Computer Aided Design of Fluidized Bed Reactor for the Production of Polypropylene

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Abstract

Fluidized bed reactor (FBR) are the most preferred reaction vessels for reactions involving gas-liquid-solid interaction as they have excellent mass transfer characteristics and exceptional heat distribution system. The fluidized bed consist of two regions: bubble and emulsion phases with an interchange coefficient for transfer of gas between regions. The computation and design of fluidized bed for the production of polypropylene was presented. Three configurations were considered for the plug flow – plug flow configuration, plug flow – mixed flow configuration and mixed flow – mixed flow configuration for the bubble and emulsion phases respectively to investigate the best configuration for highest yield of polypropylene. A computer software (ASPEN HYSIS) was used for the design the three FBR configurations. Results obtained indicated that the plug flow – plug flow configuration produced the highest yield of 51.6mole percent while the plug flow – mixed flow mode had 46.02mole percent and the mixed flow – mixed flow mode produced the lowest yield of 45.19mole percent. However, the mixed flow – mixed flow mode utilized the lowest operating temperature of 194F while the plug flow – mixed flow and plug flow – plug flow modes utilized 202F and 320F respectively, indicating that the mixed flow – mixed flow mode temperature matched plant data for 90°C (194F). The design capacity of the fluidized bed reactor (FBR) is 4813 barrel/day, 4791 barrel/day and 4639barrel/day for PFR/PFR, PFR/CSTR and CSTR/CSTR configurations respectively.

Keywords: Fluidized Bed Reactor, Polypropylene, Design, Aspen-Hysis, CSTR, PFR, Operating Temperature

1.Introduction

Polypropylene is considered as one of the important polymer products that has started to grow in a wide range among other plastics. The reason is that several materials such as steel, wood, glass, paper and other metals can be replaced by polypropylene from the point of effective cost and performance. Also, the application of polypropylene can be found from household furniture, carpets, packaging containers to pipes, automobile parts and many other products that we even cannot imagine.

Polypropylene was discovered by Paul Hogan and Robert L. Banks in 1951, in an attempt to make dimers and trimmers of ethylene and propylene with a chromium oxide catalyst for gasoline use. They accidentally produce some crystalline polypropylene and linear polypropylene. The process was planted by Philips petroleum at the beginning of 1953 (Morris, 2005). The first commercial production of polypropylene began in USA in 1957 then followed by Europe in 1958. Since the 1980s and until nowadays after passage of some 60 years from Natta and Ziegler invention, polypropylene production, consumption and application have increased and became the first common large volume among the group of thermoplastic industries used all over the world.(Moore, 1996).

In general, polymerisation of polypropylene is done by contacting propylene and Ziegler-Natta catalyst. Metallocene can be used instead of Ziegler Natta catalyst (Corradini et al, 2004). The chemical structure of polypropylene represents by the tacticity which is formed by different way, it depends on how the substituents are arranged on the polymer backbone. So polypropylene can be isotactic, actactic or syndiotactic (Paul & Robert, 1989). Polypropylene is classified into three major types: homopolymer, random copolymer, and impact copolymer. Propylene monomers are used to make homopolymer while in random and impact copolymer ethylene and propylene are used (Shariati, 1996; Gooch, 2007). The need to increase the production of polypropylene has been the headache to chemical petrochemical engineers in Nigeria over the years because of the increasing population which directly means a higher demand for the polypropylene product.

This research is timely because of the diverse applications to which the petrochemical products are being put and especially because of the demand of such products. From available data, it is seen that the total amount of polypropylene product in 1995 was 2,061 tons; 1996 was 13,129 tons, 1997 was 15,497 tons and 2012 was 140,000 tons (Khan et al., 2016; Zheng et al., 2010). Hence this study will enable us to meet up with rising demand so as to curb the problem of the lack of polypropylene which might rise in the next few years.

Therefore the focus of this research is designing a fluidised bed reactor for the production of polypropylene, due to its uniform particle mixing, uniform temperature gradients and ability to operates reactor in continuous state. The designing of this reactor incorporates the chemical engineering principles which include the material and energy balances, rate kinetics, reactor model assumptions, determination of space velocity, space time, and voidage. This design accounts for the chemical processes of polypropylene production,   heat generation per unit

volume, pressure drop, heat exchanger configurations.

2.0 Materials and Methods

2.1 Reactor Model: Plug Flow/Plug Flow Configuration

Figure 1 shows the hypothetical representation of two-phase fluidized bed reactor in plug flow/plug flow and Hysis design configurations. In a fluidized bed the bubbles surrounded by large overlapping clouds rise fast, but not much faster than the emulsion gas. Thus, these overlapping clouds may well constitute the emulsion phase (Kunii and Levenspiel, 1991). Hence it is viewed that the bed constituted two regions (bubble and emulsion), with just one interchange coefficient K_{be} to represent the up-flow of gas between regions, where u_o is the superficial velocity, u_b, u_e represent the bubble and emulsion velocity respectively. C_{Ab}, C_{Ae} is the concentration of the reactant, A in the bubble and emulsion phase.

(a) Physical PFR/PFR configuration   (b) (ASPEN HYSIS) PFR/PFR configuration
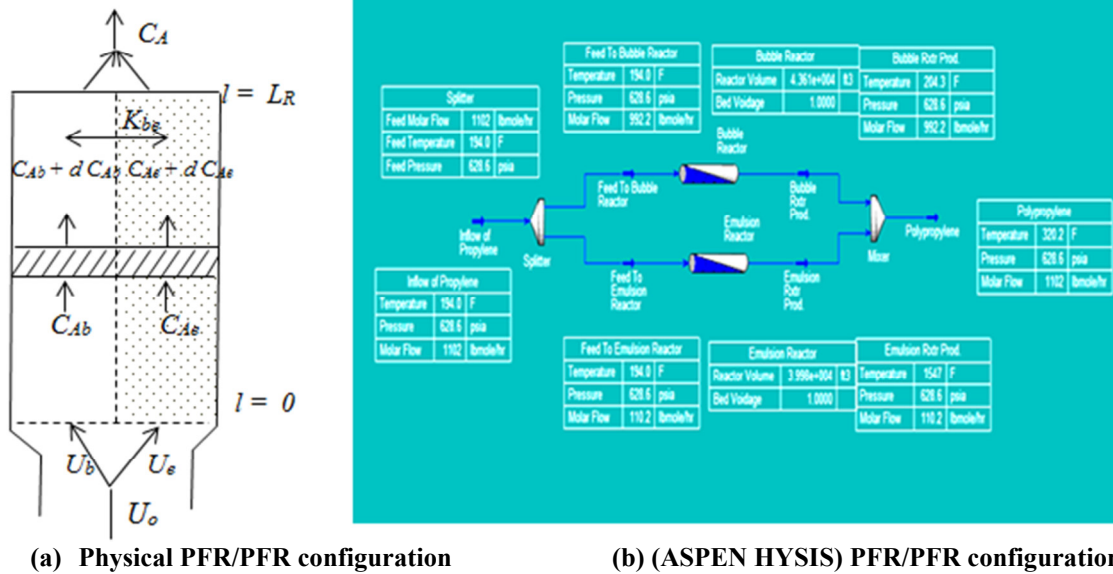
Figure 1: Hypothetical representation of PFR/PFR configuration of Fluidized bed reactor

