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CFD investigations of particle segregation and dispersion mechanisms inside a polyolefin 8-leg loop reactor of industrial scale

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ABSTRACT

The formation of polymer slugs inside loop reactors has long been a troubling issue for the polyolefin industry using slurry-phase process. The mechanism of solid phase segregation occurring in the slurry flow has been reported as one of the root causes of the formation of large polymer slugs. However, the mechanism of solid phase dispersion, which counters the solid phase segregation and retards slug formation, has not been fully understood yet especially from the aspect of fluid dynamics. Therefore, in this study we apply computational fluid dynamic (CFD) simulations to provide insightful details about these two competing mechanisms inside an 8-leg loop reactor of industrial scale. The simulations adopt the transient Eulerian–Eulerian two fluid model incorporated with the kinetic theory of granular flow to describe the slurry flow consisting of propylene in liquid state and solid polypropylene particles. The solid particles with an average diameter of 2.5 mm are found to segregate from the slurry mixture due to the centrifugal force induced by the bend geometry, forming thick particulate ropes close to the outer pipe wall. These particulate ropes are dispersed inside the vertical legs by the secondary flow, which exhibits the flow structure as a single vortex on the cross sections. The competition between the segregation and dispersion mechanisms results in numerous slurry clusters of varying solid contents. While they are circulated by the axial flow pump, the loop reactor shows fluctuating profiles of solid volume fractions and liquid velocity as well as the pump pressure output with respect to time. The simulation results reveal that the variations of pump pressure output, which is equivalent to the pump power consumption, are resultants from the varying frictions exerted by the slurry clusters. In addition, our simulation results suggest that operating loop reactors with small particle sizes can suppress the solid segregation mechanism as well as improve the uniformity of particle distributions, which consequently retards the formation of large slugs.

1. Introduction

As an important polymer material in our daily lives, polypropylene (PP) is currently produced by slurry-phase processes in the industry. The polymerization reactions are carried out inside loop reactors with the aid of solid catalysts [1]. Based on the production capability, loop reactors may consist of 4, 6 or 8 vertical pipes arranged in a closed loop. They are referred as "4-leg", "6-leg" or "8-leg" loop reactors in the industry. During a typical slurry-phase PP production process, solid catalyst particles and a certain amount of propylene monomers are first fed into a pre-polymerization reactor to initiate the polymerization reactions. The monomers polymerize on a catalyst surface, generating polymer particles of small sizes. Then these products from the pre-polymerization reactor are transported to a loop reactor, inside which the small particles continue reacting with more incoming monomers. The loop reactors are usually operated within proper pressure and temperature ranges in order to maintain the suitable polymerization rates. Under such operating conditions, the reactants including monomer and diluent solutions are present in liquid state while the produced polymer particles suspend in the liquid, resulting in a slurry flow inside loop reactors. Driven by an axial flow pump, the reacting slurry flow is circulating inside the reactor with a proper speed. As the polymerization reaction process proceeds, polymer particles gradually expand their sizes and ultimately grow to diameters ranging from 100 μm to 5 mm [2]. Nowadays, commercial plants desire to operate loop reactors with long residence times and large solid volume fractions due to economic incentives. Such strategies can not only improve the granulometry of the polymer product but also maximize the contact time of the monomer materials with catalysts; as a result, the cost of separating and recycling unreacted material in the downstream can be reduced significantly [3]. Based on the requirements for product grade, the averaged PP particle size can reach as large as 2.5 mm.

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During normal production processes, inhomogeneous distributions of the solid particles are commonly observed in loop reactors of industrial sizes, which are induced primarily by bends. The 180° and 90° bends are commonly used in loop reactors to connect horizontal or vertical pipes. When the slurry passes through these bends, solid particles migrate towards the outer pipe wall because of the centrifugal effect exerted by the curved geometry. According to the classic expression of the centrifugal force on a moving particle with tangential velocity v, $F = mv^2/r$, the centrifugal force is proportional to the mass of object. In other words, the solid segregation mechanism is significantly influenced by the density and diameter of the particle. Particularly in the PP production process, the high solid volume fractions and large particle sizes can result in severe solid segregation, forming thick layers consisting of polymer particles on the outer pipe wall. After the slurry flow has circulated inside the loop reactors for a sufficient time, these thick layers eventually develop into polymer slugs. The circulation of polymer slugs results in large pressure drop and consequently significant power consumptions by axial flow pumps [3–7]. Based on their analyses on industrial loop reactors for polyethylene (PE) synthesis, Fouarge et al. [3] reported the so-called “pump power swelling” phenomena occurring with the presence of slugs. During normal operations, the standard deviations of pump power consumptions are in the order of 1 to 10 kW. Once the slugs are formed, the pump power consumptions are swelling significantly that the standard deviation of the power peaks increases almost tenfold; in addition, the successive peaks with large fluctuations are separated by less than one minute [3]. The pump power swelling is detrimental to the production process. If it is not controlled properly, the pump power consumption can rapidly reach the safety threshold that the safety interlock system shuts down the reactor automatically. Since the average particle size of PP product is much larger than that of PE (*i.e.*, a typical size of PE particles produced by slurry process is 0.5 mm [4]), the slug formation in the PP process is more severe than that in the PE process. The tendency of operating loop reactors with long residence times and high solid volume fractions in the current industry even intensifies the frequency of slug formation.

