Hydrodynamic investigation of industrial gas-phase polyethylene reactors in two different technologies

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ABSTRACT

Gas-solid fluidized bed reactors are among the common methods to produce linear low-density polyethylene. The contact quality between two phases and the mixing of the solid particles in these reactors have significant impacts on the polymerization reaction. In this research, the hydrodynamic behavior of two reactors licensed by Basell and Mitsui companies was investigated using computational fluid dynamics. Two-fluid model with the kinetic theory of granular flow was used. The model was first validated using experimental data, and then the analyses of the Mitsui and Basell industrial reactors were carried out. The results showed that the uniformity of the gas phase volume fraction, which indicates the quality of the gas-solid contact, increases with the distance from the bed bottom in both reactors, so that at a normalized height of 0.96, the phase homogeneity reaches its maximum. At this height, the coefficient of variations of volume fraction in the Basell and Mitsui reactors are 0.4% and 1.3%, respectively, and the phase homogeneity in the Mitsui reactor is always higher than that in the Basell reactor at different heights, indicating a better contact between particles and gas. The time-averaged axial velocity of the solid particles at different heights showed that the intensity of solid particle movement is higher in the Basell reactor, so that at a normalized height of 0.72, the axial velocity of the solid particles in the Basell reactor is approximately 2 m/s, while it is approximately 1 m/s in the Mitsui reactor. Considering the axial velocity parameter, it can be concluded that the quality of solid particle mixing in the Basell reactor is higher than that in the Mitsui reactor.

KEYWORDS

Computational Fluid Dynamic, Ethylene Polymerization, Eulerian Modelling, Fluidized Bed Reactor, OpenFOAM

1. Introduction

Polyolefins are widely used in various industries. Polyethylene is the most-extensively produced polyolefin, with production methods categorized into high- and low-pressure processes. Low-pressure gas-phase processes employing fluidized-bed reactors are commonly used[1-2].

Various reactor configurations have been developed by different licensors, with the Basell and Mitsui technologies being widely used. While the overall reaction conditions are similar, differences in reactor configuration details can impact the hydrodynamics, such as solid particle mixing and gas-solid contact, which are critical in reactor performance.

The hydrodynamics of gas-solid fluidized bed reactors can be studied using two main numerical modeling approaches: Euler-Lagrange and Euler-Euler. Due to the significantly higher computational requirements of the

Euler-Lagrange method, it is not used for simulating industrial-scale fluidized bed reactors[3].

Many studies have investigated fluidized bed hydrodynamics, including a recent investigation [4] on effect of gas distributor design on bubble behavior in a lab-scale fluidized bed. However, the hydrodynamic simulation of fluidized bed reactors has rarely examined under industrial operating conditions. Most of the existing studies have been conducted on a laboratory scale and do not focus on a specific technology. Furthermore, there is a lack of research that compares the different reactor configurations and their effects on the reactor hydrodynamics.

This paper aims to investigate the hydrodynamics of two industrial reactors with distinct configurations using CFD tools. First, a suitable model is developed and validated. Subsequently, a comparative analysis of the hydrodynamic performance of the two reactors is performed using the developed hydrodynamic model.

2. Methodology

To simulate a two-phase system using the Eulerian model, the time-averaged conservation equations for mass and linear momentum are considered for each phase [5]. In addition to the primary conservation equations, the model incorporates equations describing the interactions between particle-gas, particle-particle, and particle-wall [6]. For the Eulerian simulation, a suitable rheological model is required to capture the behavior of the solid phase as a fluid-like material. In this study, the KTGF model is employed to express the aforementioned interactions [7]. The sub-models used to develop hydrodynamic model are given in Table 1.

Table 1- Closure models used in the hydrodynamic model

Model	Reference
Viscosity Model	Gidaspow [7]
Conductivity Model	Gidaspow [7]
Granular Pressure Model	Lun [6]
Frictional Stress Model	Johnson Jackson Schaeffer [8]
Radial Distribution Function	SinclairJackson[9]
Drag Model	Syamlal Obrien [10]

For simulating the industrial reactors, due to the very high volume of industrial reactors, the dimensions of the reactor were scaled down 4 times, but the properties of phases and superficial gas velocity and pressure were kept constant. General configurations of both reactors and the field of volume fraction of particles obtained from the simulation are shown in Figure 1.