Figure 1(b) shows the HYSIS design shows the inflow of propylene through a splitter which divided the feed into the two phases which is the bubble phase plug flow reactor and emulsion phase plug flow reactor respectively. The feed (monomer) from the both reactors was channelled into a mixer to give the outlet concentration of polypropylene. The mathematical model for this configuration using the law of conservation of mass on the bubble and emulsion phases, adopting the proposed assumptions yields

(a) for Bubble phase:

$$\frac{dy_{ib}}{dz} = -\frac{K_{be}L_f}{U_b}[y_{ib} - y_{ie}] \qquad (1)$$

(b) For the Emulsion phase

$$\frac{dy_{ib}}{dz} = -(-r_i)\frac{\varepsilon L_f}{U_b} + \frac{K_{be}L_f}{U_b}[y_{ib} - y_{ie}] \qquad (2)$$

2.2 Reactor Model: Plug Flow/Mixed Flow Configuration

Figure 2 depicts the hypothetical representation of two-phase fluidized bed reactor in plug flow/mixed flow and Hysis design configurations. The bed constituted two regions bubble and emulsion, with just one interchange coefficient K_{be} to represent the up-flow of gas between regions, where u_o is the superficial velocity, u_b, u_e represent the bubble and emulsion velocities respectively, K_{be} is the interchange coefficient between the bubble and emulsion phase. C_{Ab}, C_{Ae} are the concentration of the reactant, A in the bubble and emulsion phase.
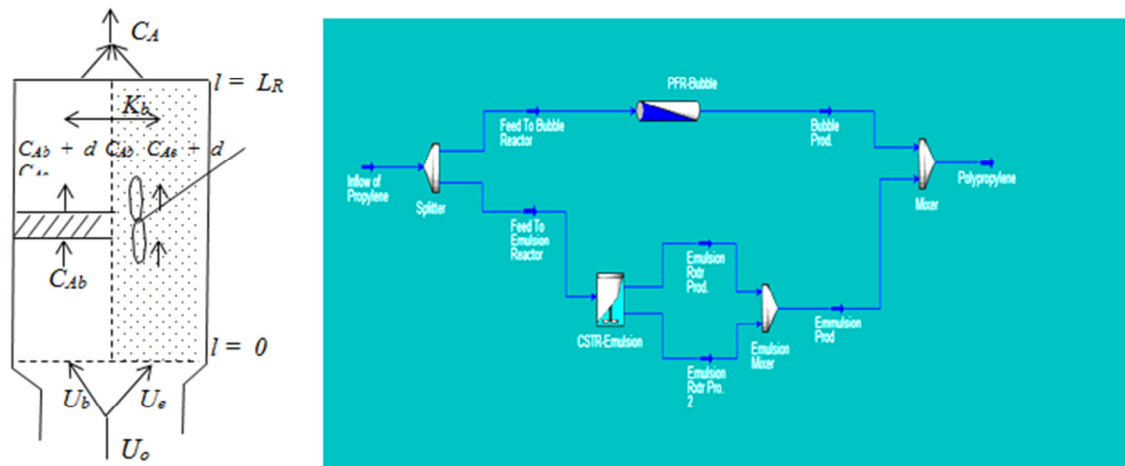
(a) Physical PFR/CSTR configuration   (b) (ASPEN HYSIS) PFR/CSTR configuration
Figure 2: Hypothetical representation of PFR/CSTR configuration of Fluidized bed reactor

The HYSIS design as shown in figure 2(b) depicts the inflow of propylene through a splitter which divided the feed into the two phases which is the bubble phase plug flow reactor and emulsion phase mixed flow reactor respectively. The feed (monomer) from the both reactors were channelled into a mixer to give the outlet concentration of polypropylene. The mathematical model for this configuration using the law of conservation of mass on the bubble and emulsion phases, adopting the proposed assumptions yields:

(a) Bubble phase:

$$\frac{dy_{ib}}{dz} = -(-r_i)\frac{\varepsilon L_f}{U_b} - \frac{K_{be}L_f}{U_b}[y_{ib} - y_{ie}]$$ (3)

(b) For the Emulsion phase

$$y_{ie} = \frac{U_e y_{ieo} - (-r_i)\varepsilon L_f z + K_{be}[y_{ib} - y_{ie}]}{U_e + K_{be}L_f z}$$ (4)

2.3   Reactor Model: Mixed Flow/Mixed Flow Configuration

Figure 3 depicts the two-phase fluidized bed reactor in mixed flow/mixed flow and Hysis design configurations. The bed constituted two regions bubble and emulsion, where u_o is the superficial velocity, u_b, u_e represent the bubble and emulsion velocities respectively, in this configuration there is no interchange coefficient between the bubble and emulsion phase. C_{Ab}, C_{Ae} are the concentration of the reactant, A in the bubble and emulsion phase.
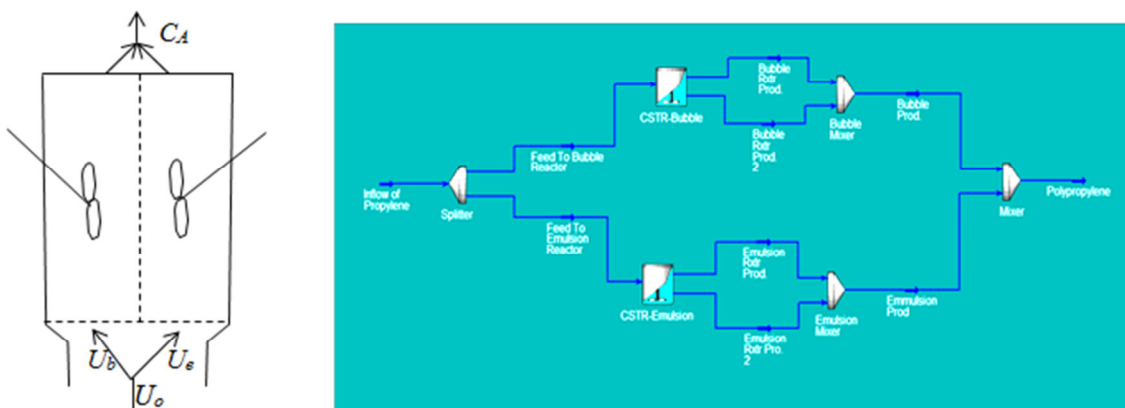
(a) Physical mixed flow/mixed flow configuration   (b) (ASPEN HYSIS) mixed flow/mixed flow configuration
Figure 3: Hypothetical representation of CSTR/CSTR configuration of Fluidized bed reactor

Figure 3(b) shows the HYSIS configuration with the inflow of propylene through a splitter which divided the feed into the two phases which is the bubble phase (mixed flow reactor) and emulsion phase (mixed flow reactor) respectively. The products from the both reactors were channelled into a mixer to give the outlet concentration of polypropylene. The mathematical model for this configuration using the law of conservation of mass on the bubble and emulsion phases, adopting the proposed assumptions yields:

(a) Bubble phase:

$$y_{ib} = \frac{U_e y_{ibo} - (-r_i)\varepsilon L + K_{be} y_{ie} L}{U_e + K_{be} L} \tag{5}$$

(b) For the Emulsion phase

$$y_{ie} = \frac{U_e y_{ieo} - (-r_i)\varepsilon L + K_{be} y_{ib} L}{U_e + K_{be} L} \tag{6}$$

2.1 Reactor Model Assumption for plug flow-plug flow (PFR/PFR) configuration
The following assumptions were made for the derivation of the fluidised reactor (FBR) model:
1. Fresh feed gas containing reactant A at C_A; enters the bed and, on contact with the fine catalyst powder, reacts there according to a first order reaction.
2. The bed consists of two regions, bubble and emulsion with the cloud and wake region negligible. We designate the reactant concentration at any level in these regions as C_{Ab}, C_{Ae}.
3. Since $U_o >> U_{mf}$, all the feed gas passes through the bed as bubbles while the catalyst resides in the emulsion phase.
4. The gas interchange rate between bubble and emulsion are given by Kbe.
5. The operation is at steady state condition.
6. The emulsion phase is at minimum fluidization velocity and reaction takes place in the emulsion phase.

