Powder Technology 270 (2015) 584–591

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

Modeling aggregation kinetics of fluidized bed spray agglomeration for porous particles

Mubashir Hussain [a,*], Jitendra Kumar [a,b], Evangelos Tsotsas [a]

[a] Chair of Thermal Process Engineering, Otto-von-Guericke University, Universitätsplatz 2, D-39106 Magdeburg, Germany
[b] Department of Mathematics, Indian Institute of Technology Kharagpur, India

ARTICLE INFO

Article history:
Received 3 September 2013
Received in revised form 9 July 2014
Accepted 10 July 2014
Available online 17 July 2014

Keywords:
Population balances
Kinetics
Aggregation
Monte-Carlo
Fluidized bed

ABSTRACT

The present work develops a comprehensive one-dimensional pure agglomeration population balance model for simulating spray fluidized bed agglomeration of porous particles. The effect of micro-processes on aggregation kinetics is analyzed using a sophisticated constant number Monte-Carlo (CNMC) approach. The CNMC is used as a virtual spray fluidized bed granulator and takes into account several micro-processes such as wetting, convective drying, imbibition, agglomeration etc. so that it is a model for the real granulator. The main components influencing the agglomeration kinetics, namely the total number of particles, the number of wet particles, the collision frequency per particle and the average wet surface coverage fraction per wet particle are modeled and incorporated in the conventional one-dimensional population balance model. Finally, the proposed population balance model is validated against the results of CNMC.

1. Introduction

Micro-interactions play a fundamental role in molding the macroscopic behavior of processes involving a dispersed system, such as spray fluidized bed granulation (SFBG). In SFBG, particles get aggregated and dried simultaneously by passing through many complex microprocesses which change the physical properties of the particles such as flowability, density or porosity, shape etc. The present work addresses the study of such micro-interactions through a micro-scale modeling approach and translating their effects onto a macro-scale level by modeling the influencing parameters.

On a macroscopic scale, particulate processes such as spray fluidized bed granulation (SFBG) are modeled by means of population balance equations (PBE), see e.g. [16]. However, a primary challenge for using population balance equation is to model the kinetics of the process. Over the years, many aggregation kinetic models have been proposed in the literature, see e.g. [2,10,14,15,23]; however, a model correlating the process conditions and material properties in rather general conditions is not yet available. The research to date has tended to focus on fitting the parameters rather than modeling.

An alternative and well suited approach for simulating particulate process is the Monte-Carlo (MC) simulation. Recent developments in the computational power have led to an increased interest in this approach. The main advantage of the MC approach lies in its generality to include multiple micro-properties of the process. This approach provides full understanding of the whole agglomeration process by accessing variables and properties (e.g. wetted surface fraction) that are even difficult to measure experimentally. However, the stochastic nature and high computational cost restrict the application of MC on a large scale.

The objective of this work is to model the aggregation kinetics of porous particles by analyzing the process using MC simulations. In the recent work of Hussain et al. [9], an effort has been made by modeling the significant process parameters in the form of an aggregation kernel by observing the MC simulations. However, previous work uses a very simplified version of constant number Monte-Carlo (CNMC) and the developed population balance model relies either on taking hypothetical values of several influencing parameters or fitting them to the MC simulations. The present work aims to develop an independent population balance model to forecast the dynamics of spray fluidized bed agglomeration process in a more realistic window of operation.

To achieve the objective we have used a comprehensive constant number Monte-Carlo (CNMC) algorithm. Moreover, the population balance models for the total number of wet particles and the total number of droplets have been revised to predict the results in general conditions. Similarly, the models for predicting the average wet surface coverage fraction and collision frequency per particle have also been generalized. The only fitting parameter in the presented population balance model (PBM) is the success fraction concerning the dissipation of kinetic energy ψ, which is taken as a constant. This work presents an independent population balance model for pure agglomeration of porous particles which correlates the process conditions and material properties to the process. Finally, it is shown that the numerical results of the

* Corresponding author. Tel.: +49 391 6752455.
E-mail address: mubashir.hussain@st.ovgu.de (M. Hussain).

http://dx.doi.org/10.1016/j.powtec.2014.07.015
0032-5910/

population balance model match very well with the results of MC simulations.

It must be pointed out that over the years MC methods have been used as a solver of PBE, see e.g. [12,13,18,19]. In the present work, the MC is used as a scaled down virtual spray fluidized bed granulator rather than as a solver of PBE. A similar approach has recently been presented by Terrazas-Velarde et al. [20–22] and Dernedde et al. [4,5]. In the present MC, the micro-processes such as collision of particles, deposition of droplets, drying of droplets, and Stokes criterion for the dissipation of kinetic energy have been modeled as in [22]. Although the CNMC used takes into account all the necessary micro-processes of SFBG, it has been simplified by neglecting breakage or fragmentation of agglomerates. Consequently, the modeling also corresponds to the pure agglomeration process.

