	42Kg/mol	The molecular weight of propylene
M_B	78Kg/mol	Molecular weight of benzene
M_C	120Kg/mol	Molecular weight of cumene
G_A	1.350Kg/s	Mass flow rate of propylene
G_B	2.508Kg/s	Mass flow rate of benzene
G_C	3.858Kg/s	Mass flow rate of cumene
$\overline{V}_A$	0.00163m^3/kg	Specific density of propylene
$\overline{V}_B$	0.00114m^3/kg	Specific density of benzene
$\overline{V}_C$	0.00116m^3/kg	Specific density of cumene
Q_A	0.00220m^3/s	Volumetric flow rate of propylene
Q_B	0.00286m^3/s	Volumetric flow rate of benzene
v_o	0.00506m^3/s	Total volumetric flow rate of reactants
C_{Ao}	0.0275mol/m^3	Initial concentration of limiting reactants
F_{Ao}	0.000140mol/s	Initial molar flow rate of limiting reactants
X_A	0.95(Dimensionless)	Maximum fractional conversion

The result was obtained from the MATLAB simulation of the flow reactors' steady-state models. At 95% fractional conversion, the CSTR and PFR functional parameters design or size specifications and their percentage difference are presented. In terms of cumene yield, the CSTR and PFR volume was 52.296m^3 and 19.771m^3 with a percentage difference of 22.6% while in terms of energy efficiency, the quantity of heat generated per unit volume of the CSTR and PFR was 0.013j/sm^3 and 0.035j/sm^3 with a percentage difference of 22.9%. The above analysis showed that in the CSTR design, more yield of cumene was achieved as indicated by its volume while in terms of energy efficiency, the PFR performed better as indicated by the quantity of heat generated per unit volume of the reactor. By implication, both reactors are suitable media for catalytic alkylation reactions and the choice of any is dependent on the designer's primary objectives. This is in agreement with the design of a CSTR for ethyl acetate production by (Wosu and Okoro, 2025) and the production of cumene in a PFR (Wosu, 2024c).

Table 4: Design Results of the CSTR and PFR Volume, Height, Diameter, Space-Time, Space Velocity, Quantity of Heat Generated and the Quantity of Heat Generated per unit Volume of the Reactors at 95% Fractional Conversion.

Reactor Design Parameters (Unit)	@ 95% Fractional Conversion		Difference (%)
	CSTR	PFR	
Volume (m^3)	52.296	19.771	22.6
Height (m)	6.343	4.652	7.7
Diameter(m)	3.217	2.326	5.7
Space-Time (s)	8.038	3.877	17.5
Space Velocity (s^{-1})	0.124	0.258	17.5
Quantity of Heat Generated (J/s)	0.694	1.804	22.2
Quantity of Heat Generated per unit volume of the Reactor (J/sm^3)	0.013	0.035	22.9

Figure 3 is a plot of the variation of CSTR and PFR volume and fractional conversion of reactant species during alkylation reaction for cumene production. This profile was obtained from the MATLAB simulation of the flow reactor steady state performance model at the same initial feed

temperature and operating temperature of 481.1k and 483k with a fractional conversion change of $0 \leq X_A \leq 0.95$at an interval of 0.05.

Plot of the CSTR and PFR Volume (V_R) and Fractional Conversion (X_A)

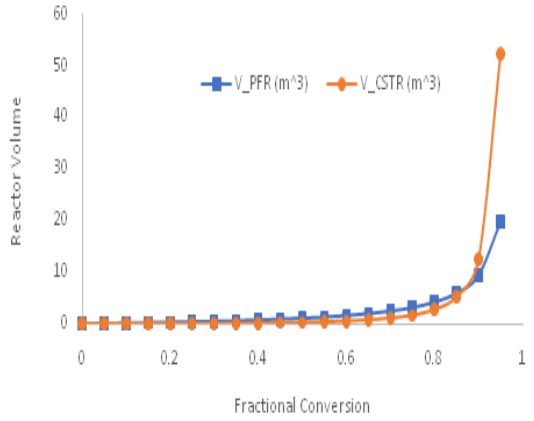


Figure 3: Plot of the CSTR and PFR Volume (V_R) and Fractional Conversion (X_A)

