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Detailed macroscopic flowsheet simulation of fluidized bed granulation process based on microscale models

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ABSTRACT

In this contribution the multiscale simulation approach for the modeling of fluidized bed spray granulation process is presented. On the macroscale the population balance model is used, whose parameters, such as size-dependent growth rate and overspray part of the suspension can be predicted from the calculations on the lower scales. On the microscale the particle motion in the apparatus is modeled by the coupled discrete element method and computational fluid dynamics. A mesoscale model is developed to calculate particle wetting with a suspension and the heat and mass transfer in the apparatus.

Keywords: Multiscale modeling, DEM, CFD, flowsheet simulation, granulation.

INTRODUCTION

The fluidized bed (FB) spray granulation is a widely used industrial production process that allows to produce particles with desired properties. During spray granulation the suspension or solution is injected into apparatus and deposited on a bed material, which is situated in fluid-like state. Afterwards, water part of suspension is evaporated and solid part remains on particle surface that leads to the continuous particle growth. Despite the wide usage of FB granulation process and the huge experimental and analytical work which has been performed in recent decades, there still exist considerable gaps in the process understanding.

In most cases the simulation of a plant performance is an ultimate goal of process modeling (1). The modeling of the FB spray granulation can be performed on different time and length scales. For the macroscopic modeling of production plants, which often consist of an interconnection of different apparatuses and process substeps, the usage of flowsheet simulation systems is state of the art. However, the flowsheet calculations are mostly based on the empirical or semi-empirical models, where the materials microproperties are poorly considered. Contrary to this, the calculations on the lower scales of the process description and the usage of the physically based models lead to the more detailed process modeling. For example, the usage of the discrete element method (DEM) on the microscale makes it possible to consider the specific microproperties of granules such as surface roughness, particle form, strength, etc. However, the transition from the macroscale to the lower scales leads to an exponential increase of computational effort. To overcome this problem and to perform a detailed modeling of the granulation plant in an appropriate time a multiscale modeling methodology can be employed.

In the case of the multiscale calculations the process is described on different time and length scales by a set of submodels which are coupled together into one global model. With an increased performance of modern computer systems also an interest to this research area is sufficiently increases. As a consequence, in the recent years a plenty of work has been done in the area of the multiscale simulation of different solids processes. Nevertheless, must of the researches were focused on some specific processes, such as drum granulators, fluidized bed reactors (2), paddle mixer-coater (3), gas-solid fluidization (4), etc.

In this contribution we present the architecture of the novel multiscale simulation system which has been applied on the fluidized bed spray granulation, but have a potential to be used for other types of solids processes.

ARCHITECTURE OF MULTISCALE ENVIRONMENT

The general architecture of the multiscale environment is illustrated in Figure 1.

