

# Modelling Of Non-Isothermal Plug Flow Reactor Adsorption Tower For Sulpur Trioxide Hydration Using Vanadium Catalyst

Goodhead T.O, Abowei M.F.N

Department of Chemical/ Petrochemical Engineering, Department of Chemical/ Petrochemical Engineering Rivers State University of Science and Technology, Rivers State University of Science and Technology Nkpolu, Port Harcourt, Rivers State, Nigeria. Nkpolu, Port Harcourt, Rivers State, Nigeria.  
Email: tgoodhead@yahoo.co.uk, fiboweng@yahoo.com

**ABSTRACT:** An isothermal plug flow reactor for the production of sulphuric acid over a range of degree of conversion,  $X_A = 0.95$  to  $0.99$  and reactor diameter,  $D_i = 0.05$  to  $0.1$ m have been designed. The reactor which operates at atmospheric pressure is capable of producing 10,000 metric tons per annum. This reactor is designed with hastelloy because it possesses an excellent corrosion and sulphuric acid resistance properties. The reactor performance models are simulated with the aid of a Computer using MATLAB (R2007b). The results provided information for the functional parameters for the reactor which include; the reactor volume, space time, space velocity, rate of heat generation per unit volume of reactor, pressure drop, and length of reactor. The relationship between these parameters and the degree of conversion are presented graphically.

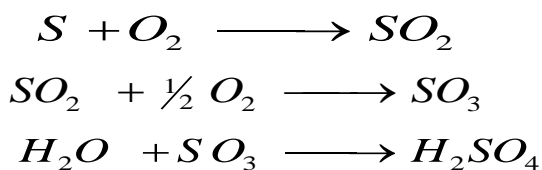
**Keywords :** Sulphur , Vanadium Catalyst, Modelling , Plug Flow Reactor

## 1 INTRODUCTION

Sulphuric acid is a very important commodity chemical and indeed, a nation's sulphuric acid production is a good indicator of its industrial strength [1]. The search for the modification in sulphuric acid production is a global concern [2]. This is due to the importance attached to the use of the acid. Therefore, this work is focused on the development of reactor types at isothermal and non isothermal conditions. Reactor types addressed in this work at the above specified conditions include.

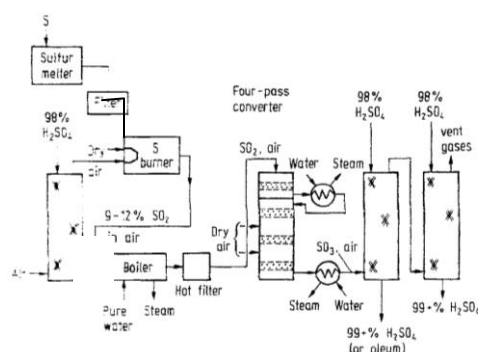
- Semi -batch reactor
- Continuous stirred tank reactors
- Plug flow reactors.

The design and operation of such equipments require rates of both physical and chemical process. The principles governing such physical process as energy transfer and mass transfer are often as important as those which govern chemical kinetics. This combination of physical and chemical operations is also a distinguishing feature of chemical engineering. Industrial chemical reactors are used to carry out chemical reactions in commercial scale. Often times in reactor design we want to know the size, type of reactor and method of operation that are best for a given reaction. Industrial scale production of sulphuric acid is dependent on the oxidation of sulphur dioxide to sulphur trioxide in fixed bed catalytic reactors. [3]. The Chemistry for the production of sulphuric acid is presented thus as follows:



Through the years, several catalyst formulations have been employed, but one of the traditional catalytic agents has been Vanadium pentoxide ( $V_2O_5$ ). Its principal applications include; ore processing, fertilizer manufacturing, oil refining, waste water processing, chemical synthesis etc. [4]. The general schematic presentation for the production of sulphuric acid is given

below.



**Figure 1.1:** Contact process for making sulfuric acid and Oleum from sulfur.

It is worthwhile to continue to research on the best hypothetical reactor unit for the production of sulphuric acid. That actually formed the basis of this thesis. The task of this thesis is to design ideal fluid-fluid contactor units that would produce sulphuric acid in commercial quantity at the lowest possible cost from gaseous sulphur trioxide and water as absorbent. The production of the acid is considered on the three principal types of reactor – semi-batch reactor, continuous stirred tank reactor and plug flow absorption reactor in a view of selecting the best absorption reactor with the best operating condition that would give the minimum capital and operational cost to achieve maximum output. In the industrial chemical process, heterogeneous fluid-fluid reactions are made to take place for one of three reasons. First, the product of reaction may be a desired material. Such reactions are numerous and can be found in practically all areas of the chemical industry where organic and inorganic syntheses are employed [5]. Fluid-fluid reactions may also be made to take place to facilitate the removal of an unwanted component from a fluid. Thus the absorption of a solute gas by water may be accelerated by adding a suitable material to the water which will react with the solute being absorbed. The third reason for using fluid-fluid systems is to obtain a vastly improved product distribution for

homogeneous multiple reactions than is possible by using the single phase alone. The area of interest in this study is of absorption with chemical reaction. Absorption is the process of removing one or more constituents of a gaseous mixture by treating it with a liquid. The necessary condition is the solubility of these constituents in the absorbing liquid. The soluble constituents of the gas mixture are called active components and the others, being practically insoluble, are called inert components [6], [7]. The reverse process of removing a gas from a solution is called stripping or desorption. The direction of mass transfer depends on the way the liquid-gas composition deviates from the mutual equilibrium state. If the concentration of the active component in a gas is higher than its concentration when it is in equilibrium with the liquid, mass transfer occurs from the gas phase to the liquid phase. On the other hand, when its concentration in the gas is lower than that corresponding to its equilibrium with the liquid, mass transfer occurs from the liquid phase to the gas phase. Absorption or stripping processes may be handled in two ways.

- a) **Statically:** This is done in order to know the equilibrium state between the phases and the deviation of the actual compositions of the two phases from the equilibrium state.
- b) **Kinetically:** This indicates the rate of the process under the given conditions or helps find conditions for running the process economically [6]. Gas absorption with reaction is usually carried out in columns. The process column requirement could be single unit, two units or multiple units, depending on choice and mixture composition. Absorption columns are vertical, cylindrical vessels containing devices that provide intimate contacting of the rising vapour (or gas) with the descending liquid. This contacting provides opportunity for the two streams to achieve some approach to thermodynamic equilibrium. Depending on the type of internal devices used, the contacting may occur in discrete steps called plates or trays, or in a continuous differential manner on the surface of a packing material [5]. The fundamental requirement of the column is to provide efficient and economic contacting at the required mass transfer rate. Individual column requirements vary from high vacuum to high pressure, from low to high liquid rates, from clean to dirty systems and so on. As a result a large variety of internal devices have been developed to fill these needs. [7]. For the case under investigation—gas absorption with chemical reaction, the following factors will determine the design method used.
  - The overall rate expression: Since materials in the two separate phases must contact each other before reaction can occur, both the mass transfer and the chemical rates will enter the overall rate expression.
  - Equilibrium solubility: The solubility of the reacting components will limit their movement from phase to phase. This factor will certainly influence the form of the rate equation since it will determine whether the reaction takes place in one or both phases.
  - The contacting scheme: In gas-liquid systems semi-batch and counter current contacting schemes predominate. In liquid-liquid systems mixed flow and batch contacting are used in addition to counter and cocurrent contacting. [5].

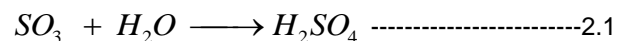
Many possible permutations of rate, equilibrium, and contacting pattern can be imagined; however, only some of these are important in the sense that they are widely used on the technical scale.

## 1.2 Definition of Problem of Study

Sulphuric acid is an important commercial commodity. Related literatures have shown that its demand for consumption has exceeded its supply [8], [1]. The traditional methods of its production in pure form could not cope with the demand [9]. The lead chamber process and the contact process have been used to produce the acid in commercial quantity. The lead chamber process produces acid of very low grade, both in purity and concentration. However, the contact process produces acid of high concentration and purity but the process of its manufacture is very expensive. This process utilizes very expensive catalyst (Vanadium pent oxide). As a result the acid from this process is equally expensive. Hence, to ensure availability and affordability of the product with acceptable quality, there is need to look for alternative methods of its production. Substantial works had been done and documented on the kinetics of sulphuric acid production [2]. Literatures have shown that direct dissolution of sulphur trioxide in water to produce the acid is not done due to very high heat of reaction occasioned in the process. Instead sulphur trioxide is absorbed in concentrated sulphuric acid to form oleum, and subsequently diluted with water to form sulphuric acid of 98%-100% concentration. Although the production of sulphuric acid is eminent and known globally, related literatures have shown that numerous treaties have been written and published on it [2]. The purpose of this research is to investigate into past works on the development of performance models for reactor types for the production of sulphuric acid, and to specifically identify and develop appropriate performance models for the areas that are deficient in past work. However, little or no known published work had been recorded for the development of performance models for the production of the acid using batch reactor, continuous stirred tank reactor, and plug flow reactor. This present work is aimed at addressing this seemingly neglected area.

