DEVELOPMENT OF MATHEMATICAL MODEL FOR A POLYETHYLENE FLUIDIZED BED REACTOR

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Abstract- **The proposed mathematical model is based on the two-phase theory of gas-solid fluidization. The two-phase model, which considers the fluidized bed reactor, consists of bubble phase and emulsion phase has proved to be the suitable model in many of the past studies. The bed is divided into several sequential sections. The model considers the combined effects of particle growth and elutriation for size distributed pre-polymer feed. In this study a complete description of polyethylene fluidized bed reactor mathematical, with the whole variables definition and a simulation with actual operation conditions was done to compare between the calculated conversion and the actual conversion. A good agreement has been observed between the model predictions and the actual plant data. It has been shown that about 0.28 % difference between the calculated and actual conversion has been achieved.**

Keywords - component; Polyethylene; Fluidized bed reactor; bubble growth model; particle size distribution; two phase modeling.

I. INTRODUCTION

The fluidized bed reactor has a unique physical design, with gas and polymer particles flowing in opposite directions. A fluidized reactor bed consists of metallic catalyst particles that are fluidized by the flow of ethylene gas, and catalyst particles (pre-polymer) are suspended in the ethylene fluid as ethylene gas is pumped from the bottom of the reactor bed to the top. The gas is fed from the base of the reactor and splits into two phases: bubble phase and emulsion phase. Prepolymer particles are fed in near the top of the reactor, and while the polymerization reaction occurs, the particles grow, increasing in weight and size. Particle segregation occurs in the reactor according to particle weight, so the full-grown polymer particles are removed at the base of the reactor. Non reacted gases leave the reactor after passing through the disengagement zone.[1] Pre-polymerization is generally carried out in continuous-stirred

tank reactors (CSTR) located before the fluidized bed reactor. Catalyst particles are fed into the CSTR along with ethylene and comonomers to yield pre-polymer. Afterwards, these pre-polymerized catalyst particles are fed into the FBR to complete the ethylene polymerization. A diagram of the industrial fluidized-bed reactor system using a CSTR as the pre-polymerization reactor is shown in fig (1). [2] In effect, the catalyst is not actually consumed, it is simply incorporated with the polyethylene product as polyethylene molecules remain stuck to the catalyst particle from which they were produced.

The conversion of ethylene is low for a single pass through the reactor and it is necessary to recycle the unreacted ethylene. Unreacted ethylene gas is removed off the top of the reactor, where it is expanded and decompressed to separate the catalyst and low molecular weight polymer from the gas. After purification, ethylene gas is then recompressed and recycled back into the reactor. Granular polyethylene is gradually removed from the bottom of the reactor as soon as reasonable conversions have been achieved. Typically, a residence time of 3 to 5 hours results in a 97% conversion of ethylene. The flow in the fluidized bed reactor can be mathematically modeled by using mole balances. [1]

Choi and Ray (1985)[3] proposed a two phase model including bubble and emulsion phases with constant bubble size. McAluey et al (1994). [5] Proposed a single phase model by modifying the Ray's model with additional assumptions. In a comparison between the two models, they have shown that the single phase assumption doesn't make considerable difference in the results obtained from the models. Hatzantonis et al.(1998)[4] in a research work developed the two phase model by considering the bubble growth effect on hydrodynamic behavior of the reactor and have shown that the developed model has a better agreement

with industrial data than single and two phase model with constant bubble size. In another work, Kiashemshaki et al. (2006) [6] developed the two phase model by considering the polymerization reaction not only in the emulsion phase but also in the bubble phase. They have indicated that about 20 % of the polymerization reaction occurs in bubble phase.
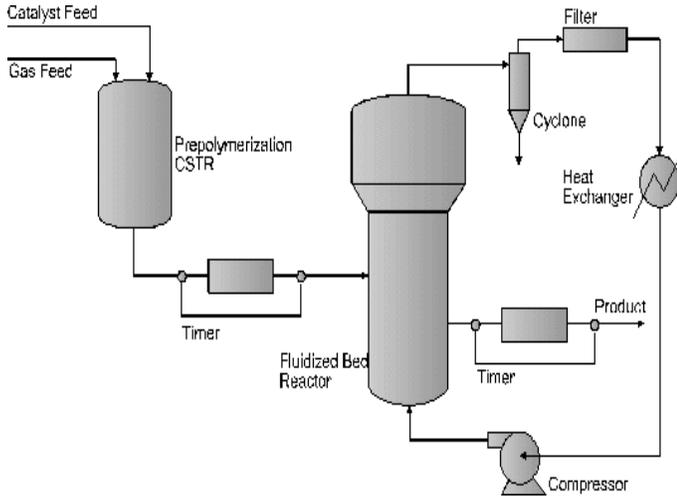

Fig (1): Industrial polyethylene production diagram (BP Chemical Technology).

In this work a two phase model including bubble and emulsion phases, which considers the bubble growth effect, is used for modeling the hydrodynamic behavior of the reactor. The double active sites Ziegler-Natta catalyst model proposed by McAuley et al. (1990) [7] has been used for simulating the kinetics of ethylene copolymerization. To control the reactor at the operating conditions, six feedback control loops with PID controllers, including anti-windup, have been used.

The advantage of the present work over the previous ones is considering the effect of bubble size and particle size distribution and catalyst properties in dynamic simulation of the reactor.