2.1.1 Material Balance
This is very important aspect of reactor design. It helps in the determination of the quantity of raw materials and products produced. It also helps in the determination of the reactor functional parameters. The principles of conservation of mass and energy were applied to achieve the aim. The general conservation equation or any process can be written as:

$$\left(\begin{array}{c}\text{Inflow of}\\\text{material/energy}\\\text{into reactor}\\\text{volume}\end{array}\right) - \left(\begin{array}{c}\text{Outflow of}\\\text{material/energy}\\\text{out of reactor}\\\text{volume}\end{array}\right) \pm \left(\begin{array}{c}\text{Generation/}\\\text{depletion by}\\\text{chemical}\\\text{reactions}\end{array}\right) = \left(\begin{array}{c}\text{Material/Energy}\\\text{accumulated}\\\text{within the}\\\text{system}\end{array}\right) \tag{7}$$

2.1.2   Material Balance Equation in the bubble phase
The principle of conservation of mass in the bubble phase is as follows:

$$\left(\begin{array}{c}\text{Rate of Inflow}\\\text{of propylene}\\\text{into differential}\\\text{bubble phase}\end{array}\right) - \left(\begin{array}{c}\text{Rate of Outflow}\\\text{of propylene}\\\text{into differential}\\\text{bubble phase}\end{array}\right) \pm \left(\begin{array}{c}\text{Rate of}\\\text{generation of}\\\text{propylene due to}\\\text{Chemical reaction}\end{array}\right) + \left(\begin{array}{c}\text{Rate of interchange}\\\text{of propylene}\\\text{between bubble}\\\text{and emulsion phase}\end{array}\right)$$

$$= \left(\begin{array}{c}\text{Accumulation of}\\\text{propylene within}\\\text{the bubble phase}\end{array}\right) \tag{8}$$

At **steady state**:
Rate of accumulation   =   0
Rate of inflow of reactant A into differential bubble phase   = $\vartheta_o C_{Ab}$
Rate of outflow of reactant A from differential bubble phase = $\vartheta_o (C_{Ab} + dC_{Ab})$
Disappearance by chemical reaction   = $(-r_A) A_R dL \varepsilon_R$
Rate of interchange of propylene between bubble and emulsion phase $= K_{be}[C_{Ab} - dC_{Ab}] A_R dL$
Where ϑ_o is the volumetric flow rate of gas, ε_R is the voidage, r_A is the reactant rate of reaction and A_R is the area of the reactor.
Substituting defined parameters into equations 2 gives

$$\vartheta_o C_{Ab} - \vartheta_o [C_{Ab} + dC_{Ab}] - (-r_A) A_R dL \varepsilon_R + K_{be}[C_{Ab} - dC_{Ab}] A_R dL = 0 \tag{9}$$

$$-\vartheta_o dC_{Ab} - (-r_A) A_R dL \varepsilon_R + K_{be}[C_{Ab} - C_{Ab}] A_R dl = 0 \tag{10}$$

Dividing through equation (4) by $A_R dL$;

$$-\frac{\vartheta_o dC_{Ab}}{A_R \, dL} - (-r_A)\varepsilon_R + K_{be}\left[C_{Ab} - C_{Ae}\right] = 0$$

But, $\dfrac{\vartheta_o}{A_R} = U_b$ Hence,

$$-U_b \frac{dC_{Ab}}{dL} = (-r_A)\varepsilon_R - K_{be}\left[C_{Ab} - C_{Ae}\right] \tag{11}$$

Similar derivation could be obtained using the emulsion phase.

$$-U_e \frac{dC_{Ae}}{dl} = (1-\delta)(1-\varepsilon_{mf})(-r_A) + K_{be}\left[C_{Ab} - C_{Ae}\right] \tag{12}$$

Where ε_R is the voidage in the bubble phase, ε_{mf} is the voidage of minimum fluidization and δ is the fraction of bed occupied by the particles.

Equations (5) and (6) are the mathematical model for the two phase fluidized beds reactor for polypropylene production in PFR/PFR configuration.

2.1.3 Derivation in Terms of Volume of Reactor (V_R)

$$-\vartheta_o \frac{dC_{AB}}{\varepsilon_R \, dV_R} = (-r_A) - K_{be}\left[C_{Ab} - C_{Ae}\right] \tag{13}$$

$$-\vartheta_o \frac{dC_{Ae}}{(1-\varepsilon_{mf}) dV_R} = (-r_A) + K_{be}\left[C_{Ab} - C_{Ae}\right] \tag{14}$$

Equation (7) and (8) represent the model in terms of volume of reactor for PFR/PFR configuration.
Since the total reactor volume, V_R is the sum of the volume occupied by the fluid and the volume occupied by the catalyst, for a catalytic reactor;

$$V_R = V_{fluid} + V_{catalyst} \tag{15}$$

where,

$$V_{fluid} = \varepsilon V_R \tag{16}$$
$$V_{cat} = (1-\varepsilon)V_R \tag{17}$$

where, ε is the void fraction or the fraction of the reactor volume occupied by the fluid and V_R is the volume of the reactor.

2.1.4 Space/Residence time and Space velocity

The mean residence time is equal to the space time and is defined as the reaction time required to process one reactor volume of feed measured at specific conditions. It is otherwise called "*holding time*"
Mathematically, it is expressed as:

$$\tau = \frac{V_{fluid}}{\vartheta_o} = \frac{\varepsilon V_R}{\vartheta_o} \tag{18}$$

Space velocity is defined as the number of reactor volume of feed at specified conditions which can be treated per unit time.
Mathematically, it is expressed as:

$$S = \frac{\vartheta_o}{\varepsilon V_R} \tag{19}$$

2.1.5 Heat Generation per unit Volume

For the case of steady flow in fluidized bed reactors, the variables that affect the heat of generation are heat of reaction (or heat of polymerization of propylene), molar feed rate, the degree of conversion and the roughness of hot pipe. This is mathematically expressed as:

$$Q = \Delta H_r \, F_{Ao} \, X_A \tag{20}$$

Where, Q is the heat flow rate (KJ/min), Hr is the heat of reaction (KJ/mol), F_{Ao} is the molar feed rate (mole/mm) and X_A is the degree of conversion
Dividing both sides of equation (14) by the volume of the reactor (V_R) the equation result to:

$$\frac{Q}{V_R} = \frac{\Delta H_r \, F_{AO} \, X_A}{V_R} \tag{21}$$

$\dfrac{Q}{V_R}$ is the heat generated per unit volume of reactor and is designated by R_q:

$$R_q \quad = \quad \frac{\Delta H_r \; F_{AO} \; X_A}{V_R} \qquad (22)$$

2.2 HYDRODYNAMIC SPECIFICATIONS

From Kunii and Levenspiel (1991), a material balance for the bed material gives:

2.2.1 Single bubble rise velocity (U_{br}) at U_{mf} is given as:

$$U_{br} \quad = \quad 0.711 \, (gd_b)^{\frac{1}{2}} \qquad (23)$$

where, g is the acceleration due to gravity (m^2/s) and d_b is the bubble diameter (m).