## 2. Kinetics Analysis

The reaction mechanism as presented in equation (2.28) showed chain reaction characteristics [10]. Gibney and ferracid reported on the photo-catalysed oxidation of  $SO_3^{2-}$  by (dimethyl-glyoximate)  $(SO_3)_2^{3-}$  and its  $(Co(dimethyl-glyoximate)(SO_3)_2)^3$  [11], [12] The work showed that the reaction



is described as irreversible bimolecular chain reaction. Further research into the works of Erikson and Huie, et al established the reaction as second order reaction with rate constant  $K_2 = 0.3 \text{ mole/sec}$  [13], [14]. Morokuma and Mugurama performed abinitio calculation and determined the energetic barrier and established conclusively that the irreversible biomolecular nature of the reaction have  $\Delta H_r = -25 \text{ kcal/mol}$  at  $25^\circ\text{C}$  [15]. Following the outcome of the work of Chenier as cited above, the rate expression for the formation and production of sulphuric acid is summarized as in equation (2.28). [1]

$$-R_A = K_2 [SO_3] [H_2O] \dots\dots\dots 2.2$$

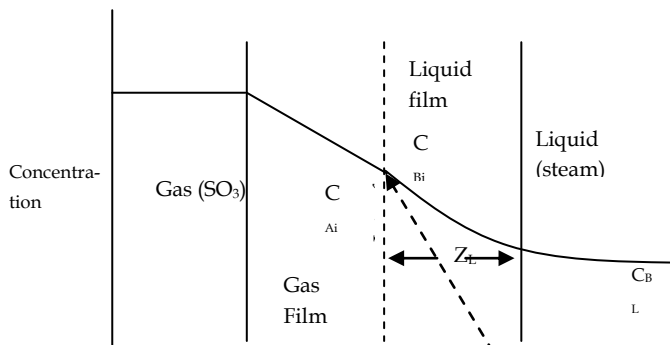
Hence from equation (2.2) the amount of SO<sub>3</sub> and H<sub>2</sub>O that have reacted at any time t can be presented as;

$$-R_A = K_2 [C_{A0} - C_{A0}X_A] [C_{B0} - C_{A0}X_A] \dots\dots\dots 2.3$$

Where

- C<sub>A0</sub> = Initial concentration of SO<sub>3</sub> (moles/Vol)
- C<sub>B0</sub> = Initial concentration of H<sub>2</sub>O ( moles/Vol)
- X<sub>A</sub> = Fractional conversion of SO<sub>3</sub>(%)
- R<sub>A</sub> = Rate of disappearance of SO<sub>3</sub> (mole/ Vol/t)

In this work, the rate expression (-R<sub>A</sub>) as in equation (2.7) will be used to develop the hypothetical semi-batch reactor, continuous stirred tank reactor and plug flow reactor design equations with inculcation of the absorption coefficient factor as recommended in the works of Van-Krevelen and Hoftyger. [16], [17]. This is achieved by modifying equation (2.3) as illustrated below. The hypothetical concentration profile of the absorption of sulphur trioxide by steam (H<sub>2</sub>O) is represented in figure.5



**Figure 2.3:** Absorption with chemical Reaction  
Distance normal to phase boundary

Sulphur trioxide (A) is absorbed into the steam (B) by diffusion. Therefore the effective rate of reaction by absorption is defined by

$$-R_A = \frac{rD_L}{Z_L} (C_{Ai} - C_{AL}) = rK_L (C_{Ai} - C_{AL}) \dots\dots\dots 2.4$$

Invoking the works of Krevelen and Hoftyzer [16], [17], the factor r is related to C<sub>Ai</sub>, D<sub>L</sub> and K<sub>L</sub> to the concentration of steam B in the bulk liquid C<sub>BL</sub> and to the second order reaction rate constant K<sub>2</sub> for the absorption of SO<sub>3</sub> in steam solution.

Thus

$$r = \frac{(K_2 D_L C_{BL})^{1/2}}{K_L} \dots\dots\dots 2.5$$

Substituting equation (2.5) into (2.4) results in

$$-R_A = (C_A) C_{BL}^{1/2} K_2^{1/2} D_L^{1/2} \dots\dots\dots 2.6$$

Previous reports showed that the amount of SO<sub>3</sub> (C<sub>A</sub>) and steam (C<sub>BL</sub>) that have reacted in a bimolecular type reaction with conversion X<sub>A</sub> is C<sub>A0</sub>X<sub>A</sub>. [18] Hence equation (2.6) can be

rewritten as

$$-R_A = K_2^{1/2} D_L^{1/2} (C_{B0} - C_{A0} X_A)^{1/2} (C_{A0} - C_{A0} X_A) = K_2^{1/2} D_L^{1/2} C_{A0}^{3/2} (m - X_A)^{1/2} (1 - X_A) \dots\dots\dots 2.7$$

Where

$$m = \frac{C_{B0}}{C_{A0}} \text{ - The initial molar ratio of reactants}$$

-R<sub>A</sub> = Rate of disappearance of SO<sub>3</sub>

K<sub>2</sub> = Absorption reaction rate constant

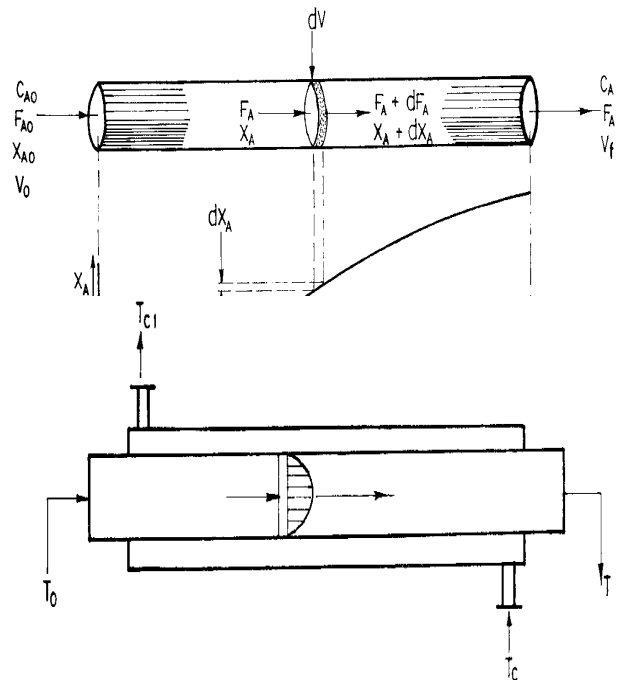
D<sub>L</sub> = Liquid phase diffusivity of SO<sub>3</sub>.

K<sub>L</sub> = Overall liquid phase mass transfer coefficient

r = Ratio of effective film thickness for absorption with chemical reaction.

### 3. Development of Performance model

In order to develop the necessary performance model equation for use in this work, we consider the reactor model as schematically presented in fig. 3.4 and 3.5, noting that a non-isothermal case is being investigated thus necessitating the use of the heat balance equation.



**Figure 3.2:** Hypothetical Heat Exchanger Unit

Considering the heat balance equation over the element of volume, dV<sub>R</sub>. The heat balance equation is given by:

$$\left\{ \begin{array}{l} \text{Rate of heat production} \\ \text{by reaction} \\ \text{within element of} \end{array} \right\} = \left\{ \begin{array}{l} \text{Rate of heat} \\ \text{flow Out of} \\ \text{element of} \end{array} \right\} + \left\{ \begin{array}{l} \text{Rate of heat removal} \\ \text{by heat transfer from} \\ \text{element of volume} \end{array} \right\} \quad (3.1)$$

For a plug flow reactor, we know the rate of heat accumulation is zero. But, Rate of heat flow out of element of volume =  $G_p C_p dT$  (3.2)

Rate of heat removal by heat transfer from element of volume

$$= U (T - T_c) dA_t \quad (3.3)$$

Rate of heat production by reaction within element of volume

$$= (-\Delta H_R) R_A dV_R \quad (3.4)$$

Substituting equation (3.2) (3.3) and (3.4) into (3.1) gives.

$$(-\Delta H_R) R_A dV_R = G_p C_p dT + U (T - T_c) dA_t \quad (3.5)$$

Where

U = Overall heat transfer coefficient, (kJ/s.m<sup>2</sup>.K)

T = Temperature of reaction mixture, (K)

T<sub>c</sub> = Temperature of cooling fluid, (K)

dA<sub>t</sub> = Effective heat transfer area in the element of volume, (m<sup>2</sup>)

G<sub>p</sub> = Total product flow rate through the reactor (Kg/s)

C<sub>p</sub> = Specific heat capacity, (KJ/Kg.K)

-ΔH<sub>R</sub> = Heat of dissolution reaction, (kJ/mole)

dT = Temperature change in the element of volume, (K)

To = Inlet temperature, (K),

Putting,

$$dA = 4dV_R/D_i \quad (3.6)$$

into equation (3.5) gives

$$\frac{4U(T - T_c)dV_R}{D_i} + G_p C_p dT = (-\Delta H_R) R_A dV_R \quad (3.7)$$

Re-arranging

$$\left[ \frac{4U(T - T_c)}{D_i} + (-\Delta H_R) R_A \right] dV_R = G_p C_p dT \quad (3.8)$$

Recall that

$$-R_A = \frac{dc_A}{dt} = K \frac{1}{2} D \frac{1}{L} C_{A0}^{\frac{3}{2}} (m - X_A)^{\frac{1}{2}} (1 - X_A) \quad (3.9)$$

$$\frac{dV_R}{dT} = f(V, T) = \frac{G_p C_p}{\left[ \frac{4U(T - T_c)}{D_i} + (-\Delta H_R) K \frac{1}{2} D \frac{1}{L} C_{A0}^{\frac{3}{2}} (m - X_A)^{\frac{1}{2}} (1 - X_A) \right]}$$

Integration of equation (3.9) using the 4<sup>th</sup> order Runge-Kutta grill method (Stroud, 1986) yields

$$V_R = V_{R0} + \Delta V_{R0} \quad (3.10)$$

Where

$$V_{R0} = 0$$

$$V_R = \Delta V_{R0} = \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4) \quad (3.11)$$

$$\left. \begin{aligned} K_1 &= \Delta T f (V_{R0}, T_0) = T (V_{R0}) \\ K_2 &= \Delta T f \left( T_0 + \frac{1}{2} \Delta T, V_{R0} + \frac{1}{2} K_1 \right) \\ K_3 &= \Delta T f \left( T_0 + \frac{1}{2} \Delta T, V_{R0} + \frac{1}{2} K_2 \right) \\ K_4 &= \Delta T f (T_0 + \Delta T, V_{R0} + K_3) \end{aligned} \right\} \quad (3.12)$$

Where

$$\Delta T = T_1 - T_0 = T_2 - T_1 = T_3 - T_2 = \dots = T_n - T_{n-1} = \text{constant}$$

### 3.1.1 Reactor Length

$$\text{From the relationship } V_R = \pi R^2 L_R \quad (3.13)$$

Combining equations (3.11) and (3.13) yields

$$L_R = V_R / \pi R^2$$

$$= \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4) / \pi R^2 \quad (3.14)$$

$$\text{Where } \pi = \text{constant} = \frac{22}{7}$$

R = Reactor radius (m)

### 3.1.2 Space Time

The space time T<sub>s</sub> for a given conversion is often used as a measure of the performance of a flow reactor. It is obtained thus,

$$T_s = \frac{V_R}{V_0} = \frac{C_{A0} V_R}{F_{A0}} = \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4) / \frac{V_0}{C_{A0}} \quad (3.15)$$

The space time (T<sub>s</sub>) measured in time unit (i.e hour or second) is the time required to process one reactor volume of feed measured at specific conditions.