In the previous works a simple CSTR model has been used for dynamic simulation and control. Simulation results indicate that this strategy promotes the control performance considerably.

The paper has been organized as follows. First a simplified process description is viewed, next reactor modeling is discussed then reactor dynamics and its control have been considered. Finally the simulation results are presented and discussed.

II. SIMPLIFIED PROCESS DESCRIPTION

a. *Catalyst preparation*: Chromium is activated at high temperature with hot air and fluidized by nitrogen. The increasing in temperature is achieved with two separate heaters, which are used to heat the gas feed, continuously activated at required temperature. The maximum temperature is 625ºC.

b. *Pre-polymerization:* Prepolymerization is generally carried out in continuous-stirred tank reactors (CSTR) located before the fluidized bed reactor. The preheated solvent is fed in to the reactor with measured amount of catalyst, anti agent and aluminum alkyl (Tri n-octyl Aluminum TnoA). Ethylene is fed continuously to the reactor and the reaction proceeds at 75 ºC and pressure of 3bar. Washing was done to remove low molecular weight fractions (Wax). Dried pre-polymer is transferred by nitrogen to storage. Nitrogen conveying system is used to transfer prepolymer to the reactor these prepolymerized catalyst particles are fed into the FBR to complete the ethylene polymerization.

c. *Polymerization*: The fluidized bed reactor has a unique physical design, with gas and polymer particles flowing in opposite directions. The gas is fed in at the base of the reactor and splits into two phases: bubble and emulsion. Catalyst or prepolymer particles are fed in near the top of the reactor, and while the polymerization reaction occurs, the particles grow, increasing in weight and size. Particle segregation occurs in the reactor according to particle weight, so the full-grown polymer particles are removed at the base of the reactor. Nonreacted gases leave the reactor after passing through the disengagement zone.[8] A diagram of the industrial fluidized-bed reactor system using a CSTR as the pre-polymerization reactor is shown in Fig (2).
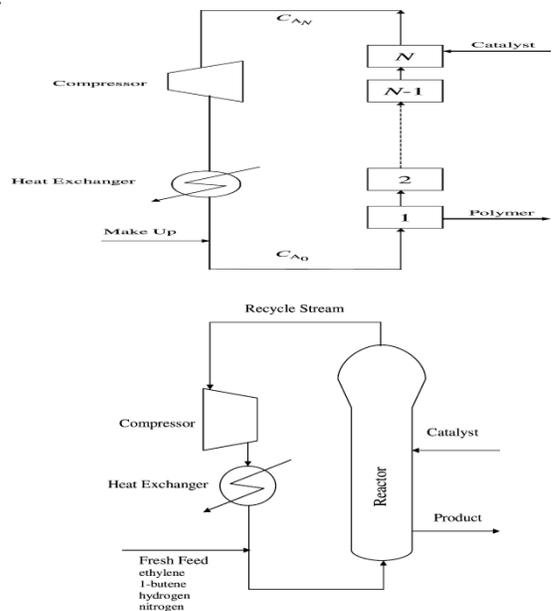

Fig (2): Industrial fluidized bed polyethylene reactor divided into i-th compartments

III.MATHEMATICAL MODEL DEVELOPMENT

The proposed mathematical model is based on the two-phase theory of gas-solid fluidization. The two-phase model, which considers the fluidized bed reactor consists of bubble phase and emulsion phase, has proved to be the suitable model for many of the past studies. Fig. (3) Shows the bubbling in fluidized bed reactor.
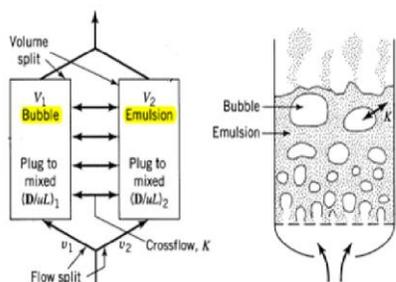

Fig (3): Two-phase model to present the bubbling in fluidized bed reactor.

A.Model Basic Assumptions
To obtain a clear understanding of the fluidized bed model, the assumptions that have been made in its development are summarized below.

1. The reactor operates at steady-state, under uniform temperature.
2. The reactor is isothermal in operation.
3. Ideal gas behavior.
4. The gas flows in plug flow, with gas interchange between phases.
5. The solids flow in CSTR (no particle segregation within the bed is considered).
6. Two phases bubble and emulsion are assumed.
7. The bed is axially divided into N compartments, each one consisting of the bubble and emulsion phases.
8. Bubbles grow continuously along the reactor height from their initial diameter until they reach the maximum stable bubble diameter.
9. The bed volume fraction occupied by bubbles and emulsion depends on the flow regime and changes along the reactor height.
10. The solids are polymer particles with a size distribution determined from the balance calculations.
11. Solids entrainment and carryover are taken into account by the model. However, particle agglomeration and breakage are not considered.
12. No chemical reaction occurs in the bubble phase which is free of solids. No chemical reaction is considered in the freeboard since the particle volume fraction in this part is considerably smaller than in the bed.
13. Bed voidage at minimum fluidizing conditions ε_{mf} is constant from the distributor until H_{mf}.
14. Catalyst particles entering the reactor are equal and uniform in size.
15. Emulsion phase remains at minimum fluidizing conditions.
16. Pre-polymerization technique is used for catalyst feeding.

