# DESIGN PROCESS OF CSTR FOR PRODUCTION OF

# **FURFURALDEHYDE**

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#### **Abstract**

A realistic academic cum industrial Isothermal continuous stirred tank reactor design, feed rate 11.51 kgs<sup>-1</sup> furfuraldehyde productions is presented. Principles of material balance and heat generated per unit volume equations were performed on the reactor system to derive model equations applied in obtaining the reactor functional parameters. Mechanical concepts of the reactor and the economics of the design were considered. The functional parameters of the reactor were computed using efficient mat-lab program version 7.7 as shown. The hydrolysis and dehydration reaction of xylan and xylose respectively to furfural is endothermic; a heating jacket is incorporated to account for the supply and maintenance of heat liberated.

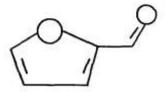
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## 1. INTRODUCTION

Design is a creative activity that integrates the elements of art and science to create something new or retrofit for existence. Some agricultural wastes [e.g peanuts seed shell] in Nigeria were subjected to titrimetric analysis for presence of furfural and results were Positive to varying degrees [Wordu and Akaranta, 1989]. The study gave obvious contributions to the local content of the economy [Nigerian Local Content Act, 2004], by designing full-scale reactor for the production of furfural.

Continuous Stirred Tank Reactor design is complemented with thermodynamics, chemical kinetics, fluid mechanics, heat transfer, mass transfer and economics as well as mechanical aspects. The perfect mixing is attained by the effect of a stirrer in the reactor which ensures contents of the reactor are properly mixed so that the temperature and concentration of the content are the same at the product stream and in the reactor. Furfural (i.e. a heterocyclic compound with an aldehyde group chemical formula is  $C_5H_4O_2$ ) is an organic compound derived from variety of agricultural by-products including corncobs, Oat hulls, wheat bran's, wood, sugarcane bagasse.



**Fig1:** Molecular structure, IUPAC name furar-2-carbaldehyde; other names are furan, furfuraldehyde, 2-furaldehyde, pyromucic aldehyde.

Furfural is produced from polysaccharide hemi-cellulose, (or pentonsans) a polymer of sugar by biphasic reaction with  $H_2SO_4$  in the present of heat (Rong et al, 2012). The hemi cellulose is heated in the presence of  $H_2SO_4$ , it undergoes hydrolysis to yield sugar of five carbon atom called xylose (pentose). The xylose is heated in the presence of  $H_2SO_4$  at the same condition; it dehydrates or undergoes cyclodehydration losing three water molecules to become furfural. The furfural and water evaporates out and are separated upon condensation.

#### 2. MATERIALS AND METHOD

#### 2.1 Rate Law, Kinetics and Process Chemistry

Furfural is produced from polysaccharide hemi-cellulose, (or pentonsans) a polymer of sugar by biphasic reaction with  $H_2SO_4$  in the present of heat (Rong et al, 2012). The hemi cellulose is heated in the presence of  $H_2SO_4$ , it undergoes hydrolysis to yield sugar of five carbon atom called xylose (pentose). The xylose is heated in the presence of  $H_2SO_4$  at the same condition; it dehydrates or undergoes cyclodehydration losing three water molecules to become furfural.

The furfural and water evaporates out and are separated upon condensation

The reaction that yield furfural from the above mentioned materials in introduction is a series first order reaction under same condition of a mineral acid and heat which are hydrolysis of the pentosans to pentose and dehydration of the pentose to furfural [4]

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### **Chemical Reaction of Furfural Production**

Pentonsans + water 
$$\xrightarrow{\Delta, Hcl}$$
 pentose (1)

$$C_5H_8O_4 + H_2O \xrightarrow{\Delta_1 Hcl} C_5H_{10}O_5$$

Pentose 
$$\xrightarrow{\Delta, Hcl}$$
 furfural + water (2)

$$C_5H_{10}O_5 \xrightarrow{\Delta,Hcl} C_5H_4O_2 + 3H_2O_1$$

# Kinetic Scheme for Furfural Production [4], [7]

Pentosan  $\xrightarrow{k_1}$  pentose  $\xrightarrow{k_2}$  furfural

Let, Pentosan = A, Pentose=B, Furfural=C

Rate of Pentosan hydrolysis:  $r_{Xylan} = \frac{dC_A}{dt} = -k_1C_A$ 

Rate of Pentose reaction [9]:  $r_{Xylose} = \frac{dC_B}{dt} = k_1 C_A - k_2 C_B$  (3)