### 3.1.3 Space Velocity

The space velocity (V<sub>s</sub>) like the space time is also a proper performance measure of flow reactors. It is the reciprocal of the space time, i.e.

$$V_s = \frac{1}{T_s} = \frac{V_0}{V_R} = \frac{F_{A0}}{C_{A0} V_R} = \frac{V_0}{\frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4)} \quad (3.16)$$

The space velocity is the number of reactor volumes of feed at specified condition which can be treated in unit time, where

V<sub>0</sub> = Volumetric flow rate (m<sup>3</sup>/sec)

F<sub>A0</sub> = Molar feed rate of SO<sub>3</sub> to the reactor (moles/sec)

C<sub>A0</sub> = Initial concentration of SO<sub>3</sub>

### 3.1.4 Heat Generation Per Reactor Volume

The heat generated per reactor volume is obtained from the relationship.

$$R_q = \frac{(-\Delta H_R) F_{A0} X_A}{V_R} \quad (3.17)$$

Substitution of question (3.11) in (3.17)) yields

$$R_q = \frac{(-\Delta H_R)F_{AO}X_A}{\frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)} \quad (3.18)$$

Where

$X_A = \text{SO}_3$  conversion

### 3.1.5 Pressure Drop Along Reactor Length

The pressure drop ( $\Delta p$ ) corresponding to the designed flow rate is often relatively small and does not usually impose any serious limitation on the condition of operation. The pressure drop must, of course be calculated as part of the performance parameter. Only for gases, at low pressure or, case of high viscosity e.g. polymers, is the pressure drop likely to have a major influence on the performance [19], [20]. Assuming Viscosity number,  $N_{vis} = 1$ , we have

$$\Delta p = 8J_h \left( \frac{L_R}{D_i} \right) \rho V^2 / 2 \quad [21] \quad (3.19)$$

Where

$J_h = \text{Friction factor} = 0.027 / (N_{RE})^{0.2} \quad (3.20)$

$L_R = \text{Length of reactor (m)}$

$D_i = \text{Diameter of reactor (m)}$

$\rho = \text{Density of reaction mixture (kg/m}^3\text{)}$

$V = \text{Linear velocity of reaction mixture (m/s)}$

$N_{RE} = GD_i / \mu \quad (3.21)$

Where

$G = \text{Mass flow rate (kg/sm}^2\text{)}$

$\mu = \text{Viscosity of mixture (kg/sm)}$

$G = G_p / S_i \quad (3.22)$

Where

$S_i = \pi D_1^2 / 4 \quad (3.23)$

$G_p = \text{Total product flow rate through the reactor (kg/sec)}$

$S_i = \text{Cross-sectional flow area inside the reactor (m}^2\text{)}$

The computation of the functional parameters of the reactor as shown in figure 2 is implemented in MATLAB, and the computer flow chart describing the computation is illustrated in figure3:

### 3.1.6 ALGORITHM FLOW CHART FOR NON-ISOTHERMAL PLUG FLOW REACTOR

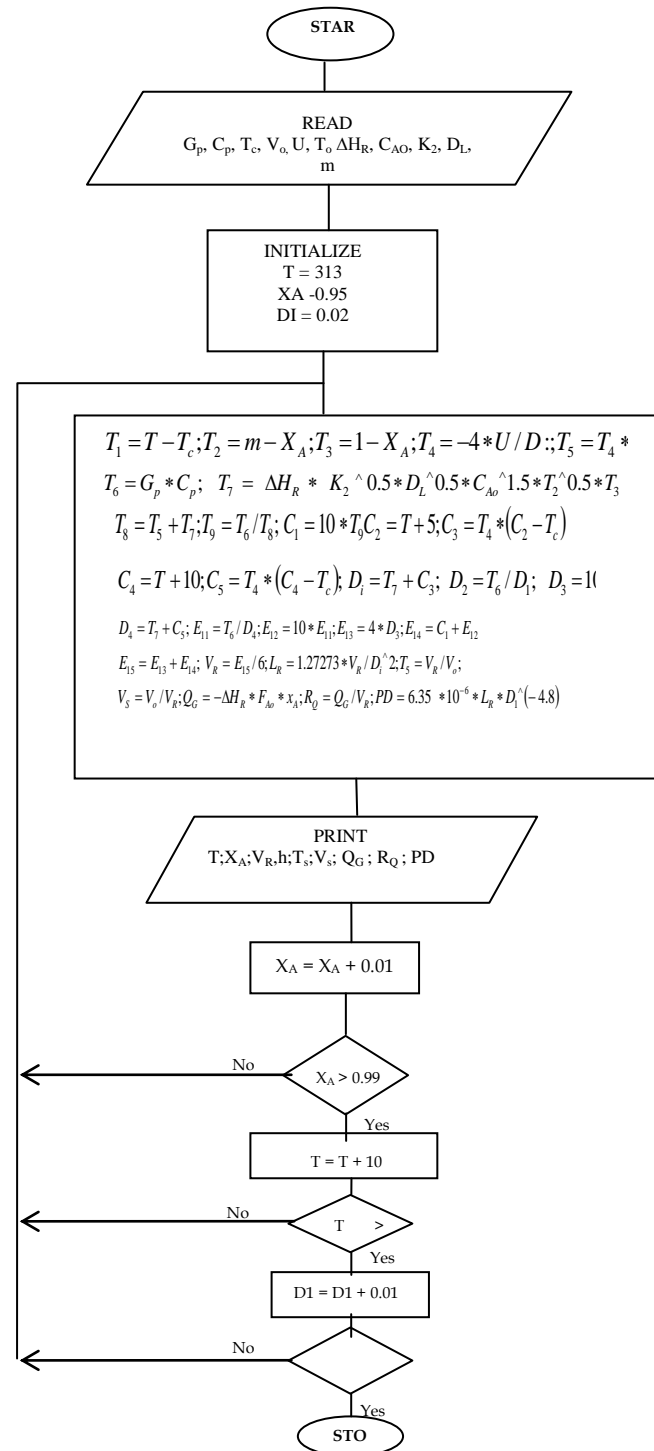


Figure3.3: flow chart describing the computation of non-isothermal PFR functional parameters

### 4. The reactor input parameters

The reactor performance models developed in section 3 contain unknown parameter such as the molar flow rate, concentration, volumetric flow rate etc. these parameters have to be determined before equations 1-10 can be evaluated.

**Table 4.1 Design data sheet.**

Quantity	Symbol	Value	Unit
Effective Heat Transfer Area	$A_t$	1.15	$m^2$
Specific Heat of product (Conc $H_2SO_4$ )	$C_p$	1.38	KJ/KgK
Specific Heat of cooling fluid	$C_{pc}$	4.2	KJ/KgK
Initial concentration of $SO_2$	$C_{A0}$	16,759	$mol/m^3$
Fractional change in volume	$\varepsilon_A$	-0.5	
Product mass flow rate	$G_p$	0.3858	Kg/sec
Operational temperature of reaction	$T$	313 to 363	K
Initial temperature of reactants	$T_0$	303	K
Initial temperature of cooling fluid	$T_0$	298	K
Heat of reaction	$\Delta H_R$	-88	Kj/mol
Overall Neat Transfer coefficient	$U$	6.945	Kj/Sec $m^2$
Product Density ( $H_2SO_4$ )	$\rho_p$	$1.64 \times 10^3$	Kg/ $m^3$
Absorption reaction rate constant	$K_2$	0.3	1/sec
Conversion degree	$X_A$	0.95 - 0.99	%
Reactant molar flow rate	$F_{A0}$	3.937	mol/sec
Cooling fluid density	$\rho_c$	1000	Kg/ $m^3$
Diameter of tubular reactor	$D_i$	0.02 to 0.1	m
Molar ratio of reactants	$m$	1.0 to 1.5	
Liquid phase diffusivity of $SO_3$	$D_L$	17	$m^2/Sec$
Volumetric flow rate of reactants	$V_0$	$2.352 \times 10^{-4}$	$m^3/Sec$

