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Mathematical Model and control for Gas Phase Olefin Polymerization in Fluidized-Bed Catalytic Reactors

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Abstract

In this study we present the developments in modeling gas-phase catalyzed olefin polymerization fluidized-bed reactors (FBR) using Ziegler-Natta catalyst. The mathematical model to account for mass and heat transfer between the solid particles and the surrounding gas in the emulsion phase is developed to calculate the concentration and temperature profile in the reactor. The effect of important reactor parameters such as superficial gas velocity, catalyst injection rate, catalyst particle growth and minimum fluidization velocity on the dynamic behavior of the FBR is investigated and compared with the constant bubble size model. The proportional integral derivative controller (PID) is also implemented to control the system under various set point changes and disturbances including the change in inlet gas temperature, with acceptable results.

Keywords: Fluidized bed reactor, Mathematical model, Dynamic studies, PID Control.

1. Introduction

The classification of polymerization reactors models are divided into two main types i.e. pseudo-homogeneous and heterogeneous models. However, heterogeneous models are most widely use in polymerization systems research in this field and concentrated mainly into three areas:.

a) Mathematical modeling for fixed bed catalyst reaction system. [1]
b) Improving the calculation of the hydrodynamics properties.[1],[2]
c) Mathematical modeling for fluidize bed catalytic reaction system. [1],[2]

The bubbling fluidized beds have extensively been studied over the past forty years and a variety of models have been proposed to describe their steady-state and dynamic behavior. Catalytic gas-phase olefin polymerization fluidized-bed reactor can be considered to consist of two distinct phases, namely the bubble and the emulsion phase. The mixing and contacting patterns of the bubble and emulsion phases are very complex and difficult to characterize, thus, various mixing models have been proposed to describe the hydrodynamic behavior of two-phase fluidized-bed reactors. So the prediction model and the main work done by many researchers for estimation of the reactor parameters are based on the two-phase fluidization theory [3], [4].

2. Problem Statement, background

Our present model is extended to account for mass transfer between the solid particles and the surrounding gas in the emulsion phase i.e. mass transfer from the bubble phase to emulsion phase and then mass transfer with chemical reactions between molecules in emulsion phase and catalyst particles. Furthermore it is a well-known fact that semi batch process is gaining wider ground in chemical industries compared with other processes. However, the control of semi batch reactor processes is more difficult because physical and chemical properties of the contents, such as heat transfer coefficient, mass transfer coefficient, emulsion concentration, emulsion temperature and rate of reaction vary from run to run and within the run [3], [5]. In this paper the aim of this work is to develop a modified mathematical model for the polymerization system and design the controller to control the temperature of the system.

3. Research Approach

3.1. Methodology

A clear operation of the polymerization system can be seen in Figure (1).

The operation of polymerization system basically occurs in three steps as, follows;

1. Bubble phase to cloud phase without chemical reaction (Step 1).
2. Cloud phase to emulsion phase without chemical reaction (Step 2).
3. Mass transfer with a chemical reaction from emulsion phase to the catalyst phase and propagation in the size and molecular weight of the polyethylene particle (Step 3).

The model developed in this work takes into account that mass transfer in these three steps without ignoring the solid phase and includes effect chemical reaction account for site activations. The details of some of the equations involved can be seen in the references [1], [2].