Rate of furfural formation: 
$$r_{furfural} = \frac{dC_C}{dt} = k_2 C_B$$
 (4)

$$k_{i} = A_{0,i} \left[ H_{2} S O_{4} \% \right]^{m_{i}} \ell \frac{-E_{A,i}}{RT}$$
(5)

$$r_i = \pm k_i C_i$$
 [9]

#### 3. METHOD

## 3.1 Development of Reactor Model

From material balance equation which applies the principle of mass conservation is the starting point of reactor design. The principle states that:

Rate of reactant flow into element of volume = Rate of reactant flow out of element of volume + Rate of reactant loss due to chemical reaction within element of volume + Rate of accumulation of reactant in element of volume [9].

Rate of reactant flow into element volume =  $F_{i,o}$ 

Rate of reactant flow out of element of volume (with respect to fractional conversion) =  $F_{i,o}(1-X_i)$ 

Rate of accumulation of reactant within element of volume  $= \frac{d}{dt}(C_iV)$ 

Rate of reactants loss due to chemical reaction =  $(-r_i)V_R$ 

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Substituting all the above into

$$F_{i,o} = F_{i,o} (1 - X_i) + (-r_i) V_R + \frac{d}{dt} (C_i V)$$

$$F_{A,O} = F_{A,O} (1 - X_A) + (-r_A) V_R + \frac{d}{dt} (C_A V)$$
(6)

Assumptions for the reactor;

- The feed is well stirred or properly mixed.
- Neglecting the inflow rate of catalyst and solvent.
- Steady state operation.
- Isothermal and non-adiabatic system.
- Constant density system.
- Cylindrical tank with hemispherical head.

Applying the assumptions where necessary into equation (1) gives:

$$F_{A,O} = F_{A,O}(1 - X_A) + (-r_A)V_R$$

$$F_{A,O} = F_{A,O} - F_{A,O} X_A + \left(-r_A\right) V_R V_R = \frac{F_{A,O} X_A}{\left(-r_A\right)}$$
 (7)

Taking the rate with respect to furfural formation

$$-r_A = r_C = k_2 C_B \tag{8}$$

Where: 
$$C_B = C_{B,O}(1 - X_A)$$
 (9)

for constant density system [9]

 $C_{BO} = C_A$  Since it's a series reaction

Substituting (9) into (8):

$$-r_{A} = k_{2}C_{A}(1 - X_{A}) \tag{10}$$

Substituting (3) into (4):

$$V_{R} = \frac{F_{A,O} X_{A}}{k_{2} C_{A} (1 - X_{A})} \tag{11}$$

 $V_R$  = Volume of the reactor  $(m^3)$ 

#### 3.2 Length of Reactor L<sub>R</sub>

Volume of a cylinder is given as:

$$V = \pi r^2 L \tag{12}$$

Equating (12) to (11):

$$\pi r^2 H = \frac{F_{A,O} X_A}{k_2 C_A (1 - X_A)} \quad H_R = \frac{F_{A,O} X_A}{\pi r^2 k_2 C_A (1 - X_A)}$$
 (13)

 $L_R$  = Length of reactor (m)

# 3.3 Dimension of Reactor Head

$$L_H = \frac{D_R}{2} \tag{14}$$

$$V_H = \pi \frac{D_R^3}{12} \tag{15}$$

Where:  $V_H$  = Volume of reactor head  $(m^3)$ ,  $L_H$  = Length of reactor head (m)

# 3.4 Resident time distribution (RTD) Space time

 $(\tau)$ .

