Jurnal
Teknologi

Full Paper

CFD MODELING OF BINARY MIXTURE HYDRODYNAMICS IN GAS-SOLID PARTICLE FLUIDIZED BED REACTOR SYSTEM

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Article history
Received
23 June 2015
Received in revised form
20 September 2015
Accepted
19 December 2015

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Graphical abstract

CONTOURS OF SOLID VOLUME FRACTION WITH DIFFERENT DRAG MODEL

Abstract

The objective of this research was to compare the effect of a binary mixture between coal, including 500, 700 and 1000-micron size, and sand, 180-micron size, on the mixing behavior in a fluidized bed system. In addition, suitable computational fluid dynamics drag models were explored, including an EMMS model, Gidaspow model and Wen & Yu model. The simulation results were compared for correctness with real plant information. The EMMS model matched well with the obtained data, This is because the employed model considers the particle cluster effect. The EMMS drag model was then used for further computational fluid dynamics simulation. The levels of mixing between sand and coal were predicted by turbulent dispersion coefficient. These coefficients of coal particle were exhibited in axial and radial direction. The highest turbulent dispersion coefficients were found in the mixture with 500 and 1000 micron coal size for radial and axial directions, respectively. The low axial turbulent dispersion coefficient and high radial turbulent dispersion coefficient were preferred for good hydrodynamics behavior.

Keywords: Fluidized bed system, binary mixture, CFD, dispersion coefficient, simulation

1.0 INTRODUCTION

A fluidization technology has been employed in various industrial scale purposes including cracking of hydrocarbons and fuel combustion due to the advantages of technology, like excellent gas-solid particle contact, uniform temperature gradient and ability to operate in a continuous system [1, 2]. The solid particles (bed) in the reactor are usually supported by a distributor, and then a gas is passed through those solid particles. Firstly, the solid particles are stationary (fixed bed) until the gas velocity is sufficient to change the solid particles to act as a fluid. This process is known as fluidization. When the solid particles are fluidized, the solid particles behave differently as gas velocity is increased. A order of transforms in the behavior of the solid particles is defined as flow regimes [3]. There are four regimes consist of bubbling, turbulence, fast fluidization and pneumatic transport. All of regimes sort of increasing gas velocities, respectively [4]. In case of bubbling regime, this regime has considered more than the other flow regimes owing to bubble characteristics. The bubble formation is the dominant characteristic of this flow regime. The bubbles coalesce as they rise through the bed which they have a pronounced positive effect on the levels of mix particles and chemical reaction conversion [1, 5].

Good mixing behavior is required in industry in order to obtain a product of an acceptable quality or to control the rate of heat and mass transfers and rate of chemical reaction conversion [6]. This phenomenon is strongly influenced by the motion of the solid particles, which depends on physical properties of solid particles. However, in the industry, the important task is to mix the solid particles with different physical properties such as shape, size and density [7]. Segregation or de-mixing occurs when a system contains solid particles with different sizes, densities, etc. Also, the improper distribution of gas velocity can cause the solid particles to separate during fluidization. The solid particles falling into the bottom of the bed are called jetsam; In contrast, the solid particles floating towards the top of the bed are called flotsam [8, 9].

Nowadays, with the enhancement of computer technology, the numerical simulation using computational fluid dynamics (CFD) technique is receiving more attention. This methodology can use to understand the hydrodynamics and other phenomena in multiphase flows. There are two main CFD methods for multi-phase flow system consisting of the Eulerian-Eulerian and Eulerian-Langragian methodes.

For the Eulerian-Lagrangian method, or discrete particle model (DPM), each individual solid particle is calculated by integrating Newton's secondary law [3]. However, this method is expensive for engineering applications due to the large amount of solid particles in the real system, which then needs a long time to solve a problem [10]. For the Eulerian-Eulerian method each phase is defined as a different continuum phases [11]. The kinetic theory of granular flow (KTGF) combined with the Eulerian-Eulerian method has been commonly be valid as constitutive equations for two phase flow [11, 12]. This model is also employed in this study.

