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Dynamic Modeling for Gas Phase Propylene Copolymerization in a Fluidized Bed Reactor

WamdafaisalElmobarak[1], Alaeldin Ibrahim Mohamed[2], Amin BabikerA.Nabi Mustafa[3]

P.G. Student, Department of Chemical Engineering, Faculty of Engineering, AL Neelain University Kh, sudan[1]
Associated Professor, Department of Chemical Engineering, Faculty of Engineering, AL Neelain University, Kh, Sudan[2]
Associated Professor, Department of Telecommunication Engineering, Faculty of Engineering, AL Neelain University, Kh, Sudan[3]

Abstract: A two-phase model is proposed for describing the dynamics of a fluidized bed reactor used for polypropylene production. In the proposed model, the fluidized bed is divided into an emulsion and bubble phase where the flow of gas is considered to be plug flow through the bubbles and perfectly mixed through the emulsion phase. Similar previous models, consider the reaction in the emulsion phase only. In this work the contribution of reaction in the bubble phase is considered and its effect on the overall polypropylene production is investigated the kinetic model is combined with hydrodynamic model in order to develop a comprehensive model for gas-phase propylene copolymerization reactor. Simulation profiles of the proposed model were compared with those of well mixed model for the emulsion phase temperature. The simulated temperature profile showed a lower rate of change compared to the previously reported models due to lower polymerization rate. Model simulation showed that about 13% of the produced polymer comes from the bubble phase and this considerable amount of polymerization in the bubbles should not be neglected in any modeling attempt.

***Keywords*:** propylene Copolymerization, Fluidized bed, Modeling, Gas phase.

I. Introduction

Gas-phase polymerization of propylene in a fluidized bed has several advantages over other polypropylene production processes due to low operating pressure and temperatures of about 75-110 ºC and 20-40 bar respectively with superficial gas velocity from 3Umf to 8Umf.The fluidized bed reactors have been modeled previously as two phase reactors to describe the performance of gas-phase propylene polymerization reactors. In these models, it was assumed that the reactions take place only in the emulsion phase due to the assumption that the bubbles are solid-free McAuley et al .assumed the polymerization reactor to be a continuously stirred tank reactor and Choi and Ray assumed the polymerization reactor comprises of two phases i.e. emulsion phase and the bubble phase. Fernandez andLona assumed a three-phase model with plug flow and Hatzantonis et al studied the effect of varying bubble size on the behavior of the reactor assuming the bubble phase was divided into N well mixed compartments in series and the size of each compartment was set equal to the bubble diameter at the corresponding bed height. In this work, a dynamic mathematical model to describe the kinetic behavior, production rate, temperature and concentration profile is done, where the reactions are assumed to occur in the bubble as well as the emulsion phase.

II. Reactor modeling

A flow diagram of gas-phase polypropylene production process is shown in Fig.1.Ziegler-Natta catalyst and triethyl aluminum co-catalyst are charged continuously to the reactor. The feed gas comprises propylene, ethylene, hydrogen, and nitrogen gases and they provide the fluidization through the distributor, as heat transfer media and also supply reactants for the growing polymer particles. The solid-free gas is then combined with fresh feed stream after heat removal and recycled back to the gas distributor with conversion per pass through the bed from 1 to 5% and the overall monomer conversion from 98%.The polypropylene product is continuously withdrawn from near the base of the reactor and above the gas distributor and the unreacted gas is recovered from the product. In this study, the bubble phase flow pattern is assumed to be plug flow while the emulsion phase is considered to be completely mixed, with the following assumptions made:

- Polymerization takes place both in the bubble and the emulsion phases.
- Mass and heat transfer resistances between the gas and solid polymer particles in the emulsion phase can be neglected (small catalyst particles and low to moderate catalyst activity.
- Radial concentration and temperature gradients in the reactor can be neglected. Based on the model assumptions the rate of reaction for each component assuming the monomers are mainly consumed through

the propagation reactions, was obtained from Mc Auley et al, and the proposed hydrodynamic correlations by Lucas et al. Kunii and Leven spiel, Mostoufi et al. Hilligardt and Werther, and Cui et al, have been used in solving the model equations for materialandenergy balance forallofthe compositionsin the bed.