B. Design Variables
1. Reactor diameter and height.
2. Initial bubble diameter (from the distributor design).
3. Solids carryover control.

C. Physical Properties
They are gas viscosity, diffusion coefficient, gas density, molecular weight; solid density, minimum fluidization voidage, Polymerization reaction constant and apparent catalyst deactivation rate constant. Simplified diagram for the computation sequence adopted is shown in fig (4).
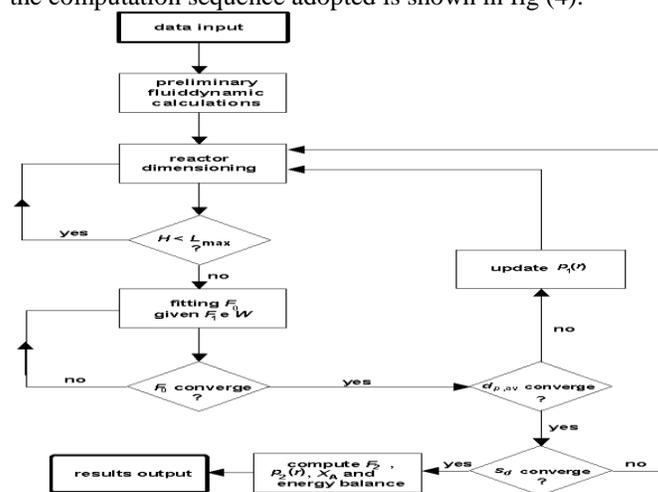

Fig (4): Simplified diagram for the computation sequence adopted.

D. Validation Analysis
The validation was carried out using process reported in (BP CHEMICALS, The Innovene Process- Chromium catalyst technology manual-(Revision 4), January 1996). [8] Data used in the validation from (Sidi Kerir for Petrochemicals Company) are shown in Table (1). Results of the validation simulations are shown in data analysis.

E.Operating Variables for Sensitivity Analysis
Identify variables affecting the model and study the effect of changing it by increasing or decreasing on output results. The variables studied for this model are:
1. Polymer particle diameter.
2. Catalyst particle diameter
3. Superficial gas velocity

4. Number of compartments in bed height.
5. Bed voidage at minimum fluidizing conditions.

TABLE (1): Operating Conditions and Simulation (Sidpec petrochemical company)

Parameter	Unit	Value
Monomer properties		
Ethylene feed concentration	mol m-3	4*10-4
Hydrogen feed concentration	mol m-3	9.6*10-5
Actual ethylene conversion per pass	%	3.33
Overall ethylene conversion	%	100
Catalyst properties		
Type of catalyst	Silica base chromium catalyst with (Al& Ti modifiers)	
Cr consumption	ppm	5ppm/ 1 ton residual polymer
Prepolymer properties		
Prepolymer density	Kgm^{-3}	2380
Prepolymer particle size	m	190*10^{-6}
Prepolymer feed rate	Kgs^{-1}	0.013
Polymer properties		
Polymer density	Kgm^{-3}	955
Polymer average particle size	m	1.166*10^{-3}
Flow rate of polymer product	Kgs^{-1}	4.16
Minimum particle size	m	1.070*10^{-3}
Maximum particle size	m	1.215*10^{-3}
Density function(PSD)	1/m	0.6489
Particle size distribution	1/m	Range from 190to1215micron
Reactor parameter		
Temperature	℃	108
Pressure	bar	21.5
Diameter	m	5
Fluidizing velocity	ms^{-1}	0.56
Bed height	m	16
Maximum reactor height	m	22
Bed voidage ε $_{mf}$	--	0.5
Inert gas properties		
Gas density		Kgm^{-3}	17.05
Composition	% volume	Ethylene	13.02
		Hydrogen	14.7
		Nitrogen	47.2
		Ethane	19.06
		Butane	6
		Butene-1	1.08*10^{-2}

F. Hydrodynamic And Transport Properties Correlations

1. Minimum Fluidizing Velocity:

The superficial gas velocity at minimum fluidization conditions is calculated from the correlations gives by Kunii and Levenspiel. [9]

$$U_{mf} = \frac{Re_{mf}\, \mu_g}{\rho_g\, d_p} \tag{1}$$

$$Ar = \frac{g\, d_p^3 \rho_g (\rho_p - \rho_g)}{\mu_g^2} \tag{1.a}$$

$$Re_{mf} = [(33.7)^2 + 0.0408\, Ar]^{0.5} - 33.7 \tag{1.b}$$

Where viscosity and density of Gas Mixture given by the following relation [10]:

$$\mu_{g,mix} = \frac{\sum y_j \mu_j\, M_j^{\frac{1}{2}}}{\sum y_j\, M_j^{\frac{1}{2}}} \tag{1.c}$$

$$\rho_g = \frac{PM}{RT} \tag{1.d}$$

2. *Bubble Growth Equations:*
   - Bubble growth diameter at corresponding bed height is calculated by the correlation given by Wen and Fan (1975). [11]

$$b_{di} = 0.14 d_p \rho_p \left(\frac{U_g}{U_{mf}}\right) h_i + d_{bo} \tag{2}$$