$$\tau = \frac{V_R}{v_o} \tag{16}$$

$$v_o = \frac{F_{A,O}}{C_A} \tag{17}$$

Substituting (11) and (9) into (5):

$$\tau = \frac{X_A}{k_2(1 - X_A)} \tag{18}$$

# 3.5 Space-Velocity (s)

$$S_{v} = \frac{1}{\tau} \tag{19}$$

Substituting (18) into (19):

$$S_{v} = \frac{k_{2}(1 - X_{A})}{X_{A}} \tag{20}$$

# 3.6 Heat Generation per Volume of Reactor

$$q_R = \frac{Q}{V_P} \tag{21}$$

$$Q = (\Delta H_r) F_{AO} X_A \tag{22}$$

Substituting (22) and (11) into (21):

$$q_R = (\Delta H_r) X_A k_1 C_A (1 - X_A) \tag{23}$$

# 3.7 Heating Jacket Design

# 3.7.1 Mass Flow Rate of Heating Fluid

$$\dot{m}_{w} = \frac{Q}{C_{pw}\Delta T} \tag{24}$$

Where:  $\Delta T = T_1 - T_2$ 

#### 3.7.2 Jacket Dimension

Height of jacket:

$$H_j = \frac{H_R}{2} \tag{25}$$

Let the pitch  $(P_i)$  between the spiral baffles be 0.2m

Numbers of Spiracles:

$$N_s = \frac{H_j}{P_j} \tag{26}$$

Length of Jacket:

$$L_{j} = N_{s} \pi D_{R} \tag{27}$$

# 3.7.3 Velocity through Channel (u):

$$u = \frac{\dot{m}_{w}}{\rho A_{j}} \tag{28}$$

# 3.7.4 Film Heat Transfer Coefficient for the Jacket

Reynolds number (Re):

$$Re = \frac{\rho u d_e}{\mu} \tag{29}$$

Prandtl number (Pr):

$$\Pr = \frac{C_p \mu}{k}$$

Where: 
$$\frac{h_j d_e}{k} = 0.023 \text{Re}^{0.8} \text{ Pr}^{0.33}$$

# **Overall Heat Transfer Coefficient:**

$$U_o = \frac{h_j h_d}{h_j + h_d} \tag{30}$$

Where:

$$h_d = \frac{1}{f_d} \tag{31}$$

# 3.8 Mechanical Design Equations

# 3.8.1 Stirrer Design

For this work, radial turbine stirrer with 6 blades is used for the two reactors.

Length of stirrer 
$$(L_{st})$$
:  $L_{st} = L_R - C$  (32)

Stirrer clearance (C): 
$$C = \frac{1}{2}to\frac{1}{6}D_R$$
 (33)

Stirrer Diameter 
$$(D_{st})$$
:  $D_{st} = \frac{1}{2}to\frac{1}{4}D_R$  (34)

Stirrer blade-width 
$$(W)$$
:  $W = \frac{1}{4} to \frac{1}{6} D_{st}$  (35)

Wall baffles 
$$(B)$$
:  $B = \frac{1}{10} to \frac{1}{12} D_R$  (36)

Power consumption 
$$(P)$$
 [10]:  $N_p = \frac{P}{n^3 D_{st}^5 \rho}$  (37)

Where  $N_p = f(\text{Re}, Fr, S_1 - S_n)$ 

$$Re = \frac{nD^2_{st}\rho}{\mu}$$
 (38)

$$Fr = \frac{n^2 D_{st}}{g} \tag{39}$$

When Re > 300, Froude number becomes a factor to determine power consumption

$$\frac{N_p}{Fr^m} = \frac{P}{n^3 D_{st}^5 \rho} \tag{40}$$

Where:

$$m = \frac{a - \log \text{Re}}{b} \tag{41}$$

Further simplification can be made at low and high Reynolds number;

If  $Re\langle 10 \rangle$ ; the flow is laminar and density is no longer a factor then;

$$\frac{N_p}{\text{Re}} = k_L \tag{42}$$

Substituting (26) into (22): 
$$N_p = k_L \frac{nD_{st}^2 \rho}{\mu}$$
 (43)

Substituting (24) into (22): 
$$P = k_L n^2 D_{st}^3 \mu$$
 (44)

