MFR Lifespan Improvement using Standard Thickness Specification Models to withstand the Effect of Temperature and Pressure during Cumene Production.

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Abstract

The production of cumene in process industries is very crucial due to its wide range of application domestically and industrially. Traditionally, cumene production is via catalytic alkylation of propylene and benzene in a mixed flow reactor (MFR). In a bid to enhance optimum production and sustainability of equipment lifespan, this research considered the development of the MFR design models from the first principle of mass and energy balance which was simulated using MATLAB R2023a version for the reactor design. The model simulation also showed the numerically, the relationship between the fractional conversion and the reactor's functional parameters. At a conversion of 0.9, the MFR volume, height, diameter, space time, space velocity, quantity of heat generated and heat generation per reactor volume were obtained as 12.386m³, 3.981m, 1.990m, 1.904sec., 0.525sec⁻¹., 0.657J/s and 0.053J/m³s respectively. Also, the standard thickness specification of the MFR based on its operating conditions such as temperature, pressure and the reactor diameter was obtained from literature models. The model results showed that for stainless steel material for construction type (304), the MFR thickness of 5.90mm is considered suitable for the reactor body (cylindrical) and head (standard ellipsoidal) in order to mitigate the impact or effect of its operating temperature, pressure or load and corrosion effect during the process. This article showed that the design and thickness specification of the MFR is crucial for optimum, continuous and sustainability of cumene production.

Keywords: MFR, Thickness Design, Cumene, Alkylation Reaction, MATLAB Simulation

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I. Introduction

The design of chemical process and equipment such as the mixed flow reactor (MFR) play a key role in the production of petrochemical product (cumene) that is utilized as a feedstock in the manufacturing of phenol, acetone, solvents in paint manufacturing, coating materials, inks, polystyrene, rubber and elastomers [1] [2] [3] [4]. For effective and optimum production of cumene from the catalytic alkylation of propylene and benzene in a MFR, the design of the reacting media (CSTR sizing and its thickness specification) is essential and must incorporate the following factors or principles such as uncontrollable cost (overall cost of materials and its properties such as compatibility, resistance to corrosion, rust or stains during reaction, oxidative resistance, conductivity or ability to control heat, thickness, weld ability complexity, fabrication) and controllable cost such as cost of operation and production [5] [1]. The production of cumene and process sustainability is very crucial in process industries because of its substantial benefits domestically and industrially, the design and thickness consideration of the MFR (reaction media) becomes very necessary for optimum production and sustainability. The choice of MFR as the reaction media is based on its design configuration and ability to facilitate continuous operation, improve mass transfer performance particularly in multiphase systems, scalability simplicity since mixing is independent on pumping rate and its ability to effectively handle solids and slurries when compared to other reactors as a result of external agitation by the configured impellers [6] [7]. The flow chemistry of the MFR enhance efficiency, sustainability and has attracted global interest as a key for chemical industries to reach net zero with the proven ability to minimize cost and energy consumption [8] [9] [10] [11]. Researchers in the past and recent past have showcased the economic viability of cumene as well as the various techniques for its production and thus; [12] in 2010 stated that cumene production in industry is via alkylation of propylene and benzene using zeolite catalyst and developed a simulation flow sheet using badger cumene technology. The research featured both alkylation reaction for cumene production and transalkylation for the removal of unwanted products. [13] in 2012 stated that the use of zeolite as catalyst during cumene production demonstrated a better performance characteristics compared to the use of solid phosphoric acid supported with alumina. Cumene can also be synthesized trans-alkylation process utilizing modified beta zeolite catalyst [14] [15]. The CSTR design

just like other process equipment design is achieved by integrating the conservation principle of material to obtain the reactor size specification [16] [17] [18] [19] [20].

To ensure continuous and sustainable process for cumene production in a MFR, this article considered the design of a MFR and its thickness analysis to ensure steady and sustainable production as well as improvement of the MFRR equipment lifespan. When considering thickness design or specification of the equipment, the material for fabrication and its mechanical strength are considered as the most common requirements [1].

Generally, for equipment (MFR) fabrication, metallic materials be it ferrous or non-ferrous are mostly utilized [5]. In this research, the stainless steel which is a ferrous metal is used as the material for the MFR thickness design and its properties such as design temperature, design pressure, design stress, welded joint efficiency, corrosion allowance, design loads, and minimum practical wall thickness must be put into consideration.

