CPFD MODEL FOR PREDICTION OF FLOW BEHAVIOR IN AN AGGLOMERATED FLUIDIZED BED GASIFIER

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ABSTRACT

Renewable energy sources have significant potential for limiting climate change and reducing greenhouse gas emissions due to the increased global energy demand. Fluidized bed gasification of biomass is a substantial contribution to meeting the global energy demand in a sustainable way. However, ash-related problems are the biggest challenge in fluidized bed gasification of biomass. Bed agglomeration is a result of interaction between the bed material and alkali metals present in the biomass ash. The agglomerates interfere with the fluidization process and might result in total de-fluidization of the bed. The study focuses on ash challenges related to the fluidization behavior in gasification of biomass. A model is developed and verified against results from previous performed experiments in a cold flow model of a bubbling fluidized bed. The commercial computational particle fluid dynamics (CPFD) software Barracuda Virtual Reactor is used for the computational study. The simulations show that the CPFD model can predict the fluidization process of an agglomerated fluidized bed gasifier.
Keywords: agglomeration, Barracuda VR, bubbling fluidized bed, CPFD simulation, flow behavior.

1 INTRODUCTION

Global warming is perhaps the most pressing environmental challenge in our time, and there is an urgent need to promote the use of renewable energy sources in order to ensure a sustainable future. The massive expansion in the use of fossil fuels and the rising fears over the effects of the increased CO_2 emissions have forced the countries to search for climate-friendly alternatives to fossil fuels [1]. Biomass-based energy is presently the largest contributor of renewable energy, and according to World Bioenergy Association, biomass annually accounts for 10.3% of the global energy supply [2]. The leading energy conversion technology for utilization of biomass fuels is fluidized bed gasification, which converts biomass into a gaseous mixture in the presence of heat and a gasifying medium [3].

Fluidized beds are noted for their high heat transfer, uniform heating and high productivity. Despite being a promising technology for sustainable heat and power generation, biomass gasification has operational problems that can restrict its commercialization [1]. Interactions between the bed material and the molten ash components cause formation of agglomerates, resulting in the ash components adhering to each other to form larger entities [4]. Bed agglomeration is the main obstacle for successful applications of biomass gasification [5]. Presence of agglomerates in the bed alters the flow behavior in the gasifier, causing changes in the fluidization properties and consequently loss of control of important operating parameters such as pressure drop, minimum fluidization velocity and bubble behavior. In the most severe cases, bed agglomeration can lead to total de-fluidization of the bed [6].

Due to the operational problems caused by bed agglomeration, extensive studies have been performed to gain more insight into the ash-related issues in biomass gasification. These research activities have provided important knowledge about ash from biomass, and the relation between ash composition and the ash melting temperatures. However, only few data are available on the ash melting and agglomeration, and its relation to the fluidization behavior

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in a biomass gasification reactor. Understanding the phenomenon of agglomeration is crucial to optimizing the design and the operation conditions of a bubbling fluidized bed gasification reactor. The objective of this work is to develop a computational particle fluid dynamics (CPFD) model that describes how the agglomerates affect the fluidization process in a bubbling fluidized bed reactor.

The model is based on theoretical and experimental studies. The commercial CPFD software package, Barracuda Virtual Reactor (VR) 17.1.0 is used for the computational study. The CPFD model is validated against previous performed experimental results carried out in a cold flow model of a bubbling fluidized bed [7].

2 BED AGGLOMERATION

Ash melting and subsequently formation of agglomerates is one of the major challenges in fluidized bed gasification of biomass [4]. Bed agglomeration occurs due to chemical reactions and physical collisions between the bed material and biomass ash with high content of alkali species. The phenomenon is illustrated in Fig. 1, which is based on [8]. Bed agglomeration happens as the inorganic alkali ash components interact with the bed material to form a sticky layer on the surface of the bed materials. As the ash particles and the bed material continue to collide, the ash coating grows thicker. Eventually, the bed particles grow towards larger agglomerates that will interfere with the fluidization process [4].