From the plot, the CSTR and PFR volume increases exponentially as the fractional conversion increases. This indicates that as more reactants are converted into products, the reactor needs to accommodate a larger volume of reaction mixture to obtain the desired conditions. This behaviour could be influenced by factors such as reaction kinetics, target product yield and the need to maintain the optimal condition of the process (Wordu and Wosu, 2019; Wosu, 2024c). At a maximum fractional conversion of 0.95, the CSTR and PFR volumes were 52.296m^3 and 19.771m^3 respectively. This profile also showed that more yield of cumene is produced in the CSTR compared to the PFR.

Figure 4 is a plot of the CSTR and PFR change in height with fractional conversion. At the same initial feed temperature and operating temperature of 481.1k and 483k respectively with a fractional conversion range of $0 \leq X_A \leq 0.95$at an interval of 0.05. According to the plot, the CSTR and PFR height increased exponentially as the fractional conversion increased. At a maximum fractional conversion of 0.95, the CSTR and PFR height were increased to 6.343m and 4.652m respectively. This result showed that the reactor height is also a function of its volume as reported by (Wordu and Wosu, 2019; Wosu, 2024b)

Plot of the CSTR and PFR Height (H_R) and Fractional Conversion (X_A)

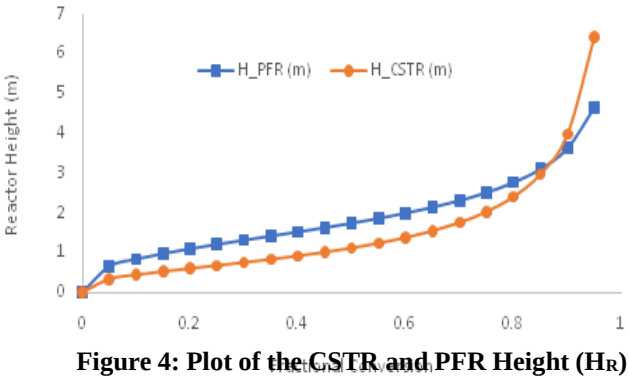


Figure 4: Plot of the CSTR and PFR Height (H_R) and Fractional Conversion (X_A)

Figure 5 represents a plot of the CSTR and PFR diameter changes with fractional conversion during the catalytic alkylation process. Just like in the case of the flow reactor volume and height, the reactor diameter also increases exponentially as the fractional conversion increases. This profile behaviour is in line with the trend for steady-state flow reactors design as reported by (Wosu, 2024b; Wosu, 2024c). At a maximum conversion of 0.95, the CSTR and PFR diameters were 3.217m and 2.326m respectively. This result showed that a reactor with a large volume and height will have a corresponding diameter as in the case of the CSTR when compared with the PFR.

Figure 6 is a plot showing the behaviour of the CSTR and PFR space-time with changes in fractional conversion obtained from the MATLAB simulation of the design models. According to the plot, there is an exponential increase in the space-time as the fractional conversion increases in both reactors. At a maximum fractional conversion of 0.95, the space-time values of 8.038 seconds and

3.877 seconds were recorded for the CSTR and PFR respectively.

Plot of the CSTR and PFR Diameter (D_R) and Fractional Conversion (X_A)

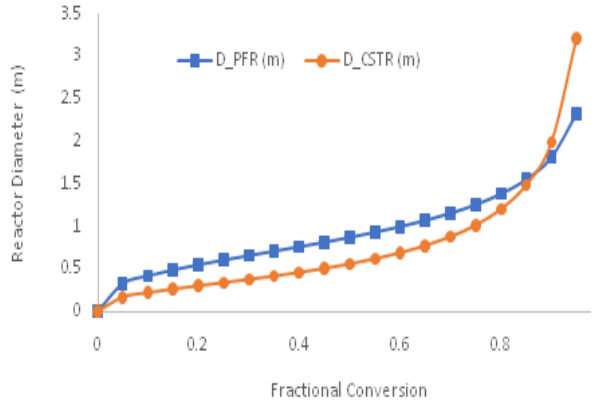


Figure 5: Plot of the CSTR and PFR Diameter (D_R) and Fractional Conversion (X_A)

This result showed that more time is spent by the element of feed in the CSTR during the alkylation process due to its design configuration and nature of reactants compared to that of the PFR. The profile behaviour showed a similar characteristic for flow reactors' steady-state operation process (Wosu, 2024b; Wosu and Ekokoje, 2025).