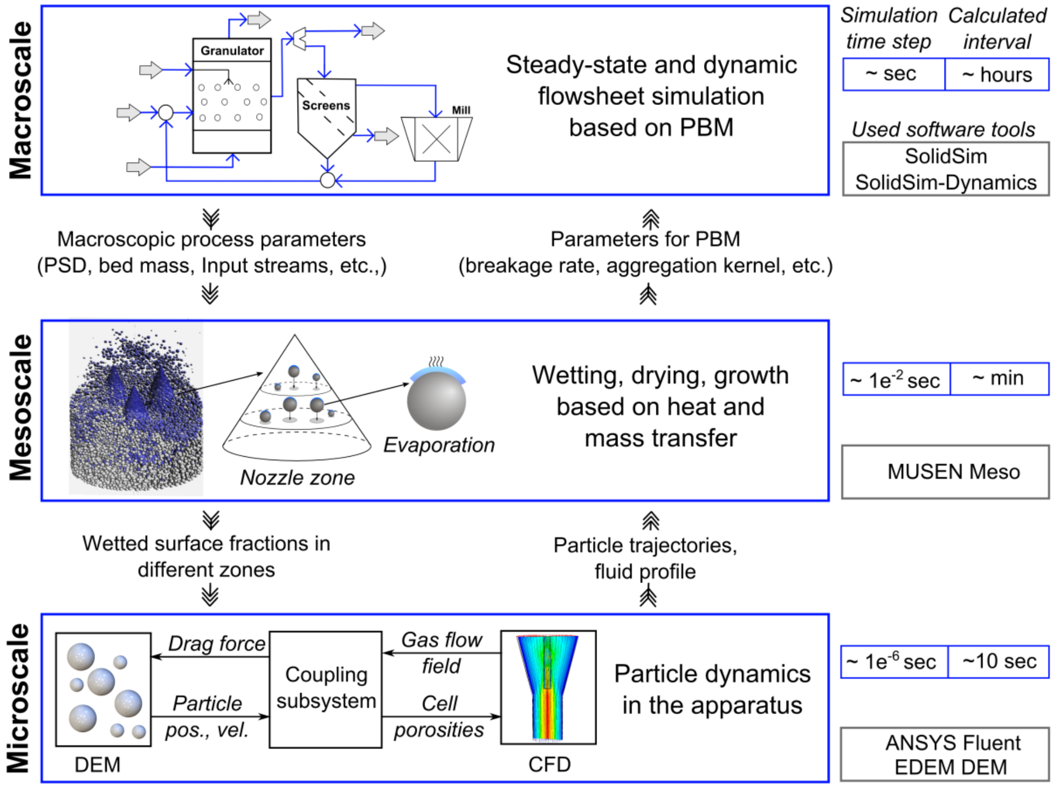

Fig. 1. Architecture of the multiscale simulation environment.

The entire environment consists of submodels on three different time and length scales, where different simulation tools are employed. On the upper hierarchical scale the process is modeled with help of the flowsheet simulation system SolidSim (5) and SolidSim-Dynamics (6). Here, the population balance models (PBM) are employed to predict the dynamics of particle population during granulation process. To approximate material specific parameters of the PBM the additional submodels are coupled to the flowsheet simulation system.

The mesoscale model is developed to calculate particle wetting by injected suspension and to calculate further drying of the liquid film. This model is based on the differential equations for the heat and mass transfer which are solved for each separate particle. From one hand, with help of the mesoscale model the wetting degree in different zones of the apparatus is approximated and transferred to the microscale. This makes it possible to consider the influence of the moisture content on the particle dynamics. From other hand, on the mesoscale the evaporation rate is approximated, as a consequence, the growth rate for each individual particle is calculated. This size-dependent growth rate is transferred into the PBM on the macroscale.

On the microscale the particle dynamics in apparatus is calculated with help of DEM coupled with a computational fluid dynamics (CFD) system. This simulation is performed for a relatively short time interval in order of seconds. The calculated particle trajectories and fluid flow profile in the apparatus are saved into the databases and transferred to the mesoscale model. In the mesoscale it is assumed that the particles repeat their trajectories cyclically during a longer time interval, in order of minutes.

DYNAMIC FLOWSHEET SIMULATION OF SOLIDS PROCESSES

As it was mentioned above, the flowsheet simulation system SolidSim-Dynamics (7) is applied to calculate the transient behavior of global granulation plant. This system has been especially developed for solids processes and allows to treat solid material properly. In a distinction to the fluid materials, solids are described by multidimensional distributed properties, as it is schematically shown in Figure 2. Therefore, during calculation it is necessary not to lose information about secondary material attributes. That is why the mathematical model of fluidized bed granulator was not solved directly, but the transformation matrix was generated from it (6). This matrix was applied to transform material streams.

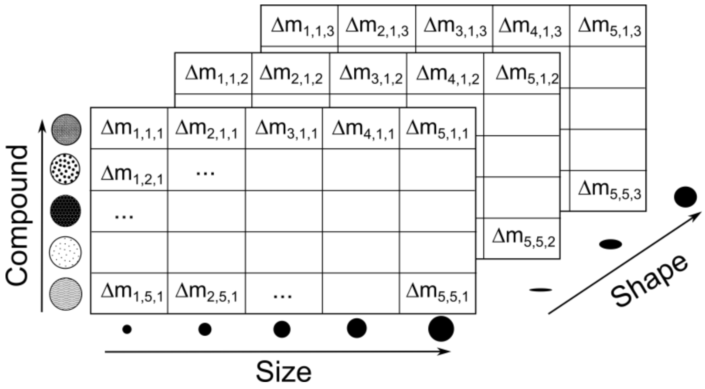

Fig. 2. Multidimensional distributed parameters of solid stream.