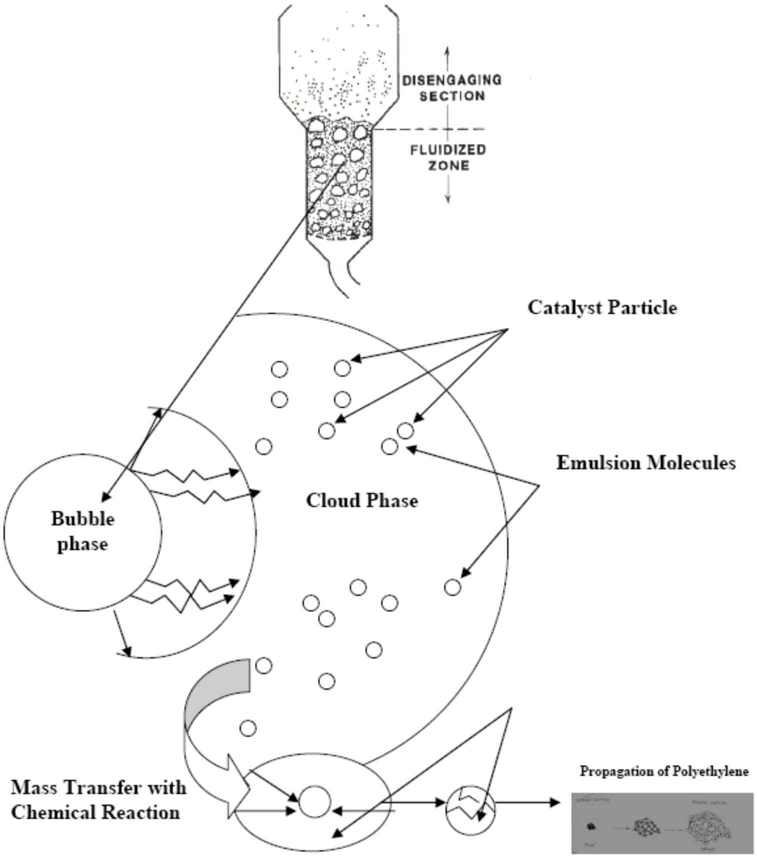

Figure (1) Operation of polyethylene system

3.2. Results& discussions

The simulation results of Figure (2) to Figure (3) show the change of monomer concentration in the bubble and cloud phases through the fluidized-bed height while the results of Figure (4) to (5) shows the change of emulsion temperature with time at certain superficial velocity and catalyst feed. Over all it can be seen that the modified model give close results as compared to the constant bubble size model at the beginning of the reaction but the behavior states change after about one hour of operation.

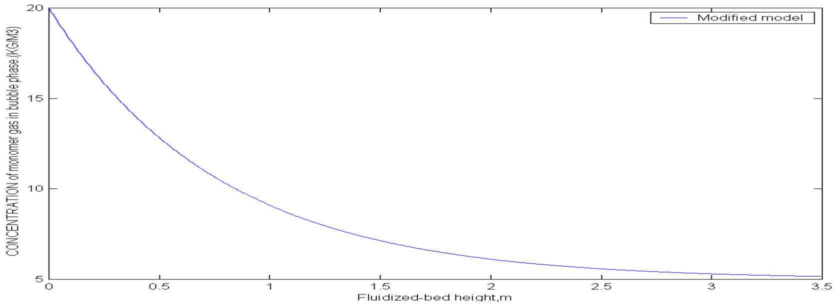

Figure (2) Monomer concentration change in bubble phase through fluidized-bed height

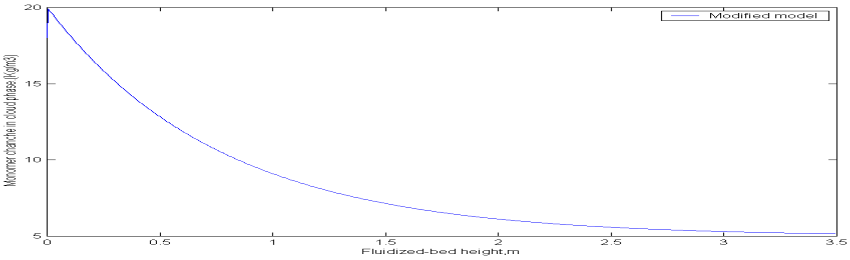

Figure (3) Monomer concentration change in cloud phase through fluidized-bed height

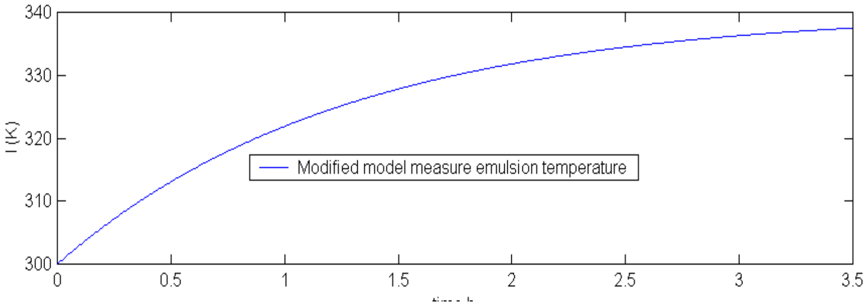

Figure (4) Emulsion temperature change with time (hr) at superficial velocity of 0.5m/sec

