

## Design of Flow Reactors for Production of Dimethyl Ether

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**ABSTRACT:** Design of flow reactors for production of dimethyl ether from the dehydration of methanol in the presence of alumina catalyst (plug flow reactor and continuous stirred tank reactor) is presented using advanced process simulation software (MATLAB). The steady state design models used in obtaining the reactor functional parameters such as volume, length, diameter, space time, space velocity were developed by performing material balance over the reactors. The temperature effect was also accounted for using the principle of conservation of energy over the reactors. The accuracy of the design parameters were ascertained by comparing predicted results with literature data of flow reactors for production of dimethyl ether. The simulation of the design models were performed using MATLAB. The reactor operates optimally at fractional conversion of 0.9 to obtain optimum values of the most significant variables/parameters (volume of PFR  $1.15\text{m}^3$ , length of the PFR 2.09m, diameter of PFR 0.838m, space time of PFR 0.311sec, space velocity of PFR  $3.21\text{sec}^{-1}$ , quantity of heat generated per unit volume of PFR  $304.634\text{J/s/m}^3$ ) and (volume of CSTR  $1.042\text{m}^3$ , length of the CSTR 1.44m, diameter of CSTR 0.959m, space time of CSTR 0.2804sec, space velocity of CSTR  $3.567\text{sec}^{-1}$ , quantity of heat generated per unit volume of CSTR  $338\text{J/s/m}^3$ ). The result obtained from the steady state simulation shows that the feed flow rate, temperature and pressure influenced the efficiency of the flow reactors.

**Keywords:** Continuous Stirred Tank Reactor, Design and Plug Flow Reactor

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### I. INTRODUCTION

Chemical engineering design is a creative activity which can be one of the most rewarding and satisfying activities undertaken by an engineer. It is the synthesis, the putting together of ideas to achieve a desired purpose. The designer starts with a particular objective in mind, and by developing and evaluating possible designs arrives at what can be considered the best way of achieving that objective (Sinnott & Towler, 2009). In the chemical industrial a design can lead to a new chemical product, new production process or improvement of an existing one. Every industrial chemical process is designed to produce a desired product from a variety of starting materials which undergoes chemical reaction. Chemical kinetics is the study of chemical reaction rates and reaction mechanisms. Chemical Reaction Engineering combines the study of chemical kinetics with the reactors in which the reactions occur (Kayode 2001).

Chemical kinetics and reactor design are at the heart of producing almost all industrial chemicals. It is primarily knowledge of chemical kinetics and reactor design that distinguishes the chemical engineer from other engineers.

This research, design of flow reactors (Plug Flow Reactors and Continuous Stirred Tank Reactor) for production of Dimethyl Ether from Dehydration of Methanol using the Alumina as Catalyst is an activity of chemical engineering which uses information, knowledge and experience from a variety of areas which includes thermodynamics, chemical kinetics, fluid mechanics, heat transfer, mass transfer economics and optimization. Chemical reaction engineering is the synthesis of all these factors with the aim of properly designing a chemical reactor (David, 1974).

The selection of reaction system that operates in the safest and most efficient manner can be the key to the economic success or failure of a chemical plant and depends on the nature of the reactants of feed materials that is if the reactant materials is liquid phase, gas-liquid phase or solid-liquid reaction.

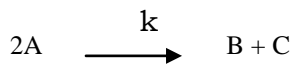
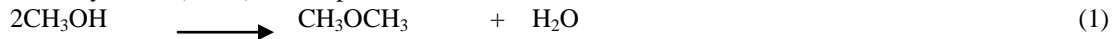
External constraints are fixed and invariable and are usually outside the designers influence. They may include physical laws, government controls, standards and codes, resources, safety regulators economic constraints etc. on the other hand, the designer have some control on internal constraints. They may include

choice of process, conditions, materials, methods, time, and personnel equipment. This research is aimed at designing a Plug Flow Reactor (PFR) and a Continuous Stirred -Tank Reactor for the production of Dimethyl Ether from dehydration of methanol (raw materials).

This research involves the use of design/performance equations, stoichiometric balance equations using first order kinetic reaction process and the condition applied in mildly exothermic.

### Reaction Kinetic Scheme

Dimethyl ether (DME) can be produced from the reaction kinetic scheme below:



Where A = methanol B = dimethyl ether

C = water

The rate equation is given by (Bondiera&Naccache, 1991) as

$$-r_A = k_0 e^{\left[ \frac{-E_0}{RT} \right]} C_A \quad (2)$$

where

$-r_A$  = Depleting rate of methanol

$C_A$  = Concentration of methanol

$K_0$  = Rate constant/pre-exponential function

$E_0$  = Activation energy

R = Gas constant

T = Standard temperature

From ideal gas equation

$$PV = nRT \quad (3)$$

$$P_i V_R = n_i RT$$

$$\frac{P_i}{RT} = \frac{n}{V_R} = C_i$$

$$C_i = \frac{P_i}{RT}$$

$$C_A = \frac{P_A}{RT} \quad (4)$$

### Development of Design Models for plug flow reactor

The following assumptions were made for the development of design/performance equations for the production of dimethyl ether.