If  $Re > 10^4$ , the flow regime is transitional or turbulent and the power consumption is independent of Reynolds number and viscosity is no longer a factor

$$N_{p} = k_{T} \tag{45}$$

Substituting (38) into (37):

$$P = k_T \rho D^5_{st} n^3 \tag{46}$$

# 3.8.2 Standard Plate Thickness [10]:

$$t = \frac{P_R D_R}{SE_j - 0.6P_R} + c \tag{47}$$

# 3.9 Solution Techniques

# 3.9.1 Operational Parameters Flow Rate

Design production rate = 4,535,929.1kg per annum.

From (1.1) and (1.2):132kg. kmol<sup>-1</sup> Of Pentosan yields 150kg. kmol<sup>-1</sup> of Pentose, also

150kg. kmol<sup>-1</sup>Of Pentose yield 96kg. kmol<sup>-1</sup>of furfural

Therefore: 4,535,926.1kg Of furfural will require 6,236,902.5kg (G) of raw feed (Pentosan)

Expressing in kg.s<sup>-1</sup>:

Molecular weight of Pentosan (A):

$$C_5H_8O_4 = (12\times5)+(1\times8)+(16\times4)$$

 $MM_A = 132$ kg. kmol<sup>-1</sup>,

$$F_{AO} = \frac{G}{MM_A}$$

$$F_{AO} = \frac{0.2 \, kg/s}{132 kg/kmol}$$

$$F_{AO} = 1.52 \times 10^{-3} \frac{kmol}{s}$$

Concentration of feeds:  $C_{\scriptscriptstyle AO} = \frac{\rho_{\scriptscriptstyle A}}{M M_{\scriptscriptstyle A}}$ 

Where:

$$\rho_A = 1424 \frac{kg}{m^3}$$

$$C_{AO} = \frac{1424 kg/m^3}{132 kg/kmol}$$

$$C_{AO} = 10.79 \frac{kmol}{m^3}$$

$$C_A = C_{A,O}(1 - X_A)$$

Where fractional conversion is 95%:

$$C_A = 10.79(1 - 0.95), C_A = 0.5395 \frac{kmol}{m^3}$$

# **Pressure of Reactor**

$$P_R = 0.01079 \frac{kmol}{dm^3} \times 0.082 atm \frac{dm^3}{kmolK} \times 448K$$
$$P_R = 0.4atm + 1atm = 1.4atm$$

### **Kinetic Parameters:**

**Table 1:** Physical properties data [12], [13]

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<b>Table 1:</b> Physical properties data [12], [13]		
PROPERTIES	VALUES	
Molar Mass	96.08gmol <sup>-1</sup>	
Appearance	Colourless oily	
Odour	Almond-like	
Density	1.16g.ml <sup>-1</sup> at 20 <sup>0</sup> C	
Melting Point	-37°C, (-35°F, 236K)	
Boiling Point	162°C, (324°F, 435K)	
Solubility in water	83g.L <sup>-1</sup>	
Flash Point	62oC, 144°F, 335K	
LD <sub>50</sub> (toxicity)	300-500mg.kg <sup>-1</sup> (oral, mice)	
Viscosity π <sup>20</sup> <sub>D</sub>	1.49	
Oxygen content. %	33%	
Freezing point	-37.6°C	
Auto-ignition	392°C	
temperature		
Partial heat of solution	+2988Cal.mole <sup>-1</sup>	
in water		
Refractive index	At 20oC 1.5261	
	At 25oC 1.5235	
Density, d <sub>4</sub> at 20°C	1.1598g.cm <sup>-3</sup>	
Vapour Density	3.3	
Heat of vaporization	42.8Kj.mol <sup>-1</sup>	
Heat Capacity	1.74J.gk	
Heat of combustion	2344Kj.mol <sup>-1</sup>	
Surface tension	40 MN/M	
Dielectric constant at	41.9	
20°C		
Explosion Limits	2.1 – 19.3	