   - Initial bubble diameter formed near the distributor is calculated from the correlations given by Kunii and Levenspiel(1991). [9]

$$d_{bo} = \frac{2.78(U_g - U_{mf})^2}{g} \tag{2.a}$$

   - When choosing a correlation for bubble size, it is important to consider the maximum size that a bubble can reach before it becomes unstable and breaks up into smaller bubbles. Davidson and Harrison (1963) [12] established that the settling velocity of the bed particles should be greater than or equal to the bubble rise velocity, U_b. The Mori and Wen[13] relation is used to obtain maximum bubble diameter.

$$d_{bm} = 0.65(S(U_g - U_{mf}))^{0.4} cm \tag{2.b}$$

   - Kunii and Levenspiel(1991)[9]correlation is used to calculate the bubble rising velocity.

$$U_{bi} = U_g - U_{mf} + 0.711(g\, d_{bi})^{\frac{1}{2}} \tag{2.c}$$

$$\delta_i = \frac{(U_g - U_{mf})}{(U_{bi} - U_{mf})} \tag{2.d}$$

   - Average bubble fraction is calculated from the correlations gives by Cui et al. (2000). [14]

$$\delta = 0.534\left(\frac{1-\exp(U_g - U_{mf})}{0.413}\right) \tag{2.e}$$

- kobayashi , et al. (1967) [15] correlation is used to calculate number of bubbles .

$$N_i = \frac{6\,S\,(H - H_{mf})}{\pi\,H\,\Delta h_i^2} \tag{2.f}$$

Where the U_{br} is given by the correlation of Grace,(1986). [16]

$$U_{br,i} = 0.711(g\,d_{bi})^{\frac{1}{2}} \tag{2.g}$$

3. n-compartment height:

Compartment height, height of i-th compartment and distance from distributor to n-compartment respectively are given by kobayashi, et al. (1965). [17]

$$\Delta h_i = 2dbo\,\frac{(2+m)^i - 1}{(2-m)^i} \tag{3}$$

$$\Delta h_1 = d_{bo} + (1 - \frac{m}{2}) \tag{3.a}$$

Where:

$$m = 1.4\,d_p\,\rho_p\,\frac{U_g}{U_{mf}} \tag{3.b}$$

$$h_n = \sum_{i=1}^{n} \Delta h_i \tag{3.c}$$

4. Height at minimum fluidizing conditions:

Height at minimum fluidizing conditions is calculated by the correlation given by Hatzanionis and Yannoulakis, (1999). [18]

$$H_{mf} = H\,(1 - \delta) \tag{4}$$

5. Maximum bubble diameter:
Haider and Levenspiel (1989) [19] correlation is used to calculate the Terminal falling velocity.

$$d_{b,max} = \frac{2\,U_t^2}{g} \tag{5}$$

$$d_p' = 2.7\,d_p \tag{5.a}$$

$$d_p^* = d_p'[\mu_g^{-2}\rho_g(\rho_p - \rho_g)g]^{\frac{1}{3}} \tag{5.b}$$

$$U_t^* = [18\,d_p^{*-2} + (2.335 - 1.744\Phi_s)\,d_p^{*-\frac{1}{2}}]^{-1} \tag{5.c}$$

$$U_t = U_t^*\,[\mu_g\,\rho_g^{-2}(\rho_p - \rho_g)\,g]^{\frac{1}{3}} \tag{5.d}$$

6. Diffusion of Ethylene:

Specchia et al. (1980) [20] correlation is used to calculate the self diffusion of ethylene.

$$D_A = \frac{U_g d_p}{8.65(1 + 19.4\,\frac{d_p}{D}^2)} \tag{6}$$

7. Mass Transfer Coefficient:

Mass transfer coefficient is calculated by the correlation given by Kunii and Levenspiel. (1969). [21]

$$K_{be,i} = [(\frac{1}{K_{bc,i}}) + (\frac{1}{K_{ce,i}})]^{-1} \tag{7}$$

$$K_{bc,i} = 4.5\,\frac{U_{mf}}{d_b} + 5.85\frac{D_A^{\frac{1}{2}}\,g^{\frac{1}{4}}}{d_{bi}^{5/4}} \tag{7.a}$$

$$K_{ce,i} = 6.78\,(\frac{\varepsilon_{mf}\,D_A\,U_b}{d_{bi}^3})^{\frac{1}{2}} \tag{7.b}$$

8. Bed Voidage:

Bed voidage is calculated by the correlation give n by Wen and Fan. (1975). [11]

$$(1 - \varepsilon) = \frac{H_{mf}\,(1 - \varepsilon_{mf})}{H} \tag{8}$$

For $\quad h \le H_{mf}$

$$(1 - \varepsilon i) = \frac{H_{mf}}{H(1 - \varepsilon_{mf})} - \frac{H_{mf}\,(1 - \varepsilon_{mf})(h - H_{mf})}{2H\,(H - H_{mf})} \tag{8.a}$$

For $\quad H_{mf} \le h \le [H_{mf} + 2(H - H_{mf})]$

9. Particle Size Distribution Of Polymer:

Grosso and Chiovetta (2005) [22] give correlation to calculate the particle size distribution of polymer and for the catalyst feed particles.