II. Materials and Methods

The materials used in this research are the raw materials or reactant feed such as propylene and benzene. The simulation tool and software used are laptop and MATLAB R2023a version and the research data were obtained from literatures, derived or calculated data and thermodynamic data. The research methodology is both quantitative and the analytical and the procedures adopted are;

- i. Development of the reaction rate kinetics
- ii. Application of the conservation law of mass and energy balance in development of the MFR design models and temperature effect model.
- iii. Design of the MFR agitator
- iv. Application of the MFR mechanical design models for thickness determination

2.2.1 Development of the Rate Law or Reaction Kinetic Models

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

$$C_3H_6 + C_6H_6 \xrightarrow{\kappa_1} C_9H_{12}$$
 (1)
The second order liquid phase alkylation reaction can be expressed symbolically as

 $A + B \xrightarrow{\kappa_1} C$

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;

 $-r_{A} = k_{o}C_{Ao}^{2}e^{-E_{/RT}}(1 - x_{A})(m - x_{A})$ (3) Where -r_A is the depleting rate of the limiting reactant, k_o is the Arrhenius constant also called pre-exponential

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/m³, X_A is the fractional conversion of specie A and m is the ratio of excess reactant and limiting reactant.

2.2 Development of MFR Design and Energy Balance Models

Consider the schematic representation of a continuous stirred tank reactor with feed and product streams



Figure 1: MFR with Mass and Heat Effect

(2)

For the MFR above, the following assumptions can be made;

- 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. The temperature within the reactor is kept at a constant value by the heat exchange medium
- vi. Constant density

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

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

The terms in equation (4) can be defined, applied and simplified at steady state process operation to yield the design models for MFR volume, height, diameter, space time and space velocity as;

$$V_{\rm R} = \frac{F_{\rm Ao} x_{\rm a}}{k_{\rm o} C_{\rm Ao}^2 e^{-E} / {\rm RT} (1 - x_{\rm A}) (m - x_{\rm A})}$$
(5)

$$H_{R} = \left[\frac{16F_{Ao}x_{A}}{\pi k_{o}C_{Ao}^{2}e^{-E/RT}(1-x_{A})(m-x_{A})}\right]^{\overline{3}}$$
(6)

$$D_{R} = \frac{\left[\frac{16F_{AO}x_{A}}{\pi k_{O}C_{AO}^{2}e^{-E}/RT_{(1-x_{A})(m-x_{A})}}\right]^{\frac{1}{3}}}{2}$$
(7)

$$\tau_{\rm CSTR} = \frac{x_{\rm A}}{k_{\rm o} C_{\rm Ao}^2 e^{-E/RT} (1-x_{\rm A})(m-x_{\rm A})}$$
(8)

$$S_{V} = \frac{k_{o}C_{Ao}^{2}e^{-E/_{RT}(1-x_{A})(m-x_{A})}}{x_{A}}$$
(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 MFR are expressed mathematically as;

$$Q = \Delta H_R F_{Ao} x_A \tag{10}$$

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

The energy balance equation can be obtained by applying the principles of conservation of energy given as;



The terms in equation (12) can be defined, applied and simplified at steady state operation to yield the temperature effect model of the process as;

 $T = \frac{\tau \Delta H_R r_i v_o + U A_c T_c + \rho v_o c_p T_o}{(13)}$

 $\Gamma = - \rho v_0 C_p + U A_c$

2.3 Design of the MFR Agitator

Usually, a clearance is allowed between the stirrer blade and the reactor height.

The length of the stirrer can be expressed mathematically as given by [5]	
$L_{st} = H_R - C$	(14)
$D_{st} = D_R - 2C$	(15)

2.4 Design of the MFR Thickness

To size the MFR thickness for optimum production of cumene via the catalytic alkylation of propylene and benzene, the material type for construction and its properties such as design temperature, design pressure, design stress, welded joint efficiency, corrosion allowance, design loads and minimum practical wall thickness must be put into consideration [5].

2.4.1 Material for construction

The stainless steel with grade (304) is utilized as the MFR material for construction. Based on its strength, quality and capability of withstanding corrosion issues that may arise during the catalytic alkylation process, since it constitute 18% and 8% minimum amount of chromium (Cr) and nickel (Ni) respectively. The properties will guarantee stable austenitic structure and good weld-ability without post-weld annealing when welding thin sections. Table 1 and 2 present the chemical and mechanical constituent of the stainless steel grade (304) type [5].

Table 1: Chemical Composition of Stainless-Steel Grade (304)										
Element	С	Si	Mn	Р	Cr	Ni	Nb	Cu	Co	Ν
% Composition	0.020	0.32	1.57	0.38	18.30	8.1	0.008	0.38	0.20	0.016

	Table 2: Mechanic	cal Properties of Stainless-S	Steel Grade (304)	1
	Mechanic	cal Properties	Elongation aft	er Fracture (A%)
	Yield Stress (MPa)	Tensile Strength (MPa)	A ₅ (%)	50mm (%)
Minimum	230	450	45	40
Maximum	330	580	NA	NA

2.4.2 Design Temperature

Traditionally, increase in temperature or heat effect during reaction greatly influence the reaction media and material for construction. In order to prevent any uncertainty, the maximum allowable design stress conventionally is usually well below the material temperature.

