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Computational study on the effect of slug dynamics on the operation of a polyolefin 8-leg loop reactor of industrial scale

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ABSTRACT

The causes and *ad-hoc* remedies associated with the formation of slugs that result in pump power fluctuation inside slurry loop reactors have been discussed in several patent literature, but studied in few research publications. The circulation of large polymer slugs inside loop reactors can induce violent fluctuations of pump power that can lead to automatic shutdown of the entire production process. In our previous work, we have developed a computational fluid dynamic (CFD) model using the Eulerian – Eulerian two fluid method to study the solid segregation and solid dispersion mechanisms inside an 8-leg loop reactor of industrial scale. Herein we adopt this model to study the response of such loop reactor to the slug circulation. The modeling results reveal that the profiles of reactor outputs, *i.e.*, solid volume fractions, velocity magnitudes and pump pressure output, demonstrate random fluctuations with small amplitudes when the reactor is in normal operations. However, these profiles show drastic fluctuations in a periodic manner once a large slug is circulating around the loop reactor. The solid dispersion mechanism governed by the secondary flow inside vertical legs cannot dissipate the slug effectively as the dispersion occurs primarily on the radial direction. Therefore, a mitigation method that offers mixing in the transverse direction is necessary to assure safe and continuous production process.

1. Introduction

Since its emergence in last century, slurry phase polymerization process has enjoyed significant commercial success in the polyolefin industry. Billion pounds of olefin polymers, *i.e.*, polyethylene (PE) and polypropylene (PP), are now being produced by such technique every year throughout the world [1]. The slurry polymerization process adopts relatively high pressure, *i.e.*, in the range of 3 to 4 MPa and suitable operating temperatures to facilitate the polymerization reactions. Under such conditions, the reactants, *i.e.*, monomers and diluent materials, are present in liquid state. The synthesized polymer particles suspend in the liquid medium, forming the particle – fluid mixture which is usually termed as “slurry”. The polymerization reactions are generally carried out inside loop reactors with the aid of designed catalysts, *i.e.*, chromium oxides, Ziegler-Natta or metallocene-types. Depending on the production capability, loop reactors may consist of 4, 6 or 8 vertical pipes which are arranged in a closed loop. They are usually referred as “4-leg”, “6-leg” or “8-leg” loop reactors by the polyolefin industry. During the normal operations, the reacting slurry is circulated around loop reactors with proper speeds so as to prevent polymer particles from settling down. The circulation is driven by one or several axial flow pumps with their impellers placed inside the reactors [2]. As the polymerization reactions proceed, polymer particles gradually grow in size leading to the preferred diameters. Within every circulation, a portion of the product slurry which is rich in solid contents of larger size is withdrawn by either settling legs [3] or continuous withdrawal mechanisms [4]. The product slurry is then sent to flash chambers to separate polymer particles and recycle the unreacted monomers and diluents.

The inhomogeneous distribution of polymer particles has been commonly observed in loop reactors of industrial scale. Such inhomogeneity is primarily initiated by the connection bends used by the loop reactors. The curving geometry of the bends induces the centrifugal force acting on the circulating slurry. In our previous study, we have demonstrated that the centrifugal force causes a net movement of polymer particles towards the outer pipe wall as they are denser than the liquid phase, which is known as “solid segregation”. In addition, the secondary flow in the liquid phase promotes the net movement as well [5]. Consequently, polymer particles segregate from the slurry and deposit on the pipe wall, forming thick particulate layers containing high solid volume fractions. After the slurry has been circulated for sufficiently long time, such

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particulate layers eventually develop into polymer slugs [6]. The slug formation has been observed extensively in loop reactors and has been reported to be detrimental to the slurry phase polymerization process. The circulation of large slugs in loop reactors can cause violent fluctuations to the pump power. According to their analyses on an industrial loop reactor producing polyethylene (PE), Fouarge et al. [7] have reported the so-called “pump power swelling” phenomenon: the pump power was fluctuating violently when slugs were detected inside the reactor. For example, the pump power was fluctuating in a range of less than 10 kW in normal operations. In comparison, such range may increase 10 folds when pump power swelling occurs [7]. If the swelling is not controlled properly, the pump power can reach the safety threshold rapidly, and the safety interlock has to automatically shut down the entire operation process [7].

Nowadays polyolefin industry desires to operate loop reactors with high solid contents due to economic incentives [7]. On one hand, such strategy 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 production yield is increased; meanwhile, the cost of separating and recycling unreacted materials in the downstream process can be reduced significantly [7,8]. On the other hand, previous reports from Fouarge et al. [7] and Marissal [6,9] have pointed out that such strategy intensifies the slug formation probabilities remarkably and consequently causes production losses. In order to prevent the frequent formation of slugs in loop reactors, the operating solid contents must be controlled below certain critical values. Such conflict of interests encourages both the academic and industrial societies to acquire fundamental understandings about the slug formation and movements as well as the consequent effects on the operation of loop reactors.