On the macroscale the growth of the particles in the fluidized bed apparatus is described by the one-dimensional PBM with the particle diameter as a property coordinate (Eq. 1).

$$\frac{\partial n(t,d)}{\partial t} = -\frac{\partial[G_e^{macro}(t,d)\cdot n(t,d)]}{\partial d} + \dot{n}_{in}(t,d) - \dot{n}_{out}(t,d), \tag{1}$$

where $\frac{\partial n(t,d)}{\partial t}$ is the change of the particles number over the time; $\dot{n}_{in}(t,d)$ and $\dot{n}_{out}(t,d)$ characterizes the particle fluxes, that are entering and leaving the apparatus, respectively; the term $G_e^{macro}(t,d)$ describes the particle growth. It can be assumed that the velocity of granule growth does not depend on the particle size (8). In this case the term $G_e^{macro}(t,d)$ can be approximated as:

$$G_e^{macro} = \frac{2\dot{M}_{susp}(1-K_{os})(1-K_w)}{\rho_p A_{tot}}, \tag{2}$$

where $\dot{M}_{susp}$ is the suspension mass stream; ρ_p is the particle density; A_{tot} is the total surface of all particles in the granulator; K_w is the water content of the suspension and K_{os} is the mass part of suspension, which leaves an apparatus as an overspray. However, the approximation given in Eq. 2 cannot always be effectively applied. Zank et al. (9) experimentally observed that the growth rate increased with increasing particle diameter. It is obvious, that such conclusion was correct just for the investigated apparatus geometry and specific process conditions. Nevertheless, it was pointed out, that depending on the size the granules can show the significant difference in growth velocity. In this contribution, the size-dependent growth kinetics has been predicted by the calculations on the microscale and the mesoscale.

CALCULATION OF HEAT AND MASS TRANSFER ON THE MESOSCALE

The mesoscale model is used to calculate thermodynamics in the fluidized bed apparatus. Here, each particle is considered as a separate entity. As the input parameters into mesoscale model the particle trajectories and fluid profiles are transferred from the microscale. The simulation on this scale is carried out for a time interval in order of minutes with a simulation time step size in order of seconds. The general sequence of the operations which are performed in each iteration is schematically shown in Fig 3.

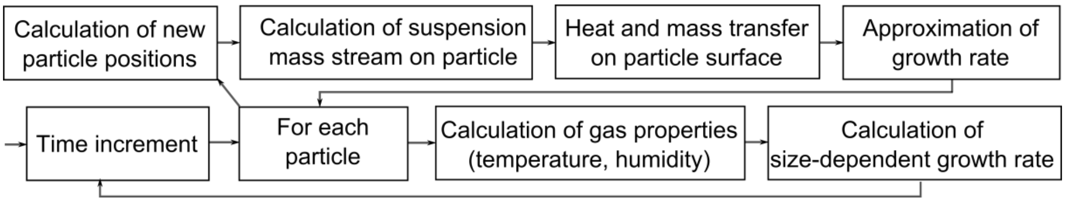

Fig. 3. Diagram of the calculation flow.

The calculation of the particle positions is based on the extrapolation of the results from the microscale under assumption that particles iteratively repeat their trajectories. To approximate the suspension mass stream which deposits onto surface of each particle the model of the spraying zone has been developed and implemented. More detailed description of this model is given in Fries et al. (10). It is assumed that a liquid film on all wetted particles has constant thickness L_{film}. Therefore, in the case, when the particle is totally wetted, than the maximal amount of the liquid M_{max} on the particle with the radius R_p is limited as it is expressed in Eq. 3, where ρ_l is a suspension density.

$$M_{max} = \frac{4}{3}\pi\left[\left(R_p + L_{film}\right)^3 - R_p^3\right]\rho_l \tag{3}$$

To predict the evaporation rate for the calculation of the growth rate, the heat and mass transfer on the particle surface is solved. The heat transfer between particle and liquid film, between liquid film and surrounded gas and between particle and gas is considered. Enthalpy streams of the sprayed suspension and evaporated liquid were also included in the model. The heat and mass transfer coefficients are calculated with help of the model proposed by Gnielinski (11) using the relative velocity between particle and gas, which has been extrapolated from the microscale model.