- i. The reactor operates at steady state
- ii. The reaction takes place in the gaseous phase with constant density.
- iii. Pressure drop along the reactor is negligible (The vessel is empty and refractory lined)
- iv. The reaction mixture is composed of 2.0 moles of methanol and products, 1 of dimethyl ether and 1 mole of water

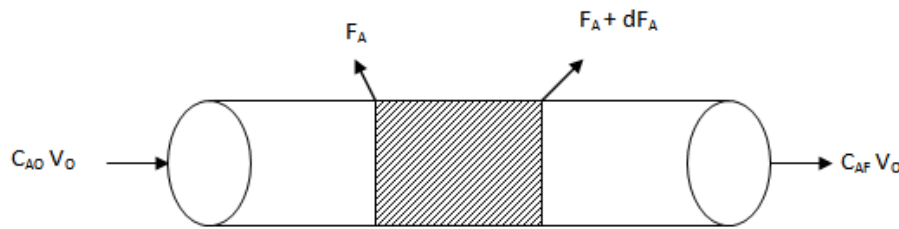


Figure 1: Plug Flow Reactor (PFR)

where

$$\begin{aligned}
 v_O &= \text{Volumetric flow rate m}^3/\text{s} \\
 C_{AO} \& C_A &= \text{Initial and final concentration of methanol} \\
 &\text{mol/m}^3, \text{ considering a unit volume of the reactor} \\
 F_A - F_A + dF_A + (-r_A) dv &= 0 \\
 dF_A + (-r_A) dv &= 0 \\
 \text{But } F_A &= F_{AO} (1 - X_A) \\
 dF_A &= -F_{AO} dX_A \\
 -F_{AO} dX_A + (-r_A) dv &= 0 \\
 F_{AO} dX_A &= (-r_A) dv
 \end{aligned} \tag{6}$$

Equation (6) accounts for A in the differential section of the reactor or volume  $dv$ . For the reactor as a whole, this expression must be integrated.  $F_{AO}$  i.e. feed rate is constant, but  $r_A$  depends on the concentration or conversion of materials.

Grouping the terms

$$\frac{dv}{F_{AO}} = \frac{dX_A}{-r_A}$$

Integrating both sides

$$\int_0^V \frac{dv}{F_{AO}} = \int_0^{X_{AF}} \frac{dX_A}{(-r_A)}$$

$$\frac{V}{F_{AO}} = \int_0^{X_{AF}} \frac{dX_A}{(-r_A)}$$

$$V_R = F_{AO} \int_0^{X_{AF}} \frac{dX_A}{(-r_A)} \tag{7}$$

$$\text{But } F_{AO} = C_{AO} V_O \tag{8}$$

$$V_R = C_{AO} V_O \int_0^{X_{AF}} \frac{dX_A}{(-r_A)} \tag{9}$$

$$\frac{V_R}{V_O} = C_{AO} \int_0^{X_{AF}} \frac{dX_A}{(-r_A)}$$

$$\tau = C_{AO} \int_0^{X_{AF}} \frac{dX_A}{(-r_A)} \tag{10}$$

### Reactor Volume ( $V_R$ ) for Plug Flow Reactor

The material balance on a differential element of the tubular reactor was rearranged to give an expression for the volume of the reactor.

$$V_R = F_{AO} \int_0^{X_A} \frac{dX_A}{k_o e^{\left[\frac{-E_o}{RT}\right]} C_A} \quad (11)$$

### Reactor Length ( $L_R$ ) for Plug Flow Reactor

The reactor volume on equation (11) expressed in terms of cross-sectional area and length was rearranged to obtain

$$L_R = \frac{4F_{AO}}{\pi D^2} \int_0^{X_A} \frac{dX_A}{k_o e^{\left[\frac{-E_o}{RT}\right]} C_A} \quad (12)$$

### Space Time ( $\tau$ ) for Plug Flow Reactor

This is the time necessary to process one reactor volume of fluid is estimated using the reactor volume expression as:

$$\tau = \frac{F_{AO} \int_0^{X_A} \frac{dX_A}{k_o e^{\left[\frac{-E_o}{RT}\right]} C_A}}{V_o} \quad (13)$$

### Space - Velocity ( $S_V$ ) for Plug Flow Reactor

This is the number of reactor volume of feed treated in a unit time and is obtained as the inverse or reciprocal of space time.