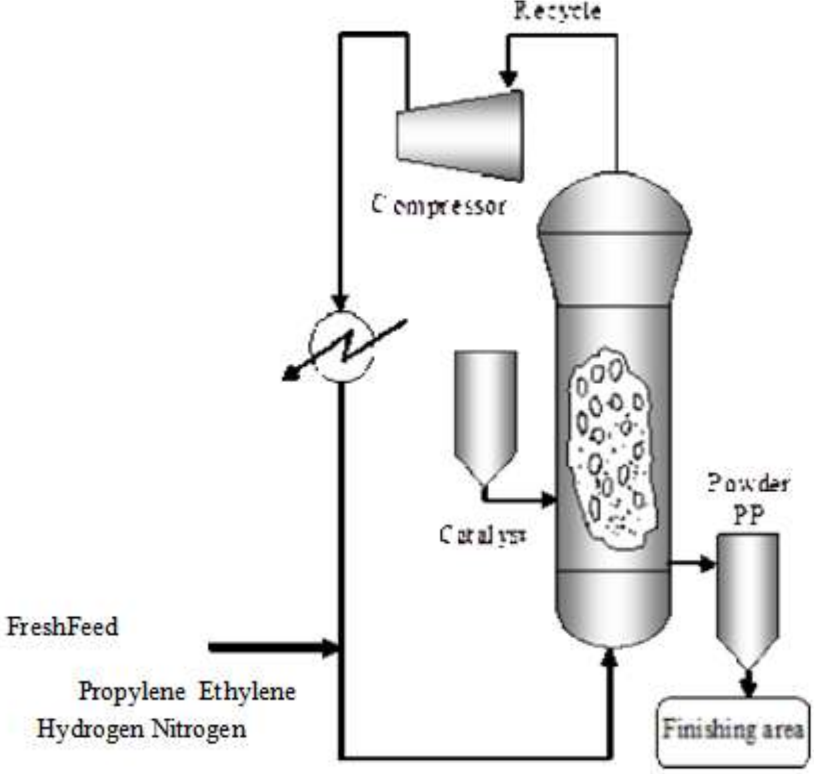

Figure1.Industrial fluidized bed polypropylene reactor.

III. Material and methodology

Simulations were carried out at the operating conditions given in Table1 where the fluidized bed reactor of poly propylene production was divided into a CSTR for the emulsion phase and a PFR for the bubble phase with heat and mass being exchanged between the two phases. A set of kinetic parameters as shown in the Table have been selected for the propylene polymerization reactions propagation and chain transfer reactions determine the polymer properties and the other reactions are less important In this work the effects of temperature and therefore activation energies on the polymerization kinetics have not been considered Fig.2 shows the evolution of the emulsion phase temperature with time where it can be noticed from this figure that the predicted polymerization temperature obtained by the new model is lower than the well mixed model results, due to the assumption of reaction occurring in the emulsion and the bubble phases and hence in the emulsion phase of present model is lower than the well mixed model (one phase model).Fig.3 shows the molecular weight distribution of the final product. This figure illustrates that the number and weight average molecular weight of the polymer increase rapidly at the beginning of the polymerization period and reach a constant value within less than three hours of production.

IV. Results and discussions

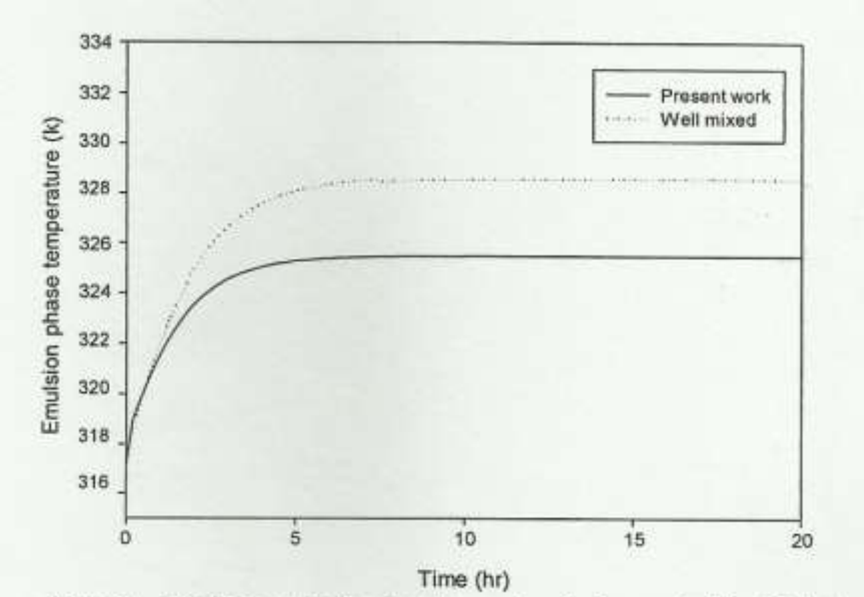

Figure 2. Evolution emulsion phase temperature in the reactor (Fcat=0.4 g/s and U_0=0.35 m/s).