For the solid particle binary mixture, the effect of interaction between two phases, or drag on the system hydrodynamics, has been extensively explored. Azizi et al. [13] found that the model of bubbling fluidized beds containing solid particles mixing with differencing in density, size, or both using Wen & Yu model were accurately predicted. Lungu et al. [8] compared the EMMS model and Gidaspow model by simulating a bubbling fluidized bed system containing solid particles with differencing in size but having same density. Their results found that the EMMS model better predicted a bed height and voidage by comparing to the real experimental data than the Gidaspow model. Chao et al. [14] investigated the effect of interaction between different solid particles. Their results found that this interaction should be considered when studying the demixing or segregation behavior in bubbling fluidized bed. Oke et al. [15] observed an increasing of lateral dispersion coefficient with the increasing of bed height.

Because the hydrodynamics behavior in fluidized bed reactor system is altered with solid particle mixing, the mixing therefore is of an essential factor. The mixing quality levels can be investigated by the turbulent dispersion coefficient. This parameter can be calculated based on the turbulence and the KTGF concepts [3]. Two types of dispersion coefficient are found in the fundamental theory. The laminar dispersion coefficient is resulted from the oscillations of individual solid particle, and the turbulent dispersion coefficient is resulted from oscillations of gas bubble/solid particle cluster [3, 16, 17]. However, from the literature review, very few studies have been reported on the effect of the binary mixture on the mixing behavior via the dispersion coefficient parameter.

In this study, the mixing hydrodynamics in two phase fluidized bed system of a binary mixture were investigated by using a commercial CFD simulation program, ANSYS FLUENT [18]. The Eulerian-Eulerian method together with the KTGF model was used to obtain results. First, the CFD simulations were developed based on the EMMS drag model, Gidaspow model and Wen & Yu model. The result from simulation was validated with available experimental records to verify the obtained simulation results. After that, the effect of a binary mixture between coal particle, including 500, 700 and 1000-micron size, and sand particle, 180-micron size, on mixing behavior in fluidized bed system was investigated based on the turbulent dispersion coefficient of coal solid particles, both in x- and y-system directions.

2.0 EXPERIMENTAL

2.1 System Geometry

The two-dimensional CFD model of a fluidized bed reactor system was constructed as shown in Figure 1. The reactor system has a 20.00 m height, 4.22 m minimum width and 7.96 m maximum width. The system mainly consisted of four inlet positions. A primary air inlet position was at the system bottom and used to flow air at 1.33 m/s gas velocity. The two coal feed positions were at the system height of 1.23 m above the primary air position with a diameter of 0.60 m. The two lower secondary air positions were at 2.37 m above the primary air position with a diameter of 0.24 m. The two upper secondary air positions were at 3.80 m above the primary air position with a diameter of 0.24 m. All of the inlet positions were fed with 30^{o} of depression. Sand solid particles were used as the bed medium in the fluidized bed reactor. It had density of 2,659 kg/m^3 and a size distribution of 75-250 micron with mean particle diameter of 180 micron. At the beginning, the sand particle was filled into the fluidized bed reactor at height of 0.61 m. The experimental coal size distribution and mean diameter were 500-1000 micron and 730 micron, respectively.

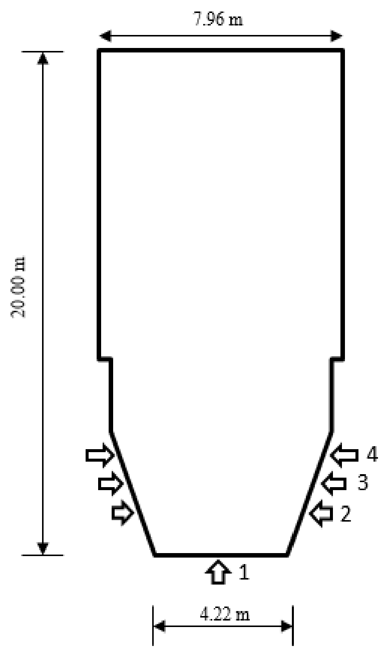

Figure 1 The fluidized bed reactor system (1) primary air, (2) coal feed, (3) lower secondary air and
(4) upper secondary air

2.2 Computational Fluid Dynamics Model

A set comprising governing equation of mass, momentum and energy transfers, available in ANSYS FLUENT, was used in this model. As stated in the introduction, the Eulerian-Eulerian numerical method was employed together with the KTFG model. This method solved the governing equations for each phase separately. In ANSYS FLUENT, the EMMS drag model was not built in module, therefore, the C programming language code was input. The other system properties are stated in Table 1. At the bottom of system, the primary air entered the fluidized bed reactor system with uniform flow distribution. At the top of system, the assumption that there was no leak of sand solid particles at the top of the reactor was set to represent the installation of a cyclone unit operation in a real experimental fluidized bed reactor system. The parameters used for CFD simulation is also shown in Table 1. In addition, Table 2 shows an overview of considered parameters in this study.