Simulations were performed by OpenFOAM v-9 on a computer with 24 CPU cores. multiphaseEulerFoam solver was used for simulations and each simulation of the reactor took around 5 to 7 days to complete (30 seconds).

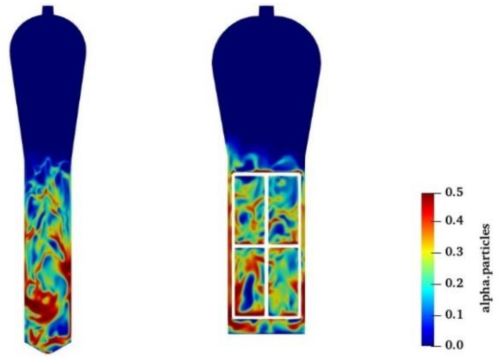

Figure 1: Contour of volume fraction of particles obtained from the simulation of the industrial reactor at t=30 s

3. Result and Discussion

To perform mesh independency study, the time-averaged volumetric fraction of the solid phase was investigated along the reactor's axial direction. After further investigation, a cell size of 10 times of particle diameter was selected (results are not shown here).

After mesh independency study, the hydrodynamic model was validated using experimental data available in Busciglio et al. [11]. One of the critical aspects in the behavior of bubbling fluidized bed reactors is the investigation of bubble characteristics, including bubble rise velocity and bubble size distribution. In this study both were studied and as an example bubble size distribution at bed height of 90 mm and gas velocity 3.4 times the minimum fluidization velocity is shown in Figure 2. The simulation could accurately predict the bubble size distribution obtained from experimental measurements.

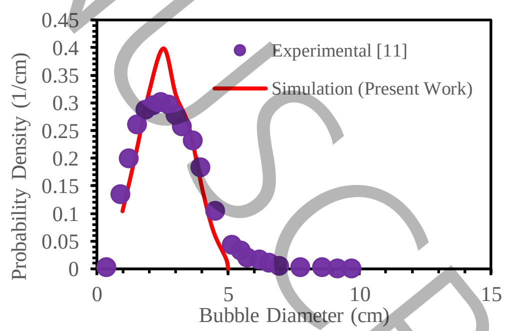

Figure 2. Comparison of the size distribution of bubbles at a height of 90 mm from the bottom of the bed and a velocity of 3.4 times the minimum fluidization velocity between simulation and experimental data [11]

Figure 3 shows the coefficient of variation of gas volume fraction (CoV) versus bed normalized height in both reactors. If Cov is reduced, the quality of gas-solid contact is increased. The gas-solid contact quality in

Mitsui technology is higher than in Basell technology, and this quality also increases with the distance from the bottom of the bed (Figure 3). Therefore, the presence of the stirrer improves the quality of gas-solid contact and the uniformity of the flow of the two phases.

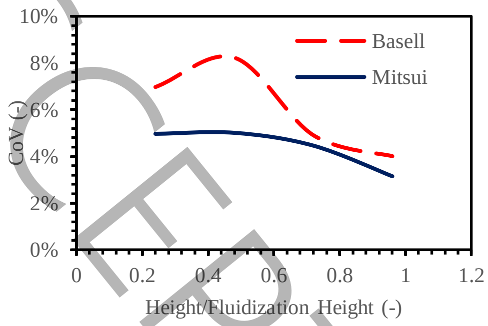

Figure 3. Comparison of the CoV related to the time averaged volume fraction of the gas phase

For evaluating the intensity of the solid mixing, axial solid velocity was considered. According to the value of the velocities, it can be seen that at a normal height of 0.72 (Figure 4), maximum velocity of solid particles in the Basell reactor is almost twice the solid particle velocity in the Mitsui reactor.