Table1: operating conditions and physical parameters for the reactor

Operating Conditions	Physical Parameters
H[m] =7 **D_t [m] = 3** **T_{in}[k] = 317** **P[bar] = 20** **Propylene Concentration [kmol/m^3] = 1** **Ethylene Concentration [kmol/m^3] = 0.1** **Hydrogen concentration [kmol/m^3] = 0.02** **Superficial gas velocity U_o[m/s] = 0.35** **Catalyst feed rate [g/s] = 0.4**	**µ[pa.s] = 1.14e-4** **ρg[kg/m^3] = 24.2** **ρs[kg/m^3] = 910** **dp[m] =500e-6**

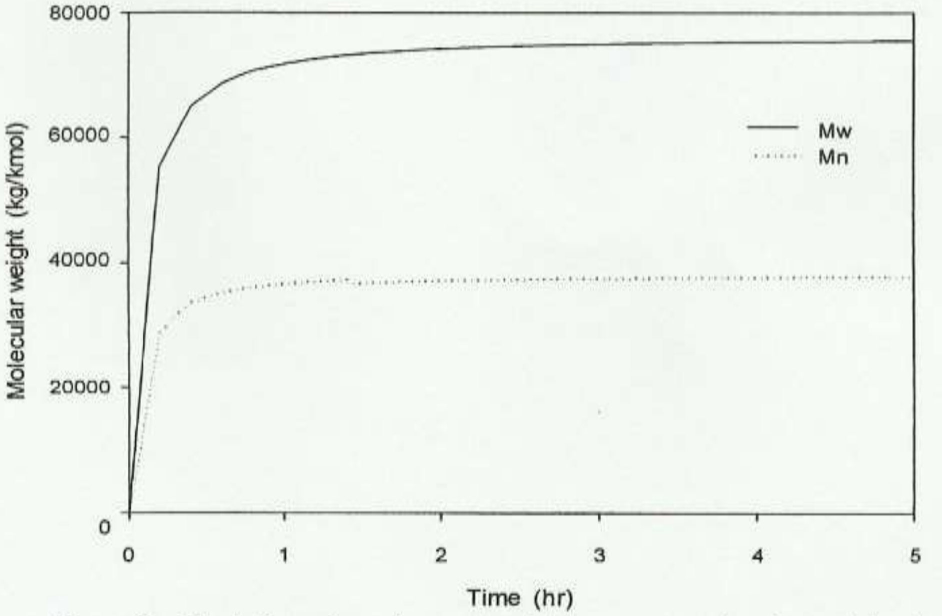

Figure 3. Evolution of number and weight average molecular weights in the reactor (Fcat=0.2 g/s and U0=0.35 m/s).