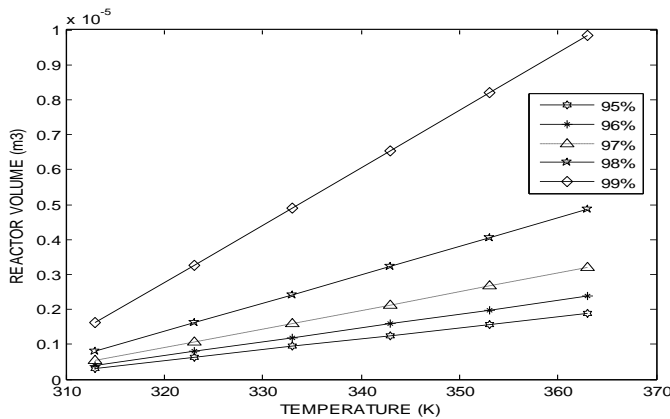
## 5. RESULTS AND DISCUSSION

### 5.1 RESULTS OF THE COMPUTATION

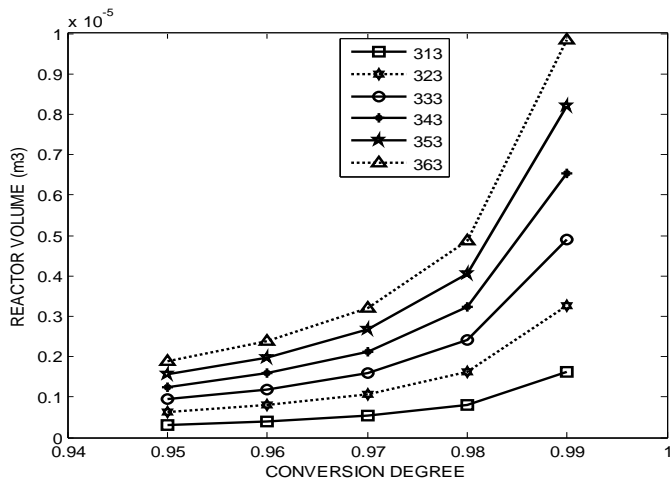
Industrial reactors for the production of sulphuric acid over a range of reaction time  $t = 60$  to  $1800$  Sec, degree of conversion  $X_A = 0.95$  to  $0.99$  and operating temperature  $T = 313$  to  $363$ K have been investigated and designed. The reactors have a capacity of  $1.389 \times 10^3$  Kg/hr of sulphuric acid. These reactors were designed with hastelloy because it has excellent corrosion and sulphuric acid resistance properties. The reactors performance models developed in chapter three were simulated with the aid of MATLAB R2007b. The results provided information for the functional reactors' parameters viz: The reactor volume and the rate of heat generation per unit volume of the continuous reactors and the semi-batch reactor. The reactor length, space time, and space velocity for the continuous reactors, while the height of reactor was obtained for the continuous stirred tank reactors and the semi-batch reactor. Similarly, information for the pressure drop in the plug flow reactor, whose diameter  $D_i$  was varied from  $0.02$  to  $0.1$  m was also obtained. Suitable heat exchangers were also designed for the isothermal reactors and the semi-batch reactor to remove the heat of reaction occasioned during the process. It is the purpose of this section to present and discuss the results of the reactor types and the heat exchangers and to compare their performance. The functional parameters of the reactors and the heat exchangers are tabulated in appendices 17, 18, 19, 20, 21, 22, 23, and 24. The results showed that the reactor volume is dependent on operating temperature  $T$  and degree of conversion  $X_A$ . The volume of the reactor would tend to infinity at 100% conversion. The variation of the reactor volume, as a result of sulphur trioxide addition to water, with reaction time, operating temperature and degree of conversion is illustrated in figures 5.1, 5.2, 5.9, 5.10, 5.13, 5.14, 5.23, and 5.29. From the results it was observed that volume of the reactors

increases with increasing reaction time and degree of conversion and decreases with increasing operating temperature. Figures 5.7, 5.8, 5.11, 5.12, 5.19, 5.20, 5.26, and 5.32 illustrated the variation of heat generation per unit volume of the reactors as a function of reaction time  $t$ , operating temperature  $T$  and degree of conversion within the limits  $t$ ,  $T$  and  $X_A$  as specified. A plot of heat generation  $R_Q$  versus operating temperature  $T$  was observed to be curvilinear. The rate of heat generation per reactor volume  $R_Q$  was found to be increasing with increasing operating temperature  $T$  within the range of  $X_A = 0.95$  to  $0.99$ . Similar plots were made  $R_Q$  versus  $X_A$  within the range of  $T = 313$  to  $363$ K. The graphs were also curvilinear with negative gradient. At fairly above 99% conversion of sulphur trioxide, there was a sharp drop tending to the abscissa of the graph. This behavior explains the infinity of the rate of heat generation per unit reactor volume at 100% degree of conversion of sulphur trioxide. Finally the rate of heat generation per unit reactor volume decreases with increasing reaction time and degree of conversion within the range of temperature as specified. Figures 5.3, 5.4, 5.15, 5.16, 5.24, and 5.30 illustrated the variation of space time with operating temperature and degree of conversion  $X_A$  as specified within the range of  $T = 313$  to  $363$ K and  $X_A = 0.95$  to  $0.99$ . The plots were curvilinear within the range of  $T$  and  $X_A$  investigated. However, for the addition of sulphur trioxide to water, the highest conversion was observed for the highest space time with the lowest operating temperature. The space time  $T_S$ , was observed to be increasing with increasing degree of conversion and decreases with increasing operating temperature within the range specified. Figures 5.5, 5.6, 5.17, 5.18, 5.25, and 5.31 illustrated the variation of space velocity with operating temperature  $T$  and degree of conversion  $X_A$  of sulphur trioxide as specified within the range  $T = 313$  to  $363$ K and  $X_A = 0.95$  to  $0.99$ . Space velocity  $V_S$  is the reciprocal of space time  $T_S$ . It is interesting to observe that the space velocity was found to be di-

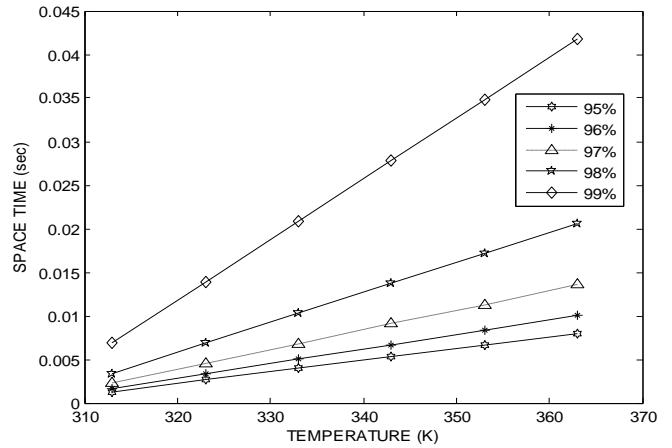
rectly proportional to the operating temperature  $T$  and inversely proportional to the degree of conversion  $X_A$ . A plot of space velocity versus operating temperature  $T$  is curvilinear, as distinct from profiles obtained for isothermal PFR which were linear with zero intercept. The difference arises from the isothermicity assumed in the design. It was observed from the results of the computation of the plug flow reactor as illustrated in Figures 5.21, 5.22, 5.27, and 5.28 that the pressure drop  $\Delta P$  decreases with decreasing degree of conversion  $X_A$  and with increasing operating temperature  $T$  within the ranges of  $T = 313$  to  $363\text{K}$  and  $X_A = 0.95$  to  $0.99$ . Also within the ranges investigated, the pressure drop  $\Delta P$  depends on the diameter of the reactor. The pressure drop increases with decreasing diameter. The pressure drop observed seems too small because of the low operating pressure as speci



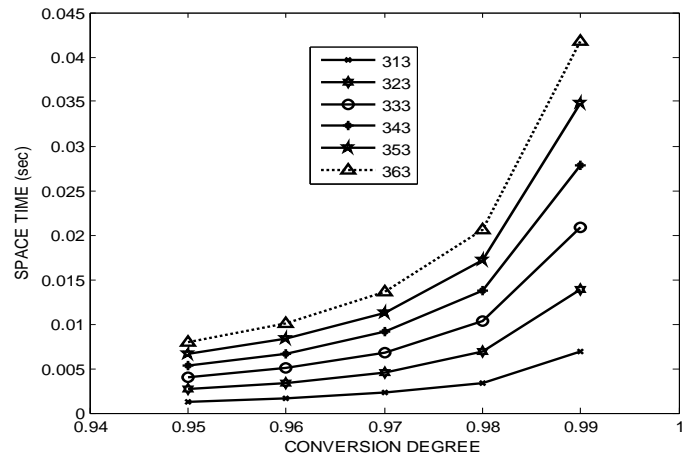
**Figure 5.1:** Plot of Reactor Volume against Temperature for Non-Isothermal PFR



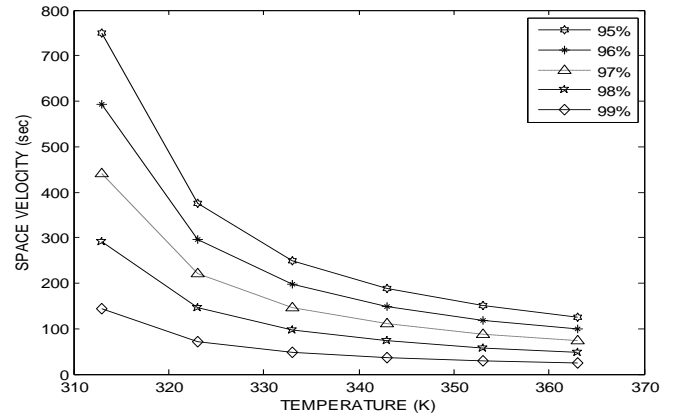
**Figure 5.2:** plots of Reactor Volume against Conversion Degree for non-Isothermal PFR



**Figure 5.3:** Plots of Space Time against Temperature for Non-Isothermal PFR



**Figure 5.4:** plots of Space Time against Conversion Degree for Non-Isothermal PFR



**Figure 5.5** Plots of Space Velocity against Temperature for non-Isothermal PFR

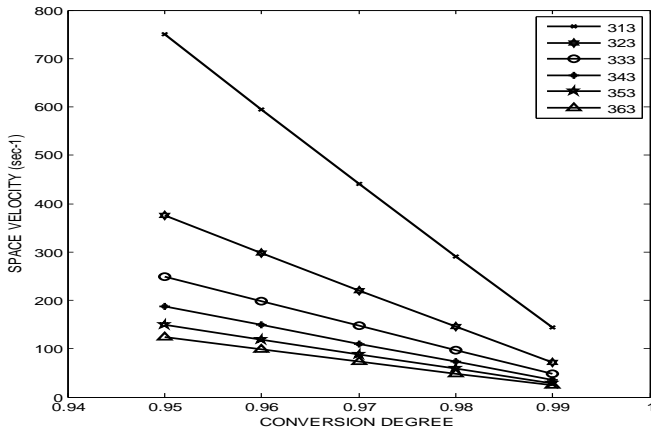


Figure 5.6: plots of Space Velocity against Conversion Degree for Non-Isothermal PFR