3.0 RESULTS AND DISCUSSION

The modeling results have been divided into two parts: the first part compares the employed hydrodynamics model with experimental data, including the system pressure drop and bed height. The second part discusses the mixing hydrodynamics of coal and sand solid particles (binary mixture). The obtained results are reported in terms of turbulent dispersion coefficient with different coal solid particle sizes.

Table 1 Summary of conditions for CFD simulation

Parameters	Values
Inlet condition	
Primary air	1.33 m/s
Lower secondary air	36.03 m/s
Upper secondary air	45.98 m/s
Coal feed	2.08 kg/s
Coal solid volume fraction	0.47
Outlet condition	
Outlet pressure	Atmosphere
Wall condition	
Restitution coefficient	0.90
Specularity coefficient	0.01
Initial condition	
Sand volume fraction	0.30
Temperature	
Sand	1213 k
Coal	1213 k
Air	1213 k
Density	
Sand	2659 kg/m^3
Coal	2000 kg/m^3
Air	0.294 kg/m^3
Viscosity	
Air	4.636 x 10^{-5} kg/m s

3.1 Model Validation

As shown in Figure 2, the computed time-average of sand size 180 micron distribution with difference drag model were different. Note that the employed computational cell and step time in this simulation were already performed the independent study.

Table 2 Overview of the parameters consideredin this study

Parameters	Value
Drag model	EMMS, Gidaspow, Wen&Yu
Coal solid particle size	500, 700, 1000 micron
Turbulent dispersion coefficient	x, y direction

From the contour, it is clearly found that when the EMMS model was used, the heterogeneous structures were found to be in agreement with the bed expansion data. At the bottom and top of system, the dense phase at and the dilute phase were observed. In contrast, when the Gidaspow and Wen & Yu models were used, most of the sand solid particles moved up to the top of the fluidized bed reactor.

Table 3 compares the obtained pressure drop and bed expansion data of sand solid particles between simulation results and real experimental data.

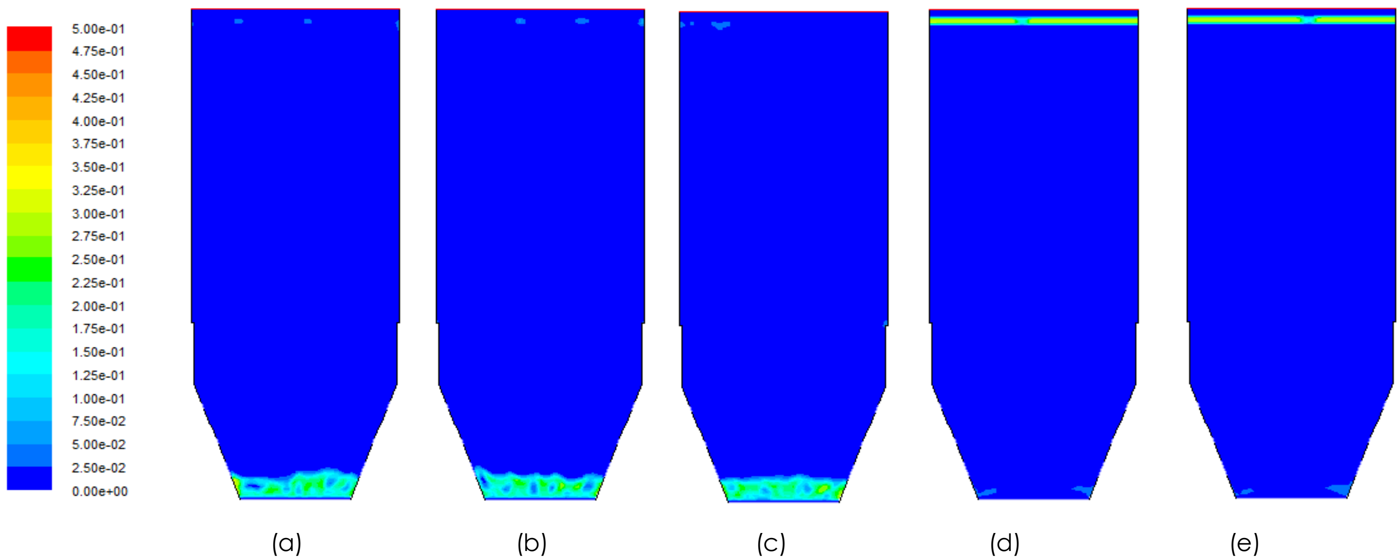

Figure 2 Contours of sand volume fraction for (a) EMMS drag model at 50 s, (b) EMMS drag model at 55 s, (c) EMMS drag model at 60 s, (d) Gidaspow drag model at 60 s and (e) Wen & Yu drag model at 60 s