2.2.2 Bubble Velocity U_b is given as:

$$U_b = \quad U_o - U_{mf} + U_{br} \qquad (24)$$

2.2.3 Bed fraction in bubbles, δ in (m^3 bubbles/m^3 bed) is given as
(Choi and Ray, 1988):

$$\delta = \quad \frac{U_o - U_{mf}}{U_b} \qquad (25)$$

For $U_b \gg U_{mf}$, we can use:

$$\delta = \quad \frac{U_o}{U_b} \qquad (26)$$

2.2.4 Catalyst Bed Height:

The catalyst bed height is expressed as;

$$H_f = \frac{W}{\rho s \, A_R \, (1 - \varepsilon_f)} \qquad (27)$$

where, W is the mass of solid (catalyst) on the bed, ρs is the density of solid (catalyst) A_R is the cross-sectional area of the bed, ε_f is the void fraction.

2.2.5 Rise Velocity of Emulsion phase

The rise velocity in the emulsion phase is given as:

$$U_e \quad = \quad \frac{U_{mf}}{\varepsilon_{mf}} \qquad (28)$$

Where, ε_{mf} is the voidage at minimum fluidization velocity and U_{mf} is the bed height at minimum fluidization velocity.

2.2.6 Interchange, Volume between bubble and cloud, or Cloud and emulsion

The expressions for bubble cloud circulation and the Higbei theory for cloud – emulsion diffusion, the interchange of gas between bubble and cloud is:

$$K_{bc} \quad = \quad 4.5 \quad \left(\frac{u_{mf}}{d_b} \right) + 5.85 \quad \left(\frac{D^{\frac{1}{2}} \, g^{\frac{1}{4}}}{d_b^{\frac{5}{4}}} \right) \qquad (29)$$

and between cloud-wake and emulsion

$$K_{ce} \quad = \quad 6.77 \quad \left(\frac{E_{mf} \, D U_{br}}{d_b^3} \right)^{0.5} \qquad (30)$$

And for interchange coefficient between bubble emulsions is (Kunii and Levenspiel, 1991):

$$\frac{1}{K_{be}} \quad = \quad \left(\frac{1}{K_{ce}} + \frac{1}{K_{bc}} \right) \qquad (31)$$

The volume of solids in bubbles per volume of bed is roughly estimated to be:

$$f_b \quad = \quad 0.001 \text{ to } 0.01 \qquad (32)$$

where, $f_b + f_c + f_e = f_{total} = 1 = \varepsilon_f$ \qquad (33)

2.3 RATE KINETIC EVALUATION

The kinetic rate expression for the polypropylene is approximately given as (Fait *et al,* 1995);

$(-r_A) = K_p [M] C$ (34)

where, M is the number of active site per gram of catalyst, K_p is the propagation rate constant and C is the concentration of monomer.

Let $\quad k = k_p M$ and $C = C_A$;

$$\frac{dM}{dt} = \quad (-r_A) = k C_A$$ (35)

where, k = rate constant of reaction

The rate constant varies with temperature in accordance with the Arrhenius expression given as:

$$k = k_o \exp.\left[E_{cat}/RT\right]$$ (36)

Therefore, $\quad \dfrac{dM}{dt} = \quad (-r_A) = K_o \exp.\left[E_{cat}/RT\right] C_A$

where, $C_A = C_{Ao}(1 - X_A)$ (37)

Substituting $\quad (-r_A) = k_o \exp.\left[E_{cat}/RT\right] C_{AO}(1 - X_A)$ (38)

where, k_o is the frequency factor or pre-exponential constant, E_{cat} is the activation energy, R is the universal gas constant T is the reaction temperature, C_{Ao} is the Initial concentration of propylene and X_A is the fractional conversion of propylene.

2.4 ENERGY BALANCE

Consider the steady state heating of a continuous flow of solids F_o (Kg/s) at temperature T_p by a hot gas in a single fluidized bed entering at temperature T_{gi} as shown in Figure 4. We neglect heat loss to the surroundings, reasonable for commercial scale fluidized bed reaction applying the energy balance.
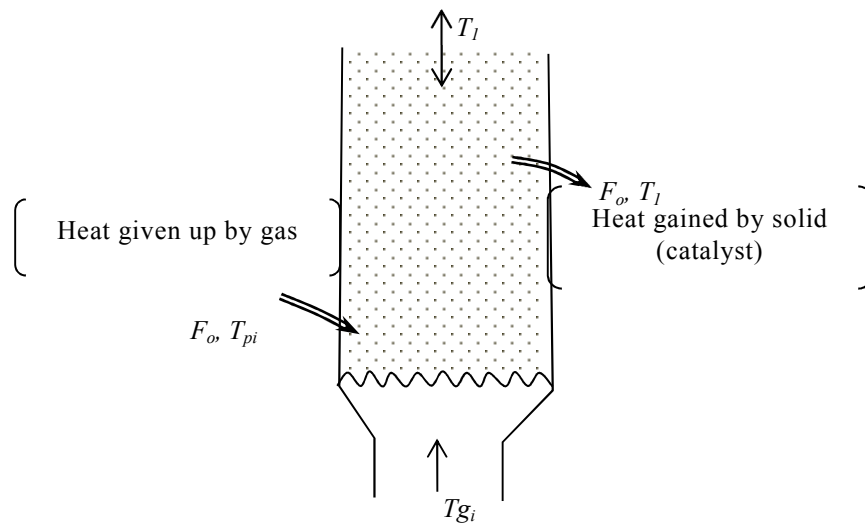

Figure 4Continuous heat exchange between solids and fluidizing gas

Assuming that the exit gas, bed solids and existing solids are all at the same temperature T_1.

Heat inflow with gas $\quad = \quad A_t U_o \rho_g C_{pg} T_{gi}$

Heat inflow with catalyst $\quad = \quad F_o \rho_s C_{ps} T_{pi}$

Heat outflow with gas $\quad = \quad A_t U_o \rho_g C_{pg}, T_1$

Heat outflow with solids $\quad = \quad F_o \rho_g C_{pg}, T_1$

Combining the terms into equation (3.34) gives

$A_t U_o \rho_g C_{pg} T_{gi} + F_o \rho_s C_{ps} T_{pi} = A_t U_o \rho_g C_{pg} T_1 + F_o \rho_s C_{pg}, T_1$ (39)

$A_t \rho_g U_o Cp_g Tg_i - A_t \rho_g U_o Cp_g T_1 = F_o \rho_s Cps T_1 - F_o C_{pg}, \rho_s T_{p1}$

$A_t U_o \rho_g C_{pg} (Tgi - T1) = F_o \rho_s C_{ps}(T_1 - T_{pi})$ (40)

Making T_1 the subject of the formulae.