**Table 2:** Kinetics parameters for the production of furfural

[3]		
Pre- exponential	Activation energy(E <sub>A,0</sub> )	Reaction order of the
$value(A_{O,i})$ $(s^{-1})$	$(\frac{J}{kmol})$	hydronuim concentration in the acid(m <sub>i</sub> )
$3.27 \times 10^{14}$	137,300	1.85
1.608×10 <sup>22</sup>	211,300	0.06

Taking the temperature of the reaction  $175^{\circ} C$ :

$$T = 175^{\circ} C \approx 448K$$

Hydronuim ion concentration as 0.3%:  $[H^+] = 0.03$ 

$$R = 8.314 \frac{J}{mol K}$$

$$k_1 = 4.88 \times 10^{-5} \, \text{s}^{-1}$$

$$\begin{split} k_1 &= \left[0.03\right]^{1.85} \times 3.27 \times 10^{14} \, s^{-1} \times \ell^{\left[\frac{-137,300 \frac{J}{mol}}{8.314 \frac{j}{molK} \times 448 K}\right]}, \\ k_2 &= \left[0.03\right]^{0.06} \times 1.608 \times 10^{22} \, s^{-1} \times \ell^{\left[\frac{-211,300 \frac{J}{mol}}{8.314 \frac{j}{molK} \times 448 K}\right]}, \\ k_2 &= 3.00 \times 10^{-3} \, s^{-1} \end{split}$$

#### **Reactor Head Dimension**

Where:

$$D_R = 6m$$

$$H_H = \frac{D_R}{2},$$

$$H_{H}=\frac{6m}{2},$$

$$H_H = 3m$$

$$V_H = \frac{2}{3}\pi(r_R)^3,$$

$$V_H = 0.67 \times 3.142 \times (3)^3$$

$$V_H = 56.8m^3$$

# Heat generated per unit volume [5], [9]:

$$q_R = (\Delta H_r) X_A k_2 C_{AO} (1 - X_A)$$

Where:  $\Delta H_R = -277,6\dot{0}4,400 \text{ J. kmol}^{-1}$ 

$$q_R = \left(-277,604,400 \frac{J}{kmol}\right) \times 0.95 \times 3.0 \times 10^{-3} \, s^{-1} \times 10.79 \frac{kmol}{m^3} \left(1 - 0.95\right)$$

$$q_R = 426,837.6 \text{ J. m}^3 \text{s}^{-1}$$

Mat lab 7.7 is used to solve the design equations to give the functional parameters of the reactor such as Volume of reactor, space velocity, space time and length of reactor.

# 3.10 Heating Jacket Design [5],[9]

# Mass Flow Rate of Heating Fluid

$$\dot{m}_{w} = \frac{Q}{C_{pw}\Delta T}$$

Where: 
$$Q = (\Delta H_R) F_{A,O} X_A$$
  
 $Q = \left(277,604,400 \frac{J}{kmol}\right) \times 1.09 \times 10^{-3} \frac{kmol}{s} \times 0.95$ 

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$$Q = 287,459.36 \frac{J}{s}$$
,  $C_{pw} = 1.851 \frac{KJ}{kgK}$  At  $200^{\circ} C$ 

The heating fluid enters the jacket at  $200^{\circ} C$  and leaves at  $45^{\circ} C$ 

$$\Delta T = T_1 - T_2$$

$$\Delta T = 200^{\circ} C - 50^{\circ} C$$

$$\Delta T = 150^{\circ} C \approx 423K$$

$$\dot{m}_{w} = \frac{287.46 \, KJ/s}{1.851 KJ/kgK \times 423K}$$

$$m_{\rm w} = 0.\dot{3}7~{\rm kg.\,s^{-1}}$$

#### **Jacket Dimension**

Height of jacket:

$$H_j = \frac{H_R}{2}$$

$$H_j = \frac{1.8m}{2}$$

$$H_j = 0.9m$$

Let the pitch  $(P_i)$  between the spiral baffles be 0.2m

Numbers of spiracles:

$$N_s = \frac{H_j}{P_j}$$

$$N_s = \frac{0.9m}{0.2m}$$

$$N_s = 4.5 \approx 5$$

Length of Jacket:

$$L_i = 94.3m$$

Area of jacket: Let, the space between the jacket and the reactor be  $\Delta b = 0.3m$ 

$$A_j = 0.3m \times 0.2m$$

$$A_i = 0.06m^2$$

Hydraulic diameter  $(d_a)$ :

$$d_e = \frac{4(0.3 \times 0.2)}{2(0.3 + 0.2)},$$

$$d_e = 0.24m$$

# Velocity through channel (u): $u = \frac{\dot{m}}{\rho A_i}$

Where;, 
$$\rho = 1000 \text{kg. m}^3$$
,  $u = \frac{0.37 \frac{kg}{s}}{1000 \frac{kg}{m^3} \times 0.06 m^2}$ 

$$u = 6.17 \times 10^{-3} \frac{m}{s}$$

# Film Heat Transfer Coefficient for the Jacket

Reynolds number (Re):

$$Re = \frac{\rho u d_e}{\mu}$$

$$\mu = 134.5 \times 10^{-6} \, Pa.s$$

$$Re = \frac{1000 \times 0.48 \times 0.24}{134.5 \times 10^{-6}}$$

$$Re = 8565055$$

Prandlts number 
$$(Pr)_{:} Pr = \frac{C_p \mu}{k}$$

Where:
$$C_p = 1.939 \text{ KJ. kg}^{-1} \text{K}^{-1}$$

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$$k = 663.31 \times 10^{-3} \frac{W}{m.K}$$

$$Pr = \frac{1.939 \times 134.5 \times 10^{-6}}{663.31 \times 10^{-3}}$$

$$Pr = 0.39$$

$$\frac{h_j d_e}{k} = 0.023 \text{Re}^{0.8} \, \text{Pr}^{0.33}$$

Ignoring correction factor or taking it as 1

$$\frac{h_j \times 0.24}{663.31 \times 10^{-3}} = 0.023(856505.5)^{0.8} (0.39)^{0.33}$$

$$h_i = 2597W.m^{-2}K^{-1}$$

#### **Overall Heat Transfer Coefficient**

$$U_o = \frac{h_j h_d}{h_j + h_d}$$

Where;

$$h_d = \frac{1}{f_d}$$

Where,

$$f_d = 0.0025 \frac{m^2 C}{W}$$

$$h_d = \frac{1}{0.0025}$$

$$h_d = 400 \frac{W}{m^{2^{\circ}} C}$$

$$\therefore \frac{1}{U_o} = \frac{1}{2597} + \frac{1}{400}$$

$$U_o = 346.62 \frac{W}{m^{-2} C^{-1}}$$

# Heat Transfer Area of the Jacket

$$A = \frac{Q}{U_o \Delta T_{lm}}$$

$$\Delta T_{lm} = \frac{200 + 50}{2}$$

$$\Delta T_{lm} = 125^{\circ} C$$

$$A = \frac{287,459.36 \frac{J}{s}}{346.62 \frac{W}{m^{-2} C^{-1}} \times 125^{\circ} C}$$

$$A = 6.63m^2$$

# Mechanical Design Aspect of the Reactor[1]

# Stirrer Design

Stirrer clearance (C):

$$C = \frac{1}{6}D_R$$

$$C = \frac{6m}{6}$$

$$C = 1.0m$$

Stirrer length  $(L_{st})$ 

$$L_{st} = H_{R} - C$$

$$L_{st} = 1.8m - 1.0m$$

$$L_{st} = 0.8m$$

Diameter of stirrer  $(D_{st})$ 

$$D_{st} = \frac{D_R}{4}$$

$$D_{st} = \frac{6m}{4}$$

$$D_{st} = 1.5m$$

Stirrer blade width (W)

$$W = \frac{D_{st}}{5}$$

$$W = \frac{1.5m}{5}$$

$$W = 0.3m$$

Wall baffle

$$W = \frac{D_R}{10}$$

$$W = \frac{6m}{10}$$

$$W = 0.6m$$

Power consumption

$$Re = \frac{nD^2_{st}\rho}{\mu}$$

Using the viscosity of water since the mixture is water-base;  $\rho = 1424 \text{kg.} \, \text{m}^3$ 