$$P_b(d_p) = \frac{(3\,d_p^5\,\rho_p^2\,\chi_{cat}^2)}{d_{po}^6\,\rho_{cat}^2\,(1 - \chi_{cat})} * \frac{\left(1 + \left(\frac{d_p^3}{d_{po}^3}\right)\left\{\left(\frac{\rho_{cat}}{\rho_p} - 1\right)\right\}\right)\exp\left(\rho_p\,\chi_{cat}\,(d_p^3 - d_{po}^3)\right)}{\rho_{cat}\,d_p^3(1 - \chi_{cat})} \tag{9}$$

$$P_o(r) = \int_{d_{po}}^{d_p} P_b(d_p)d_p \; d(d_p) \; [\int_{d_{po}}^{d_p} P_b(d_p)d(d_p)]^{-1} \quad (9.a)$$

For $H_{mf} \leq h \leq [\, H_{mf} + 2(H - H_{mf})]$

10. The flow rate of solids of all sizes removed from the bed:

The flow rate of solids of all sizes removed from the bed by the gas flow is calculated by Geldart (1986) [23]

$$F_2 = S \int_{d_{pmin}}^{d_{p\,max}} K^\bullet(d_p) \, P_b(d_p) \, d(d_p) \quad (10)$$

Where the Elutriation constant is calculated as follows:

$$K^\bullet(d_p) = 23.7 \, \rho_g \, U_g \, exp \left(\frac{-5.4 \, U_t(d_p)}{U_g} \right) \quad (10.a)$$

$$K(d_p) = K^\bullet(d_p) \, \frac{S}{W} \quad (10.b)$$

Kunii and Levenspiel(1991) [9] correlation is used to calculate the weight of solids in the bed.

$$W = S \, H \, (1 - \varepsilon) \, \rho_{cat} \quad (10.c)$$

11. The Ethylene Polymerization Rate:

The ethylene polymerization rate was adopted, based on the model used by Choi and Ray (1985) [3]and McAuley *et al.* (1994) [4]

$$r_{pi} = K_p C_{ei} \, \chi_{cat} \, \rho_p V_{ei} \, (1 - \varepsilon_i) \, M_e \quad (11)$$

This rate expression assumes that the ethylene concentration at the catalyst sites is proportional to C_e, the concentration in the emulsion gas. Since monomer diffusion rates, both to the polymer particles and within them (Floyd *et al.,* 1986a, b, 1987) [24], are fast relative to the reaction kinetics, the ethylene dissolved in the polymer phase is in equilibrium with the ethylene in the emulsion gas. Hutchinson and Ray (1990) [25] have shown that Henry's law applies to the solubility of ethylene in polyethylene at the conditions in the reactor. Hence, the proportionality assumption is valid. The rate constant, k_p includes the Henry's law constant for ethylene partitioning between the two phases. We neglect the mild effect of temperature on the Henry's law constant and assume that *k,* displays Arrhenius behavior.

$$R_{pi} = rpi \int_{d_{pmin}}^{d_{pmax}} P_b(dp) \, d(dp) \quad (11.a)$$

$$K_p = k_{po} \exp - \left(\frac{E_a}{R\,T} \right) \quad (11.b)$$

Catalyst deactivation is included in the kinetic model described by Khang and Lee (1997) [26] as following relations:

$$K_{p,actual} = K_p \exp(-k_d) \quad (11.c)$$

Where

$$A_i = K_p \; C_{e,i} M_e \; r^3 \, \chi_{cat} \quad (11.d)$$

$$\tau = \frac{1}{A_i}(r^3 - (\frac{d_{p,o}}{2})^3) \quad (11.e)$$

12. Mass Balance Around The N-Th Compartmen:t

Tanaka (1967) [27] give correlation for the Material balance around the n-th compartment

$$k' = \frac{K_{be} \, (U_b - \frac{U_{mf}}{\varepsilon_{mf}})}{(U_b + \frac{2 \, U_{mf}}{\varepsilon_{mf}})} \quad (12)$$

$$S \, U_g \, C_{b,i-1} = (k' V_{bi} \, (C_{b,i} - C_{e,i})) + S U_g C_{b,i} \quad (12.a)$$

$$K' \, V_{bi} \, (C_{b,i} - C_{e,i}) = R_{pi} V_{ei} \quad (12.b)$$

McAuley et al. (1994) [4] give correlation to calculate the Volume of compartment phases

$$V_{bi} = S \, \Delta h_i \delta_i \quad (12.c)$$

$$V_{ei} = S \, \Delta h_i \, (1 - \delta_i) \quad (12.d)$$

13. The Population Balance:

The population balance is based on a mass balance for particles of size between r and *r + dr*, as presented by Kunii and Levenspiel (1969, 1991) [18, 9]

$$F_1 + F_2 + F_o - \sum_{i=1}^{n} R_{pi} = 0 \quad (13.a)$$

Kim and Choi (2001) [28] give correlation for Rate of increase in particle diameter.

$$\Re(d_p) = d\left(\frac{dp}{dt}\right) = \frac{d_{po} \, \rho_{cat} \, R_p}{3(1-\varepsilon) \, d_p^2 \, \rho_p} \quad (13.b)$$

Overall Mass Balance:

$$F_o P(d_p) - F_1 P_b(d_p) - W\, K(r) P_b(d_p) - W \frac{d\, \Re\,(d_p) P_b(d_p)}{d(dp)} +$$

$$3W\, \Re\, (dp) \frac{P_b(d_p)}{(d_p)} = 0 \quad (13.c)$$

$$F_1 + F_2 + F_o - \int_{dpo}^{dp} \frac{3W}{r} \Re\, (d_p) \frac{Pb(dp)}{d_p}\, d(d_p) = 0 \quad (13.d)$$

14. Conversion of Ethylene

Kunii and Levenspiel(1991) [9] correlation is used to calculate the Conversion of ethylene per pass.

$$XA = \frac{22.4 \sum R_P\, T * 1000}{U_g * 3600 * (YC2/100) * (1.013 * P) * S * 273 * 28} \quad (14)$$

$$X_A = \frac{C_{Ain} - C_{Aout}}{C_{Ain}} \quad (14.a)$$

III. RESULT AND DISCUSSION

The model was solved using Microsoft Excel. The model equations were for the operating conditions shown in table (1) and the fluidized bed reactor was divided into ten compartments. Each compartment consists of two phases, bubble phase and emulsion phase.