2. Monte-Carlo algorithm

The process of spray fluidized bed agglomeration for porous particles is simulated with the help of a CNMC algorithm. Micro-processes such as collision of particles, addition of binder droplets, convective drying of droplets, penetration of droplets into the pores (called imbibition) etc. are incorporated in the algorithm. The structure of the algorithm is based on the work of Dernedde et al. [4,5] and Hussain et al. [9] whereas the models for micro-processes have been taken from [22]. The flow chart of the CNMC approach is given in Fig. 1.

In order to simulate particle collisions we have discretized the surface area of any primary particle into 6 sectors. The area of each sector is approximately set equal to the area blocked by a single primary particle on a successful collision. Moreover, the area of each sector is further subdivided into 5 small areas called *positions*. The area of each position is approximately set equal to the surface footprint of a droplet. This means, in a droplet deposition event one position is set as completely 'occupied or wet'.

In each time step of the CNMC algorithm, either a binary collision between particles or a droplet deposition on a particle is selected according to the probability of occurrence of these events. In order to compute the time step, at first the total number of events (sum of total number of collisions among particles and total droplet deposition) taking place in a unit time is calculated. Then, the time required to complete one event is computed by taking the reciprocal of the total number of events per unit time, which serves as the time step, see [9]. During each time step of MC, we carry out the selected event and update the time. If a droplet addition event takes place, then a droplet is added onto a particle and the algorithm starts counting its deposition time. If a collision event takes place, then a collision between a randomly chosen pair of particles is simulated. If particles strike at wet position/s in a wet collision and the kinetic energy of the colliding particles is dissipated by the liquid layer, then colliding particles form a new agglomerate. It is important for our subsequent discussion to mention and to clarify that by wet collision we mean a collision in which at least one wet particle (either partially or completely wet) is involved. Hence, in the present definition of wet collision, one or both wet particles may collide at dry positions. For a better understanding, we now briefly describe some important processes that appear in the CNMC algorithm. For the detailed structure and working of the algorithm see [9,22].

2.1. Collision frequency

The frequency of collision per particle f_c, which is required to compute the total collision rate of particles in each time step, is calculated using the model presented by Buffière & Moletta [3],

$$f_c = F_c\left[1-\left(\frac{\phi_{\exp}}{\phi_{\mathrm{fix}}}\right)\right]\left(\frac{\phi_{\exp}}{\phi_{\mathrm{fix}}}\right)^2 u_g. \tag{1}$$

In Eq. (1), u_g is the superficial fluidization velocity and ϕ_{fix} and ϕ_{exp} are the solid volume fractions of the expanded and fixed beds, respectively. The pre-factor F_c is taken to be 45, as given in [22].

2.2. Droplet deposition

Once a decision to deposit a droplet is made, we select a particle according to its surface area from the distribution of particles. In a fluidized bed, we expect that a particle with a larger surface area is more probable to catch the droplet, which makes size dependent wetting more logical. After selecting a particle, a dry position is randomly selected from the unblocked positions of the particle and the particle is marked as 'wet'.

2.3. Binary collision

If a collision event is selected, then two particles are randomly chosen from the distribution of particles and a collision between them is made. For executing the collision, we randomly select a position on

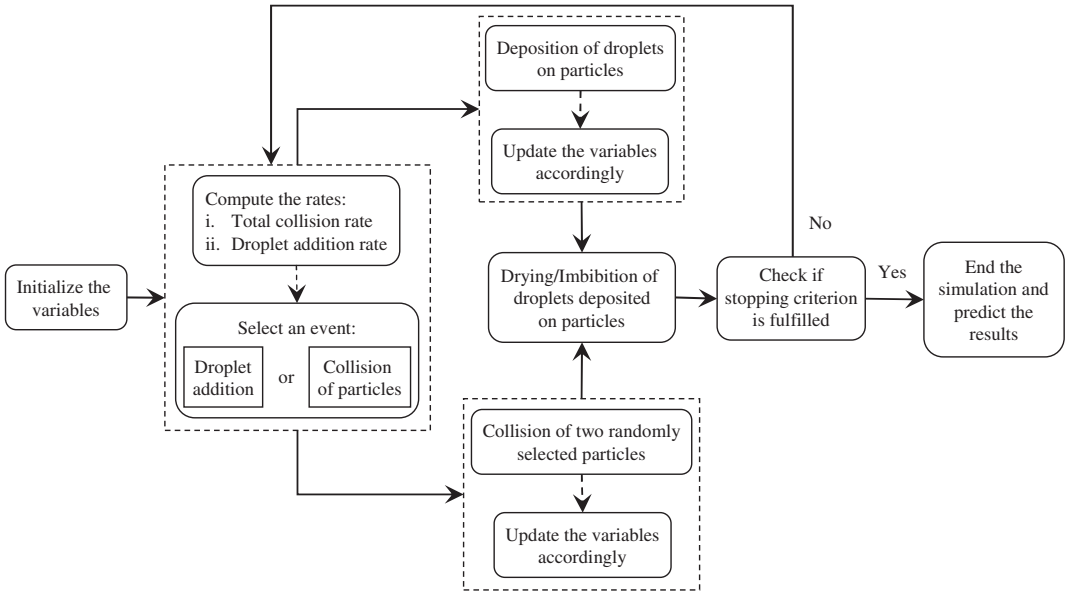

Fig. 1. CNMC flow chart.