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Review

Advances in Mathematical Modeling of Gas-Phase Olefin Polymerization

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Abstract: Mathematical modeling of olefin polymerization processes has advanced significantly, driven by factors such as the need for higher-quality end products and more environmentally-friendly processes. The modeling studies have had a wide scope, from reactant and catalyst characterization and polymer synthesis to model validation with plant data. This article reviews mathematical models developed for olefin polymerization processes. Coordination and free-radical mechanisms occurring in different types of reactors, such as fluidized bed reactor (FBR), horizontal-stirred-bed reactor (HSBR), vertical-stirred-bed reactor (VSBR), and tubular reactor are reviewed. A guideline for the development of mathematical models of gas-phase olefin polymerization processes is presented. **Keywords:** modeling; olefin; gas phase; kinetics

1. Introduction

Polyolefin or polyalkene, which is one of the most popular thermoplastic polymers, are formed from the monomer of the alkene group, which possesses a double bond. The most common monomers used to produce this polyolefin are ethylene and propylene. The polyolefin formed through the polymerization of ethylene is either in the form of polyethylene (PE), high-density polyethylene (HDPE), or low-density polyethylene (LDPE), and another type of polyolefin can be produced through a similar procedure from the monomer propylene in the form of polypropylene (PP). Meanwhile, copolymerization of these two monomers produces a polyolefin, which is in the form of ethylene-propylene diene monomer (EPDM). These polyolefins are in high demand and widely used in several sectors, such as automobiles, packaging, construction, and textiles. As reported by Szabó (2015) [1], the annual consumption of polyolefin per capita in the European continent is expected to increase significantly from 88 kg per person in 2015 to 120 kg per person in 2030 with an increment of 36 percent. Figure 1 summarizes the total consumption per capita in three parts of the European continent for the years 2015, 2020, and 2030.

As shown in Figure 1, Western European countries such as France, Italy, and the United Kingdom are considered to be the biggest consumers of this polyolefin compared with their neighbors located in central and Eastern Europe. This is due to the localization of several polyolefin industries, such as SO.T.AC SRL and Montello SPA in Italy, Borgeois in France, Vital Parts Ltd. in the United Kingdom, and Warm-On Gmbh, and Co.Kg in Germany. In regard to this high demand for polyolefins, the performance of the current polymerization process needs to be reviewed and improved, starting from the selection of monomers and catalyst up to the production of end products.