Chapter 12
Computational Modeling of Gas-Solids Fluidized-Bed Polymerization Reactors

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ABSTRACT

Gas-solids flows have numerous industrial applications and are also found in natural processes. They are involved in industries like petrochemical, polymer, pharmaceutical, food and coal. Fluidization is a commonly used gas-solids operation and is widely used in production of polyethylene. Polyethylene is one of the most widely used thermoplastics. Over 60 million tons are produced worldwide every year by both gas-phase and liquid-phase processes. Gas-phase processes are more advantageous and use fluidized-bed reactors (e.g., UNIPOL™ PE PROCESS and Innovene process) for the polymerization reactions. In this work a chemical-reaction-engineering model incorporating a given catalyst size distribution and polymerization kinetics along with the quadrature method of moments is used to predict the final polymer size distribution and temperature. An Eulerian-Eulerian multi-fluid model based on the kinetic theory of granular flow is used to solve the fluidized-bed dynamics and predict behavior such as particle segregation, slug flow and other non-ideal phenomena.

INTRODUCTION

Polymers have various applications in automotive industry, packaging, chemical, construction, electrical, packaging, and agriculture. Widely used polymers fall in the category of thermoplastics and thermosets. The major thermoplastics include low density polyethylene (LDPE), polypropylene (PP), poly vinyl

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chloride (PVC), high density polyethylene (HDPE), polyethylene terephthalate (PET), polystyrene (PS) and polyamide (PA). Important thermoplastics include polyurethanes (PU), phenolics and epoxy resins. Various commercial reactors are used for the production of thermosets and thermoplastics. These include stirred tank reactors, fluidized-beds, plug flow reactors, loop reactors, bubble columns and multizone circulating reactors. These fall in the category of gas-solids systems (fluidized-beds, stirred tanks), gas-liquids (bubble columns), and gas-solid-liquids (slurry reactors).

When one surveys the total polymerization marketplace today, thermoplastics represent the major portion of the total production volume. Polyolefins, in turn, represent roughly 60 percent of all the thermoplastics produced and sold in the world today. The major types of polyolefins include polypropylene, high-density polyethylene, linear low-density polyethylene, low-density polyethylene, metallocene polyethylene and polypropylene, and various co-polymers and elastomers. The polyolefin family of products serves a wide variety of end-use markets in the major sectors of packaging, automotive, construction, medical, wire and cable and others. Unlike the incremental technological developments more common in other polymers, polyolefin technology developments are significant and routinely leapfrog the existing ones. These tremendous developments in technology impact the whole industry as a unit as well as the high profit sectors. Multiphase reactors and the associated catalyst technology play a key role in polyolefin businesses.

Polyethylene is the most widely used polyolefin in a wide range of applications. For example, it is used to manufacture plastic bags, electrical insulation, plastic tubing, bottles and packaging materials, and has the advantages of low price, flexibility of molding, and ease of disposal and recycling (Kaneko et al., 1999). Over 60 million tons of polyethylene is produced annually worldwide. It can be produced using gas-phase and liquid-phase processes. In general the gas-phase processes are more advantageous than liquid-phase processes. The activity of most catalysts is approximately 1000 Kg polymer per gram of catalyst and the final polymer need not be separated from the catalyst. In liquid-phase processes the olefin needs to be dried and separated from the solvent (Xie et al., 1994). Earlier technologies produced polyethylene at high pressures (~ 3000 atm). With the advent of catalysts like Ziegler-Natta and metallocene, polyethylene can be produced at low pressures (~ 20 atm). The available commercial gas-phase reactors are fluidized beds (UNIPOL and Innovene process), vertical stirred-beds (NOVOLEN process), horizontal stirred-beds (AMOCO process) and multizone circulating reactors (Basell process). Of all reactor types, fluidized-beds have become popular due to its excellent mass and heat transfer characteristics.

Although there are several advantages with gas-solids fluidized-bed polymerization reactors, there are also some disadvantages, which researchers are trying to understand and solve. In fluidization we generally encounter particles of different sizes and/or densities. When gas flows through a bed of such particles different phenomena are observed. Consider a gas-solids system where the density of the particles is the same (as is the case for gas-phase polyethylene polymerization), but they have two different sizes. The dynamic response of one particle size is different from the other primarily due to the size dependence of the drag force exerted by the gas phase. As a general rule, the drag force for a given gas velocity on small catalyst particles will be much larger than on large polymer particles. When the gas flow rate is operated at velocities between the minimum fluidization velocity of the smaller and larger particles a phenomenon known as *segregation* (Bokkers et al, 2004; Fan, 2006; Fan & Fox, 2008; Kim & Choi, 2001; Mahdi et al., 2002) is observed. Fluidized beds operated at velocities higher than the minimum fluidization of all particles results in a well-mixed system. However, at high gas velocities particles can escape out of the top of the reactor. This phenomenon is called *entrainment* or *elutriation* (Baerns, 1966; Baron et al., 1987; Briens et al., 1992). The other important phenomena occurring in fluidized-bed polymeriza-