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$$W = 1791.2 \times 10^{-6} Pa.s$$

Taking 
$$n = \frac{90r}{\text{min}}$$

The stirrer type is a radial turbine with 6 blades

$$Re = \frac{90/60 \times (1.5)^2 \times 1424}{1.7912 \times 10^{-2}}$$

$$Re = 2,683,117.46$$

Since  $\text{Re} \rangle 10^4$ , the flow regime is turbulent and the power consumption is independent of the Reynolds number.

$$N_P = K_T$$

Where  $K_T = 6.30$  (Peters M.S, 2004)

$$P = K_T \rho D^5_{st} n^3$$

$$P = 6.30 \times \frac{1424}{1000} \times (1.5)^5 \times (90/60)^3$$

$$P = 0.229KW \approx 0.23KW$$

# **Standard Plate Thickness**

$$t = \frac{P_R D_R}{SE_i - 0.6P_R} + c$$

$$p_R = 1.4atm \times 1.013 \times 10^5 Nm^{-2} = 141,855pa$$

$$D_R = 6m$$

$$S = 66,900 \times 10^3 \ pa$$

$$E_{i} = 0.6$$

$$c = 0.0032$$

$$t = \frac{141,855 \times 6m}{66,900 \times 10^3 \times 0.6 - 0.6 \times 141,855} + 0.0032$$

$$t = 0.024m$$

#### **Material Selection [1]**

Based on the following factors;

Corrosion resistant

Temperature

Allowable pressure

Mechanical properties such brittleness, low thermal conductivity.

PH

Heat transfer rate

Austenitic stainless steel is selected as the material for constructing and fabrication of the reactor.

Carbon steel is selected for the heating jacket

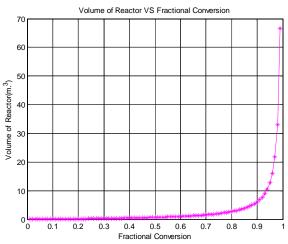
# **Costing of the Reactor[10]**

Using the correlation chart, the purchase cost is \$70,000. In Nigeria equivalent at the exchange rate of 150 naira to \$1, The purchase cost is 10,500,000 naira.

#### 4. RESULTS AND DISCUSSION

Mat lab (7.7) was used to simulate the reactors parameters and the results presented on graphs.

The discussion is on the graphs plotted with result of simulation using Mat lab. The graphs are;



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Fig 1 plot of volume of reactor against fractional conversion

The plots shows that volume of the reactor increases slowly at different fractional to a point where there is a rise in the volume increase till it gets to infinity.

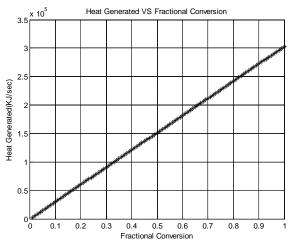


Fig 2 plot of heat generated against fractional conversion

The graph gives a straight line negative graph which shows that the heat generated is directly proportional to fractional conversion

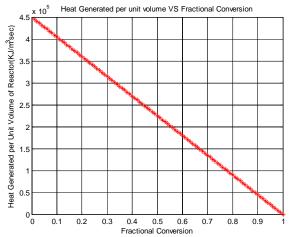


Fig 3 plot of Heat generated per unit volume against fractional conversion

The graph gives a negative straight line graph which shows that the heat generated is directly proportional to fractional conversion

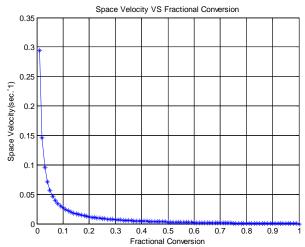
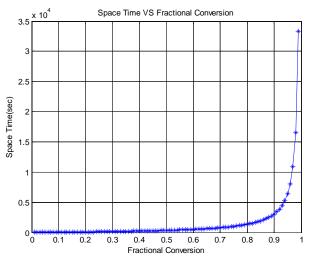


Fig 4 Plot of space velocity against fractional conversion



**Fig 5** plot of space time against fractional conversion. The graph shows that the time taken to react one reactor volume of feed increases with the fractional conversion slowly to a point, it increases till it goes to infinity.