As results from the mesoscale the following parameters are obtained:

- normalized size-dependent growth rate (12) and overspray part of suspension, which are transferred into the macroscale;
- wetting surface fractions φ in different zones of the apparatus, which is transferred to the microscale. This parameter is defined as a ratio between the particle surface covered with the liquid film to the total particle surface.

MICROSCALE MODEL

The microscale calculations are based on the discrete element method (DEM), whereby each particle considered as a separate entity. Coupling of the DEM with the CFD system makes it possible to calculate particle dynamics in the fluid field (13). The general coupling scheme is shown in Fig. 4.

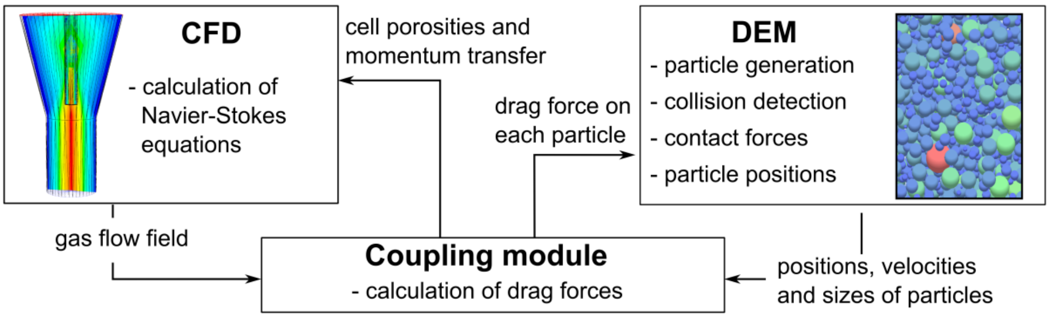

Fig. 4. Coupling scheme between DEM and CFD systems.

In the each simulation step of the DEM the collisions between particles are analyzed and equations describing the contact forces are solved. In this study the soft sphere contact model according to Hertz, Mindlin and Tsuji (10). However, this model was developed for dry particles and cannot be effectively used for the simulation of a spray granulation process, where the injected liquid can have a significant influence on the particle dynamics (14).

To consider the influence of the liquid film, the interaction distance, where the contact detection and force calculation are performed, was increased by the thickness of the liquid film L_{film}, as it is schematically shown in Fig 5. For each new contact the coordinates of colliding partners are analysed and, based on the results from mesoscale, the wetted surface fraction of particles φ in the current zone of the apparatus is approximated. The different contact scenarios are examined: two particles are dry, one of them is wet or both of them are wet.

According to the probabilities expressed in Fig. 5 the each new contact is arranged to one of possible collision types. If it is considered that at least one of the contact partners behaves as wet material, than the capillary and viscous forces acting due to liquid layer squeezing and forming liquid bridge are calculated. The wet collision is considered to be finished when the rupture of the liquid bridge occurs.

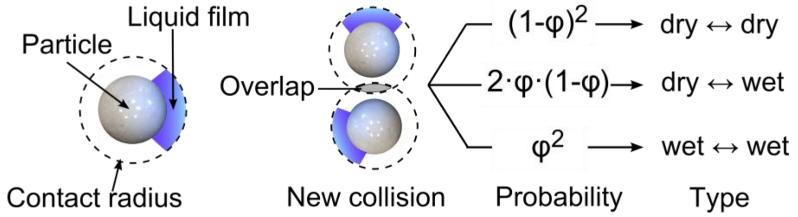

Fig. 5. Contact scenarios for the modeling of collisions between wetted particles.

During microscale calculations the trajectories of all particles are saved into the database which is afterwards transferred to the mesoscale. The usage of the DEM related to the huge volume of the generated data, especially in the case when a large amount of particles is modeled on the microscale. To minimize the volume of the stored data and to increase the speed of data access operations, the advanced data storage format has been developed (15). The CFD calculations have been done in the commercial system ANSYS Fluent. For these calculations and for the mesoscale simulations the fluidized bed apparatus has been discretized into different types of cells (mesh). The CFD calculations have been performed on the irregular grid. However, on the mesoscale the Cartesian grid type has been used. Therefore, the data received from the CFD system have been converted into the Cartesian grid type.