$$S_V = \frac{1}{\tau}$$

$$S_V = \frac{V_o}{F_{AO} \int_0^{X_A} \frac{dX_A}{k_o e^{\left[\frac{-E_o}{RT}\right]} C_A}} \quad (14)$$

where  $X_A$  = Fractional conversion of methanol  
 $v_o$  = Volumetric flow rate

### Selectivity $S_{DME}$

The selectivity enables the prediction of the product produced from the reaction and was introduced in other to determine reaction conditions that minimize the unwanted product  $H_2O$  from the reaction. The selectivity of the reaction product was obtained using the expression given by Fogler (1999), Coulson & Richardson (1999).

$$S_{DME} = \frac{\text{Amount of desired product formed}}{\text{Amount of all products}} \quad (15)$$

### Yield (Y)

The product distribution as reaction proceeds in each reaction was obtained using the expression for relative or instantaneous yield (Coulson & Richardson, 1991).

$$Y_{DME} = \frac{N_{DME}}{N_M} = \frac{F_{DME}}{C_M} \quad (16)$$

$$Y_{DME} = S_{DME} X_{DME} \quad (17)$$

Energy Balance

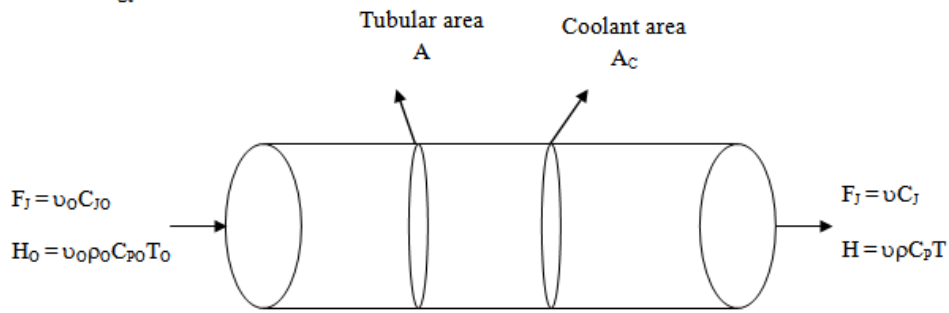


Figure 2: Energy Balance for Plug Flow Reactor

Figure 2 shows a hypothetical representation of a Plug Flow Reactor (PFR) indicating the energy balance, taking a differential balance on the enthalpy flow between Z and Z+ dz for a tube of length L and diameter D. A shell balance is made on the differential element of volume dv between Z and Z + dz. Species flow Fj and enthalpy flow in and out of this volume is balanced by the steady flow energy equation.

$$O = [UA_t \rho C_p T]_Z - [UA_t \rho C_p T]_{Z+dz} + A_t (-\Delta H_R) \gamma_i dz - UP_w (T - T_c) dz \quad (18)$$

Where

$$A_t = \text{cross sectional area of the tube} = \left[ \frac{1}{4} \pi D^2 \text{ for cylindrical tube} \right]$$

$$dv = A_t dz$$

Heat transfer occurs across the external wall of the tube, with area dAc

$$dA_c = P_w dz$$

Where, Pw is the perimeter length of the wall of the tube.

The heat transfer rate in the element is dQ = UPw dz [T - Tc]

For constant flow density and tube diameter between z and z + dz, we obtain

$$O = A_t UC_p \rho [T_Z - T_{Z+dz}] + A_t [-\Delta H_R] \gamma_i dz - UP_w (T - T_c) dz \quad (19)$$

Taking limit as dz  $\longrightarrow$  0

$$\text{Lim } (T_Z - T_{Z+dz}) \text{ as } dz \longrightarrow 0 \longrightarrow = -\frac{dT}{dZ} \cdot dz$$

Dividing through by dZ, we obtain

$$UA_t \rho C_p \frac{dT}{dZ} = A_t (-\Delta H_R) \gamma_i - UP_w (T - T_c) \quad (20)$$

For multiple reaction,

$$U \frac{dT}{dZ} = \sum_{i=1}^R \frac{-\Delta H_R}{\rho C_p} \gamma_i - \frac{UP_w}{\rho C_p A_t} (T - T_c) \quad (21)$$

Development of Design Models for CSTR

Consider the schematic representation of a continuous stirred tank reactor with feeds and product as shown in figure 2

Assumptions

- i. Runs at steady state with continuous flow of reactant and products.
- ii. The feed assumes a uniform composition throughout the reactor.
- iii. Balance can be made about the entire volume of the reactor.

- iv. The reacting mixture is well stirred.
- v. The composition of the exit stream is the same as that within the reactor.
- vi. Shaft work by the impeller or the stirrer is negligible.
- vii. The temperature within the reactor is kept at a constant value by the heat exchange medium.