The main problem with ash melting and agglomeration in fluidized beds is the issue of de-fluidization. The agglomerated ash-particles (Fig. 2) differ considerably from the bed particles in shapes, sizes and densities, and are therefore difficult to fluidize adequately. At the time of de-fluidization, a sudden decrease in the pressure drop over the bed is observed as the sticky and cohesive agglomerated ash particles form small volumes in the bed. These volumes are not fully fluidized, leading to improper circulation of the biomass and thereby non-uniform temperature distribution and decreased heat transfer in the bed. Inside the de-fluidized volumes, the temperatures will be increased, which in turn increases the stickiness of the particle surfaces resulting in enhanced agglomeration [7].

The poor mixing and the decreased heat transfer that occur due to bed agglomeration change the bubble behavior in the bed. While normal fluidization conditions give well-distributed bubble frequency through all sections along the bed, the fluidization in the agglomerated bed is characterized by instabilities with frequent bubbling and channeling of fluid. Eventually, the bed takes a sluggish appearance. The unwanted collapse of the fluidized bed is rarely recognized until sudden de-fluidization occurs, and might lead to shutdown of the whole installation [4]. Figure 3 illustrates the bubble behavior in a normal fluidized bed compared to the bubble behavior in an agglomerated fluidized bed.

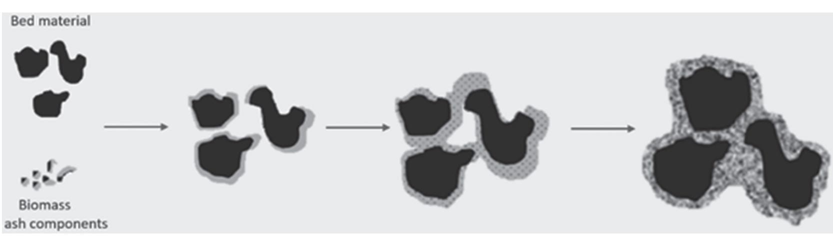

Figure 1: Formation of agglomerates.

Figure 2: Agglomeration of silica sand particles.

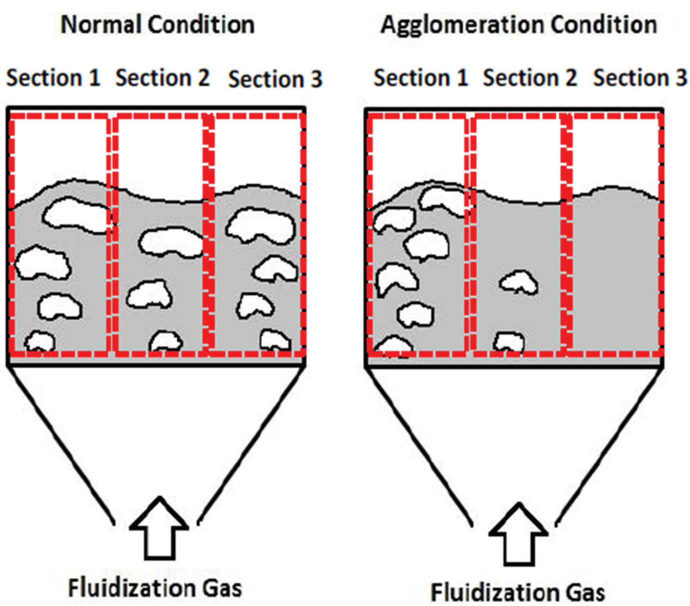

Figure 3: Bubble frequency in a fluidized bed [9].

3 MODEL DEVELOPMENT

3.1 Model description

The CPFD software package Barracuda VR 17.1.0 was used to simulate the flow characteristics in an agglomerated bubbling fluidized bed. Barracuda VR uses the Multiphase Particle In-Cell (MP-PIC) approach that is based on the Eulerian–Lagrangian approach, where the transport equations are solved for the continuous fluid phase and each of the discrete particles are tracked through the calculated fluid field. The fluid–particle interaction is considered as source terms in the transfer of mass, momentum and energy between the two systems. CPFD simulations are hybrid numerical methods where the Eulerian approach is used for solving the fluid phase, and the Lagrangian computational particle approaches for the modeling of the particle phase [10]. Chladek *et al.* [11] and Jayarathna *et al.* [12] describe the transport equations in detail.

The Barracuda software package includes several drag models. In order to find the most suitable model for the simulations of flow characteristics in an agglomerated fluidized bed gasifier, different drag models were tested. The best fit between the numerical model (simulation) and the experimental results was achieved with the Wen–Yu drag model. Wen–Yu drag model is based on a variety of experiments performed by Richardson and Zaki [13]. The correlation developed from the experimental data achieved by Richardson and Zaki [13] is valid when the internal forces are negligible, meaning that the viscous drag forces dominate the flow behaviour.

