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Euler-Lagrange model of particles circulation in a spout-fluid bed apparatus for dry coating

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ABSTRACT

The main objective of the study was to develop a model describing the flow of particles (cores) in an apparatus operating within the range of the fast circulating dilute spout-fluid bed. The greatest emphasis was placed on the selection of appropriate description of the particle-wall interactions (impact model or fixed values of restitution coefficients). Its influence on the dispersed phase velocity in the draft tube and annulus of the apparatus was investigated. Results obtained from computer simulations were compared with our own experimental data. The use of equations calculating normal and tangential restitution coefficient resulted in a noticeable improvement in the accuracy of results only in the area of the draft tube in relation to the fixed restitution coefficient approach. It was found that the flow hydrodynamics and apparatus geometry favour computing of low restitution coefficients in the annular zone.

1. Introduction

Spouted bed apparatuses were created as a modification of classical fluidized bed devices [1]. They have made it possible to carry out various processes on materials with diameters up to a few millimetres (Geldart class D) [2]. This is related to the unique characteristics of the bed flow in such devices. Gas fed only through a hole in the apparatus's axis carries particles in the so-called spout zone. Then they form a fountain above the surface of the bed and fall freely into the annular zone, where they are again entrained to the spout zone. Considering the movement of particles, the two zones are fundamentally different. In the central part we are dealing with pneumatic transport, high flow velocities of both phases and low concentration of solids. On the contrary, in the annular one a loosely packed bed is formed [3]. As a result of such an operating mode, from the very beginning spout bed apparatuses were used in many fields of the industry. Due to the intense particle movement in the spout zone, spouting is widely used for drying viscous materials such as pastes, slurry [4,5] and grains with high moisture content [6], and in the food industry for dehydration of fruit and vegetables [7]. This type of equipment is used for pyrolysis, combustion and gasification of waste materials for instance: biomass, sludge, plastics and tires [8–12]. A comprehensive overview of classic spout bed apparatuses can be found in the article of Moliner et al. [3].

In comparison to the fluidized bed, the arranged movement of particles makes the spout bed apparatuses ideal for coating in the pharmaceutical and food industries [13]. A coating is applied in the spout zone and the material is dried in the annular zone. In classic spout bed apparatuses, the particles are taken to the spout zone from any part of the annular zone, which results in their different moisture content and random distribution of the residence time in the coating zone [14]. The solution to this problem is the use of a draft tube, which physically separates both zones and thus organizes particle circulation. They can only be taken into the spout zone within a short distance between the bottom edge of the draft tube and the bottom of the apparatus [15]. In addition, the draft tube reduces the minimum spouting velocity and allows the use of high beds (no maximum spoutable bed depth). In the case of equipment with a coating nozzle placed in the bottom of the apparatus, the introduction of an additional fluidizing air stream in the bottom part of the annular zone (spout-fluid bed system with draft tube), prevents agglomeration of viscous particles in the area closest to the nozzle. Such a system called the Wurster apparatus is considered the best for periodic coating of fine granular materials [13,16].

Experimental testing of spout-fluid bed apparatuses allows for a collection of limited process data. In principle, it is not possible to measure basic flow quantities such as velocity fields of both phases and porosity [17]. Moreover, almost every measurement method is a factor disturbing the natural flow under investigation. These are arguments in favour of replacing them with computational methods, devoid of these limitations. For several decades there has been an increase in

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the popularity of computational fluid dynamics (CFD) used to describe complex multiphase flows, which is related to the dynamic development of software and hardware.

Multiphase system models are usually divided into two main groups: the Eulerian-Eulerian (EE) and Eulerian-Lagrangian (EL) [3]. The basic difference between them concerns the description of the dispersed phase elements. Models belonging to the first group are based on the assumption that both the solid phase and the dispersed phase are interpenetrating continua [18]. The phases present in the computational cell are described by the same system of balance equations and their effects are treated together (flow characteristics are averaged on the basis of the volume fraction). Based on EL method, the flow of dispersed phase elements is modelled using the motion equation for each particle separately. This requires an involvement of significant computing power and operating memory, which is why it is not used for a very large number of particles [3]. The current computational power of computers allows for modelling systems that do not exceed several million elements of the dispersed phase [19].

Fluid and spouting beds are characterized by granular flows with a high concentration of the dispersed phase. Therefore, according to EL, this type of flows is usually described using the DEM technique (*Discrete Element Method*), which was used for the first time to simulate rock movements [20]. The basics of the DEM algorithm were described by Tsuji et al. [21] and Hoomans et al. [22], respectively, in the *soft-sphere* and *hard-sphere* variants. The use of the pure DEM model for apparatus modelling in chemical engineering was, however, limited, as it did not take into account the hydrodynamic forces resulting from the interaction of the fluid in which solid particles move. Their description in the case of simulating the processes taking place in the spouting bed apparatuses required a combination of two groups of models: DEM for solid particles and CFD for the fluid. The increase in computational capabilities of computers has led to the development of DEM-CFD modelling over the last twenty years, making it a very useful tool for testing hydrodynamics of complex granular flows.