#### Volume of Continuous Stirred Tank Reactor ( $V_R$ )

The Material Balance can be stated as follows

$$V_R = \pi \left( \frac{D_R}{2} \right)^2 L_R \quad (22)$$

For a CSTR,

$$\text{Let } \frac{L_R}{D_R} = 2 \quad (23)$$

$$D_R = \frac{L_R}{2} \quad (24)$$

Combining equation (22) and (24) yields

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

$$V_R = \frac{\pi L_R^3}{16}$$

$$\therefore L_R = \left( \frac{16V_R}{\pi} \right)^{1/3} \quad (25)$$

Substituting equation (11) into (25) yields

$$L_R = \left[ \frac{16 F_{AO} X_A}{\pi \cdot K_O^{-E/RT} C_{AO} (1 - X_A)} \right]^{1/3} \quad (26)$$

#### Diameter of Continuous Stirred Tank Reactor ( $D_R$ )

From equation (24)

$$D_R = \frac{L_R}{2}$$

Substituting equation (26) into (24) yields

$$D_R = \frac{\left[ \frac{16 F_{AO} X_A}{\pi \cdot K_O^{-E/RT} C_{AO} (1 - X_A)} \right]^{1/3}}{2} \quad (27)$$

#### Space Time ( $\tau_{CSTR}$ ) for Continuous Stirred Tank Reactor

This is defined as the ratio of reactor volume and volumetric flow rate

$$\tau_{CSTR} = \frac{V_R}{v_o} \quad (28)$$

Substituting equation (11) into (13) yields

$$\tau_{CSTR} = \frac{F_{AO} X_A}{K_O^{-E/RT} C_{AO} (1 - X_A) v_O} \quad (29)$$

$$F_{AO} = C_{AO} v_O \quad (30)$$

Substituting equation (30) into (29) yields

$$\tau_{CSTR} = \frac{X_A}{K_O^{-E/RT} (1 - X_A)} \quad (31)$$

### Space Velocity ( $S_V$ ) for Continuous Stirred Tank Reactor

This is defined as the reciprocal of space time.

$$S_V = \frac{1}{\tau_{CSTR}} \quad (32)$$

Substituting equation (32) into (31) yields

$$S_V = \frac{K_O^{-E/RT} (1 - X_A)}{X_A} \quad (33)$$

### Heat Generated Per Unit Volume of Continuous Stirred Tank Reactor

$$Q = \Delta H_R F_{AO} X_A \quad (34)$$

Q = Quantity of Heat (j/s)

$\Delta H_R$  = Heat of reaction (KJ/mol)

$F_{AO}$  = Flow Rate of Species (mol/s)

$X_A$  = Fractional Conversion of Species

Dividing through by  $V_R$

$$\frac{Q}{V_R} = \frac{\Delta H_R F_{AO} X_A}{V_R} \quad (35)$$

$$q = \frac{\Delta H_R F_{AO} X_A}{V_R} \quad (36)$$

Where q = quantity of heat generated per unit volume of the reactor

$$0 = \rho V_O C_p T_O - \rho V_O C_p T - (-r_A) V_R (\Delta H_R) - UA_C (T - T_C)$$

By rearranging and factorization

$$\rho V_O C_p (T - T_O) = -(-r_A) V_R (\Delta H_R) - UA_C (T - T_C)$$

Dividing through by  $\rho V_O C_p$

$$T - T_O = -\frac{(-r_A) V_R (\Delta H_R)}{\rho v_O C_p} - \frac{UA_C (T - T_C)}{\rho v_O C_p} \quad (37)$$

But  $\frac{V_R}{v_O} = \tau$  (space time)

$$T - T_O = \tau \frac{-\Delta H_R r_A}{\rho C_p} - \frac{UA_C (T - T_C)}{\rho v_O C_p} \quad (38)$$

### Stirrer Design

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

The length of the stirrer can be obtained as follows

$$L_{st} = L_R - C \quad (\text{Perry et al., 2008}) \quad (39)$$

where

$L_R$  = Length of reactor

$C$  = Clearance

$L_{st}$  = Length of Stirrer

The diameter of the stirrer can be obtained from the equation

$$D_{st} = D_R - 2C \quad (\text{Perry et al., 2008}) \quad (40)$$

$D_R$  = Diameter of the Reactor

$D_{st}$  = Diameter of the Stirrer

### Mechanical Design

This enables us to determine which material type of the flow reactors will be most economically suitable for optimum production, thereby maximizing efficiency of the reactors.