In general, the drag force caused by the fluid on the particles is calculated from:

$$F_p = m_p \cdot D \cdot \left(u_f - u_p\right) \tag{1}$$

where m_p is the particle mass, D the drag function, u_f the superficial velocity of the fluid and u_p the superficial velocity of the particles. The Wen–Yu drag function is dependent on the fluid and the particle properties and is expressed by the drag coefficient (C_d):

$$D = \frac{3}{8} \cdot C_d \cdot \frac{\rho_f \cdot \left(u_f - u_p\right)}{\rho_p \cdot r_p} \tag{2}$$

where ρ_f and ρ_p is the density of the fluid and the particle, respectively, and r_p the particle radius. C_d is a function of Reynolds number *(Re)* and the fluid volume fraction *(θ_f)*, and is determined according to a set of conditions shown in eqn (3).

$$C_d = \begin{cases} \dfrac{24}{Re} \cdot \theta_f^{n_0} \; 0.5 < Re \\ . \\ \dfrac{24}{Re} \cdot \theta_f^{n_0} \cdot \left(c_0 + c_1 \cdot Re^{n_1}\right) 0.5 \le Re \le 1000 \\ . \\ c_2 \cdot \theta_f^{n_0} \; Re > 1000 \end{cases} . \tag{3}$$

Reynolds number is determined by

$$Re = \frac{2 \cdot \rho_f \cdot r_p \cdot \left(u_f - u_p\right)}{\mu_f} \tag{4}$$

where μ_f is the viscosity of the fluid. More detailed information of the Wen–Yu drag model are presented by Wen and Yu [14].

3.2 Computational setup

The cold flow model of the fluidized bed used in the experimental study is shown in Fig. 4.

A three-dimensional Cartesian coordinate system was used to describe the cylindrical column with a height of 140 cm and a diameter of 8.4 cm. In the present study, the static bed height was 21 cm. The computational grid is shown in Fig. 5. The mesh size was 0.01 m x 0.01 m x 0.01 m and the number of control volumes was 13,284. Isothermal temperature at 300 K was used, and the fluidizing gas was air at atmospheric pressure that was flowing through the gas distributor from the bottom of the column. The total pressure was monitored at positions 3.5 cm (P1) and 13.5 cm (P2) above the distributor. The simulation was run for 50 s with a time step of 0.001 s. The simulation parameters are summarized in Table 1. The Wen–Yu drag model was selected, and the coefficient values c_0, c_1, c_2, n_0 and n_1 were equal to 1.0, 0.15, 0.44, –2.65 and 0.687, respectively.

Quartz sand with a Solid density of 2,650 kg/m^3 was used as bed material. The particle size of the sand ranged from 150 μm to 340 μm with a mean diameter of 175 μm. The particle size distribution was determined by sieving analysis. The maximum close pack volume fraction was set to 0.54, which was calculated based on the ratio of the bulk density and the particle density. The maximum momentum from the redirection of particles collision was

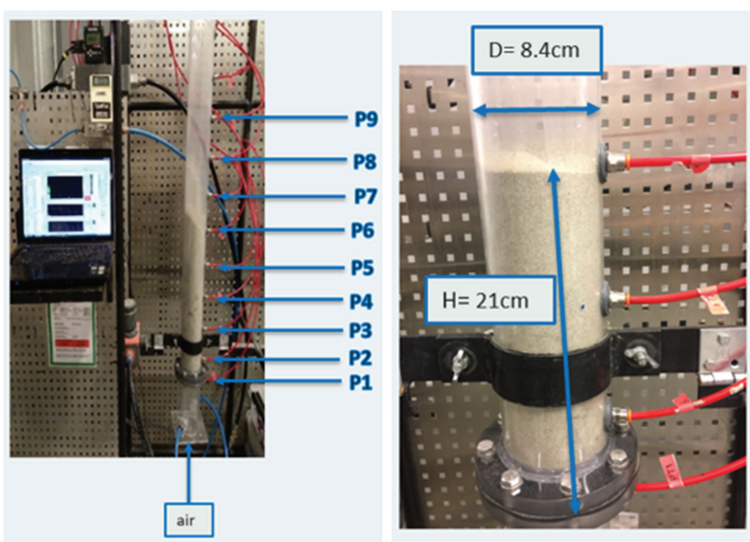

Figure 4: Cold flow model of bubbling fluidized bed.