$A_t \rho_g U_o C_{pg} T_{gi} + F_o \rho_s C_{ps} T_{pi} = F_o \rho_s C_{ps} T_1 + A_t \rho_s U_o C_{pg} T_1$

$= T_1 (F_o \rho_s C_{ps} + A_t \rho_s U_o C_{ps})$

$$T_1 \quad = \quad \frac{A_t \, \rho_g \, U_o \, C_{pg} \, T_{gi} \; + \; F_o \, \rho_s \, C_{ps} \, T_{pi}}{F_o \, \rho_s \, C_{ps} \, T_{pi} + A_t \, \rho_g \, U_o \, C_{pg}} \tag{41}$$

where, F_o is the volumetric flow rate of catalyst, T_p is the entry temperature of catalysts, T_{gi}, is the entry temperature of gas and T_1 is the exit temperature.

2.5 GAS TEMPERATURE PROFILE WITH CATALYST BED HEIGHT

Assuming plug flow for the gas stream and quasi steady state condition, the change of gas temperature with catalyst bed height is given by heat balance in equation (1)

$$- \rho_g \, Cp_g \, U_o \, d \, T_g = \quad \frac{6\left(1-\varepsilon_f\right)}{Q_s \, d_\rho} H_f \, \left[T_g - T_p\right] dz \tag{42}$$

$$\frac{d T_g}{dz} \quad = \quad \frac{6\left(1-\varepsilon_f\right)}{Q \, d_\rho} H_f \, \left(T_g - T_p\right) \tag{43}$$

$T_g = T_{gi,}$ at $z = 0$

Catalyst Bed Temperature with Time

Applying equation (3.34) to the whole bed during a short time interval dt gives:

$- \rho_g \, Cp_g \, U_o \, d \, (T_{gi} - T_p) \, dt = \quad \rho_g \, Cp_g \, (1 - E_f) \, L_f = dT_p$

$$\frac{d \, T_p}{dt} \quad = \quad \frac{\rho_g \, C_{pg} \, U_o \, (T_{gi} - T_{pi})}{\rho_g \, C_{pg} \, (1 - \varepsilon_f) \, H_f} \tag{44}$$

$B_C \quad T_p = \quad T_{po} \quad$ at $t = 0$

2.6 EFFICIENCY OF HEAT UTILIZATION

The efficiency of heat utilization of gas and solid in the system are then:
For Gas:

$$\eta_g = \quad \frac{\text{temperature drop of gas}}{\text{maximum possible temperature drop}} = \quad \frac{T_{gi} - T_1}{T_{gi} - T_{pi}} \tag{45}$$

For Solids:

$$\eta_s = \quad \frac{\text{temperature rise of solid}}{\text{maximum possible temperature rise}} = \quad \frac{T_1 - T_{p1}}{T_{gi} - T_{pi}} \tag{46}$$

$$= \quad 1 - \eta_g \tag{47}$$

2.7 OPERATING PARAMETERS

The models developed was applied in the design of the fluidized bed reactor using the operating parameters depicted in Table 1.

Table 1: Operating data of Fluidized Bed Reactor (Khan *et al*, 2016 and westerink *et al*,1988)

COMPOSITION		
	Propylene	**Polypropylene**
Molecular Weight	42.08g	42.08g
Normal Boiling Point	-	-47.67^{o}C
Temperature	-	-91.06^{o}C
Pressure	-	4555kpa
Composition (Mole)	0.548	0.452
REACTION		
Type of reaction	Heterogeneous reaction	
Activation Energy, E	7.04X10^4 J/mol	
Pre-exponential Factor	1.2X10^4 m^3/mols	
Stoichiometric Ratio	1:1	
FEED STREAM		
Temperature	90°C	
Pressure	4334kpa	
Mass Flow rate	21040kg/hr	

REACTOR (PFR-PFR SYSTEM)		
	Bubble Reactor	**Emulsion Reactor**
Reactor type	PFR	PFR
No of tubes	10	10
Molar Flow Rate	992.2Ibmol/hr	110.2Ibmol/hr
Total Volume	13289.28 m^3	12192m^3
Length	0.9859m	0.940m
REACTOR (PFR-CSTR SYSTEM)		
Reactor type	PFR	CSTR
No of tubes	10	-
Molar Flow Rate	992.2Ibmol/hr	110.2Ibmol/hr
Total Volume	12100.56m^3	193.761m^3
Length	1.699m	-
REACTOR (CSTR-CSTR SYSTEM)		
Reactor Type	CSTR	CSTR
Molar Flow Rate	992.2Ibmol/hr	110.2Ibmol/hr
Total Volume	193.7766m^3	161.452m^3

3.0 RESULTS AND DISCUSSION

Table 2 shows results obtained from three fluidized bed reactor configuration: plug flow – plug flow (PFR/PFR), plug flow – mixed flow (PFR/CSTR), mixed flow – mixed flow (CSTR/CSTR) configuration adapted to the process simulation software (ASPEN HYSIS). The polypropylene yield, temperature and pressure for the three configurations are presented in table 2.

Table 2 Comparison of predicted results for the three configurations

PARAMETERS	REACTOR CONFIGURATIONS		
	PFR/PFR	**PFR/CSTR**	**CSTR/CSTR**
Polypropylene yield (mole fraction %)	51.60%	46.02%	45.19%
Conversion of propylene (mole %)	48.40%	53.98%	54.81%
Temperature (F)	320F	201F	194F
Pressure (psi)	4334kpa	4334kpa	4334kpa
No of tubes	10	10	10

The plug flow – plug flow mode gave the highest yield of 51.6%, while that of the plug flow – mixed flow and mixed flow – mixed flow configuration modes were 46.02% and 45.19% respectively. The temperature distribution for the three modes were 320F, 201F and 194F as for plug flow – plug flow (PFR/PFR), plug flow – mixed flow (PFR/CSTR) and mixed flow – mixed flow (CSTR/CSTR) configurations respectively. These indicate that the plug flow – plug flow (PFR/PFR) configuration produced the highest yield reaction with very high temperature distribution as compared with that of plug flow – mixed flow (PFR/CSTR) and mixed flow – mixed flow (CSTR/CSTR) configurations. The propylene conversion for the three configurations of fluidized bed reactor are depicted in Table 2, the conversions are 48.40mole%, 53.98mole% and 54.81mole% for plug

flow – plug flow, plug flow – mixed flow, mixed flow – mixed flow respectively. The number of tubes used in the design were the same for the three configurations. Other parameters are presented in table 3.