A plot of the CSTR and PFR Space Time (τ) and Fractional Conversion (X_A)

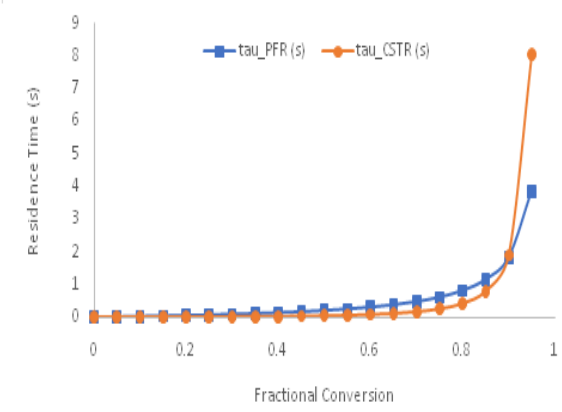


Figure 6: Plot of the CSTR and PFR Space Time (τ) and Fractional Conversion (X_A)

Figure 7 is a profile variation of the CSTR and PFR space velocity with fractional conversion within the range of $0 \leq X_A \leq 0.95$. This profile was obtained from the MATLAB simulation of the steady-state flow reactor models at the same process condition. Here, an exponential decrease in the space velocity was observed as the fractional conversion increased during the process in both reactors. This profile behaviour follows a similar trend of flow reactors' steady-state design operation as reported by (Wosu, 2024c). At a maximum fractional conversion of 0.95, the space velocity recorded in the CSTR and PFR was 0.125sec^{-1} and 0.258sec^{-1}. This behaviour justified the mathematical relationship between the space-time and the space velocity. The PFR space velocity as observed is higher than that of the CSTR.

Plot of the CSTR and PFR Space Velocity (S_V) and Fractional Conversion (X_A)

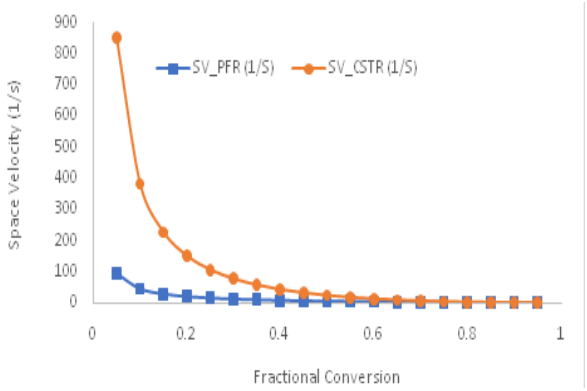


Figure 7: Plot of the CSTR and PFR Space Velocity (S_V) and Fractional Conversion (X_A)

Figure 8 is the profile behaviour of the CSTR and PFR quantity of heat generated with a change in fractional conversion within the range of$0 \leq X_A \leq$ 0.95 during the alkylation process for cumene production which follows the trend for steady-state flow reactor operation as recently reported by (Wosu and Okoro, 2025). According to the plot, there is a linear increase in the quantity of heat generated as the fractional conversion increases. At a maximum conversion of 0.95, the quantity of heat generated in the CSTR and PFR were 0.694j/s and 1.804j/s respectively. The PFR here, showed better performance characteristics in terms of energy

efficiency as indicated in the large quantity of heat generated when compared to that of the CSTR.