For flow reactors (plug flow reactor and continuous stirred tank reactor) of a given;

- i. Operating pressure (P)
- ii. Operating temperature (T)
- iii. Material type
- iv. Welds are fully graphed:  $J= 1$
- v. Design pressure  $P_i$

### For cylindrical section

Determination of minimum thickness (e) is given as

$$e = \frac{P_i D_i}{2JF - P_i} \quad (\text{Sinnotts\&Towler, 2009}) \quad (41)$$

where

$J$  = welded joint efficiency

$F$  = design stress

Thickness (t) = e + Corrosion Allowance (42)

### For Doomed Head

Try a Standard Dish-Head (Torispherical)

Determination of minimum thickness (e) is given as

$$e = \frac{P_i R_i C_s}{2JF - P_i (C_s - 0.2)} \quad (\text{Sinnotts\&Towler, 2009}) \quad (43)$$

where

$R_s = D_i$

$C_s$  = Stress Concentration Factor

$$C_s = \frac{1}{4} \left[ 3 + \sqrt{\frac{R_c}{R_k}} \right] \quad (\text{Sinnotts\&Towler, 2009}) \quad (44)$$

where  $P_k$  = knuckle radius = 6%  $R_c$

Thickness (t) = e + corrosion allowance

### For Standard Ellipsoidal Head

Determination of minimum thickness (e) is given as

$$e = \frac{P_i D_i}{2JF - 0.2P_i} \quad (\text{Sinnotts\&Towler, 2009}) \quad (45)$$

Thickness (t) = e + Corrosion Allowance

### For Flat Head

Determination of minimum thickness (e) is given as



$$e = C_p D_c \sqrt{\frac{P_i}{f}} \quad (\text{Sinnotts\&Towler, 2009}) \quad (46)$$

where

$C_p = 0.4$  (full face gasket)

$D_c =$  Bolt circle diameter

Thickness (t) e + Corrosion Allowance

### Costing of Flow Reactors

The capital cost of a Plug Flow Reactor and continuous flow stirred tank reactor unit is given by

$$\text{Cost} = \$200,000 \left( \frac{V_R}{1000} \right)^{0.6} \quad (47)$$

According to John, (2007) where  $V_R$  is the volume of PFR/ CSTR in  $m^3$ . The above equation is for a life of 20 years with no salvage values.

### Determination of Design Parameters

#### Mass Flow Rate of Reactants and Products (G)

The mass flow rate of reactants and products can be calculated as follows: using a given production rate

Mass flow rate of methanol ( $G_A$ )

$$G_A = \frac{M_A}{M_C} \times G_C \quad (48)$$

Where

$G_C =$  Mass flow of DME (product of interest) in kg/s

$M_A =$  Molecular weight of methanol (kg/mol)

$M_C =$  Molecular weight of DME (kg/mol)

Mass flow rate of alumina catalyst ( $G_B$ )

$$G_B = \frac{M_B}{M_C} \times G_C \quad (49)$$

where

$G_B =$  Mass flow rate of alumina catalyst (kg/s)

$M_B =$  Molecular weight of alumina catalyst (kg/mol)

Mass flow rate of water ( $G_D$ )

$$G_D = \frac{M_D}{M_C} \times G_C \quad (50)$$

where

$G_D =$  Mass flow rate of water(kg/s)

$M_D =$  Molecular weight of water(kg/mol)

#### Specific Density of Reactants and Products ( $\bar{V}$ )

This is defined as the reciprocal of density of various species.

Specific volume of Methanol ( $\bar{V}_A$ )

$$\bar{V}_A = \frac{1}{\rho_A} \quad (51)$$

where

$\bar{V}_A =$  Specific volume of methanol ( $m^3/kg$ )

$\rho_A =$  Density of methanol ( $kg/m^3$ )

Specific Volume of Alumina Catalyst ( $\bar{V}_B$ )

$$\left(\bar{V}_B\right) = \frac{1}{\rho_B} \quad (52)$$

where

$\bar{V}_B$  = Specific volume of alumina catalyst ( $\text{m}^3/\text{kg}$ )

$\rho_B$  = Density of alumina catalyst ( $\text{kg}/\text{m}^3$ )

### Volumetric Flow Rate of Reactants and Products ( $Q_A$ )

This is defined as the product of mass flow rate and specific density.