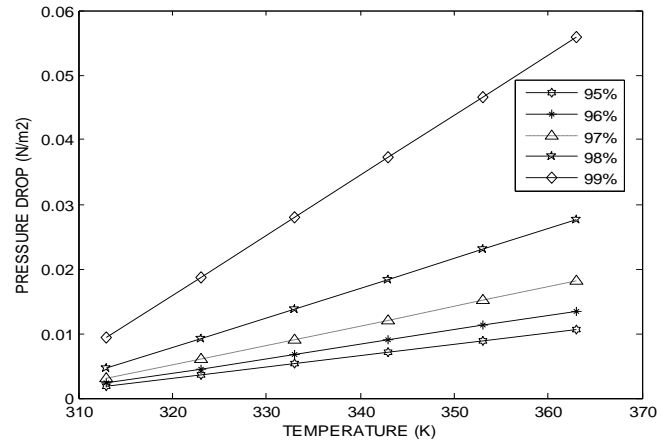


Figure 5.8 Plot of Pressure Drop against Temperature for non-Isothermal PFR

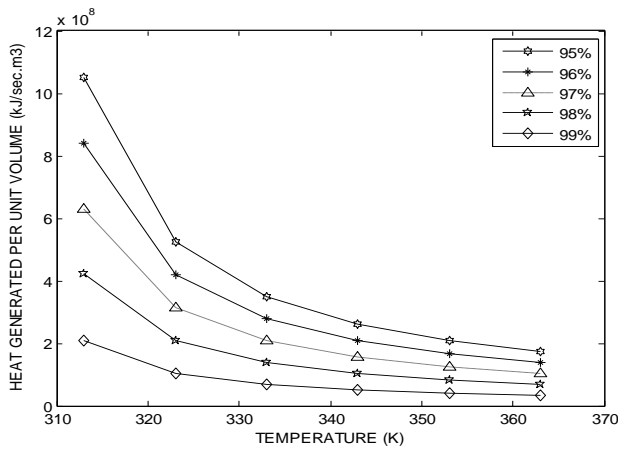


Figure 5.7: Plots of Heat Generated per unit Volume against Temperature for non-Isothermal PFR

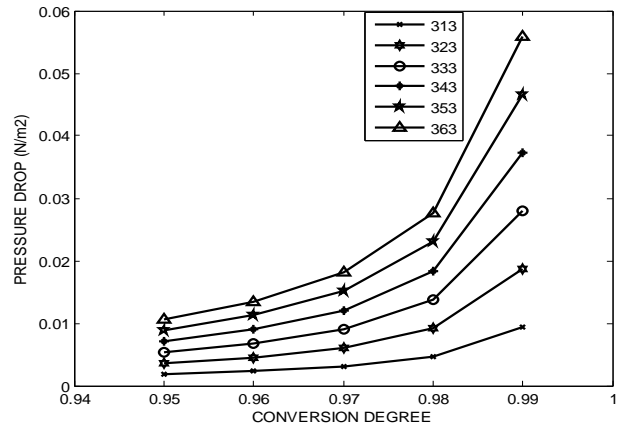


Figure 5.9: plot of Pressure Drop against Conversion Degree for non-Isothermal PFR

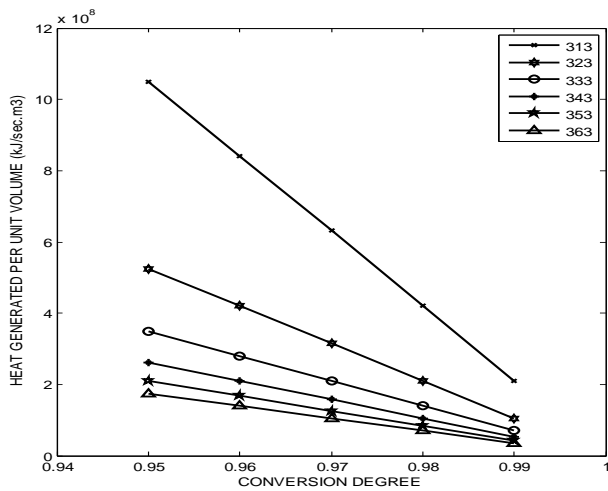


Figure 5.7 plot of Heat Generated per Unit Volume against Conversion Degree for non-Isothermal PFR

## 5.2 DISCUSSIONS

The consideration of non-isothermity of the reactors is a reasonable assumption as long as the operation of the reactors is within the sonic limit. An observation deduced from this work is that the operating temperature tends to influence the reactor performance. Generally the operation is favoured by low temperature. This confirms the reason why heat exchangers should be incorporated in the design. The consideration of the optimum limit of degree of conversion  $X_A$  from 0.95 to 0.99 is reasonable because at 100% conversion of sulphur trioxide, the functional parameters of the reactors will all tends to infinity. In this case the dimensions of the reactors have no limit. Work free days of 65 is allowed to produce the specified quantity i.e.  $1.389 \times 10^3 \text{Kg/hr}$  of sulphuric acid. Sulphur trioxide,  $\text{SO}_3$  can be produced by catalytic oxidation of sulphur dioxide using vanadium pentoxide as catalyst. From the results of the computation for the non-isothermal CSTR it was found that; if the degree of conversion,  $X_A$  was 0.95, the operational temperature,  $T$  was 313K, the reactor volume,  $V_R$  were  $2.5957\text{E-}05\text{m}^3$  and  $7.8263\text{E-}06\text{m}^3$  when the reactant molar ratio,  $m=1.0$  and 1.5 respectively but increase of  $X_A$ , and  $T$  resulted in increase of the reactor volume up to  $1.1432\text{E-}04$  to  $1.2781\text{E-}03\text{m}^3$  when  $m=1.0$ ,  $T=363\text{K}$  and  $X_A= 0.95$  to 0.99 and  $3.4469\text{E-}05$  to  $1.7897\text{E-}04\text{m}^3$  when  $m=1.5$ . The results of the computation for non-isothermal PFR showed that, if the opera-



tional conditions were as specified above and the diameter,  $D_i$  of the reactor tube was 0.02m, the reactor volume,  $V_R$  were  $5.36E-07m^3$  and  $1.5028E-07m^3$  when the reactant molar ratio,  $m=1.0$  and  $1.5$  respectively but increase of  $T$ ,  $X_A$ , and  $D_i$  resulted in increase of the reactor volume, up to  $3.218E-06$  to  $3.634E-05m^3$  when  $m=1.0$ ,  $T=363K$ ,  $D_i=0.1m$  and  $X_A=0.95$  to  $0.99$  and  $9.1071E-07$  to  $4.6796E-06m^3$  when  $m=1.5$ . The semi-batch reactor results showed that, if the reaction time,  $t$  was 60 sec, and degree of conversion,  $X_A$  was 0.95, the reactor volume,  $V_R$  were  $0.0226m^3$  and  $0.0760m^3$  when the reactant molar ratio,  $m=1.0$  and  $1.5$  respectively but increase of  $t$  and  $X_A$  resulted in increase of the reactor volume up to  $0.6910$  to  $0.0610 m^3$  when  $m=1.0$ ,  $t=1800$  sec and  $X_A=0.95$  to  $0.99$  and  $2.2939$  to  $0.4411m^3$  when  $m=1.5$ . At any given reaction time the semi-batch reactor volume decreases with increase in degree of conversion. Similarly, at any given conversion degree the semi-batch reactor volume increases with increase in reaction time. This is due to its peculiar mode of operation. Such behaviour is expected of a semi-batch reactor since it holds a batch of one reactant while the second reactant is gradually introduced into the reactor during the processing period. From the results of the computation for the isothermal CSTR it was found that, if the degree of conversion,  $X_A$  was 0.95, the reactor volume,  $V_R$  were  $6.84E-05m^3$  and  $2.06E-05m^3$  when the reactant molar ratio,  $m=1.0$  and  $1.5$  respectively but increase of  $X_A$  resulted in increase of the reactor volume up to  $7.965E-04m^3$  to  $1.115E-04m^3$  when  $X_A=0.99$  and  $m=1.0$  to  $1.5$ . The results of the computation for isothermal PFR showed that, if the degree of conversion,  $X_A$  was 0.95 and the reactor diameter  $D_i$  was 0.02m, the reactor volume,  $V_R$  were  $7.20E-06m^3$  and  $2.39E-05m^3$  when the reactant molar ratio,  $m=1.0$  and  $m=1.5$  respectively but increase of  $X_A$  and  $D_i$  resulted in increase of the reactor volume, up to  $7.20E-06m^3$  to  $1.609E-05m^3$  when  $m=1.0$ ,  $D_i=0.1$ , and  $X_A=0.95$  to  $0.99$  and  $2.39E-05$  to  $1.149E-04m^3$  when  $m=1.5$ . The various functional parameters of the reactors are all related to  $X_A$  and the reactor dimensions. From the results of the computation for the heat exchangers of the semi-batch reactor and the isothermal PFR showed that, if the degree of conversion,  $X_A$  was 0.95, the quantity of heat generated,  $Q$  was 329,1332KJ, and heat transfer area,  $A$  was  $26.06948m^2$ , but increase of  $X_A$  resulted in increase of quantity of heat generated up to 342.9914KJ but leads to slight decrease in heat transfer area up to  $26.02067m^2$  when  $X_A=0.99$ . From the results of the computation for the isothermal CSTR external heat exchanger showed that, while the conditions and quantity of heat generated were as stated above, the heat transfer area was  $680.5788m^2$ , but increase of  $X_A$  resulted in increase of heat transfer area up to  $709.2347m^2$  when  $X_A=0.99$ . For the jacketed semi-batch reactor and the double pipe heat exchanger unit for the isothermal PFR, the heat transfer areas were not adversely affected by the degree of conversion. Comparison analysis of the results obtained for the heat exchanger units for the various reactor types showed that the heat transfer area for the jacketed reactors were by 26 times smaller than the external shell-and-tube heat exchanger. Comparison analysis of the results obtained for the reactor types confirms that, the CSTR operating under the same design conditions is the least capital intensive, and it requires a smaller volume. The semi-batch reactor which relatively requires a larger volume and reaction time under the same working conditions would demand higher labour cost compared to CSTR and PFR. Within the limitation of the operating conditions of the non-isothermal PFR, agreement with

isothermal PFR performance is satisfactory. The results so obtained for the plug flow reactors suit industrial purpose better than those obtained for the continuous stirred tank reactors. The reactor volumes obtained were reasonable and were in accordance with literature data on experimental units. Critical examination of the results of the reactor types gives the following analysis:

- a. At the same degree of conversion, change in operating temperature from 313 to 363K curvilinearly increase the reactor volume and space time of the non-isothermal PFR, while the rate of heat generation per reactor volume and space velocity decreases curvilinearly by the same proportion.
- b. At the same operating temperature, change in degree of conversion,  $X_A$  from 0.95 to 0.99 curvilinearly increases the reactor volume and space time of the non-isothermal PFR, while the rate of heat generation per reactor volume and space velocity decreases by the same proportion.
- c. At the same degree of conversion, change in operating temperature from 313 to 363K linearly increases the pressure drop of the non-isothermal PFR, while at the same operating temperature, change in degree of conversion,  $X_A$  from 0.95 to 0.99 curvilinearly increases the pressure drop. But, as the reactor diameter increases the change in pressure drop becomes very gradual.