The hard-sphere method assumes that all interactions between particles are binary and immediate (the contact time is infinitely small) and contact forces are impulsive [22,23]. Particles have a spherical shape and their shape is preserved after collision. The basic dependencies used in this method are the momentum and energy balances before and after collision. During the point contact between the bodies, they undergo normal and tangential deformations resulting from the elasticity forces. Particle velocities after collision are determined by the velocity before collision, restitution coefficients and friction. If the values are known, the kinematics of particles after collision can be determined. At the stage of setting the boundary conditions, each wall with the condition “reflect” is described by two restitution coefficients: normal and tangential to the wall surface.

$$e_{n,t} = \frac{V_{r\ n,t}}{V_{i\ n,t}} \tag{1}$$

Indices n and t show the normal and tangential direction, and symbols r and i indicate the incident and rebound velocity. The value of the coefficient equal to unity means that the momentum exchange due to the collision was carried out without loss of kinetic energy. The second extreme value, equal to zero, indicates in turn the total loss of momentum by the particle and the full conversion of the kinetic energy of the particle into other forms of energy (friction, elastic or plastic deformation). Details of the hard-sphere model can be found in [14,22–24]. The hard-sphere model can be used successfully if the concentration of the dispersed phase is low [23]. Its application concerns both particle-particle and particle-wall collisions.

The soft-sphere method assumes that particles can be microdeformed in the contact point area as a result of friction and stresses. Deformations cause “numerical” displacement of two bodies, i.e. deformation. The greater the deformation, the greater the contact force between the bodies will be achieved [23]. Modelling of collisions using the soft-sphere method is a complex task. Detailed analysis of contact mechanics is presented in [24,25]. The theory of mechanical collisions distinguishes three main types: elastic, elastic-plastic and plastic. The elastic collision is treated in the same way as in the *hard-sphere* model. During a plastic collision, the energy is dispersed in the material in the form of plastic deformations. The elastic-plastic collision is a transient state between the two mentioned above; both types of interaction are present.

Models used to describe the contact force and the corresponding deformation vary depending on the nature of the interactions occurring during a collision. For the elastic collisions, Hertz theory can be applied with sufficient precision [25], while the other types of collisions are well described by deformation theory by Mindlin and Deresiewicz [26]. These theoretical models are complex and difficult to implement in numerical calculations, which is why, apart from purely theoretical solutions, simplified phenomenological models were developed, which satisfactorily reflected the relationship between deformation and contact force [17]. Traditionally used solutions include the models *linear-spring* and *spring-dashpot* proposed by Walton [27]. Thornton et al. [28] applied Hertz's theory to the modelling of force-deformation relations in the normal direction and Mindlin–Deresiewicz's theory in the tangential direction. The model has been coined in the literature as the Hertz–Mindlin–Deresiewicz model [24]. The collisions in which the adhesion forces play an important role were described by Johnson et al. [29] and Thornton [30]. For non-elastic collisions, a number of model proposals have been put forward, resulting in analytical formulas being applied to the normal and tangential restitution coefficient. These models are particularly convenient for CFD-DEM modelling and will be discussed separately in Section 2.2 of this study.

In relevant literature numerous articles can be found which describe the DEM-CFD modelling of spout-fluid bed apparatuses used, among others, for the purposes of granulation [31–33], mixing [34,35], wet coating [36,37], drying [38], and chemical reactions [39]. Very interesting and comprehensive studies of Zhong et al. [40] and Moliner et al. [3] describe the latest research on theoretical fundamentals and applications of CFD-DEM modelling of non-spherical particle systems and classic spouted bed devices respectively. The influence of such phenomena as Saffman's force and Magnus' effect [39,41,42] or the lift force on the movement of particles is also studied [43]. For micro-powders, electrostatic interactions and Brown movements are also taken into account [44]. In the past, due to the number and complexity of model equations and the low computational capabilities of computers, computing time was reduced by simplifying geometry to a two-dimensional form [20,22,45,46]. In later studies 3D geometry was used more often [12,34,40,47]. Efforts are now being made to develop efficient calculation algorithms for more complex geometries [48]. The aforementioned researchers modelling spouting and fluidization focused on the description of interactions between elements of the dispersed phase, because in case of its high concentration, collisions between particles significantly are predominant in relation to collisions with walls of the apparatus.

Szafran et al. [49,50] presented an innovative design of the spout-fluid bed apparatus with an internal bed circulation used for dry coating of fine powder materials, which is a further development of Wurster's concept [51]. Thanks to its specific design, the hydrodynamics of the coated particles flow differs significantly in comparison to that of classic spouting apparatuses. The device works with a fast-circulating dilute bed regime, at low concentration and high velocity of coated particles in all zones of the apparatus, which shortens the process time and reduces the agglomeration, especially for micro-powders from group C of the Geldart classification [52]. Due to the high degree of dilution of the dispersed phase [53], a simplified DEM model called DPM (Discrete Phase Model) can be used, which only takes into account the collision of particles with the apparatus walls. The main problem here is the proper description of this phenomenon. At present, there are no reports of studies concerning this type of modelling of spouting apparatuses.