SIMULATION EXAMPLE

The developed multiscale modeling approach was used for the detailed calculation of the continuous fluidized bed spray granulation process, which is shown in Fig. 6.

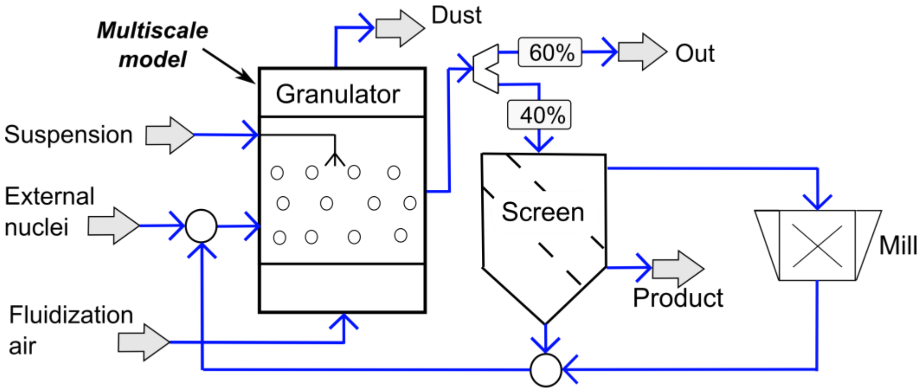

Fig. 6. Flowsheet of fluidized bed granulation process.

In the first stage the global production process has been simulated up to the steady-state. For these calculations the assumption of the size-independent growth rate (Eq. 2) was done. According to the obtained steady-state results, such as particle size distribution and mass of the holdup, external material streams into the apparatus, etc. the microscale model has been generated.

In the second stage the microscale simulations were performed for a time interval of 9 seconds. The obtained particle trajectories and fluid profiles were saved to the databases. Afterwards, the mesoscale calculations were carried out for a time interval of 300 seconds and the wetting surface fractions in different zones of apparatus have been obtained. This data were transferred back to the microscale to perform more precise estimation of the particle dynamics. Finally, after a set of reiterations the interscale convergence has been reached and the calculated size-dependent growth rate has been transferred to the PBM. On the left-hand side of Fig. 8 the comparison between size-independent growth rate (Eq. 2) and growth rate calculated with a multiscale model is shown. It can be seen that the smaller particles have a higher growth velocity. It is related to the top-down configuration of the three nozzle zones and a partial segregation of the bed material. In comparison to the coarse granules, the smaller granules have a larger residence time in the upper layers of the bed and, as a consequence, a bigger amount of the suspension can be deposited on their surfaces. The right-hand diagram in Fig. 8 compares the particle size distributions in the fluidized bed apparatus at the steady-state which were obtained using empirical and multiscale models.

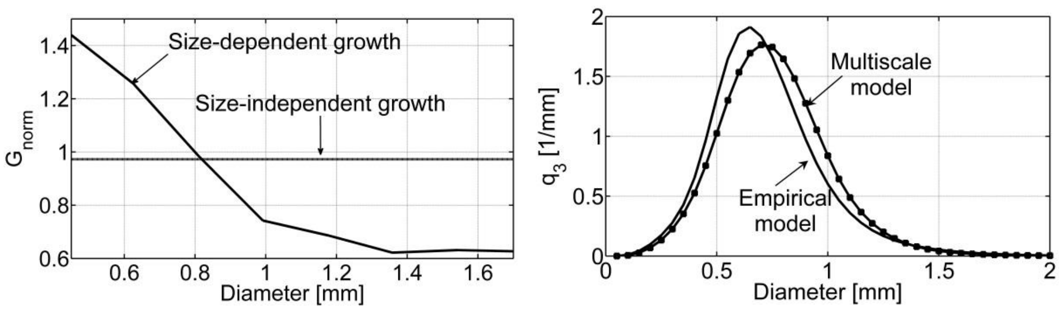

Fig. 7. Simulation results: normalized growth-rate (left) and comparison between semi-empirical and multiscale model (right).

CONCLUSIONS

In this contribution the architecture of the multiscale simulation approach for the modeling of fluidized bed spray granulation is presented. The proposed multiscale environment consists of simulation systems on three different time and length scales and allows to perform detailed simulations of granulation plants by considering the physically-based material micro properties.

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