# Novel multiscale simulation environment for modeling of fluidized bed granulation

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Citation: AIP Conference Proceedings **1542**, 1126 (2013); doi: 10.1063/1.4812134
View online: http://dx.doi.org/10.1063/1.4812134
View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1542?ver=pdfcov
Published by the AIP Publishing

# Novel Multiscale Simulation Environment for Modeling of Fluidized Bed Granulation

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**Abstract.** In this contribution the architecture of a novel simulation environment,which has been developedfor the multiscale modeling of fluidized bed spray granulation,is presented. The novel environment describes the granulation process on four different time and length scales. On the one hand, it allows to predict dynamics of the global production process, whereby, on the other hand, material properties can be considered.

**Keywords:** Multiscale model, simulation environment, flowsheet simulation, DEM, population balance, fluidized bed.
**PACS:** 47.55.Lm, 81.20.Ev, 02.60.Cb

## INTRODUCTION

The fluidized bed spray granulation process is widely used in the solid industry to produce particulate products with desired properties. To understand the dynamics of the production process,to optimize the process and to theminimize energy consumption the numerical simulation can be effectively used. Such simulation can be carried out on different time and length scalesregarding the process description.

For the modeling of industrial scale granulation plants in most cases empirical or semi-empirical population balance models (PBM) are used [1]. The application of such macroscale models does not allow to consider material micro-properties or specific process parameters. But due to the relatively small amount of computations, it ensures to obtain a numerical solution in appropriate time.

Contrary to this, the usage of the discrete element method (DEM) on the microscale leads to more detailed prediction of the process behavior. However, the transition to the lower scales of the process description results in the exponential increase of the computational volume. Therefore, it is impossible to perform the microscale calculations of the global production process even for short time intervals.

The models of different apparatuses and processes in solids industry can be distinguished by detailing levels and application purposes.The joining between submodels on the different scales into one multiscale model can be used as an effective strategy to perform modeling of the global process with high detailing grade [2]. The multiscale models have been previously used in the solids industry for the simulation of different processes, such as drum granulation, fluidized bed reactors [3], paddle mixer-coater [4], fluidized bed agglomeration [5], rotor based granulator [6], general agglomeration model [7], fluidized bed granulation [8], etc. However, no general simulation framework has been developed which will be applicable for different types of solids processes.

## MULTISCALE SIMULATION ENVIRONMENT

In order to combine the process description on the different time and length scales the MUltiscale Simulation ENvironment with acronym MUSEN has been developed at our institute. This environment is used to control the simulation of all submodels, to analyze the interscale convergence and to realize data transfer. In Fig. 1 the schematic representation of the program architecture is shown. The developed system consists of submodels which are allocated on the four different scales. To perform simulation several commercial tools (EDEM, ANSYS Fluent, Matlab, SolidSim) have been extended with additional software components and simulation subsystems.

### Macroscale level

For the macroscale calculations of solids processes the dynamic flowsheet simulation system “SolidSim-

*Powders and Grains 2013*
AIP Conf. Proc. 1542, 1126-1129 (2013); doi: 10.1063/1.4812134

Dynamics" has been applied [9]. The temporal change of the PSD, which occurs due to the continuous transport of the particles in the state space, has been described by the one-dimensional populationbalance equation (PBE) with particle diameter as internal coordinate.

The parameters, which determine the dynamics of the PBE, such as the size-dependent growth rate [8], coalescence kernel [5] and breakage rate are obtained from the modeling on the lower simulation scales.