2.4.3 Design Pressure

The MFR design just like design of other process equipment design must be made in such a way that it will overcome the maximum allowable pressure that will be applied during the process operation. Traditionally, the design pressure is about 5 to 10% higher than the operating pressure [5]. This will help alleviate extraneous actions during minor disturbance. Also, the design pressure should constitute the fluid pressure.

2.2.4 Design Stress

The maximum allowable stress that will be applied on the MFR also called the normal design strength is very important as well as the use of a standard or accurate stress factor that will control the effect of loading, uncertainty, material quality, design techniques and operation. This will enhance optimum yield, safe operation and improve equipment lifespan.

2.4.5 Welded Joint Efficiency

The lifespan of MFR also depend greatly on the type of welds, its quality and the type of welded joint used. The above factors can be taken into consideration by visual inspection and the use of radiography. For MFR construction, the butt joint is recommended under ASME BPV code sec. VII D1.

2.4.6 Corrosion Allowance

The impact of corrosion on process equipment during shutdown or operation is major threat to equipment lifespan. To enhance sustainability and improve equipment lifespan, acceptable corrosion allowance must be considered during thickness specification before the fabrication stage. The corrosion allowance usually depends on the material for construction to be used, nature of reactant species or processes involved as well as past experiences from similar processes. For MFR fabrication with stainless steel material type (304), a corrosion allowance of 4.00mm is conventionally used [21].

2.4.7 Design Load

During MFR operation, both internal and external loads which could be seen as major or minor loads are bound to occur. The MFR design should be capable enough to overcome any load (internal or external) forces that could emanate. Usually, major loads are the noticeable static loads, design pressure, total vessel weight and reactant components in it as well as wind loads and seismic loads while the minor loads are loads from shock, local stresses from support or connecting pipes and structures within, coefficient of expansion of the materials, stress due to temperature and pressure changes as well as bending moment must be put into consideration to improve functionality and lifespan of the MFR during operation or shutdown.

2.4.8 Minimum Practical Wall Thickness

Conventionally, for an equipment design and fabrication, a minimum thickness allowance is essential in order to improve the equipment rigidity, manage stresses from equipment weight and external loads connected with it.

Usually, the thickness of reacting vessels such as the MFR is a function of its diameter and corrosion allowance [5].

Consider the MFR in figure 2 for cumene production with inlet (feed) and outlet (product) streams as well as the reactor operating parameters such as temperature (T), pressure (P) and diameter (D_R).



Figure 2: Design of the MFR Thickness

The MFR thickness design models to be applied for determination of the reactor column body (cylindrical) and head (torispherical, standard ellipsoidal and flat) head are presented in equation (16), (17), (19) and (21) by [17] as;

Reactor Column Body (Cylindrical)
$$e = \frac{P_i D_i}{2JF - P_i}$$
(16)Reactor Column Head (Torispherical) $e = \frac{P_i D_i C_s}{2JF - P_i (C_s - 0.2)}$ (17) $C_s = \frac{1}{4} \left[3 + \sqrt{\frac{R_i}{R_k}} \right]$ (18)Reactor Column Head (Standard Ellipsoidal) $e = \frac{P_i D_i}{2JF - 0.2P_i}$ (19)

Reactor Column Head (Flat)

$$e = c_p D_c \sqrt{\frac{P_i}{F}}$$
⁽²⁰⁾

The total thickness of the reactor's body and heads as shown in equation (16), (17), (19) and (20) is given as

Thickness (t) = e +corrosion allowance.

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 3 and 4 respectively were computed and simulated using MATLAB.

alues	Description
13.9Kg/m ³	Density of propylene
76Kg/m ³	Density of benzene
62Kg/m ³	Density of cumene
314Nmmol ⁻¹ K ⁻¹	Gas Constant
	3.9Kg/m ³ 76Kg/m ³ 52Kg/m ³ 814Nmmol ⁻¹ K ⁻¹

(21)

Data	Values	Description	References
Т	483K	Operating temperature	[2]
k _o	$6.510 \times 10^3 \mathrm{s}^{-1}$	Frequency factor	[2]
k _i	$4.124 \times 10^{-3} \mathrm{s}^{-1}$	Rate constant	[2]
$-r_A$	$1.305 \times 10^{-5} \text{ mol/m}^{3/s}$	Reaction rate	[22]
E	52564KJ/Kmol	Activation energy	[22]

III. Result and Discussion

The results and discussion of the MFR design, the relationship between the fractional conversion and process functional parameters as well as the thickness design or specification of the reactor are presented in this section.