Table 3 Comparison of the obtained pressure drop and bed expansion data of sand solid particles between simulation results and real experimental data

Drag model	Pressure drop (Pa)	Bed height (m)
EMMS model	4726.57	0.90
Gidaspow model	5817.25	-
Wen&Yu model	5652.53	-
Experimental	4800.00	0.92

From the results, the Gidaspow and Wen & Yu drag models were found to be unsuccessful for predicting the hydrodynamics of sand solid particles. This is because neither drag models consider the effect of a dense solid particle concept on gas-solid particle interface force [5, 8, 16, 19]. On the other hand, both pressure drop and bed expansion of fluidized bed system were captured by the EMMS model. The EMMS model (Energy Minimization Multi-Scale) calculated the interaction between gas-sold particles (drag) using a concept of dense solid particle, or particle cluster concept. This drag model has already proven its correctness to determine the coexistence of the dilute and dense flows by many researchers, for example, Chalermsinsuwan et al. [16]. They found that in the dense phase, the EMMS drag model gave realistic results of the obtained system pressure drop, solid particle flux and particle density than the conventional drag between sand and FCC particles. Zhou and Wang [20] used the EMMS drag model to simulate a binary mixture as it could predict the dynamical behavior of segregation and mixing in a fluidized bed (CFB) reactor system.

3.2 Turbulent Dispersion Coefficient

The EMMS drag model together with the KTGF model were used to estimate turbulent dispersion coefficients of different coal solid particle sizes mixed with sand solid particles. In this study, the quasi-steady state results were found after 50 s. However, the results with time-averaged range between 60-80 s were selected to represent this system. As stated above, there are two kinds of dispersion coefficient with solid particle mixing in fluidization: the turbulent and the laminar ones. The turbulent dispersion coefficient (D_i) can be acquired as a function of the Lagrangian integral time scale (T_L) of the solid particle motion and the normal Reynolds stresses as described below [3, 16, 17,21]:

$$D_i = \overline{v_i^{'} v_i^{'}} T_L \qquad (1)$$

$$T_L = \int_0^{\infty} \frac{\overline{v_i^{'}(t) v_i^{'}(t+t^{'})}}{\overline{v_i^{'} v_i^{'}}} dt^{'} \qquad (2)$$

where $\overline{v_i^{'} v_i^{'}}$ is the normal Reynolds stresses or the mean square of solid particle fluctuating velocity which refers as a characteristic of turbulence motion. The normal Reynolds stresses are applied to represent the turbulence of the dispersion coefficient. A subscript "*i*" refers to the radial (x-) and the axial (y-) system directions. Normally, the turbulent dispersion coefficient in radial direction is lower than the one in the axial direction or flow direction for CFB [16, 17, 21]. The high radial turbulent dispersion coefficient and low axial turbulent dispersion coefficient are required for good mixing behavior inside the reactor system.

Figure 3 displays a comparison of turbulent dispersion coefficients with various coal solid particle sizes. In the radial direction, all of coal solid particle sizes had similar values of radial turbulent dispersion coefficients at the height between 0.70-1.10 m, which implies that the mixing in the dense region among coal solid particle sizes was similar. At the height of 2.00 m or the dilute region, the radial turbulent dispersion coefficients increased with the decrease of coal solid particle size. This is because the small solid particles can spread easily in the lateral direction due to their low weight as shown in Figure 4, which implies high solid fluctuation or mixing [22]. In the axial direction, the axial turbulent dispersion coefficients with different coal solid particle sizes were also similar at the height between 0.70-0.90 m. At the height above 1.10 m or bed front, the axial turbulent dispersion coefficients increased with the increase of coal solid particle size. This is because the large solid particles mainly moving up at the reactor center and moving down at the reactor wall as shown in Figure 4. In the radial direction, less solid particle spreading was observed.