1. Effects of superficial gas velocity

Industrial fluidized-bed polyethylene reactors are operated at superficial gas velocities ranging from 3 to 6 times the minimum fluidization velocity (Wagner et al., 1981). [29]The major effect of an increase in the superficial velocity, Ug, is a reduction in the time required for a given quantity of gas to pass through the bed.
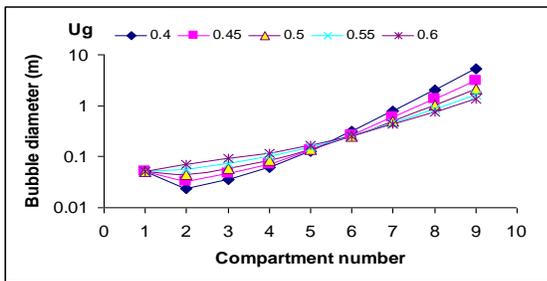

Fig (5): Effect of superficial gas velocity on bubble diameter of i-th compartment.

Fig (5) illustrates the effect of superficial gas velocity on the bubble diameter at different compartments number. As can be seen, an increase in the superficial gas velocity results in a decrease in bubble maximum diameter for the maximum

recommended number of compartments as shown in McAluey et al. (1994).[5]who also used 10compartement through model simulation because using small number of compartment did not provided a strong particle segregation.

Fig (6) shows axial profile for the effect of the superficial gas velocity on the diffusion coefficient and the percent ethylene conversion. As the superficial gas velocity increases the ethylene diffusion coefficient increases.

However, high gas velocities reduce the conversion of monomer per pass through the reactor, and can lead to greater elutriation of small particles from the bed. Elutriated particles are prevented from passing out of the reactor and into the gas recycle system using a velocity reduction zone at the top of the reactor where entrained particles are given the opportunity to drop back into the bed. Particle return may also be aided by a cyclone (Wagner et al., 1981). [29]
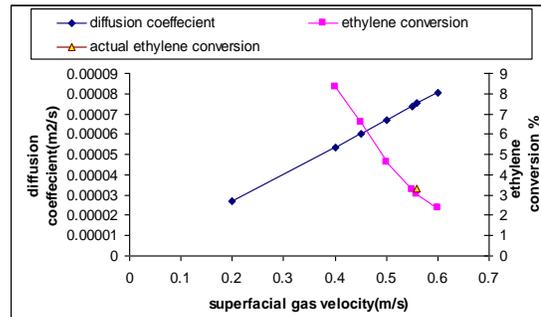

Fig (6): Effect of superficial gas velocity on ethylene diffusion coefficient and ethylene conversion.

2. Effects of bubble size

Fig. (7) Shows that by increasing the compartment number the bubble diameter increase and the total number of bubbles in the compartment decrease. Through model simulation in equation (3) which calculates the height of compartment as the bubble diameter increases the compartment height increase which leads to divide the bed into small number of compartments.
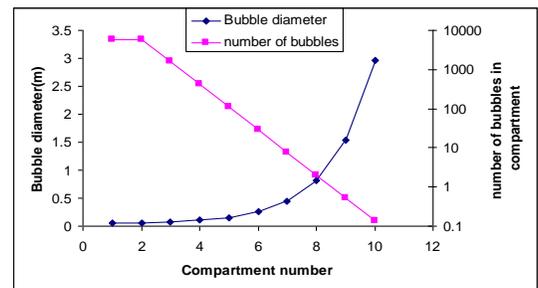

Fig (7): Effect of compartment number on bubble growth rate and number of bubbles of each.

3. Effect of bed height

The simulation shows that there is a highly active reaction zone in the top of the reactor, the ethylene conversion decreases by increasing the bed height. It is clear from Fig (8) that both polymerization rate and single pass ethylene conversion decreased with the increasing the bed height. This trend is similar to that found by Fabiano and Lona (2002) [30].