3.1 MFR Design Results

The design results of the MFR for the production of cumene is presented in table 5.

Table 5: Design Results of MFR Design Volume, Height, Diameter, Space Time, Space Velocity and
Quantity of Heat generated Per Unit Volume of the Reactor at various Fractional Conversion and
Operating Temperature

X _A	T(K)	$V_R(m^3)$	H _R (m)	$D_R(m)$	τ _{MFR} (s)	$S_V(s^{-1})$	Q(J/s)	q(J/m ³ s)
0.10	481.1	0.017	0.442	0.221	0.003	382.920	0.073	4.298
0.20	481.1	0.043	0.603	0.301	0.007	151.280	0.146	3.396
0.30	481.1	0.084	0.754	0.377	0.013	77.215	0.219	2.560
0.40	481.1	0.153	0.920	0.460	0.024	42.547	0.292	1.910
0.50	481.1	0.275	1.119	0.560	0.042	23.637	0.365	1.326
0.60	481.1	0.516	1.380	0.690	0.079	12.607	0.438	0.849
0.70	481.1	1.070	1.760	0.880	0.165	6.078	0.511	0.478
0.80	481.1	2.752	2.411	1.206	0.423	2.364	0.584	0.212
0.90	481.1	12.386	3.981	1.990	1.904	0.525	0.657	0.013

Table 5 represents the MFR design results for cumene production via catalytic alkylation of propylene and benzene. Using MATLAB R2023a, simulation were run at constant temperature (481.1K) and varying fractional conversions between 0.1 and 0.9. At maximum conversion of 0.9, the optimum value of the MFR functional parameters such as volume, height, diameter, space time, space velocity, quantity of heat generated as well as the quantity of heat generated per unit volume of the reactor was 12.386m³, 3.981m, 1.990m, 1.904s, 0.525s⁻¹, 0.657J/s and 0.013J/m³s respectively.

3.1.1 Profile of MFR Volume (V_R), Height (H_R), Diameter (D_R) and Fractional Conversion (X_A)



Figure 3: Graph of MFR volume (VR), Height (HR), Diameter (DR) and fractional conversion (XA)

Figure 3 is a profile of MFR functional parameters (volume, height and diameter) with an increase in fractional conversion of the reactant species during cumene production from the catalytic alkylation of propylene and benzene. The profile was generated from MATLAB simulation of the MFR design models. From the profile, the design quantities (V_R , H_R and D_R) displayed an exponential increase as the fractional conversion increases and at a maximum conversion of 0.9, the volume, height and diameter of the MFR were 12.386m³, 3.981m and 1.990m respectively.



3.1.2 Profile of MFR Residence Time (T) and Fractional Conversion

Figure 4: Graph of Residence Time (τ) and Fractional Conversion (X_A)

Figure 4 indicate that the residence time also called the space time increases exponentially as the fractional conversion increases during the alkylation process. This signifies that more yield of the target product increases as the conversion of feed increases with time. At a fractional conversion of 0.1, 0.5 and 0.9, the residence time spent by the reactant species in the reactor was 0.003 seconds, 0.042seconds and 1.904seconds respectively.

3.1.3 Profile of Space Velocity (Sv) and Fractional Conversion (XA)



Figure 5: Graph of Space Velocity (Sv) and Fractional Conversion (XA)

Figure 5 depitch the mathematical correlation between the residence time and the space velocity. The space velocity is said to be the reciprocal of space time. It is the time required to process a unit volume of the feed at inlet condition. From figure 4, the space velocity dsplayed an exponential decrease as the fractional conversion increases. The significance of this is that more conversion of the feed material or more yield of the target product

(cumene) will be produced at least value of the space velocity. At space velocity of 382.920sec⁻¹, 23.637sec⁻¹ and 0.525sec⁻¹, the volume of the reactor which depends on the yield of target product (cumene) were 0.017m³, 0.275m³ and 12.386m³ respectively.





Figure 6: Graph of Quantity of Heat (Q), Quantity of Heat Generated per unit volume (q) and Fractional Conversion (X_A).