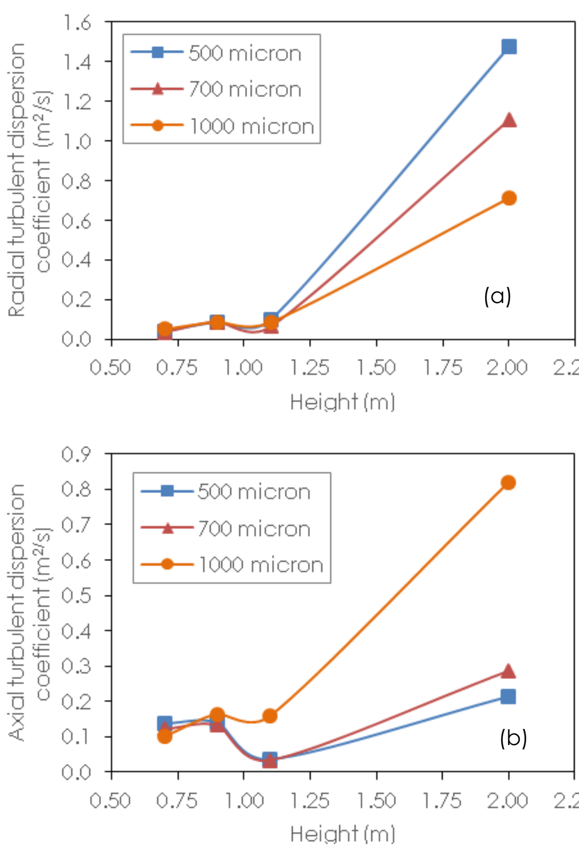

Figure 3 Turbulent dispersion coefficient with different coal solid particle sizes (a) radial direction and (b) axial direction

For the system hydrodynamics, the solid particles settled mainly at the reactor bottom, while some of them dispersed above the bed front. The sand solid particles were dispersed more than the coal solid particles due to their density and size. From the figure, it can also be concluded that the axial turbulent dispersion coefficients were comparable to the radial ones in the dense region. This is because the axial and radial mixing behavior is quite similar in the dense zone of fluidized bed reactor system. In the dilute region, the radial turbulent dispersion coefficients were higher than the axial ones due to the low available force and empty moving space above the bed front.