Table 3 Volume of fluidized bed reactor (FBR) for the three configurations

Dimension	Reactor Configurations		
	PFR/PFR	PFR/CSTR	CSTR/CSTR
Volume of reactor (cm^3)	25481.28	12294.321	355.2286
Length of reactor (cm)	19.2599	16.19	---

Table 4. Comparison of the Reactor's configuration yield in terms of barrel/day

Reactor	Yield (barrel/day)
PFR-PFR	4813
PFR-CSTR	4791
CSTR-CSTR	4639

The differences in the yield achieved, the yield obtained in the plug flow-plug flow reactor configuration is higher than the yields obtained in mixed flow-mixed flow and mixed flow-plug flow reactor configuration. The high operating temperature of the plug flow-plug flow configuration ensures a high mass transfer rate, which is required for high yield.

3.2 EFFECT OF TEMPERATURE ON THE REACTOR IN THE BUBBLE AND EMULSION PHASE
3.2.1 Bubble Phase
Figure 5a shows that the temperature increases with increase in reactor length. At higher velocity of the gas, there is an increase in temperature along the reactor length. As the gas velocity is increased, these bubbles often lose their shape as they move forward to burst at the bed surface. Thus the increase in temperature is due to the fact that large volume of gas is being fed into the reactor. The increase in temperature and velocity causes bubble rise and mass transfer of the reactant gases takes place as they flow in and out of the bubble to contact the solid particles which contain higher concentration in the emulsion phase where the reaction product is formed. The reaction is an exothermic reaction resulting in increasing temperature progression.
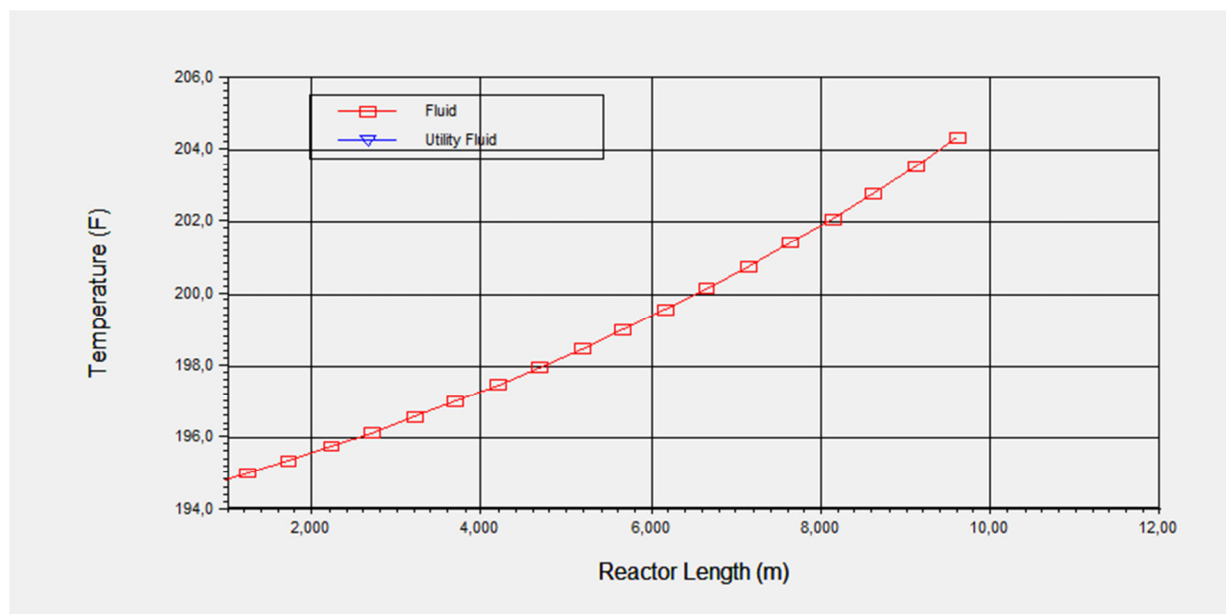

Figure 5a Effect of temperature in the Bubble phase for plug flow – plug flow configuration
3.2.2 Emulsion Phase
In figure 5b the temperature in the emulsion phase is far higher than the temperature in the bubble phase that is from 37.8^{o}C – 482°C because reaction takes place in this phase. There was a rapid increase in temperature from 37.8^{o}C – 454°C along the reactor length from 1.2m to 1.9m. As a result of an increase in the temperature, the fluidized behaviour of the propylene or reactor particles progressively shift from A to B, where the reaction occurs and then the temperature became steady along the length of the reactor. Thus products is formed at this stage because of the higher concentration of the catalyst domicile in the emulsion phase inherent with low input velocity. This behaviour also explains why isothermal conditions is assumed for fluidized bed reactor
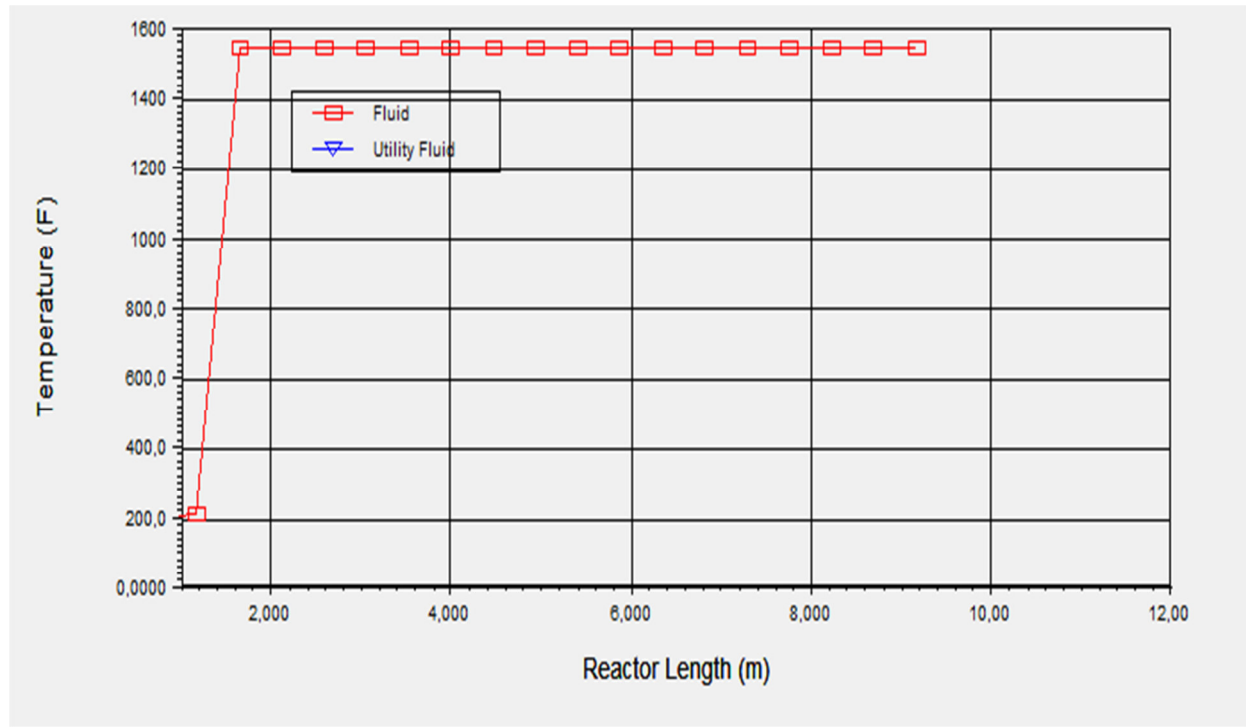
Figure 5b Effect of Temperature in the emulsion phase for plug flow