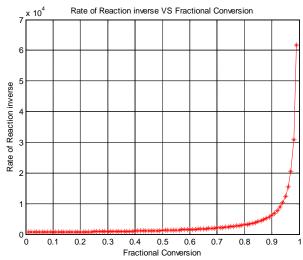


Fig 6 plot of rate inverse against fractional conversion

The graph for the reactor shows a steady rate till a point the rate starts to reduce till it gets to infinity. The graph can be use as a model to determine the volume of the reactor at any fractional conversion. This is done by multiplying the flow rate by the area under the curve from the point of the required fractional conversion.

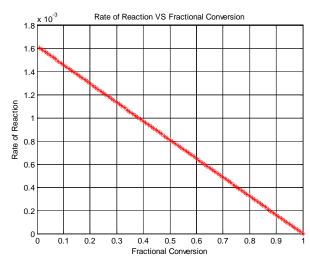


Fig 7 Plot of Rate of reaction against fractional conversion

The plot of rate of reaction against fractional conversion for the reactor produced a negative straight line graph which shows that the rate of reaction is directly proportional to fractional conversion.

# 5. CONCLUSION

The design process accommodates the general principles of material and heat balances, rate law, kinetics, economics and mechanical aspects to bring to bear the designing of the CSTR of capacity. This is a typical pragmatic design that can be operationalised by private sector.

# **NOMENCLATURE**

 $\Delta$  = Heat

 $K_1, k_2 = Rate constant$ 

 $r_{xylan}$  = Rate of xylan hydrolysis

 $r_{xylosee}$  = Rate of xylose dehydration

 $r_{\text{furfural}} = \text{Rate of furfural hydrolysis}$ 

C<sub>A</sub>= Final concentration of A

 $C_B$ = Final concentration of B

C Final concentration of B

C<sub>C</sub>= Final concentration of C

C<sub>AC</sub>= Initial concentration of A

C<sub>BO</sub>= Initial concentration of B

C<sub>CO</sub>= Initial concentration of C

t = Time

A<sub>Oi</sub>= Pre-exponential factor

E<sub>Ai</sub>= Activation energy

R = Gas constant

T = Temperatue

F<sub>iO</sub>= Initial molar flow rate of specie i

X<sub>i</sub>= Fractional conversion of specie i

 $V_R$ = Volume of reactor

r<sub>i</sub>= Initial concentration of C

V<sub>R</sub>= Volume of reactor

F<sub>AO</sub>= Initial molar flow rate of specie

 $\pi = Pie$ 

r = Radius

 $L_H = Length of reactor$ 

 $V_H = Volume of reactor head$ 

L = Length

RTD = Resident Time Distribution

 $\tau = Space$ 

 $S_v = Space velocity of reactor$ 

 $q_R$  = Heat generated per unit volume of reactor

 $L_{ST}$  = Length of stirrer

C = Clearance of stirrer

 $D_{St}$  = Diameter of stirrer

B = Wall baffle

P = Power

 $N_p = Power number$ 

n = Number of revolution

 $\rho = Density$ 

f = Function

 $R_e = Reynold number$ 

 $f_r$  = Froude number

 $S_n$  = Reactor dimension number

 $\mu = Viscosity$ 

 $\dot{m} = Mass flow rate$ 

 $\Delta H_R$  = Heat of reaction

 $\Delta T$  = Change in Temperature

 $H_i$  = Height of the jacket

 $L_i$  = Length of the jacket

 $P_i$  = Pitch of the spiracles

 $A_i$  = Area of heating jacket

d<sub>e</sub> = Hydraulic diameter

u = Velocity

Pr = Prandlt number

k = Thermal conductivity

 $h_i$  = Film heat transfer of the heating jacket

 $h_d$  = Film heat transfer coefficient of dirt

 $f_d = Dirt factor$ 

 $U_0$  = Overall transfer coefficient

 $\Delta T_{lm} = Log mean temperature$ 

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