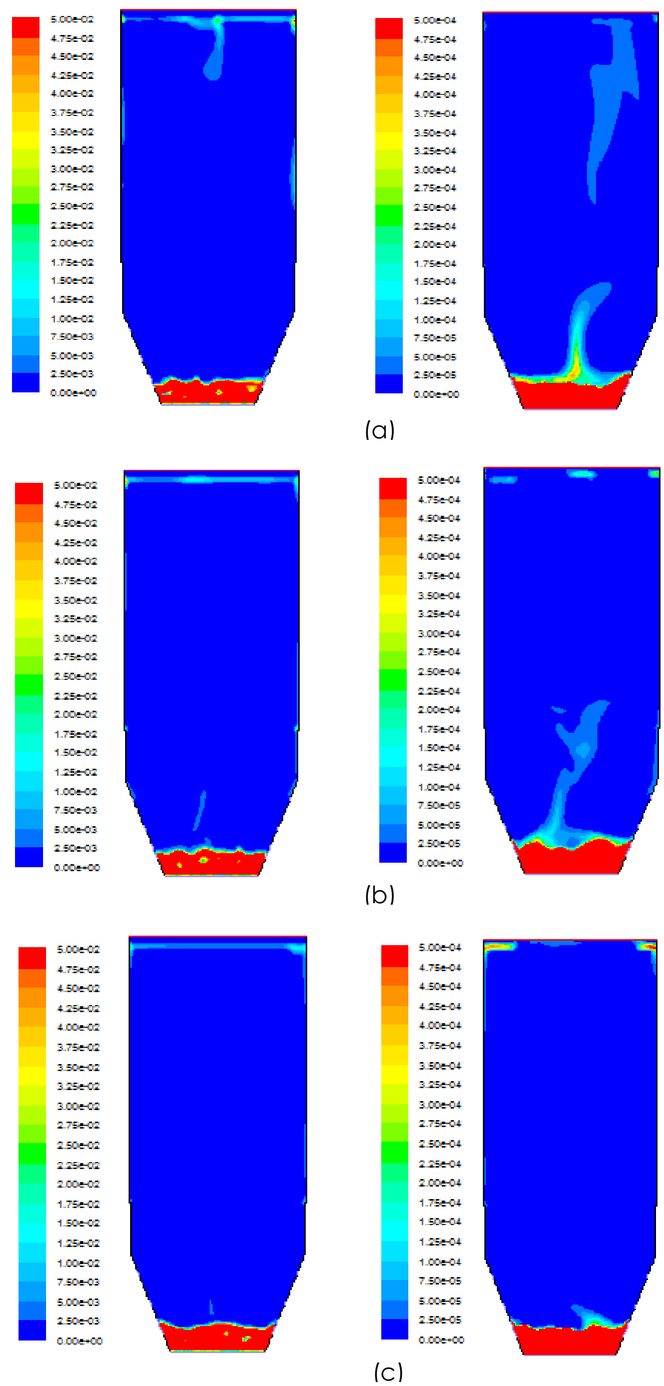

Figure 4 Contours of sand (left) and coal (right) solid volume fractions at 75 s (a) sand 180 µm : coal 500 µm, (b) sand 180 µm : coal 700 µm and (c) sand 180 µm : coal 1000 µm

4.0 CONCLUSION

The CFD model combined with the EMMS model and the KTGF was be able to simulate the major characteristics of binary mixture flow because the EMMS model considered the effect of dense solid particle, or particle cluster. For the system hydrodynamics, the solid particles settled mainly at the reactor bottom, while some of them dispersed above the bed front. The sand solid particles were dispersed higher than the coal solid particles due to their density and size. The obtained model was then used to calculate the turbulent dispersion coefficients. All of the obtained turbulent dispersion coefficients for coal solid particles were discussed in radial and axial directions. The effect of a binary mixture between coal and sand on axial and radial turbulent dispersion coefficients was exhibited in opposite directions. The highest turbulent dispersion coefficient in radial direction was found in the mixture with 500 micron coal size while the highest turbulent dispersion coefficient in axial direction was found in the mixture with 1000 micron coal size. The low axial and high radial turbulent dispersion coefficients were preferred for good mixing behavior inside this fluidized bed reactor system.

Acknowledgements

The Ratchadaphiseksomphot Endowment Fund 2015 of Chulalongkorn University (CU-58-059-CC), the Thailand Research Fund (TRG5780205), the Chulalongkorn University Grant to Commemorate the 72nd Anniversary of the Birth of His Majesty King Bhumibala Aduladeja and the D.A. Research Center Co. Ltd are gratefully acknowledged.

References

[1] Chalermsinsuwan, B., Gidaspow, D. and Piumsomboon, P. 2011. Two- And Three-Dimensional CFD Modeling Of Geldart A Particles In A Thin Bubbling Fluidized Bed: Comparison Of Turbulence And Dispersion Coefficients. *Chemical Engineering Journal.* 171: 301-313.

[2] Chalermsinsuwan, B., Kuchonthara, P. and Piumsomboon, P. 2009. Effect Of Circulating Fluidized Bed Reactor Riser Geometries On Chemical Reaction Rates By Using CFD Simulations. *Chemical Engineering and Processing*. 48(1): 165-177.

[3] Samruamphianskun, T., Piumsomboon, P. and Chalermsinsuwan, B. 2012. Computation Of System Turbulences And Dispersion Coefficients In Circulating Fluidized Bed Downer Using CFD Simulation. *Chemical Engineering Research And Design*. 90(12): 2164-2178.

[4] Chalermsinsuwan, B., Boonprasop, S., Nimmanterdwong, P. and Piumsomboon, P. 2014. Revised Fluidization Regime Characterization In High Solid Particle Concentration Circulating Fluidized Bed Reactor. *International Journal of Multiphase Flow*. 66: 26-37.

[5] Zhansheng, S., Wei, W. and Jinghai, L. 2011. A Bubble-Based EMMS Model For Gas–Solid Bubbling Fluidization. *Chemical Engineering Science*. 60(22): 5541-5555.

[6] Sahoo, A. and Roy, G. K. 2008. Mixing Characteristics Of Irregular Binaries In A Promoted Gas–Solid Fluidized Bed: A Mathematical Model. *The Canadian Journal of Chemical Engineering*. 86(1): 53-61.

[7] Norouzi, H. R., Mostoufi, N. and Gharebagh, R. S. 2012. *Effect of fines on segregation of binary mixtures in gas–solid fluidized beds. Powder Technology*. 225: 7-20.