3.3 EFFECT OF PRESSURE ON THE REACTOR IN THE BUBBLE AND EMULSION PHASE
3.3.1 Bubble Phase and Emulsion Phase
The effect of pressure is depicted in figure 6a and 6b. Observing the trend of the plot the pressure in both phases remains constant throughout the reaction along the length of the reactor. The pressure is set at 4334kpa to maintain the reaction at the desired phase for the selected temperature.
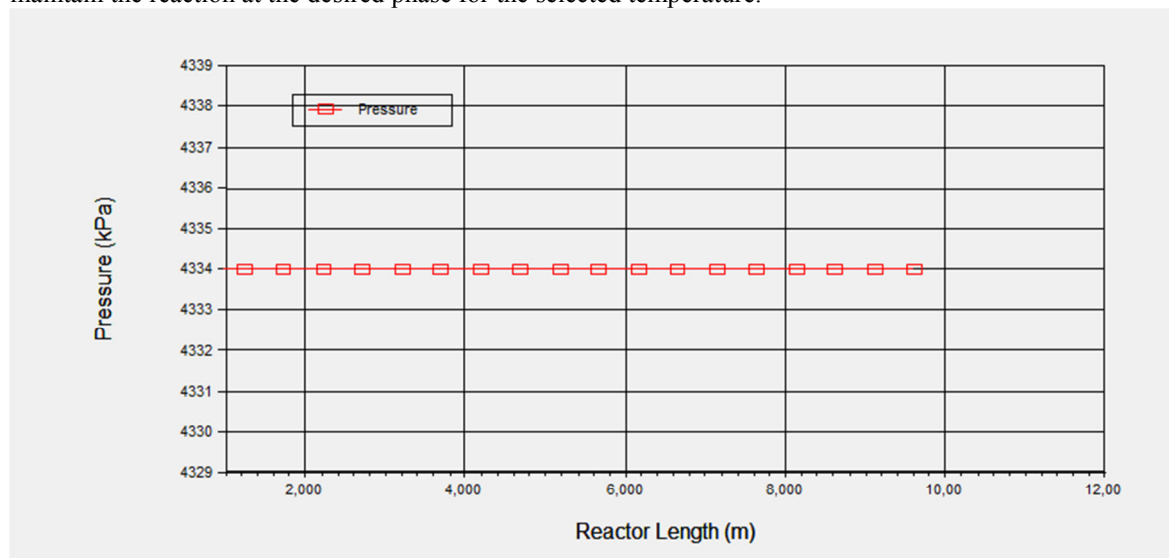

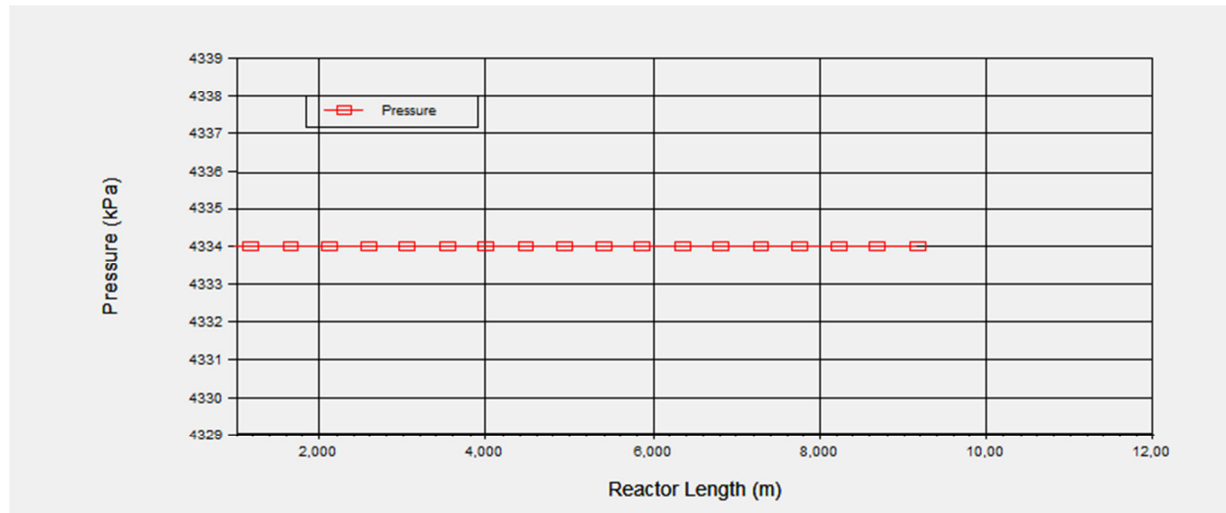**Figure 6a Effect of pressure in the bubble phase**

Figure 6b Effect of pressure in the emulsion phase

3.4 EFFECT OF ENTHALPY ON THE REACTOR IN THE BUBBLE AND EMULSION PHASE
3.4.1 Emulsion Phase
From the plot in Figure 7a, the various changes in enthalpy along the reactor length. There is sharp increase of enthalpy along the reactor length from 1.20m to 1.60m then a step increase to the apex point at about 2.30m where a reaction product is obtained. Therefore there is rapid decrease in enthalpy along the reactor's length. Rapid reaction occur within the first two meters because of fresh catalyst activity and thereafter decreases due to catalyst deactivation. This happens in the emulsion phase where reaction is assumed to occur. Stability is obtained after the formation of product.
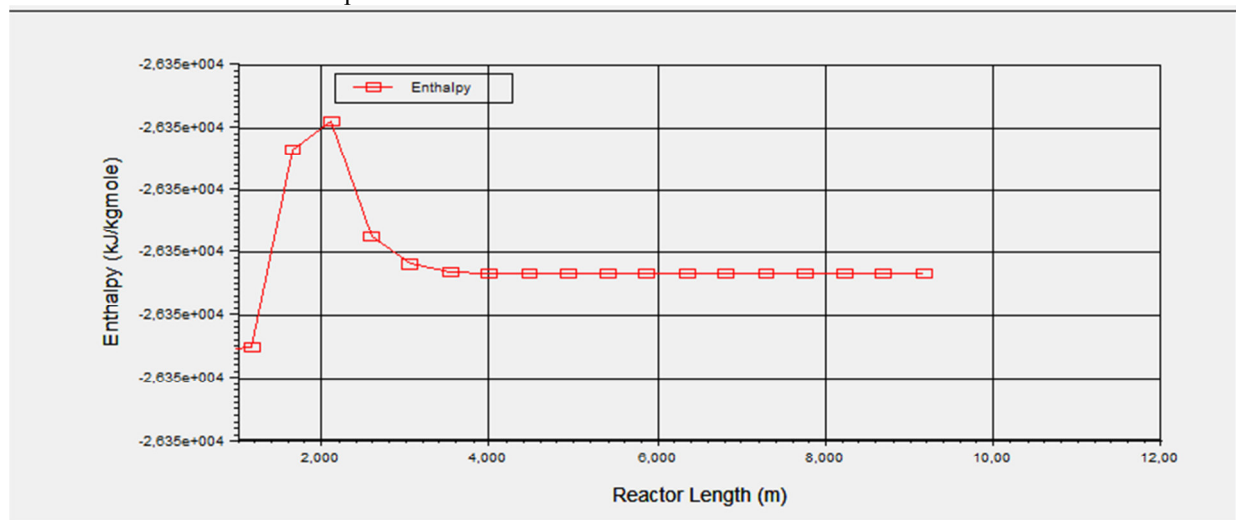