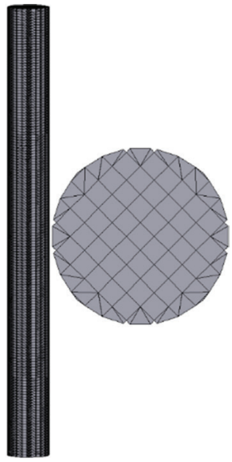

Figure 5: Computational grid.

Table 1: Simulation parameters.

Parameter	Value
Number of grid cells	13,284
Static bed height	21 cm
Fluidizing agent	Air
Type of flow	Isothermal @ 300 k
Superficial gas velocity	0.02: 0.005: 0.15 m/s
Simulation time for each flowrate	50 s
Drag model	Wen–Yu
Drag coefficients (c_0, c_1, c_2, n_0, n_1)	Default values

assumed to be 40%, the normal-to-wall and tangential-to-wall momentum retention were 0.3 and 0.99, respectively. The particle properties are listed in Table 2.

The flow behavior in an agglomerated fluidized bed was studied by comparing three different CPFD simulations, where agglomerates were present in the bed. The different cases were defined with 5%, 10% and 15% of agglomerates. In order to simulate agglomerates, a coarser

Table 2: Particle properties.

	Property			
Particle	**Mean diameter (µm)**	**Density (kg/m^3)**	**Sphericity**	**Close pack volume fraction**
Bed material	175	2,650	0.86	0.54
Agglomerates	N/A	1,506	0.6	N/A

grid was used and the number of grid cells was reduced from 13,284 to 5,782. The size of the agglomerates was limited by the chosen grid, which allowed a maximum particle size of 1.0 cm. The agglomerates ranged from 0.5 cm to 1.0 cm in diameter, with density equal to 1,506 kg/m^3. The density of the agglomerates was determined based on mass and volume [7].

4 RESULTS AND DISCUSSION

The Wen–Yu drag model was used in the CPFD simulations. The model was validated by customizing it to the previous performed experimental results for sand particles with a mean diameter of 175 µm [7]. The pressure drop in the bed was plotted as a function of the superficial air velocity. As the superficial velocity is steadily increased, the bed expands slightly. The drag caused by the fluid on the particles increases and at some point, the particles begin to move. At a certain velocity, the particles will be suspended by the upward-flowing fluid [15]. This state is referred to as the minimum fluidization and the corresponding superficial velocity is the minimum fluidization velocity (u_{mf}). Figure 6 compares the simulation with the experimental result. The simulated minimum fluidization velocity was 0.039 m/s, which is slightly higher than the experimental value of 0.035 m/s.

The deviation between the simulation and the experiment can be related to how the characteristics of the particles influence on the fluidization processes, and how the numerical model accounts for the particle size distribution. Barracuda uses the MP-PIC-based Euler–Lagrangian approach, which means that instead of tracking each individual particle in the bed separately, particles with the same properties are grouped into parcels. Each parcel is represented by one computational particle, in which the equation for motion is solved as the discrete particle moves through the flow field [16]. Another explanation for the deviation might be erroneous assumptions for the drag model coefficients, c_0, c_1, n_0 and n_1. The value of c_2 will not influence on the results as it only has significance when $Re > 1{,}000$. Which is not the case for the present work. In order to find the model that shows the best agreement with the experimental results, several simulations with different values for the coefficients were performed. Finally, the default values provided in Barracuda were chosen for all the coefficients. In Fig. 6, it is seen that the simulation has a significant peak in the pressure drop at the onset of fluidization. However, the pressure drop decreases quickly after fluidization and stabilizes at approximately the same value as in the experiment, corresponding to the weight of the particles [11].