4. Effect of polymer particle size

Fig (9) shows that by increasing the polymer particle size the particle size distribution increase. This trend is similar to that found by Omid and Hassan (2008). [31]
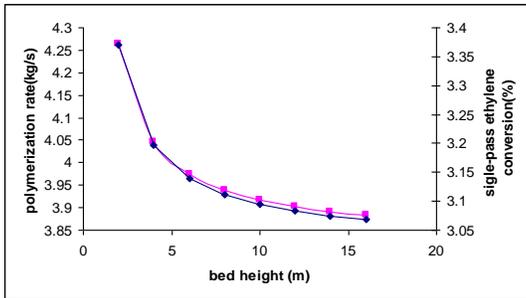

Fig (8): Effect of bed height on ethylene single pass conversion and polymerization rate along the bed height.
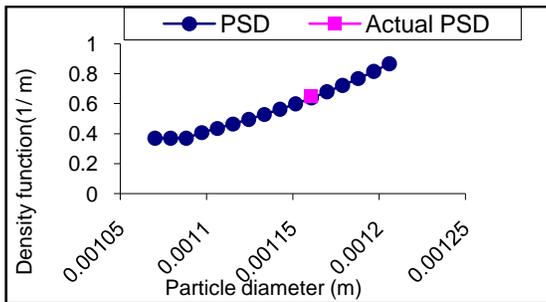

Fig (9): Effect of particle diameter on particle size distribution

5. Effect of feed catalyst properties

Fig (10) illustrates the effect of pre-polymer particle size and the polymer particle size on the particle size distribution. And it shows that by increasing the pre-polymer particle size the particle size distribution decreases.

And Fig (11) shows the effect of catalyst feed rate on the ethylene conversion and the particle size distribution of polymer particles. It indicates that as the catalyst feed rate increase the ethylene conversion and particle distribution increase. Kim and Choi (2001) [28] elutriated that increasing

catalyst feed rate decrease particle residence time due to increasing production rate and hence polymer particle size distribution shifted to the left (smaller sizes). And also for the ethylene conversion as expected higher catalyst feed rates leads to higher polymerization rates and height conversion. This trend is similar to that found by McAuley et al. (1994). [5]

6. Ethylene conversion

A comparison between the calculated conversion and the actual conversion was shown in fig (12). Good agreement has been observed between the model predictions and the actual plant data. It has been shown that about 0.28 % difference between the calculated and actual conversion has been achieved.
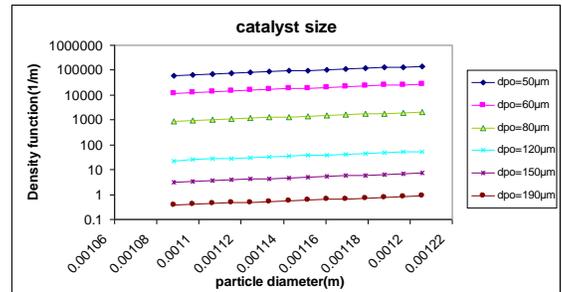

Fig (10):Effect of initial catalyst size on the particle size distribution in the bed.
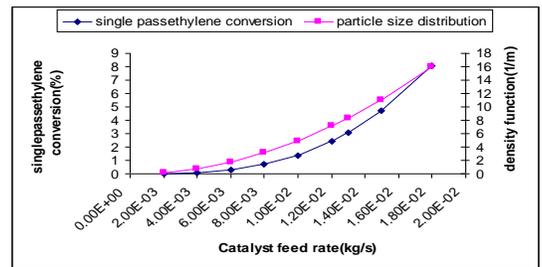

Fig (11): Effect of catalyst feed rate on ethylene single pass conversion and particle size distribution of polymer
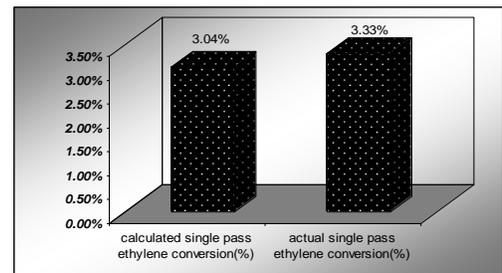

Fig (12): Comparison between actual and calculated ethylene conversion for single pass.

7. *Operating Variables for sensitivity analysis*

Fig(14) shows the senstivity analysis of the mathematical model using multiplication factors of (0.5,1,and 1.5) for the variables affected the model.

Regarding to catalyst particle diameter,decreasing its value will incresase tremendously the single pass ethylene conversion(by about 4000 fald) on the other hand increasing catalyst particle diameter 50% will decrease the single pass ethylene conversion to about 1% of its original value.

Regarding to the superficial gas velocity on increasing this value the single pass ethylene conversion decreases. This is understandable since the contact time decreases.

From the result shown it is clear that the single pass ethylene conversion is not senstive to change in superficial gas velocity but heighly senstive to catalyst particle diameter.

Also regarding the effect of total number of compartment it is clear that increasing total number of compartment in the bed leads to increase of single pass ethylene conversion. This can be atibuted to increasing the number of compartment in the bed results in better segregation of the polymer product. It is accordance to McCauley et al. (1994)[5]
On the other hand increasing bed voidage incrasing single pass ethylene conversion. This can be atibuted to increase bed voidage would increase contact surface.
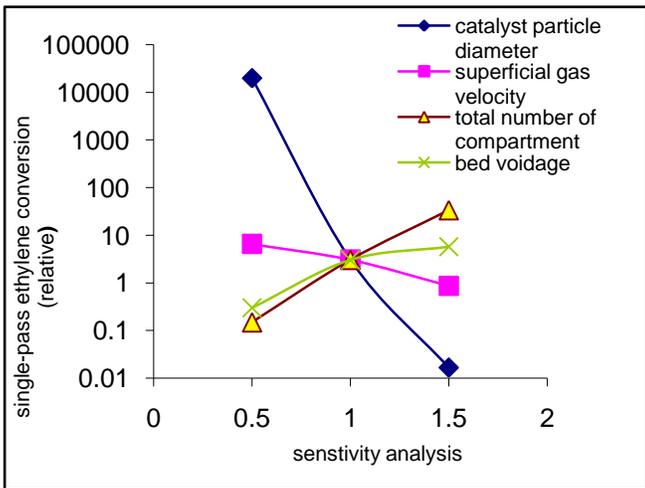

Fig (13): sensitivity analysis for ethylene conversion

CONCLUSION

Mathematical model based on the two phase theory of gas phase fluidization has been developed.the model

considered the combined effect of particle growth and elutriation for size distribution for polymer feed. The model has been validated and showed a good agreement with the actual plant data, model has found to that single pass ethylene conversion is senstive to catalyst particle diameter, number of compartment and bed voidage and changing in superficial gas velocity has no significant effect on model.