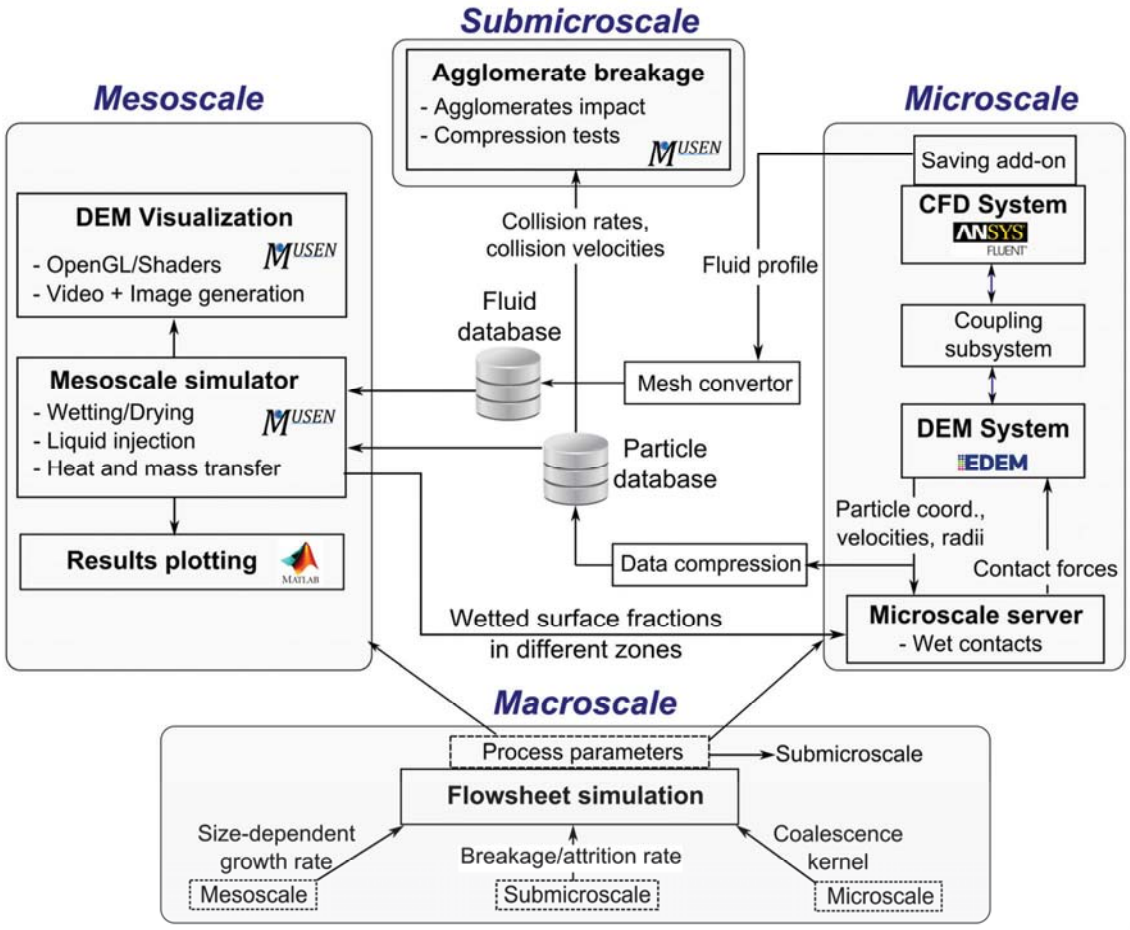


**FIGURE 1.** Architecture of the multiscale simulation environment.

## Microscale level

The microscale calculations are based on the discrete element method (DEM) for particle dynamics coupled with a CFD system for the fluid dynamics. By the DEM each particle is considered as a separate entity and in each simulation time step the Newtonian equations of motion are solved. Coupling between CFD and DEM systems allows to predict particle and fluid dynamics.

During the fluidized bed spray granulation processes the suspension is being injected into the apparatus and the solid part of the suspensionis deposited onthe bed material. This leads to the sufficient change of the particle dynamics. In order to consider the influence of the liquid film, the microscale server has been developed. In the each simulation time step of the DEM,the server receives the comprehensive information about the particles and calculates additional capillary and viscous forces caused by the liquid.

To distinguish between dry and wet contacts, the wetting surface fraction φ isused. It is defined as a ratio between particle surface covered by liquid to the total particle surface.

Each new interparticle collision is assigned toone of three possiblecontact types:

- "dry-dry", with probability $(1-\varphi)^2$;
- "dry-wet", with probability $2\varphi(1-\varphi)$;

- "wet-wet", with probability $\varphi^2$.

To simulate the wet surface properly, the contact radius of thesolid particle isincreased by the thickness of the liquid film. The collision is supposed to be finished when the rupture of the liquid bridge occurs.

The calculations with the help of the DEM and CFD approach are performed for the time interval in the order of seconds. As results from the microscale simulation the following parameters are obtained and transferred to the submodels on the other scales:

- particle trajectories (→mesoscale);
- collision properties (→submicroscale);
- sticking rate (→macroscale).

For the CFD calculations (in ANSYS Fluent) and for the mesoscale simulations the apparatus is discretized into different types of discrete cells (mesh). The CFD calculations are performed on the irregular grid. Therefore, the data, which are received from the CFD system, are converted into the Cartesian grid type, which is used on the mesoscale. For this purpose the mesh convertor tool has been developed (Fig. 1).

The usage of the DEM related to the huge volume of the generated data, which should be stored for further analysis and post-processing. 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 and implemented into the simulation environment [10].

## Mesoscale Level

On the mesoscale the particle wetting and the heat and the mass transfer occurring in the apparatus are calculatedfor the time interval in order of minutes.The particle trajectories, the fluid profiles and the macroscopic process parameters are transferred as the input parameters into the mesoscale. The mesoscale simulations are carried out for much longer time intervals compared to the microscale calculations. Therefore, it is assumed that the particles iteratively repeat their trajectories.

For the prediction of the particle wettingthe simplified model of the nozzle zone has been developed and implemented [11]. The wetting region is represented as a cone zone, which is discretized throughout a height into a set of layers. The amount of liquid which is depositedon the particle depends on suspension mass stream, relative position of the particle in the wetting region, particle cross-cut surface and porosity in the upper layers. The implemented mesoscale simulator allows to defineseveralnozzles in one apparatus, to specify their geometry and to consider that theparticles can be simultaneously located in the multiple wetting regions.