[8] Lungu, M., Zhou, Y., Wang, J. and Yang, Y. 2015. A CFD Study Of A Bi-Disperse Gas–Solid Fluidized Bed: Effect Of The EMMS Sub Grid Drag Correction. *Powder Technology*. 280: 154-172.

[9] Zhong, H., Gao, J., Xu, C. and Lan, X. 2012. CFD Modeling The Hydrodynamics Of Binary Particle Mixtures In Bubbling Fluidized Beds: Effect Of Wall Boundary Condition. *Powder Technology*. 230: 232-240.

[10] Lee, B. E., Tu, J. Y. and Fletcher, C. A. J. 2002. On Numerical Modeling Of Particle–Wall Impaction In Relation To Erosion Prediction: Eulerian Versus Lagrangian Method. *Wear*. 252(3-4): 179-188.

[11] Upadhyay, M. and Park, J. H. 2015. CFD Simulation Via Conventional Two-Fluid Model Of A Circulating Fluidized Bed Riser: Influence Of Models And Model Parameters On Hydrodynamic Behavior. *Powder Technology*. 272: 260-268.

[12] Sun, J., Wang, J. and Yang, Y. 2012. CFD Investigation Of Particle Fluctuation Characteristics Of Bidisperse Mixture In A Gas–Solid Fluidized Bed. *Chemical Engineering Science*. 82: 285-298.

[13] Azizi, S., Hosseini, S. H., Ahmadi, G. and Moraveji, M. 2010. Numerical Simulation Of Particle Segregation In Bubbling Gas-Fluidized Beds. *Chemical Engineering and Technology*. 33(3): 421-432.

[14] Chao, Z., Wang, Y., Jakobsen, J. P., Fernandino, M. and Jakobsen. H. A. 2010. A Binary Kinetic Theory Of Granular Flow Model For Fluidized Beds. *7th International Conference on Multiphase Flow. ICMF 2010: Tampa. FL USA*.

[15] Oke, O., Lettieri, P., Salatino, P., Solimene, R. and Mazzei, L. 2014. Numerical Simulations Of Lateral Solid Mixing In Gas-Fluidized Beds. *Chemical Engineering Science*. 120: 117-129.

[16] Chalermsinsuwan, B., Piumsomboon, P. and Gidaspow, D. 2009. Kinetic Theory Based Computation Of PSRI Riser: Part I-Estimate Of Mass Transfer Coefficient. *Chemical Engineering Science*. 64(6): 1195-1211.

[17] Jiradilok, V., Gidaspow, D. and Breault, R. W. 2007. Computation Of Gas And Solid Dispersion Coefficients In Turbulent Risers And Bubbling Beds. *Chemical Engineering Science.* 62(13): 3397-3409.

[18] FLUENT 6.3 User's Guide. [online]. From: https://www.sharcnet.ca/Software/Fluent6/html/ug/main_pre.htm. [Accessed on 20 September 2015].

[19] Hong, K., Wang, W., Zhou, Q., Wang, J. and Li, J. 2012. An EMMS-based Multi-fluid Model (EFM) For Heterogeneous Gas–Solid Riser Flows: Part I. Formulation Of Structure-Dependent Conservation Equations. *Chemical Engineering Science.* 75: 376-389.

[20] Zhou, Q. and Wang, J. 2015. CFD Study Of Mixing And Segregation In CFB Risers: Extension Of EMMS Drag Model To Binary Gas–Solid Flow. *Chemical Engineering Science*. 122: 637-651.

[21] Jiradilok, V., Gidaspow, D., Damronglerd, S., Koves, W. J. and Mostofi. R. 2006. Kinetic Theory Based CFD Simulation Of Turbulent Fluidization Of FCC Particles In A Riser. *Chemical Engineering Science*. 61(17): 5544-5559.

[22] Jiradilok, V., Gidaspow, D., Breault, R. W., Shadle, L. J., Guenther, C. and Shi, S. 2008. Computation Of Turbulence And Dispersion Of Cork In The NETL Riser. *Chemical Engineering Science*. 63(8): 2135-2148.

[23] Kashyap, M., Chalermsinsuwan, B. and Gidaspow, D. 2011. Measuring Turbulence In A Circulating Fluidized Bed Using PIV Techniques. *Particuology*. 9(6): 572-588.