Plot of the CSTR and PFR Quantity of Heat Generated (Q) and Fractional Conversion (X_A)

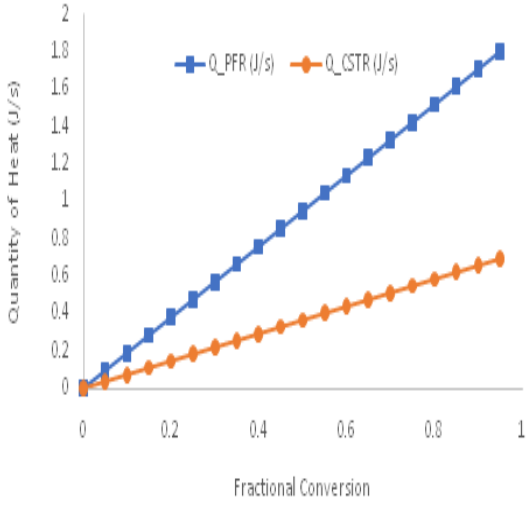


Figure 8: Plot of the CSTR and PFR Quantity of Heat Generated (Q) and Fractional Conversion (X_A)

Figure 9 is the profile or relationship between the CSTR and the PFR quantity of heat generated per unit volume of the reactors with changes in fractional conversion within the range of$0 \leq X_A \leq 0.95$. The profile showed that the quantity of heat generated per unit volume of the reactors decreases as the fractional conversion increases during the process. This justifies the mathematical relationship between the quantity of heat generated per unit volume of reactors and fractional conversion (Wosu, and Okoro, 2025). At a maximum fractional conversion of 0.95, the quantity of heat generated per unit volume of the CSTR and PFR were 0.013j/sm^3 and 0.035j/sm^3 respectively. Here the PFR showed better performance characteristics as it conserves more heat at the end of the process compared to that of the CSTR.

Figure 10 is the relationship or variation of the CSTR and PFR operating temperature and the fractional conversion during the cumene production. with a fractional conversion change within the range of $0 \leq X_A \leq 0.95$ X_A. From the plot, changes in fractional conversion do not affect the operating temperature in both reactors since the operating temperature is within the range or standard for an alkylation reaction (isothermal process).

Plot of the Quantity of Heat Generated per unit Volume of the CSTR and PFR (q) with Fractional Conversion (X_A)

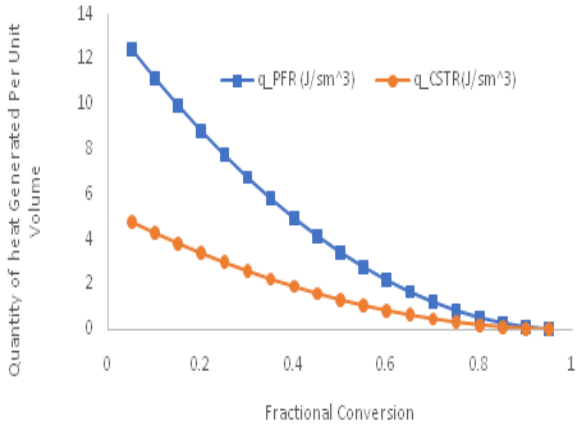


Figure 9: Plot of the Quantity of Heat Generated per unit Volume of the CSTR and PFR (q) with Fractional Conversion (X_A)

However, an operating temperature below or above the standard range will result in loss of materials, low yield and purity of the target product, or even thermal runaway during the process. This behaviour is in agreement with the results obtained from Wosu, 2024b.

CONCLUSION

The research considered the design of CSTR and PFR also known as flow reactors for the production of 100,000 tons per year of cumene from the catalytic alkylation of propylene and benzene. The conservation principle of mass and energy was explored in the development of the flow reactors' performance or design models. The models were simulated at the same initial feed and operating

condition of the reactors and fractional conversion variation from 0 to 0.95 at an interval of 0.05.

At a maximum fractional conversion of 0.95, the volume of the CSTR and PFR was 52.296m^3 and 19.771m^3 respectively with a percentage difference of 22.6% while the quantity of heat generated per unit volume of the CSTR and PFR was 0.013j/sm^3 and 0.035j/sm^3 with a percentage difference of 22.9%.