APPENDIXES

APPENDIX 17A: NON-ISOTHERMAL-PFR ( m=1; Di= 0.02m)							
T(K)	XA	VR m3	LR (m)	TS (sec)	VS (sec-1)	Rq (KJ/sec.m3 )	ΔP (N/m2)
		*10-5				*108	
313	0.95	0.0536	0.0017	0.0023	438.4074	6.1423	1.5497
323	0.95	0.1074	0.0034	0.0046	219.0502	3.0690	3.1015
333	0.95	0.1612	0.0051	0.0069	145.9311	2.0446	4.6555
343	0.95	0.2150	0.0068	0.0091	109.3715	1.5324	6.2117
353	0.95	0.2690	0.0086	0.0114	87.4357	1.2250	7.7701
363	0.95	0.3230	0.0103	0.0137	72.8118	1.0201	9.3307
313	0.96	0.0750	0.0024	0.0032	313.5242	4.4389	2.1669
323	0.96	0.1502	0.0048	0.0064	156.6085	2.2173	4.3381
333	0.96	0.2255	0.0072	0.0096	104.3033	1.4767	6.5136
343	0.96	0.3010	0.0096	0.0128	78.1506	1.1065	8.6933
353	0.96	0.3766	0.0120	0.0160	62.4589	0.8843	10.8773
363	0.96	0.4523	0.0144	0.0192	51.9978	0.7362	13.0657
313	0.97	0.1156	0.0037	0.0049	203.4248	2.9101	3.3397
323	0.97	0.2316	0.0074	0.0098	101.5588	1.4528	6.6896
333	0.97	0.3479	0.0111	0.0148	67.6033	0.9671	10.0496
343	0.97	0.4646	0.0148	0.0198	50.6255	0.7242	13.4199
353	0.97	0.5816	0.0185	0.0247	40.4388	0.5785	16.8004
363	0.97	0.6990	0.0223	0.0297	33.6476	0.4813	20.1913
		*10-4					
313	0.98	0.0213	0.0068	0.0091	110.4506	1.5963	6.1510
323	0.98	0.0427	0.0136	0.0182	55.0715	0.7959	12.3365
333	0.98	0.0642	0.0204	0.0273	36.6116	0.5291	18.5566
343	0.98	0.0859	0.0273	0.0365	27.3815	0.3957	24.8119
353	0.98	0.1077	0.0343	0.0458	21.8433	0.3157	31.1028
363	0.98	0.1296	0.0412	0.0551	18.1511	0.2623	37.4296
313	0.99	0.0608	0.0194	0.0259	38.6528	5.6435	17.5767
323	0.99	0.1227	0.0391	0.0522	19.1718	2.7992	35.4368
333	0.99	0.1855	0.0591	0.0789	12.6775	1.8510	53.5899
343	0.99	0.2494	0.0794	0.1060	9.4300	1.3768	72.0455
353	0.99	0.3144	0.1001	0.1337	7.4811	1.0923	90.8140
363	0.99	0.3805	0.1211	0.1618	6.1815	0.9025	109.9061

APPENDIX 17A: NON-ISOTHERMAL-PFR (m=1; Di= 0.05m)							
T(K)	X <sub>A</sub>	V <sub>R</sub> m <sup>3</sup>	L <sub>R</sub> (m)	T <sub>S</sub> (sec)	V <sub>S</sub> (sec <sup>-1</sup> )	R <sub>q</sub> (KJ/sec.m <sup>3</sup> )	ΔP (N/m <sup>2</sup> )
		<b>*10<sup>-5</sup></b>				<b>*10<sup>8</sup></b>	
313	0.95	0.0536	0.0003	0.0023	438.7756	6.1475	0.0030
323	0.95	0.1072	0.0005	0.0046	219.3264	3.0729	0.0061
333	0.95	0.1609	0.0008	0.0068	146.1767	2.0480	0.0091
343	0.95	0.2146	0.0011	0.0091	109.6018	1.5356	0.0122
353	0.95	0.2683	0.0014	0.0114	87.6569	1.2281	0.0153
363	0.95	0.3221	0.0016	0.0137	73.0269	1.0231	0.0183
313	0.96	0.0749	0.0004	0.0032	313.8925	4.4441	0.0043
323	0.96	0.1499	0.0008	0.0064	156.8848	2.2212	0.0085
333	0.96	0.2250	0.0011	0.0096	104.5490	1.4802	0.0128
343	0.96	0.3001	0.0015	0.0128	78.3810	1.1097	0.0171
353	0.96	0.3752	0.0019	0.0160	62.6802	0.8874	0.0213
363	0.96	0.4505	0.0023	0.0192	52.2130	0.7392	0.0256
313	0.97	0.1154	0.0006	0.0049	203.7931	2.9154	0.0066
323	0.97	0.2310	0.0012	0.0098	101.8351	1.4568	0.0131
333	0.97	0.3467	0.0018	0.0147	67.8492	0.9706	0.0197
343	0.97	0.4625	0.0024	0.0197	50.8561	0.7275	0.0263
353	0.97	0.5785	0.0029	0.0246	40.6603	0.5817	0.0329
363	0.97	0.6946	0.0035	0.0295	33.8631	0.4844	0.0395
313	0.98	<b>*10<sup>-4</sup></b>	0.0011	0.0090	110.8190	1.6017	0.0121
323	0.98	0.0212	0.0022	0.0181	55.3481	0.7999	0.0242
333	0.98	0.0425	0.0032	0.0271	36.8577	0.5327	0.0363
343	0.98	0.0638	0.0043	0.0362	27.6125	0.3991	0.0484
353	0.98	0.0852	0.0054	0.0453	22.0654	0.3189	0.0606
363	0.98	0.1066	0.0065	0.0544	18.3673	0.2655	0.0728
		0.1281				<b>*10<sup>7</sup></b>	
		0.0603	0.0031	0.0256	39.0217	5.6973	0.0343
313	0.99	0.1209	0.0062	0.0514	19.4493	2.8397	0.0687
323	0.99	0.1820	0.0093	0.0774	12.9251	1.8871	0.1034
333	0.99	0.2434	0.0124	0.1035	9.6629	1.4108	0.1384
343	0.99	0.3052	0.0155	0.1298	7.7055	1.1250	0.1735
353	0.99	0.3675	0.0187	0.1562	6.4006	0.9345	0.2089
363	0.99						

APPENDIX 17A: NON-ISOTHERMAL-PFR ( m=1; Di= 0.1m)							
T(K)	X <sub>A</sub>	V <sub>R</sub> m <sup>3</sup>	L <sub>R</sub> (m)	T <sub>S</sub> (sec)	V <sub>S</sub> (sec <sup>-1</sup> )	R <sub>q</sub> (KJ/sec.m <sup>3</sup> )	ΔP (N/m <sup>2</sup> )
		<b>*10<sup>-5</sup></b>	<b>*10<sup>-3</sup></b>			<b>*10<sup>8</sup></b>	<b>*10<sup>-3</sup></b>
313	0.95	0.0536	0.0682	0.0023	438.8984	6.1492	0.0273
323	0.95	0.1072	0.1365	0.0046	219.4185	3.0742	0.0547
333	0.95	0.1608	0.2048	0.0068	146.2585	2.0492	0.0820
343	0.95	0.2144	0.2730	0.0091	109.6786	1.5367	0.1094
353	0.95	0.2681	0.3413	0.0114	87.7306	1.2292	0.1368
363	0.95	0.3218	0.4097	0.0137	73.0986	1.0241	0.1641
313	0.96	0.0749	0.0954	0.0032	314.0152	4.4458	0.0382
323	0.96	0.1498	0.1908	0.0064	156.9769	2.2225	0.0764
333	0.96	0.2248	0.2862	0.0096	104.6308	1.4814	0.1147
343	0.96	0.2998	0.3817	0.0127	78.4578	1.1108	0.1529
353	0.96	0.3748	0.4772	0.0159	62.7539	0.8885	0.1912
363	0.96	0.4498	0.5728	0.0191	52.2847	0.7402	0.2295
313	0.97	0.1153	0.1469	0.0049	203.9158	2.9171	0.0588
323	0.97	0.2308	0.2938	0.0098	101.9272	1.4581	0.1177
333	0.97	0.3462	0.4408	0.0147	67.9310	0.9718	0.1766
343	0.97	0.46180.	0.5880	0.0196	50.9329	0.7286	0.2356
353	0.97	57740.69	0.7352	0.0245	40.7340	0.5827	0.2946
363	0.97	31	0.8825	0.0295	33.9348	0.4855	0.3536
		<b>*10<sup>-4</sup></b>					
313	0.98	0.0212	0.0003	0.0090	110.9418	1.6034	0.1081
323	0.98	0.0424	0.0005	0.0180	55.4402	0.8013	0.2164
333	0.98	0.0637	0.0008	0.0271	36.9397	0.5339	0.3248
343	0.98	0.0849	0.0011	0.0361	27.6894	0.4002	0.4333
353	0.98	0.1062	0.0014	0.0452	22.1392	0.3200	0.5419
363	0.98	0.1276	0.0016	0.0542	18.4391	0.2665	0.6507
						<b>*10<sup>7</sup></b>	<b>*10<sup>0</sup></b>
313	0.99	0.0601	0.0008	0.0255	39.1445	5.7153	0.0003
323	0.99	0.1204	0.0015	0.0512	19.5415	2.8531	0.0006
333	0.99	0.1808	0.0023	0.07690.	13.0072	1.8991	0.0009
343	0.99	0.2415	0.0031	1027	9.7400	1.4221	0.0012
353	0.99	0.3023	0.0038	0.1285	7.7797	1.1359	0.0015
363	0.99	0.3634	0.0046	0.1545	6.4728	0.9451	0.0019