Volumetric Flow Rate of Methanol ( $Q_A$ )

$$Q_A = G_A \bar{V}_A \quad (53)$$

where

$Q_A$  = Volumetric flow rate of methanol ( $\text{m}^3/\text{s}$ )

$G_A$  = Mass flow rate of methanol ( $\text{kg}/\text{s}$ )

$\bar{V}_A$  = Specific volume of methanol ( $\text{m}^3/\text{kg}$ )

Volumetric flow rate of Alumina Catalyst ( $Q_B$ )

$$Q_B = G_B \bar{V}_B \quad (54)$$

where

$Q_B$  = Volumetric flow rate of alumina catalyst ( $\text{m}^3/\text{s}$ )

$G_B$  = Mass flow rate of alumina catalyst ( $\text{kg}/\text{s}$ )

$\bar{V}_B$  = Specific volume of alumina catalyst ( $\text{m}^3/\text{kg}$ )

**Table 1:** Design Data

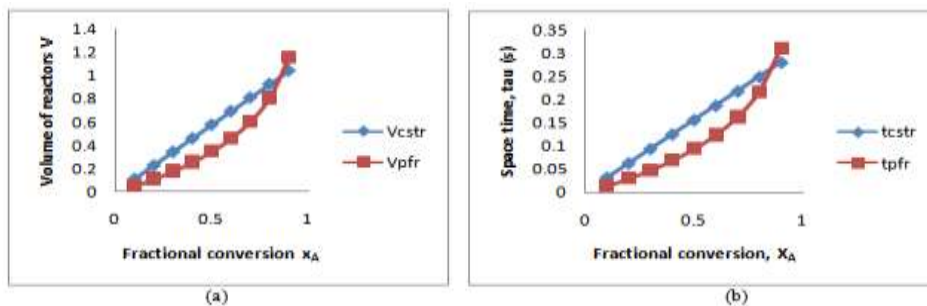
Data/parameter	Values	Description
$M_A$	64kg/mol	Molecular weight of methanol
$M_B$	100kg/mol	Molecular weight of alumina catalyst
$M_C$	46kg/mol	Molecular weight of DME
$M_D$	18kg/mol	Molecular weight of water
$G_C$	1.93kg/s	Mass flow rate of DME
$G_A$	2.69kg/s	Mass flow rate of methanol
$G_B$	4.20kg/s	Mass flow rate of alumina catalyst
$G_D$	0.76kg/s	Mass flow rate of water
$\bar{V}_A$	0.00126 $\text{m}^3/\text{kg}$	Specific volume of methanol
$\bar{V}_B$	0.885 $\text{m}^3/\text{kg}$	Specific volume of alumina catalyst
$Q_A$	0.00339 $\text{m}^3/\text{s}$	Volumetric flow rate of methanol
$Q_B$	3.717 $\text{m}^3/\text{s}$	Volumetric flow rate of alumina catalyst
$V_O$	3.720 $\text{m}^3/\text{s}$	Sum of volumetric flow rate of reactants
$C_{AO}$	0.4107 $\text{mol}/\text{m}^3$	Initial concentration of methanol
$F_{AO}$	1.53 $\text{mol}/\text{s}$	Initial molar flow rate of methanol
$X_A$	0.9(dimensionless)	Fractional conversion

**Table 2:** Data Obtained from Literature

Data	Values	Description	References
$T_0$	498k	Initial temperature of feed	Irene et al., (2013)
$K_0$	$1.21 \times 10^6 \text{ kmol}/(\text{m}^3 \text{ cat.hkpa})$	Pre-exponential factor	Bondiera & Naccache (1991)
E	80.48kj/mol	Activation energy	Bondiera & Naccache (1991)
T	533k	Operating temperature of the reactor	Bondiera & Naccache (1991)
$C_p$	2.53j/mol k	Specific heat capacity of propylene oxide	Bondiera & Naccache (1991)
T	24		Dagde & Harry, (2016)
L	6m	Length of catalyst bed	Dagde & Harry, (2016)
$\Delta H_R$	256j/mol	Change in heat of reaction	

**Solution Techniques**

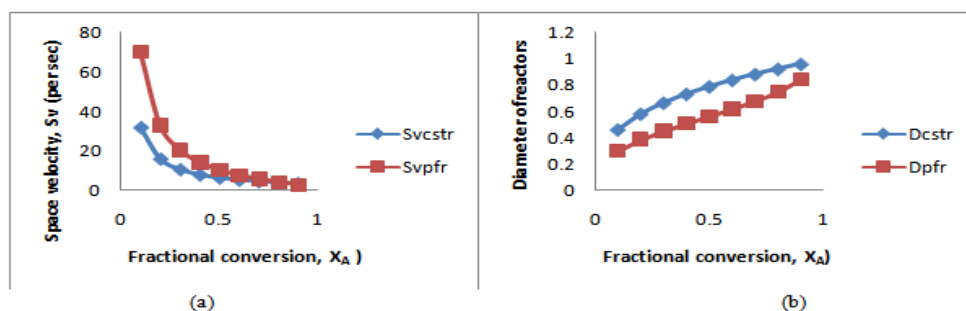
The models were solved numerically using 4<sup>th</sup> order Range-Kutta algorithm. The functional parameters of the flow reactors i.e. continuous stirred-tank reactor and plug flow reaction were compared to ascertain the better performed reactor. The pressure drop is one of the characteristics of the plug flow reactor was studied and profiles taken versus degree of conversion.