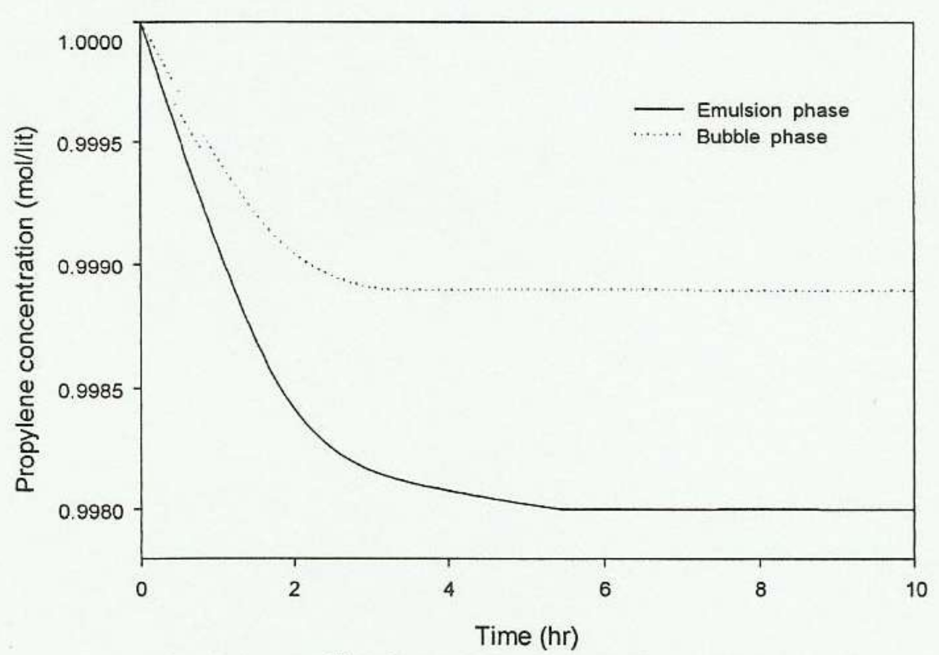

Figure 4. Profile of propylene concentration in the reactor

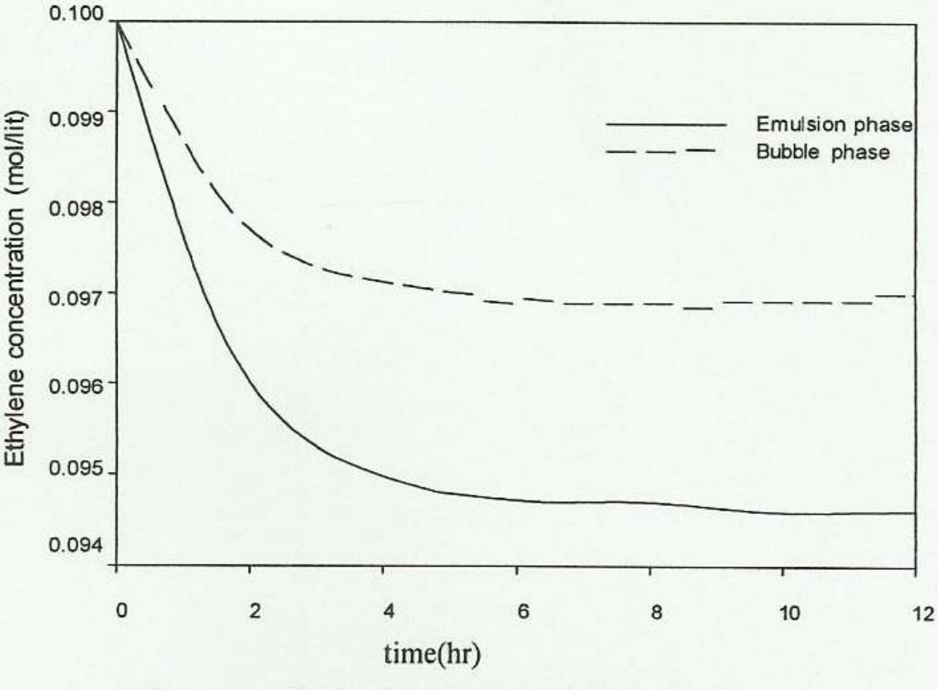

Figure 5. Profile of ethylene concentration in the reactor.

Fig.2 shows the evolution of the emulsion phase temperature with time where it can be noticed from this figure that the predicted polymerization temperature obtained by the new model is lower than the well mixed model results. Fig.3 shows the molecular weight distribution of the final product. Profiles of the concentration of propylene and ethylene in the emulsion and bubble phases are shown in Figs.4and5 where the concentrations of propylene and ethylene in the bubble phase are higher and their rate of change which is proportion al to the rate of consumption of ethylene are lower those in the emulsion phase. This indicate that the emulsion contains about 88% of the catalyst while the bubbles carry about 12% of the catalyst and hence the apparent reaction rate is higher in the emulsion than that in the bubble phase.

V. Conclusion

A fluidized bed reactor model for polypropylene production using the dynamic two-phase concept of fluidization combined with proper kinetic model is presented in this study to provide a better understanding of the reactor performance and shown that about 13% of the polymer is produced in the bubble phase which is an appreciable amount that needs to be considered in all future models of the system.

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