APPENDIX 17B: NON-ISOTHERMAL-PFR ( m=1.5; Di= 0.02m)							
T(K)	X <sub>A</sub>	V <sub>R</sub> m <sup>3</sup>	L <sub>R</sub> (m)	T <sub>s</sub> (sec)	V <sub>s</sub> (sec <sup>-1</sup> )	R <sub>q</sub> (KJ/sec.m <sup>3</sup> )	ΔP (N/m <sup>2</sup> )
313	0.95	1.5028e-007	4.7835e-004	6.3894e-004	1.5651e+003	2.1928e+009	0.4341
323	0.95	3.0056e-007	9.5671e-004	1.2779e-003	7.8254e+002	1.0964e+009	0.8682
333	0.95	4.5084e-007	1.4351e-003	1.9168e-003	5.2169e+002	7.3092e+008	1.3023
343	0.95	6.0112e-007	1.9134e-003	2.5558e-003	3.9127e+002	5.4819e+008	1.7364
353	0.95	7.5140e-007	2.3918e-003	3.1947e-003	3.1302e+002	4.3855e+008	2.1704
363	0.95	9.0168e-007	2.8701e-003	3.8337e-003	2.6085e+002	3.6546e+008	2.6045
313	0.96	1.8897e-007	6.0150e-004	8.0343e-004	1.2447e+003	1.7622e+009	0.5458
323	0.96	3.7794e-007	1.2030e-003	1.6069e-003	6.2233e+002	8.8109e+008	1.0917
333	0.96	5.6690e-007	1.8045e-003	2.4103e-003	4.1489e+002	5.8739e+008	1.6375
343	0.96	7.5587e-007	2.4060e-003	3.2137e-003	3.1116e+002	4.4055e+008	2.1834
353	0.96	9.4484e-007	3.0075e-003	4.0172e-003	2.4893e+002	3.5244e+008	2.7292
363	0.96	1.1338e-006	3.6090e-003	4.8206e-003	2.0744e+002	2.9370e+008	3.2751
313	0.97	2.5296e-007	8.0519e-004	1.0755e-003	9.2980e+002	1.3301e+009	0.7307
323	0.97	5.0592e-007	1.6104e-003	2.1510e-003	4.6490e+002	6.6506e+008	1.4614
333	0.97	7.5888e-007	2.4156e-003	3.2265e-003	3.0993e+002	4.4337e+008	2.1921
343	0.97	1.0118e-006	3.2208e-003	4.3020e-003	2.3245e+002	3.3253e+008	2.9227
353	0.97	1.2648e-006	4.0260e-003	5.3775e-003	1.8596e+002	2.6602e+008	3.6534
363	0.97	1.5178e-006	4.8312e-003	6.4530e-003	1.5497e+002	2.2169e+008	4.3841
313	0.98	3.7900e-007	1.2064e-003	1.6114e-003	6.2058e+002	8.9692e+008	1.0948
323	0.98	7.5800e-007	2.4128e-003	3.2228e-003	3.1029e+002	4.4846e+008	2.1895
333	0.98	1.1370e-006	3.6192e-003	4.8342e-003	2.0686e+002	2.9897e+008	3.2843
343	0.98	1.5160e-006	4.8256e-003	6.4456e-003	1.5515e+002	2.2423e+008	4.3790
353	0.98	1.8950e-006	6.0320e-003	8.0570e-003	1.2412e+002	1.7938e+008	5.4738
363	0.98	2.2740e-006	7.2384e-003	9.6683e-003	1.0343e+002	1.4949e+008	6.5685
313	0.99	7.4174e-007	2.3610e-003	3.1537e-003	3.1709e+002	4.6297e+008	2.1426
323	0.99	1.4835e-006	4.7221e-003	6.3073e-003	1.5855e+002	2.3148e+008	4.2851
333	0.99	2.2252e-006	7.0831e-003	9.4610e-003	1.0570e+002	1.5432e+008	6.4277
343	0.99	2.9670e-006	9.4441e-003	1.2615e-002	7.9273e+001	1.1574e+008	8.5702
353	0.99	3.7087e-006	1.1805e-002	1.5768e-002	6.3418e+001	9.2594e+007	10.7128
363	0.99	4.4504e-006	1.4166e-002	1.8922e-002	5.2849e+001	7.7161e+007	12.8553

APPENDIX 17B: NON-ISOTHERMAL-PFR (m=1.5; Di= 0.05m)							
T(K)	X <sub>A</sub>	V <sub>R</sub> m <sup>3</sup>	L <sub>R</sub> (m)	T <sub>S</sub> (sec)	V <sub>S</sub> (sec <sup>-1</sup> )	R <sub>q</sub> (KJ/sec.m <sup>3</sup> )	ΔP (N/m <sup>2</sup> )
313	0.95	1.5141e-007	7.7111e-005	6.4373e-004	1.5534e+003	2.1764e+009	0.0009
323	0.95	3.0281e-007	1.5422e-004	1.2875e-003	7.7672e+002	1.0882e+009	0.0017
333	0.95	4.5422e-007	2.3133e-004	1.9312e-003	5.1781e+002	7.2548e+008	0.0026
343	0.95	6.0562e-007	3.0844e-004	2.5749e-003	3.8836e+002	5.4411e+008	0.0034
353	0.95	7.5703e-007	3.8555e-004	3.2187e-003	3.1069e+002	4.3529e+008	0.0043
363	0.95	9.0844e-007	4.6266e-004	3.8624e-003	2.5891e+002	3.6274e+008	0.0052
313	0.96	1.9075e-007	9.7150e-005	8.1102e-004	1.2330e+003	1.7457e+009	0.0011
323	0.96	3.8151e-007	1.9430e-004	1.6220e-003	6.1650e+002	8.7285e+008	0.0022
333	0.96	5.7226e-007	2.9145e-004	2.4331e-003	4.1100e+002	5.8190e+008	0.0033
343	0.96	7.6301e-007	3.8860e-004	3.2441e-003	3.0825e+002	4.3642e+008	0.0043
353	0.96	9.5376e-007	4.8575e-004	4.0551e-003	2.4660e+002	3.4914e+008	0.0054
363	0.96	1.1445e-006	5.8290e-004	4.8661e-003	2.0550e+002	2.9095e+008	0.0065
313	0.97	2.5617e-007	1.3046e-004	1.0891e-003	9.1815e+002	1.3135e+009	0.0015
323	0.97	5.1233e-007	2.6093e-004	2.1783e-003	4.5907e+002	6.5673e+008	0.0029
333	0.97	7.6850e-007	3.9139e-004	3.2674e-003	3.0605e+002	4.3782e+008	0.0044
343	0.97	1.0247e-006	5.2186e-004	4.3566e-003	2.2954e+002	3.2836e+008	0.0058
353	0.97	1.2808e-006	6.5232e-004	5.4457e-003	1.8363e+002	2.6269e+008	0.0073
363	0.97	1.5370e-006	7.8279e-004	6.5349e-003	1.5302e+002	2.1891e+008	0.0087
313	0.98	3.8625e-007	1.9671e-004	1.6422e-003	6.0894e+002	8.8009e+008	0.0022
323	0.98	7.7250e-007	3.9343e-004	3.2844e-003	3.0447e+002	4.4005e+008	0.0044
333	0.98	1.1587e-006	5.9014e-004	4.9266e-003	2.0298e+002	2.9336e+008	0.0066
343	0.98	1.5450e-006	7.8686e-004	6.5688e-003	1.5223e+002	2.2002e+008	0.0088
353	0.98	1.9312e-006	9.8357e-004	8.2111e-003	1.2179e+002	1.7602e+008	0.0110
363	0.98	2.3175e-006	1.1803e-003	9.8533e-003	1.0149e+002	1.4668e+008	0.0132
313	0.99	7.7002e-007	3.9217e-004	3.2739e-003	3.0545e+002	4.4596e+008	0.0044
323	0.99	1.5400e-006	7.8434e-004	6.5478e-003	1.5272e+002	2.2298e+008	0.0088
333	0.99	2.3101e-006	1.1765e-003	9.8217e-003	1.0182e+002	1.4865e+008	0.0131
343	0.99	3.0801e-006	1.5687e-003	1.3096e-002	7.6361e+001	1.1149e+008	0.0175
353	0.99	3.8501e-006	1.9608e-003	1.6370e-002	6.1089e+001	8.9193e+007	0.0219
363	0.99	4.6201e-006	2.3530e-003	1.9643e-002	5.0908e+001	7.4327e+007	0.0263