**Figure 3:** Plots of (a) Volume of reactor and (b) Space time against Fractional Conversion for PER & CSTR

Figure 3 depicts volume of reactors and Space time against fractional conversion, respectively. Generally at ambient temperature, the volume of the reactors increased as the fractional conversion increased. For CSTR, there was linear increase of volume with fractional conversion  $x_A$  while for PFR; there was exponential increase of volume of reactor with  $X_A$ . At 0.9 conversion,  $V_{PFR} = 1.16\text{m}^3$  and  $V_{CSTR} = 1.04\text{m}^3$ . The volume of plug flow reactor is greater than that of the continuous stirred-tank reactor. Hence, more yields at same condition as obtained from plug flow reactor than CSTR. PFR is a better performed reactor.

Space time for the reactors (PFR and CSTR) against  $X_A$  according to Figure 3(b) shows that the space time increases as fractional conversion increase for both reactors but for PFR, the space time was higher with values 0.31secs and 0.28secs respectively as compared with continuous stirred tank reactor. The results proved that PFR is a better performed reactor.



**Figure 5** Plot of (a) Space Velocities and (b) Diameter of Reactor against Fractional Conversion for both PER & CSTR

Figure 5(a) showed that there is a relationship of space velocity of reactors against  $X_A$  that the space velocity is highest at least  $X_A$  and lowest at highest  $X_A$ . At  $X_A = 0.9$ , PFR has the least value of space velocity than the CSTR. This shows that the PFR was the best reactor for the reaction process at lower space velocity, the highest the volume of reactor, the more products gotten, and the more profit.

Figure 5(b) showed that diameter of the CSTR and PFR with  $X_A$  at constant temperature (298k) and that though the dimensions of the CSTR and PFR are not the same, the diameters generally increases as fractional conversion does. This give values at 0.9 conversion as 0.96m and 0.84m respectively for CSTR and PFR.

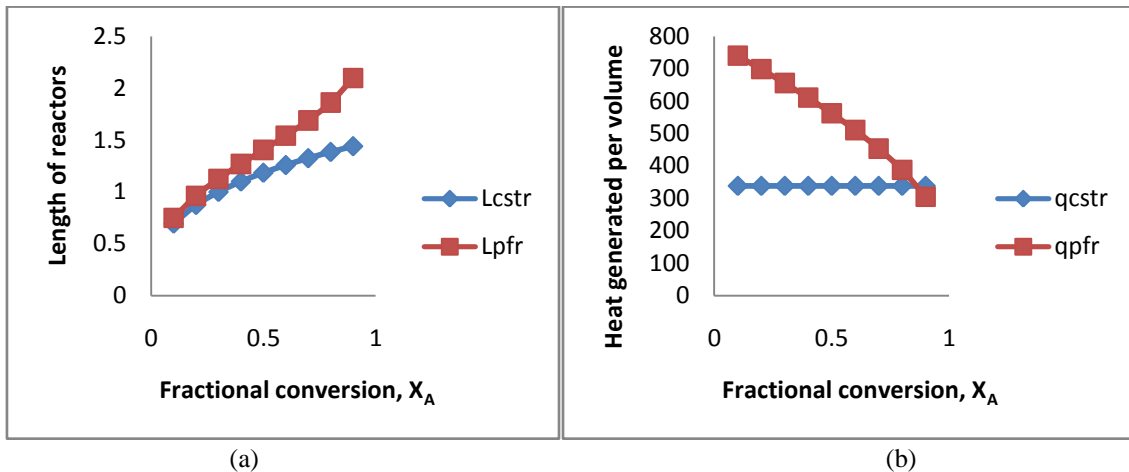


Figure 7 Graph of (a) Length of reactors (b) Heat Generated per volume against Fractional conversion for both PER & CSTR

Figure 7(a) depicts the profile of the length of the reactors (PFR and CSTR) against fractional conversion. The length of reactors generally increased as the  $X_A$  and values of length at  $X_A = 0.9$  were respectively for CSTR and PFR were 1.44m and 2.10m. Due to high length of PFR give rise to high volume produced, hence better performed reactor as compared to CSTR. Figure 7(b) Plots of Heat Generations for PFR & CSTR against Fractional Conversion Heat generated per unit volume of reactors (CSTR and PFR) is one of the characteristics of the flow reactor that predicts conservation of energies and how it can reduce cost. Figure 7(b) shows the heat generated per unit volume against the fractional conversion. The heat generated per unit volume decreased as  $X_A$  increased. For quantity of heat generated per unit volume (q) decreased, then energy is geared towards conservation and hence maximize profit from the graph, at  $X_A = 0.9$ ,  $q_{PFR} = 304.63 \text{ kW/m}^3$  and  $q_{CSTR} = 338.25 \text{ kW/m}^3$ . This informed us that at  $X_A = 0.9$ , the productivity was at highest level and the heat generated per unit volume was at least and PFR gave the least value of q and maximized profit. Note also that the heat generated per unit volume of CSTR is steady throughout the  $X_A$ .