To calculate the evaporation process, the system of differential equations for the description of air temperature, mass of liquid film, temperature of liquid film, particle temperature and air humidity has been formulated [9].The Reynolds number, which is needed for the approximation of heat and mass transfer coefficients, depends on the relative velocity between particle and fluid and it is obtained based on the results received from the microscale.

The calculation of the evaporation rate from the surface of each separate particle allows to predict its growth rate and to approximate size-dependent growth rate of the whole particle assembly. This size-dependent growth rate is normalized and transferred to the macroscale model [8]. Another output parameter from the mesoscale model is the wetted surface fraction in the different regions of an apparatus. These values are transferred into the microscale to consider the influence of the liquid film on the particle dynamics.

For the interactive representation of the mesoscale results the hardware accelerated visualization system has been developed. This system allows to reacha high level of the visual quality with the further data export into image and video files [12].

## Submicroscale Level

To investigate breakage behavior of agglomerates and to obtain breakage function for the population balance model, the calculationsof representative agglomerates on the submicroscale has been performed. For this purpose, the novel simulation tool has been developed.The particle collision velocities and collision frequencies are transferred from the microscale into the submicroscale. According to collision dynamics, the probability based simulation of collisions is carried out and the breakage characteristics are obtained.

The simulation system on the submicroscaleis based on the DEM, whereby an agglomerate is represented as a set of primary particles connected with solid bonds (see Fig. 2). For the calculation of the forces and moments in the solid bonds the bonded particle model has been used [13].

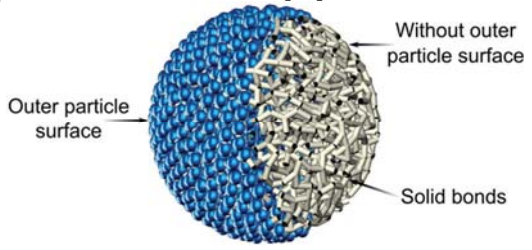


**FIGURE 2.** Agglomerate and its internal structure.

As the bond breakage criteria the maximum of shear and tensile stresses are analyzed. If one of the stresses exceeds the bond strength, then the bond breaks and is removed from the calculation procedure. In the case when the simulation step is not chosen appropriately such discrete event can lead to the significant increase of particle velocity and to the divergence in the system. Therefore, after each iteration the analysis of the system state is performed and possible reduction of the step size is made.

## MAIN CALCULATION AGLORITHM

The calculations on the different scales are carried out sequentially, whereby submodelsare simulated for different time intervals. In Fig. 3 the general flowchart of the main simulation algorithm is represented.

According to the macroscopic process parameters the microscale model is created and calculations are performed for the time interval $T_{micro}$, which is in the order of seconds. Afterwards, the control is transferred into the mesoscale where thermodynamics in the apparatus is simulated for the time interval $T_{meso}$(in order of minutes) and the interscale convergence is analyzed. As the convergence criteria the deviations of transferred parameters on the successive iterationsare used. Therefore, it is necessary to perform at least two iterations on the micro and mesoscales.

In the case, when the agglomerate breakage should be considered, the simulation on the submicroscale should be performed. The simulation time interval $T_{submicro}$is much shorter in comparison to $T_{micro}$ and is in the order of 1-2 seconds. However, the calculations on the submicroscale should be repeated iteratively with different initial conditions.

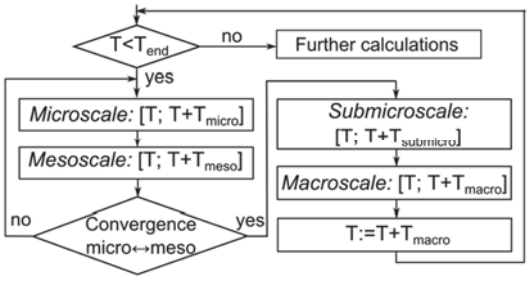


**FIGURE 3.** Flowchart of the main simulation algorithm.

Finally, the flowsheet simulation of the global production process is carried out on the macroscale. The magnitude of the time interval $T_{macro}$ depends on the change of main process parameters and can be in the order of ~30-60 min.

## CONLUSION

In this contribution the architecture of the novel multiscale simulation environment for particle systems is presented. The developed environment combines different commercial simulation tools and extends them with additional software components and modeling subsystems forrunning simulation on different time and length scales. Such architecture allows to perform modeling of the global production process considering specific process parameters and different material microproperties of solids.

The proposed environment has been effectively applied for the simulation of the growth and aggregation inthe fluidized bed apparatus. However, in the current implementation there still exist a large number of assumptions and neglected effects. Nevertheless, the component-based organization of the environment allows to extend it easily with new functional relationships and simulation subsystems.

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