NOMENCLATURE

Ar   Archimedes number
A_i For each compartment (correspond to an exponential decayment in polymer particle growth rate)
C_{Aout} Ethylene outlet concentration (mol)
C_{Ain} Ethylene inlet concentration (mol)
C_{ei} Monomer concentration in emulsion phase i-th compartment (mol m^{-3})
d_p Polymer average particle size(m)
d_p^* Dimensionless particle size
Dp_{min} Minimum particle diameter (m)
dp_{max} Maximum particle diameter (m)
d_{po} Catalyst particle size (m)
d_{bo} Bubble diameter near distributor(m)
$d_{b,max}$ Maximum stable bubble diameter(m)
d_{bm} Bubble diameter (m)
d_b Bubble diameter at (h)height i-th compartment (m
D_A Diffusion coefficient for ethylene (m^{2}s^{-2})
D   Reactor diameter (m)
E_a Activation energy (J mol^{-1})
F_o Catalyst (prepolymer) feed rate (kg s^{-1})
F_1 Flow rate of polymer product (kg s^{-1})
F_2 Flow rate of solids removed by elutriation (kgs^{-1})
g   Gravitational acceleration(ms^{-2})
h   Bed axial coordinate
H   Bed height (m)
H_{mf} Bed height at minimum fluidizing conditions (m)
h_n Distance from the distributor to n-compartment (m)
Δh_1 Initial compartment height (m)
Δh_i Height of i-th compartment (m)
i-th   Compartment number
$K_{bc,I}$ Coefficient of gas interchange between bubble and cloud phases i-th compartment(S^{-1})
$K_{e,i}$ Coefficient of gas interchange between cloud and emulsion phases i-the compartment(S^{-1})
$K_{b,i}$ Coefficient of gas interchange between bubble and emulsion phases, over all mass   transfer coefficient i-th compartment (S^{-1})
$K'(r)$ Elutriation constant as a function of r (kg m^{-2} s^{-1})
$K(r$ Elutriation constant (s^{-1})
K_p Reaction rate constant (m^3 kg$_{cat}^{-1}$ s^{-1})
k_{po} Preexponential factor (m^3 kg$_{cat}^{-1}$ s^{-1})
k_d Apparent catalyst deactivation rate constant (s^{-1})
M_j Molecular weight of component j (kg mol^{-1})
m   Proportionality constant relating the bubble diameter Re$_{mf}$ Reynolds's number at minimum fluidizing condition
N_i Number of bubbles in i-th compartment
n   Total compartment number
$P_{b(d)}$ Particle size distribution in reactor as a function of r (m^{-1})
$P_o(r)$ Particle size distribution of feed catalyst (m^{-1})
r_{pi} Reaction rate in i-th compartment (kg s^{-1})
R   Gas constant (J mol^{-1}K^{-1})
R_{pi} Reaction rate for whole solid phase i-th compartment (Kg s^{-1})
r_{cat} Catalyst particle radius(m)
r   Polymer particle radius (m)
S   Crosses sectional area (m^2) S= $\pi D^2/ 4$
T   Temperature (K)
$U_{br,i}$ Velocity i-th compartment (ms^{-1})
U_t Terminal velocity of falling particles (m s^{-1})
U_t^* Dimensionless Terminal falling velocity coefficient

$U_t(d_p)$ Terminal velocity of falling particles as function of particle diameter(s^{-1})

U_{bi} Velocity of bubble rising up thought the bed i-th compartment (m s^{-1})

U_{mf} Minimum fluidizing velocity (m s^{-1})

U_g Fluidizing gas velocity (m s^{-1})

V_{ci} Volume of cloud phase i-th compartment (m ^{3})

V_{bi} Volume of bubble phase i-th compartment (m ^{3})

V_{ei} Volume of emulsion phase i-th compartment (m ^{3})

W   Weight of solids in the bed (Kg)

X_A Ethylene conversion

χ_{cat} Catalyst mass fraction in polymer particle

y_j Mole fraction of component j

Greek letters

ρ_p Polymer density (kgm^{-3})

ρ_g Gas density (kg m^{-3})

ρ_{cat} Catalyst density (kg m^{-3})

ρ_J Density of component j(kg m^{-3})

ℜ (dp)Rate of increase in particle diameter (ms^{-1})

τ   Growth time for polymer particles

μ_g Gas viscosity (kg m^{-1} s^{-1})

μ_j Viscosity of component j (kg m^{-1} s^{-1})

ε_i Bed voidage , i-th compartment

ε Bed voidage

ε_{mf} Bed voidage at minimum fluidizing conditions

δi Bubble fraction for i-th compartment

Φ_s Spherisity for sphere particles

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