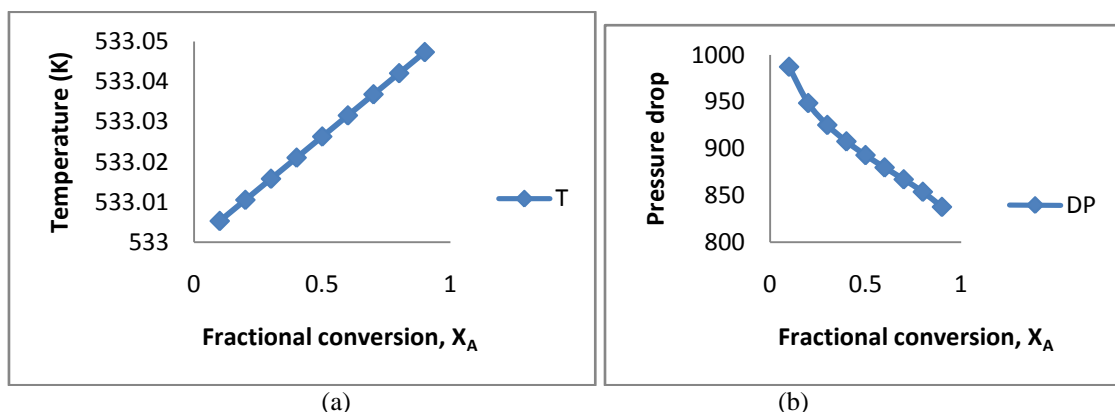


Figure 9 Plots of (a) Temperature distribution and (b) Pressure Drop against Fractional Conversion of CSTR.

Figure 9(a) shows the energy balance profile of CSTR against fractional conversion. The temperature increased from  $T=533\text{K}$  at  $X_A = 0.9$  increased in temperature, indicates that the reaction was endothermic.

Figure 9(b) depicts the pressure drop (kpa) against fractional conversion. The pressure drop decreased as  $X_A$  increased. This is the characteristic of plug flow reactor. Hence at  $X_A = 0.1$ ,  $\Delta p = 987\text{kpa}$  and increased to  $X = 0.9$ ,  $\Delta p = 837.5\text{kpa}$

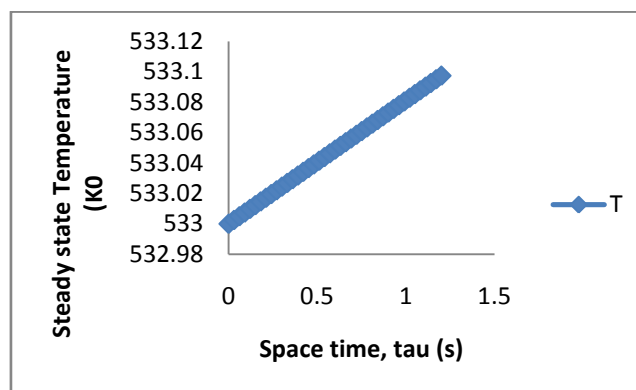


Figure 11 Plots of Steady State Temperature of PFR against Space Time

Figure 11 shows profile of temperature of PFR against space-time. There is increase of temperature as fractional conversion increases. Comparatively, the heat increased for PFR is small compared to that of CSTR. The steady state temperature profile is a good criterion to investigate the performance of the reactors PFR in better performed than the CSTR because the heat increase is very small compared to the heat of CSTR.

## II. CONCLUSION

Flow reactors (plug flow reactor and continuous stirred tank reactor) can be designed to produce 50,000.00 metric tons per year of Dimethyl Ether using dehydration of methanol in the presence of alumina catalyst. The reaction occurs at temperature not exceeding 533K. At 0.9 fractional conversion, the plug flow reactor had more yield than the continuous stirred tank reactor. This is also true with the space time, space velocity, and length of reactor. The heat generated per unit volume decreases with increase in the fractional conversion for the plug flow reactor. This means that most of the heat energy is geared towards conversion. This characteristic of plug flow reactor helps to maximize profit. The heat generated per unit volume remains almost constant against the fractional conversion for a CSTR. This is also evidence in the cost of production: under the same operating conditions, Continuous Stirred Tank Reactor costs more than the Plug Flow Reactor.

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