Plot of the CSTR and PFR Temperature (T) and Fractional Conversion (X_A)

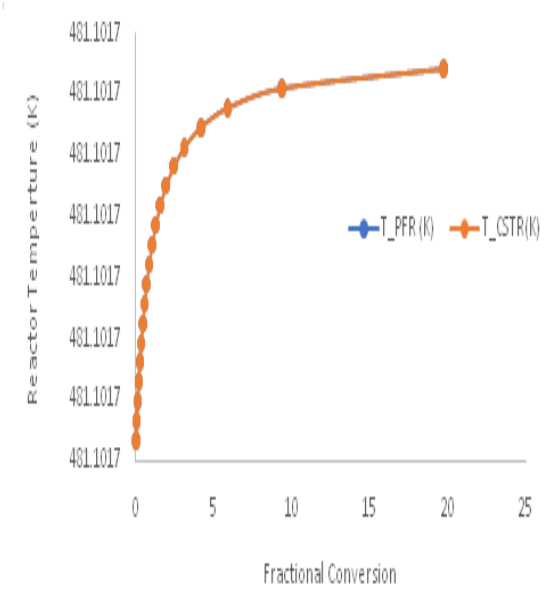


Figure 10: Plot of the CSTR and PFR Temperature (T) and Fractional Conversion (X_A)

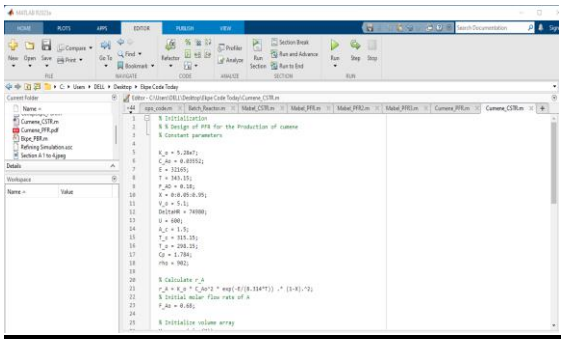
The comparative analysis of the flow reactors' performance showed that in the CSTR design, more yield of cumene is produced as indicated by the reactor volume while in terms of energy efficiency, the PFR showed a better performance as indicated by the quantity of heat generated per unit volume of the reactor. This research showed that both the CSTR and PFR are suitable for cumene production and the choice of either reactor depends on the designer's primary objectives.

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	S

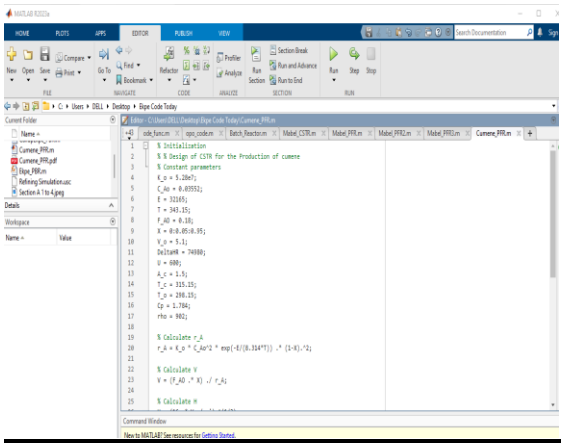
The MATLAB simulation code of the flow reactors (CSTR and PFR) is presented in Appendix A and B.

Appendix A



```
% Display volumes
disp('Volume of the PFR at each step:');
disp('X      Volume (m^3)');
disp([X', V']);

% Calculate H
H = (16 .* V ./ pi).^(1/3);

% Calculate D
D = H ./ 2;

% Calculate τ_CSTR
tau_CSTR = V ./ V_o;

% Calculate SV
SV = 1 ./ tau_CSTR;

% Calculate Q
Q = DeltaHR * F_AO .* X;

% Calculate q
q = (DeltaHR * F_AO .* X) ./ V;

% Calculate T_R
T_R = (tau_CSTR .* r_A .* V_o + U * A_c * T_c + rho * V_o * Cp * T_o) ./ (rho * V_o * Cp + U * A_c);
```

Appendix B



```
% Calculate D
D = H ./ 2;

% Calculate τ_CSTR
tau_CSTR = V ./ V_o;

% Calculate SV
SV = 1 ./ tau_CSTR;

% Calculate Q
Q = DeltaHR * F_AO .* X;

% Calculate q
q = (DeltaHR * F_AO .* X) ./ V;

% Calculate T_R
T_R = (tau_CSTR .* r_A .* V_o + U * A_c * T_c + rho * V_o * Cp * T_o) ./ (rho * V_o * Cp + U * A_c);
```

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