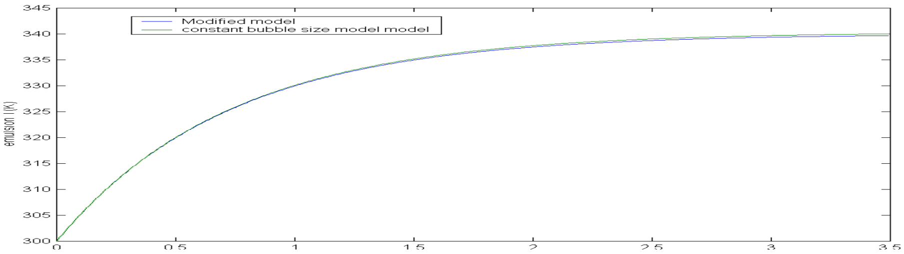

Figure (5) Emulsion temperature change at catalyst feed of 0.005gm/sec

The simulation results for closed loop control implementation of the PID controller for controlling the temperature of the polyethylene system can be seen in Figures (6) to (8). The performance of the controller is investigated through studies under nominal operating conditions in Figure (6) and set point tracking states in Figure (7) and external disturbance including the change to the inlet temperature of the gas, in Figure (8). The integral absolute errors (IAE) of the responses are shown in Table (1). From these results it can be seen that the control effects is aggressive and the process output oscillate around the set point in all the three cases. However, the results are acceptable as it is within the upper and lower limits set point for the temperature of the system and the offsets are small.

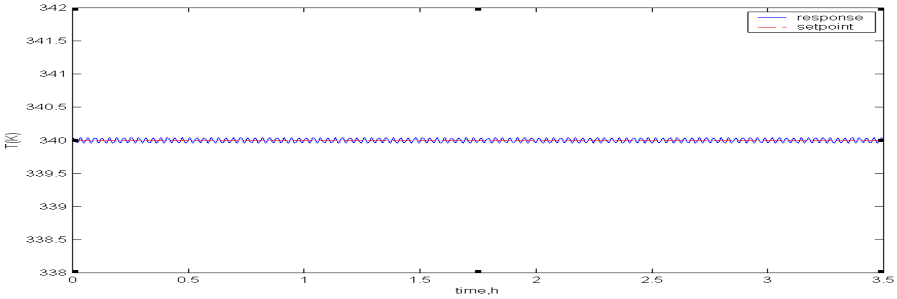

Figure (6) Controller response of PID controller for nominal operating condition study

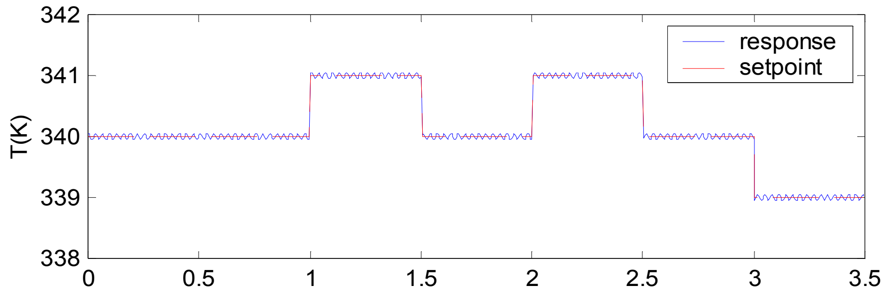

Figure (7) Controller response of PID controller for set point tracking

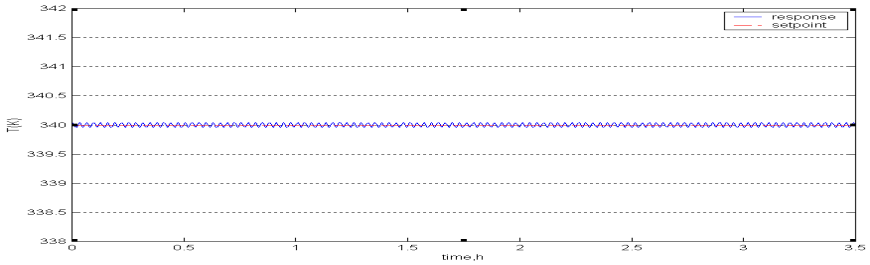

Figure (8) Controller response of PID controller for external disturbance rejection study

Table (1): Integral absolute error for controller performance.

Studies	***IAE***
Nominal operating condition	*0.05125*
External disturbance changes	*0.0544*
Set point changes	*0.0533*

4. Conclusions and future work

The present modified mathematical model of the fluidized bed is developed to give a clear picture about the effects of the all changes happening in the bubble phase and cloud phase for monomer concentration change through the fluidized-bed height. It also, shows the effects of superficial velocity and catalyst feed on the emulsion temperature. The control of the system using conventional PID is found to be acceptable but our future work involves designing advanced controllers such as the neural net work controllers to obtain improved and better performance for the controlled system.

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