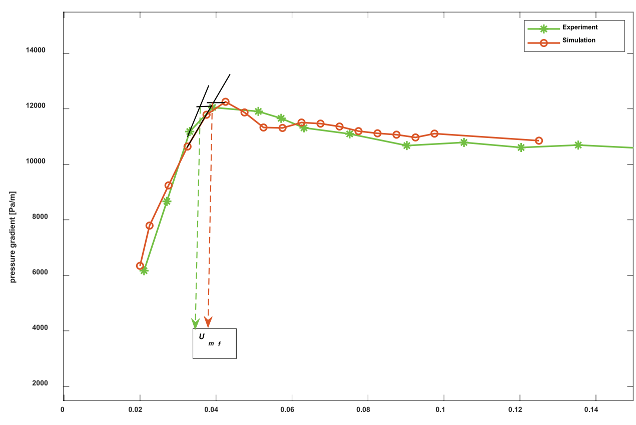

Figure 6: Pressure drop as a function of increasing superficial air velocity.

The result shows that the validated CPFD model describes the fluidization of the sand particles with good agreement, and the model was used to simulate the fluidization conditions in an agglomerated fluidized bed. Figure 7 shows how bed agglomeration changes the fluidization characteristics of the bed. Smooth fluidization is a result of hydrodynamic, gravitational and inter-particle forces. When agglomerates are present in the bed, the inter-particle forces take control over the bed behavior, and the agglomerates will interfere with the fluidization process. As the sticky particles grow into larger entities, the particles lose their original weight and are no longer able to be fluidized by the initial gas velocity. Under fluidized conditions, the pressure drop through the bed is equal to the total hydrostatic pressure of the bed, but due to channeling and agglomerated zones, agglomerated fluidized beds are characterized by lower pressure drop than normal fluidized beds.

The decreased pressure drop in the agglomerated fluidized beds indicates that the beds are not completely fluidized, as the bubbles collapse at the bottom of the bed instead of passing through the entire bed. Figure 8 illustrates the distribution of the particle species in the agglomerated fluidized bed, initially (Fig. 8a) and after fluidization (Fig. 8b). Blue color indicates bed

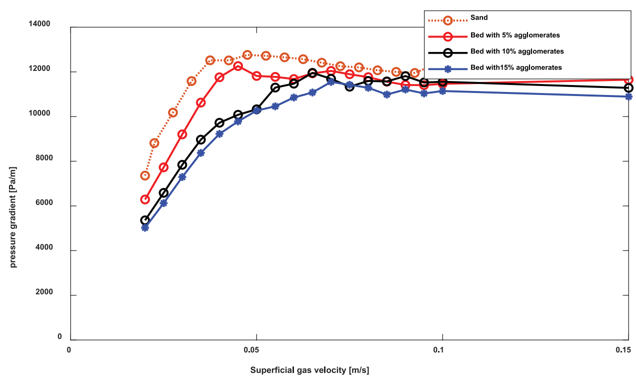

Figure 7: Simulation of fluidization in normal and agglomerated fluidized bed.

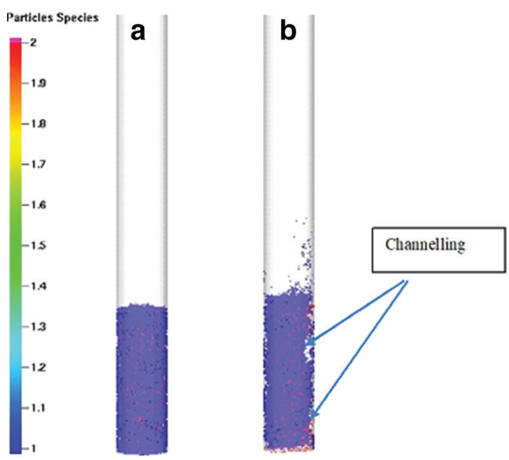

Figure 8: (a) Initial particle species and (b) particle species after fluidization.

particles, while red color indicates agglomerates. The bed material are in motion at the top of the bed, while the agglomerates remain at the bottom and one side of the column resulting in the gas flowing in channels. In biomass gasification, agglomeration causes improper circulation of the biomass and non-uniform temperature distribution in the bed. The non-uniform temperature distribution forms zones with de-fluidized volumes and increased temperatures. Higher temperatures increase the stickiness of the particle surfaces and might result in enhanced formation of agglomerates. Eventually, the bed takes a sluggish appearance.

5 CONCLUSION

The objective of this study was to develop a CPFD model for simulation of the flow behavior in an agglomerated fluidized bed gasifier. The simulations were performed using the commercial CPFD software package Barracuda VR.

The agglomerates consist of a large amount of primary particles clustered together. They have irregular shapes, sizes and structures, and are therefore difficult to fluidize and handle adequately.