Figure 6 is a plot of heat quantities generated during the alkylation process and MFR volume. According to the plot, the quantity of heat generated increases linearly as, the fractional conversion or reactor volume increases while the quantity of heat generated per unit volume of the reactor demonstrated an exponential decrease as the fractional conversion and reactor volume increases. At maximum fractional conversion of 0.9, the values of the quantity of heat generated and the quantity of heat generated per unit volume of the reactor were 0.694J/s and 0.053J/m³s respectively.

3.2 MFR Agitator Design

The design or specification of the MFR Agitator is presented in table 6.

Table 6: MFR Agitator Design			
MFR Agitator Parameter	Specification (Unit)		
Height of Agitator	2.981m		
Diameter of Agitator	0.990m		

Table 6 represents the sizing results of the MFR agitator height and diameter. The MFR agitator is crucial for uniform mixture or composition of the feed in the reactor during the alkylation process. The design of the MFR agitator in terms of height and diameter is dependent on the reactor height and diameter as well as minimum practical allowance or clearance. For a clearance of 1m, the MFR agitator was obtained as 2.981m and 0.990m respectively.

3.3 Design of the MFR Thickness

The thickness design or specification of the MFR is presented in table 9.

Table 7: Design of the MFR Thickness			
Thickness Parameter	Specification (Unit)		
Column Body	-		
Cylindrical	3.90mm		
Column Head Doomed	-		
Torispherical	5.84mm		
Ellipsoidal	3.90mm		
Flat	39.12mm		

Table 7 is the mechanical or thickness design of the MFR column body and head obtained from the application of the thickness design models. From the table, a column body (cylindrical body) of 3.90mm thickness was obtained while various thicknesses were obtained for the column head (torispherical, ellipsoidal and flat head). For the purpose of economics, efficiency and uniformity, a thickness of 3.90mm for the cylindrical body and column head (ellipsoidal) is recommended as the thickness for MFR construction using stainless steel material type (304) as the material for construction. The thickness was obtained by considering certain factors such as material type for construction, operating temperature and pressure, column diameter, design load, stresses, corrosion allowance welded joint efficiency, etc. The above factors were considered to ensure sustainability and improve the lifespan of the MFR for continuous operation and production of cumene.

IV. Conclusion

The research considered the design and simulation of MFR for the production of cumene from the catalytic alkylation of propylene and benzene. The design models were developed from the first principle of mass and energy balance and simulated using MATLAB R2023a version. The MFR thickness for stainless steel material type (304) construction was obtained for the column body (cylindrical) and head (ellipsoidal) in a bid to ensure continuous production, sustainability and improvement of equipment lifespan due to its ability to withstand the effect of temperature, pressure, internal and external loads as well as corrosion effect on the equipment during operation or shutdown.

Symbol	Definition	Unit
А	Propylene	-
В	Benzene	-
С	Cumene	-
K_1	Kinetic rate constant	s ⁻¹
-r _A	Depletion rate of the limiting reactant	mol/m ³ /s
C _A	Concentration of reactant specie A	mol/m ³
C _B	Concentration of reactant specie B	mol/m ³
Т	Reaction time	S
C _{AO}	Initial concentration of specie A	mol/m ³
C _{BO}	Initial concentration of specie B	mol/m ³
М	Mole ratio of initial concentration of species	Dimensionless
Ko	Arrhenius or pre-exponential constant	s ⁻¹
Е	Activation energy	KJ/kmol
Т	Operating temperature	Κ
R	Gas constant	j/molk
F _{AO}	Initial molar flow rate of feed	mol/s
V _R	Volume of the reactor	m ³
H _R	Height of the reactor	М
D _R	Diameter of the reactor	М
X _A	Fractional conversion of specie A	Dimensionless
Q	Quantity of heat generated	J/s
Q	Quantity of heat per unit reactor volume	J/m ³ s
ΔH_{P}	Heat of reactor	KJ/mol
τ	Space time	S
$\mathbf{S}_{\mathbf{V}}$	Space velocity	s ⁻¹
Vo	Initial volumetric flow rate	m ³ /s
C _p	Specific heat capacity	J/molK
A _C	Area of heat exchange	m ²
U	Heat transfer coefficient	W/m ² K

Fable	8:	Nomenclature
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T _o	Feed initial temperature	Κ
T _c	Coolant temperature	Κ
$ ho_{ m i}$	Density of species	Kg/m ³
L _{st}	Length of stirrer	М
С	Clearance	М
D _{st}	Diameter of the stirrer	М
Е	Minimum thickness	Mm
Pi	Design pressure	N/mm ²
Di	Column diameter	М
J	Welded joint efficiency	N/mm
F	Design stress factor	Dimensionless
Cs	Stress concentration factor	Dimensionless
C _p	Full face gasket (0.4)	Dimensionless
D _c	Bolt circle diameter	Mm

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