In current stage, experimental investigations on polymer slugs inside loop reactors are still confronting challenges. Loop reactors of pilot scale usually have good homogeneity in terms of particle distributions in fluid flow. According to the invention proposed by Marissal [6], these loop reactors have short cumulative settling distance which is below the critical value that can lead to slug formation. Therefore, slugs are usually not observed inside loop reactors of pilot scale. Experimental studies on loop reactors of industrial scale are limited by the expenses and more importantly the safety issues. Alternatively, according to literature publications, computational fluid dynamics (CFD) analyses have turned out to be an economic and effective approach to study the slurry flow inside loop reactors [5,10–12].

In our previous work, we have developed a CFD model to study the solid segregation and dispersion mechanisms inside an 8-leg loop reactor of industrial scale. The model adopts the Eulerian–Eulerian two–fluid model to describe the slurry flow and incorporates the kinetic theory of granular flow (KTGF) to describe the particle motions and interactions in the solid phase. Such model has successfully predicted the fluctuating profiles of the reactor outputs, *i.e.*, solid volume fraction, liquid phase velocity and pump pressure output, under the developing stage of slug formation [5]. In this study, we continue our work to investigate the response of such loop reactor to the circulations of large polymer slugs. In the first part of this study, the CFD simulations are carried out to study the slurry flow when the loop reactor is in normal operations. In the second part, a large polymer slug is introduced to the loop reactor. The corresponding reactor outputs, *i.e.*, distributions of the solid phase, velocity magnitudes of the liquid and solid phases, pressure output of the axial flow pump and *etc.*, are analyzed while such slug is circulated inside the loop reactor. The simulation results reveal the “pump power swelling” phenomenon and explain the fluctuating profiles from the aspect of fluid mechanics. According to our knowledge, there are no open reports so far that have applied CFD simulations to analyze the slug motions inside loop reactors of industrial scale. This work may enhance the fundamental understanding of slug circulations on the operations of polyolefin loop reactors and may help the polyolefin industry to address the pump power swelling issue.

2. Reactor dimensions and fluid properties

The 8–leg loop reactor used in this study is identical as the one in our previous work. The dimensions of the loop reactor are taken from US Patent 2004/0116625 [1]. The reactor consists of eight vertical legs, seven 180° bends and two 90° bends, as seen in Fig. 1(A). The axial flow pump and the guiding vane, as illustrate in Fig. 1(C) and (D), locate inside a horizontal pipe between the 1st and 8th legs as shown in Fig. 1(B). The inner diameter of all the pipes (D) is 0.56 m (22″ pipe). The radius of all the 180° bends and the two 90° bends are 1.83 m and 1.22 m, respectively.

Table 1 lists the physical properties of the slurry and the operating parameters of the loop reactor used by this study. As one aim of this study is to compare the effect of particle size on the operations of loop reactors with our previous work, the properties of fluid and particles and the operating conditions are identical as those in the previous study [5]. The loop reactor was operated with a relatively high solid volume fraction as $C_v = 0.23$, corresponding to solid weight fraction as 39% approximately. The polymer particles were assumed to have average diameter (D_p) as 0.5 mm, which is a typical grade for PE and PP products. The rotational speed of the axial flow pump was adjusted to 180 rad/s; such rotation drove the slurry to circulate around the loop reactor with an average velocity as 7.7 m/s. Since the infusing and withdrawing rates were much smaller compared to the circulating rate, the inflows from the inlet and outflows from the outlet were not considered by the numerical model. The other details about the geometry and operation of the loop reactor are introduced in our paper, as seen in reference [5].

3. Numerical model

3.1. Brief introduction to the model

The slurry flow inside the loop reactor is described by the Eulerian–Eulerian two fluid model in this work. The numerical model takes the assumption that the liquid phase is incompressible and Newtonian; in addition, the model treats the solid phase as a continuous fluid. The flow behavior of the solid phase is described by the kinetic theory of granular flow (KTGF). The parameters associated with the solid phase are estimated through the solid temperature. The momentum exchange between the two phases is described by the empirical drag law proposed by Gidaspow et al. [13]. The large Reynolds number of the liquid phase ($Re_l = \rho_l v_l D/\mu_l = 3.25 \times 10^7$, in which $v_l = 7.7$ m/s is the average circulation velocity of the liquid phase; D is the diameter of the pipe) indicates that the slurry flow inside the loop reactor is in the fully-developed turbulent regime. The RNG k-ε model was selected to describe the turbulent flow as it enhances the prediction of swirling flows compared to the standard k-ε model.

The surfaces of all pipes, pump impellers and the guiding vane were specified with wall boundary conditions. For these wall boundaries, the liquid phase was imposed with the no-slip condition while the solid phase was imposed with the partial slip condition proposed by Johnson and Jackson [14,15].

Equations of CFD models used in this work are listed in Table 2. The details about the governing equations and the boundary conditions can be found in our previous paper as listed in reference [5].

3.2. Model setup

The modeling work was carried out using the commercial CFD package ANSYS Fluent 15. The rotation of the pump was modeled by the moving reference frame mode in Fluent. Such method enables the steady-state solutions of pump motions at each time step. After performing a mesh dependence study, a computational mesh consisting of about 3.1 million computational cells was used by the model.

In the first part of this study, we applied this numerical model to analyze the slurry flow when the loop reactor was under normal