The simulations show that bed agglomeration influences the fluidization characteristics of a bubbling fluidized bed. The pressure drop decreases and the minimum fluidization velocity increases when agglomerates are present in the bed. Moreover, the formation of agglomerates cause large instabilities with uneven distribution of bubbles and channeling that lead to loss of fluidization. When channeling occurs in the bed, there is less contact between gas and particles and the heat and mass transfer operation is weakened. Consequently, de-fluidized zones occur, which in turn can lead to unscheduled shutdowns of the whole installation.

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REFERENCES

[1] Sansaniwal, S.K., Rosen, M.A. & Tyagi, S.K., Global challenges in the sustainable development of biomass gasification: an overview. *Renewable and Sustainable Energy Reviews*, **80**, pp. 23–43, 2017. https://doi.org/10.1016/j.rser.2017.05.215

[2] World Bioenergy Association, *WBA Global Bioenergy Statistics*, 2017.

[3] Basu, P., *Biomass Gasificaion, Prolysis and Torrefaction*, 2nd edn., Academic Press Inc.: UK, 2013.

[4] Bartles, M., Lin, W., Nijenhuis, J., Kapteijn, F. & Ommen, R., Agglomeration in fluidized beds at high temperaures: Mechanisms, detection and prevention. *Progress in Energy and Combustion Science*, **34(5)**, pp. 633–666, 2008. https://doi.org/10.1016/j.pecs.2008.04.002

[5] Wang, L., Weller, C.L., Jones, D.D. & Hanna, M.A., Contemporary issues in thermal gasification of biomass and its application to electricity and fuel production. *Biomass and Bioenergy*, **32(7)**, pp. 573–581, 2008. https://doi.org/10.1016/j.biombioe.2007.12.007

[6] Khadilkar, A.B., Rozelle, P.L. & Pisupati, S.V., Investigation of fluidized bed agglomerate growth process using simulations and SEM-EDX characterization of laboratory-generated agglomerates. *Chemical Engineering Science*, **184**, pp. 172–185, 2018. https://doi.org/10.1016/j.ces.2018.03.035

[7] Furuvik, N.C.I.S., Jaiswal, R. & Moldestad, B.M.E., Flow behaviour in an agglomerated fluidized bed gasifier. *International Journal of Energy and Environment*, **10(2)**, pp. 55–64, 2019.

[8] Moradian, F.A., *Behaviour in Fluidized-Bed Combustion and Gasification of Biomass and Waste Fuels*, Thesis for the Degree of Doctor of Philosophy, University of Borås, Sweden, 2016.

[9] Montes, A., *Factors Affecting Bed Agglomeration in Bubbling Fluidized Bed Biomass Boilers*, Electronic Thesis and Dissertation Repository, September 2014.

[10] Thapa, R.K. & Halvorsen, B.M., Stepwise analysis of reactions and reacting flow in a dual fluidized bed gasification reactor. *WIT Transactions on Engineering Sciences*, **82**, pp. 37–48, 2014.

[11] Chladek, J., Jayarathna, C.K., Moldestad, B.M.E. & Tokheim, L.A., Fluidized bed classification of particles of different size and density. *Chemical Engineering Science*, **177**, pp. 155–162, 2018. https://doi.org/10.1016/j.ces.2017.11.042

[12] Jayarathna, C.K., Moldestad, B.E. & Tokheim, L.A., Validation of results from Barracuda® CFD modelling to predict minimum fluidization velocity and pressure drop of Geldart A particles. *Proceedings of the 58th SIMS Conference*, 2017.

[13] Richardson, J.F. & Zaki, W.N., Sedimentation and fluidisation: Part I. *Chemical Engineering Research and Design*, **75**, pp. S82–S100, 1997. https://doi.org/10.1016/s0263-8762(97)80006-8

[14] Wen, C. & Yu, Y., Mechanics of fluidization. *Chemical Engineering Progress Symposium Series*, **62**, pp. 100–111, 1966.

[15] Kunii, D. & Levespiel O., *Fludization Engineering*, 2nd edn., Butterworth-Heinemann: USA, 1994.

[16] Crowe, C.T., Schwarzkopf, J.D., Sommerfield, M. & Tsuji, Y., *Multiphase Flows with Droplets and Particles*, 2nd edn., Taylor & Francis Group: USA, 2012.