**APPENDIX 17B: NON-ISOTHERMAL-PFR (m=1.5; Di= 0.1m)**

T(K)	X <sub>A</sub>	V <sub>R</sub> m <sup>3</sup>	L <sub>R</sub> (m)	T <sub>S</sub> (sec)	V <sub>S</sub> (sec <sup>-1</sup> )	R <sub>Q</sub> (KJ/sec.m <sup>3</sup> )	ΔP (N/m <sup>2</sup> )
313	0.95	1.5179e-007	1.9326e-005	6.4535e-004	1.5496e+003	2.1710e+009	7.7431e-006
323	0.95	3.0357e-007	3.8652e-005	1.2907e-003	7.7478e+002	1.0855e+009	1.5486e-005
333	0.95	4.5536e-007	5.7978e-005	1.9360e-003	5.1652e+002	7.2367e+008	2.3229e-005
343	0.95	6.0714e-007	7.7304e-005	2.5814e-003	3.8739e+002	5.4275e+008	3.0972e-005
353	0.95	7.5893e-007	9.6630e-005	3.2267e-003	3.0991e+002	4.3420e+008	3.8715e-005
363	0.95	9.1071e-007	1.1596e-004	3.8721e-003	2.5826e+002	3.6183e+008	4.6459e-005
313	0.96	1.9136e-007	2.4364e-005	8.1359e-004	1.2291e+003	1.7402e+009	9.7617e-006
323	0.96	3.8271e-007	4.8728e-005	1.6272e-003	6.1456e+002	8.7010e+008	1.9523e-005
333	0.96	5.7407e-007	7.3092e-005	2.4408e-003	4.0971e+002	5.8007e+008	2.9285e-005
343	0.96	7.6542e-007	9.7456e-005	3.2543e-003	3.0728e+002	4.3505e+008	3.9047e-005
353	0.96	9.5678e-007	1.2182e-004	4.0679e-003	2.4583e+002	3.4804e+008	4.8808e-005
363	0.96	1.1481e-006	1.4618e-004	4.8815e-003	2.0485e+002	2.9003e+008	5.8570e-005
313	0.97	2.5726e-007	3.2755e-005	1.0938e-003	9.1427e+002	1.3079e+009	1.3123e-005
323	0.97	5.1451e-007	6.5509e-005	2.1875e-003	4.5713e+002	6.5395e+008	2.6247e-005
333	0.97	7.7177e-007	9.8264e-005	3.2813e-003	3.0476e+002	4.3597e+008	3.9370e-005
343	0.97	1.0290e-006	1.3102e-004	4.3751e-003	2.2857e+002	3.2698e+008	5.2494e-005
353	0.97	1.2863e-006	1.6377e-004	5.4689e-003	1.8285e+002	2.6158e+008	6.5617e-005
363	0.97	1.5435e-006	1.9653e-004	6.5626e-003	1.5238e+002	2.1798e+008	7.8741e-005
313	0.98	3.8873e-007	4.9494e-005	1.6527e-003	6.0505e+002	8.7448e+008	1.9830e-005
323	0.98	7.7745e-007	9.8988e-005	3.3055e-003	3.0253e+002	4.3724e+008	3.9660e-005
333	0.98	1.1662e-006	1.4848e-004	4.9582e-003	2.0168e+002	2.9149e+008	5.9491e-005
343	0.98	1.5549e-006	1.9798e-004	6.6110e-003	1.5126e+002	2.1862e+008	7.9321e-005
353	0.98	1.9436e-006	2.4747e-004	8.2637e-003	1.2101e+002	1.7490e+008	9.9151e-005
363	0.98	2.3324e-006	2.9697e-004	9.9165e-003	1.0084e+002	1.4575e+008	1.1898e-004
313	0.99	7.7994e-007	9.9305e-005	3.3161e-003	3.0156e+002	4.4030e+008	3.9787e-005
323	0.99	1.5599e-006	1.9861e-004	6.6321e-003	1.5078e+002	2.2015e+008	7.9574e-005
333	0.99	2.3398e-006	2.9791e-004	9.9482e-003	1.0052e+002	1.4677e+008	1.1936e-004
343	0.99	3.1197e-006	3.9722e-004	1.3264e-002	7.5391e+001	1.1007e+008	1.5915e-004
353	0.99	3.8997e-006	4.9652e-004	1.6580e-002	6.0313e+001	8.8059e+007	1.9894e-004
363	0.99	4.6796e-006	5.9583e-004	1.9896e-002	5.0261e+001	7.3383e+007	2.3872e-004

**6. CONCLUSION**

Reactors have been designed for the production of ten thousand metric tons per year of sulphuric acid. Computer programs were developed and utilized to simulate the reactors performance models over a temperature interval of T=313 to 363K, and conversion degree, X<sub>A</sub>=0.95 to 0.99. For the plug flow reactors and the semi-batch reactor, additional variable of reactor diameter of 0.02 to 0.1m and reaction time of 60 to 1800sec respectively were used. From the results of computation, it is clearly established that:

**For the non- isothermal PFR**

- a. When the diameter of the reactor, Di=0.02m, degree of conversion, X<sub>A</sub>=0.95, operational temperature, T=313K, the volume of the reactor, V<sub>R</sub> are 5.360E-07m<sup>3</sup> and 1.5028E-07m<sup>3</sup>, the space time, T<sub>S</sub> are 2.2789E-03sec and 6.3894E-04sec, the reactor length, L<sub>R</sub> are 1.7055E-03m and 4.7835E-04m, the rate of heat generation per reactor volume, R<sub>Q</sub> are

6.1423E08KJ/sec.m<sup>3</sup> and 2.1928E09KJ/sec.m<sup>3</sup> and the pressure drop, ΔP are 1.5497N/m<sup>2</sup> and 0.4341N/m<sup>2</sup> for the reactant molar ratio, m=1.0 and 1.5 respectively.

- b. When the degree of conversion, X<sub>A</sub>=0.99 for the same lower reactor diameter, and operational temperature as specified above, the reactor volume, V<sub>R</sub> are 6.080E-06m<sup>3</sup> and 7.4174E-07m<sup>3</sup>, the space time, T<sub>S</sub> are 2.585E-02sec and 3.1537E-03sec, the reactor length, L<sub>R</sub> are 1.9345E-02m and 2.3610E-03m, the rate of heat generation per reactor volume, R<sub>Q</sub> are 5.6435E08KJ/sec.m<sup>3</sup> and 4.6297E08KJ/sec.m<sup>3</sup>, and the pressure drop, ΔP are 17.5767N/m<sup>2</sup> and 2.1426N/m<sup>2</sup> for the reactant molar ratio, m=1.0 and 1.5 respectively.
- c. When the reactor diameter, Di=0.02m, degree of conversion, X<sub>A</sub>=0.95, at the upper limit of operating temperature, T=363K, the reactor volume, V<sub>R</sub> are 3.230E-06m<sup>3</sup> and 9.0168E-07m<sup>3</sup>, the space time, T<sub>S</sub> are

- 1.3733E-02sec and 3.8337E-03sec, the reactor length,  $L_R$  are 1.0277E-02m and 2.8701E-03m, the rate of heat generation per reactor volume,  $R_Q$  are 1.0201E08KJ/sec.m<sup>3</sup> and 3.6546E08KJ/sec.m<sup>3</sup>, and the pressure drop,  $\Delta P$  are 9.3307N/m<sup>2</sup> and 2.6045N/m<sup>2</sup> for the reactant molar ratio,  $m=1.0$  and 1.5 respectively.
- d. When the degree of conversion,  $X_A=0.99$  for similar conditions as in (c) above, the reactor volume,  $V_R$  are 3.805E-05m<sup>3</sup> and 4.4504E-06m<sup>3</sup>, the space time,  $T_S$  are 0.1618sec and 1.8922E-02sec, the reactor length,  $L_R$  are 0.1211m and 1.4166E-02m, the rate of heat generation per reactor volume,  $R_Q$  are 9.025E07KJ/sec.m<sup>3</sup> and 7.7161E07KJ/sec.m<sup>3</sup>, and the pressure drop,  $\Delta P$  are 1.099E02N/m<sup>2</sup> and 12.8553N/m<sup>2</sup> for the reactant molar ratio,  $m=1.0$  and 1.5 respectively.
- e. From 2(a) – (d) above, the reactor volume, space time, reactor length and the pressure drop were greater at the upper limits of conversion degree. While the rate of heat generation per reactor volume decreases as conversion degree increases.
- f. When the reactor diameter,  $D_i=0.1m$ , degree of conversion,  $X_A=0.95$ , operational temperature,  $T=313K$ , the reactor volume,  $V_R$  are 5.360E-07m<sup>3</sup> and 1.517E-07m<sup>3</sup>, the space time,  $T_S$  are 2.2789E-03sec and 6.4535E-04sec, the reactor length,  $L_R$  are 6.820E-05m and 1.9326E-05m, the rate of heat generation per reactor volume,  $R_Q$  are 6.1492E08KJ/sec.m<sup>3</sup> and 2.171E09KJ/sec.m<sup>3</sup> and the pressure drop,  $\Delta P$  are 2.730E-05N/m<sup>2</sup> and 7.7431E-06N/m<sup>2</sup> for the reactant molar ratio,  $m=1.0$  and 1.5 respectively.
- g. When the reactor diameter,  $D_i=0.1$ , the degree of conversion,  $X_A=0.99$  for the same lower operational temperature as specified in (f) above, the reactor volume,  $V_R$  are 6.01E-06m<sup>3</sup> and 7.7994E-07m<sup>3</sup>, the space time,  $T_S$  are 2.5552E-02sec and 3.3161E-03sec, the reactor length,  $L_R$  are 7.6491E-04m and 9.9305E-05m, the rate of heat generation per reactor volume,  $R_Q$  are 5.7153E07KJ/sec.m<sup>3</sup> and 4.4030E08KJ/sec.m<sup>3</sup>, and the pressure drop,  $\Delta P$  are 3.0647E-04N/m<sup>2</sup> and 3.9789E-05N/m<sup>2</sup> for the reactant molar ratio,  $m=1.0$  and 1.5 respectively.
- h. When the reactor diameter,  $D_i=0.1$ , degree of conversion,  $X_A=0.95$  at the upper limit of operational temperature,  $T=363K$ , the reactor volume,  $V_R$  are 3.218E-06m<sup>3</sup> and 9.1071E-07m<sup>3</sup>, the space time,  $T_S$  are 1.370E-02sec and 3.8721E-03sec, the reactor length,  $L_R$  are 4.097E-04m and 1.1596E-04m, the rate of heat generation per reactor volume,  $R_Q$  are 1.0241E08KJ/sec.m<sup>3</sup> and 3.6183E08KJ/sec.m<sup>3</sup> and the pressure drop,  $\Delta P$  are 1.641E-04N/m<sup>2</sup> and 4.6459E-05N/m<sup>2</sup> for the reactant molar ratio,  $m=1.0$  and 1.5 respectively.
- i. When the degree of conversion,  $X_A=0.99$  for similar conditions as in (h) above, the reactor volume,  $V_R$  are 3.634E-05m<sup>3</sup> and 4.6796E-06m<sup>3</sup>, the space time,  $T_S$  are 0.1545sec and 1.9896E-02sec, the reactor length,  $L_R$  are 4.6251E-03m and 5.9583E-04m, the rate of heat generation per reactor volume,  $R_Q$  are 9.451E06KJ/sec.m<sup>3</sup> and 7.3383E07KJ/sec.m<sup>3</sup>, and the pressure drop,  $\Delta P$  are 1.8531E-03N/m<sup>2</sup> and

2.3872E-04N/m<sup>2</sup> for the reactant molar ratio,  $m=1.0$  and 1.5.

- j. From 2(f) – (i) above, the reactor volume, space time, reactor length and the pressure drop were greater at the upper limits of conversion degree. While the rate of heat generation per unit reactor volume decreases as conversion degree increases.

### Generally,

At the lower limits of operating conditions (i.e. operational temperature,  $T=313K$ , and conversion degree,  $X_A=0.95$ ) increase in reactor diameter leads to corresponding increase in reactor volume and space time. While the reactor length, the rate of heat generation per reactor volume and the pressure drop decrease as reactor diameter increases. However, at the upper limits of operating conditions (i.e. operational temperature,  $T=363K$  and conversion degree,  $X_A=0.99$ ) increase in reactor diameter leads to decrease in reactor volume, space time, reactor length and pressure drop. While the rate of heat generation per reactor volume increases with increase in reactor diameter.

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