Figure 7a Effect of enthalpy in the emulsion phase for PFR-PFR
3.4.2 Bubble Phase
We can observe in Figure 7b that there is a step increase of enthalpy with respect to reactor length from 2m to 9m followed by a rapid increase of enthalpy.
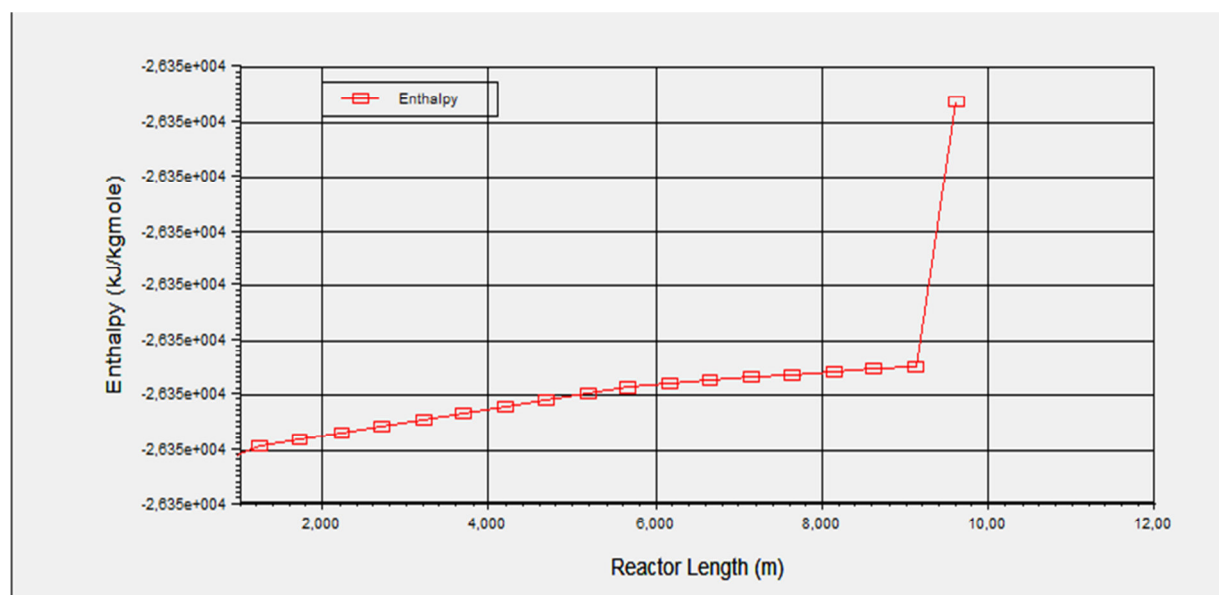
Figure 7b Effect of enthalpy in the bubble phase for PFR-PFR

The step increase along the reactor's length is as a result of slow or no reaction taking place in this phase. Thus the heat supplied to the reactor is being increased gradually for the gas bubble formation. Bubbles of gas rise rapidly and burst on the surface, and the emulsion phase is thoroughly agitated, as a result there is rapid increase in heat quantity contained in the reactor at the bed surface.

4.0 CONCLUSION

A comparative simulation study was carried out using process simulation software (ASPEN HYSIS). Fluidized bed reactor was designed for gas-liquid-solid interaction in polypropylene production. The fluidized bed reactor consist of two regions: bubble and emulsion with an interchange coefficient (k_{be}) for transfer of gas between regions.

Three configurations of fluidized bed reactor: plug flow - plug flow (PFR/PFR) configuration, plug flow – mixed flow (PFR/CSTR), and mixed flow – mixed flow (CSTR/CSTR) were considered. Comparing the yields of polypropylene obtained from the three configurations of the fluidized bed reactor, the plug flow – plug flow (PFR/PFR) configuration was observed to be more efficient, productive and suitable for the design of fluidized bed reactor. The temperature distribution for the mixed flow – mixed flow (CSTR/CSTR) configuration was considered the best at 90°C, this value is in agreement with plant data obtained from Eleme Petrochemical Company.

REFERENCES

Choi, K., Ray, W.H (1998), *Dynamic Behaviour of CSTR for Gas Phase Polymerization of Propylene,* BocaRaton, florids, CRC press 2707, China.

Corradini, P., Bisico, V., Cavallo, L., Guerra G.,Vacatello M. & Venditto V (1992), Molecular Catalysis*, American Institute of Chemical Engineers*, **74**: 433-442.

Fait, A., Resconi, L., Piemontesi, F., Colonnest, M., Rychlicki, H. & Zeeigler, R., (1995), Synthesis and olefin polymerization catalysis, *American Institute of Chemical Engineers,* **28:** 6667-6676

Gooch, J.W. (2007), *Encyclopedic Dictionary of Polymers,* 3rd Edition, Springer Publisher, USA., P200.

Khan, J.H.M., Mohd, A. Z. & Igbal, M. M. (2016), Developed hybrid model for propylene polymerization at optimum reaction conditions, *Chemical Engineering Division* **47**:3-25

Kunii, D., Levenspiel, O. (1991), *Fluidised Engineering;* 2nd edition, Butterwork Heinemann, USA.

Levenspiel, O. (1999), *Chemical Reaction Engineering* 3rd Edition, Butter Worth Publisher, Singapore, Pp 460-467

McAuley, K.B., Mc Donald, D.A. & Mclellan P.J. (1995), Effect of Operating conditions stability of polypropylene reactor, *American Institute of Chemical Engineers Journal,* **41**: 868-873.

Moore, E. (1996) *Polypropylene Characterization and Applications*, Cincinnati, OH/Gardner Publisher, New York.

Morris, J. (2005), *History of science and large molecules,* Chemical Heritage Foundation, New York.

Paul, J., Robert, L.B. (1989), Methods of producing polypropylene and High-Density Polyethylene, *American Chemical Society,* New York, **47:** 110-213

Ray, S., Gavin, T. (2009), *Chemical Engineering Design*, 5th Edition, Butter Worth Publisher, London, P$_P$ 310-

315.

Shariati, A. (1996), *Kinetic Modelling of Slurry Polymerization of Ethylene with a Supported Zeigler-Natta Catalyst,* Queens University, Kingston, Ontario, ABC International group, Canada.

Stroud, K.A. & Dexter, J.B. (2007), *Engineering Mathematics,* 7th Edition, Palgrave Macmillan Publisher, New York, P.987.

Westerink, E.J.& Westerterp, K.R. (1988), Safe Design and Operation of Fluidised Bed Reactors, *Chemical Engineering Science,* **45:** 333-354

Zheng, L., Peilin, S. & Wei, W. (2010), Industrial loop reactor for catalytic propylene polymerization*, American Chemical Society,* **55:** 385-526.