Besides the solid segregation mechanism, there exists the solid dispersion mechanism inside loop reactors, which counters solid segregation and retards slug formation. On one hand, the solid segregation mechanism results in thick layers consisting of polymer particles, which may eventually develop into slugs; on the other hand, the solid dispersion mechanism alleviates the solid segregation by dispersing those thick layers. Currently, there are few discussions in literature focusing on the dispersion mechanism in loop reactors but a number based on pneumatic conveying systems. The solid particles segregate from the solid–gas mixture in pneumatic conveying system as well, forming a so-called particulate rope in this field. Recent papers published by Levy's group demonstrated the bends used in pneumatic conveying systems can generate secondary flow in the form of a single vortex [8] or double vortices [9] on cross sections. The particulate ropes are dissipated by the combined effects of such secondary flow and turbulent dispersions. Since the behavior of slurry flow inside loop reactors is analogous to that of the gas–solid flow inside pneumatic conveying systems in some extent, the bends used by loop reactors should also generate secondary flow to disperse the thick layers of polymer particles.

Since the competition between solid segregation and dispersion mechanisms determines the slug formation crucially, a comprehensive understanding of these two mechanisms is important to the PP industry as well as the other polyolefin industries involving loop reactors. In 1993, Zacca and Ray [10] proposed a model that simplified the loop reactor as a continuous stirred tank (CSTR). Although this model is robust and efficient in terms of modeling polymerization reactions with heat and mass transfer, it neglects the solid–liquid flow behavior by assuming the flow is homogeneous [10]. In order to understand the segregation and dispersion mechanisms, numerical modeling using computational fluid dynamics (CFD) is necessary to reveal the liquid–solid flow. Generally, there are two approaches that can be used to model the solid–liquid flow; they are the Lagrangian and the Eulerian approaches. The Lagrangian approach tracks the motions of individual particles and takes account of particle–particle and particle–fluid interactions by solving the equations of motion. As the loop reactors of industrial scale usually contain billions of particles, this approach requires massive computational efforts thus is challenging even with the aid of supercomputing. The Eulerian approach treats the solid phase as continuous and solves an additional set of continuity and momentum equations for the solid phase. It requires less amount of computational resource compared to the Lagrangian approach, thus it is practical to be adopted to study loop reactors of industrial scales. In previous studies, Shi *et al.* developed a numerical model using steady-state Eulerian–Eulerian model to reveal the liquid–solid flow inside a 2-leg loop reactor of pilot scale. Although their simulations have predicted particulate layers close to the outer wall of 90° bends, the segregation phenomenon was not severe because of the small sizes of particles as well as the small scale of the loop reactor [11].

In this work, we have adopted the transient Eulerian–Eulerian model to study the solid segregation and dispersion mechanisms inside an 8-leg loop reactor of industrial scale. The simulations have revealed the fluctuating profiles of several important parameters for loop reactor operations, *i.e.*, solid volume fractions, velocity magnitude and pressure output. The results indicate that the fluctuations are generated by the competition between the segregation and dispersion mechanisms inside the loop reactor. The effect of particle sizes on the solid segregation mechanism is also discussed in this paper. According to our knowledge, there are no open reports so far that perform CFD simulations on loop reactors of industrial scales. This work may help the academic and industrial communities to understand the complex liquid–solid flow behavior inside loop reactors.

2. Reactor dimensions and flow properties

The geometry of the 8-leg loop reactor used in this study is taken from the US Patent 2004/0116625 [12]. The reactor consists of eight vertical legs, seven 180° bends and two 90° bends, which are arranged into two sections. The legs and bends are numbered sequentially around the reactor. The index starts from the discharge of the axial flow pump and ends at the pump's suction. As shown in Fig. 1, the 1st, 6th, 7th, and 8th legs are located on the front pipe section. The axial flow pump dwells inside a horizontal pipe of 1.22 m long between the 1st and 8th legs. The other legs are located on the rear pipe section. These two pipe sections are connected by two 180° bends named as the 2nd and 6th bends, respectively.

During normal operations, the slurry flow is circulated inside the loop reactor by the axial flow pump. When it leaves the discharge of the axial flow pump, the slurry enters the 1st bend which is 90° and flows upward into the 1st vertical leg. Then it flows into the 2nd bend on top where the axial flow direction shifts to 90° from the yz plane to the xz plane. On the exit of this bend, the slurry shifts its axial flow direction of 90° again and enters the rear pipe section. One by one, it passes through the 2nd leg, 3rd bend, 3rd leg, 4th bend, 4th leg, 5th bend and 5th leg in sequence. Among them, the 3rd and 5th bends are the bottom bends located on the ground while the 4th bend is a top bend. The 2nd and 4th legs are the descending legs in which the slurry is flowing downward. In contrast, the 3rd and 5th legs are the ascending legs where the slurry flows upward. After it leaves the 5th leg, the slurry enters the 6th bend on top and changes its axial flow direction similar to that in the 2nd bend. On the exit of this bend, the slurry flows back to the front pipe section. In this section, the slurry continues to pass through the 6th leg, 7th bend, 7th leg, 8th bend, 8th leg and 9th bend sequentially and finally enters the pump suction region. Among these legs and bends, the 1st, 7th and 9th bends are located on the ground while