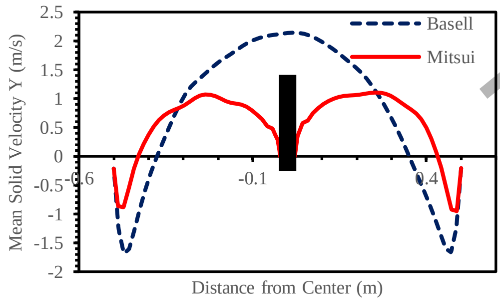

Figure 4. Comparison of the time averaged solid phase velocity (from 10 to 30 seconds) in the axial direction and at a normal height of 0.72.

Therefore, this higher velocity of solid particles in Basell technology indicates more mixing of solid particles in this reactor.

4. Conclusion

The study investigated the hydrodynamics in industrial fluidized bed reactors used for linear low-density polyethylene production: the Basell and the Mitsui reactors. The results showed that the gas-solid contact quality was better in the Mitsui reactor compared to the Basell reactor. For instance, at normalized bed heights of 0.96, CoV was 4% for Basell and 1.3% for Mitsui. In addition, across all bed heights, the Mitsui reactor demonstrated a lower CoV, suggesting better gas-solid contact quality. In terms of solid particle mixing, the Basell reactor showed higher axial solid particle velocities and more intense solid mixing compared to the Mitsui reactor. In conclusion, the hydrodynamic comparison showed that the quality and uniformity of the two-phase contact in the reactor used in Mitsui technology was higher than the Basell reactor. On the other hand, it was observed that the solid particles in the Basell reactor were moving at a higher velocity in the axial direction, resulting in better mixing of the solid particles.

5. References

[1] P. Galli, G. Vecellio, Polyolefins: The most promising large-volume materials for the 21st century, Journal of Polymer Science Part A: Polymer Chemistry, 42(3) (2004) 396-415.

[2] S. Schneiderbauer, S. Puttinger, S. Pirker, P. Aguayo, V. Kanellopoulos, CFD modeling and simulation of industrial scale olefin polymerization fluidized bed reactors, Chemical Engineering Journal, 264 (2015) 99-112.

[3] M. Khan, M. Hussain, Z. Mansourpour, N. Mostoufi, N. Ghasem, E. Abdullah, CFD simulation of fluidized bed reactors for polyolefin production–A review, Journal of Industrial and Engineering Chemistry, 20(6) (2014) 3919-3946.

[4] K. Jang, Y. Feng, H. Li, Investigation of Bubble Behavior in Gas-Solid Fluidized Beds with Different Gas Distributors, Chemical Engineering & Technology, 44(4) (2021) 723-731.

[5] T.B. Anderson, R. Jackson, Fluid mechanical description of fluidized beds. Equations of motion, Industrial & Engineering Chemistry Fundamentals, 6(4) (1967) 527-539.

[6] C.K. Lun, S.B. Savage, D. Jeffrey, N. Chepurniy, Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flowfield, Journal of fluid mechanics, 140 (1984) 223-256.

[7] D. Gidaspow, Multiphase flow and fluidization: continuum and kinetic theory descriptions, Academic press, 1994.

[8] P.C. Johnson, R. Jackson, Frictional–collisional constitutive relations for granular materials, with application to plane shearing, Journal of fluid Mechanics, 176 (1987) 67-93.

[9] J. Sinclair, R. Jackson, Gas-particle flow in a vertical pipe with particle-particle interactions, AIChE journal, 35(9) (1989) 1473-1486.

[10] M. Syamlal, T.J. O'Brien, Computer simulation of bubbles in a fluidized bed, in: AIChE Symp. Ser, Publ by AIChE, 1989, pp. 22-31.

[11] A. Busciglio, G. Vella, G. Micale, L. Rizzuti, Analysis of the bubbling behaviour of 2D gas solid fluidized beds: Part II. Comparison between experiments and numerical simulations via digital image analysis technique, Chemical Engineering Journal, 148(1) (2009) 145-163.