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Original Research Paper

Multiscale simulation of fine grinding and dispersing processes: Stressing probability, stressing energy and resultant breakage rate

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ABSTRACT

Wet grinding is an important unit operation in many industrial fine grinding and dispersing processes. The main aim of this study is the development of a multiscale modelling method to predict and optimize grinding and dispersing processes in wet operated stirred media mills. In the first part of this paper, numerical CFD-DEM studies on the meso and macro scale were carried out with the focus on the acting forces, stressing probability, grinding media motion and the stressing energy distribution of a stirred media mill. The stressing probability of product particles between the grinding media was investigated at varying relative velocities in normal direction as well as at different conditions of grinding bead rotation. The determination of the stressing energy distribution on the macro scale is discussed exemplarily for a disc stirrer at three different rotational velocities. Thus, the increase in stressing frequency and energy at higher rotational speed was quantified. Moreover, the transfer of the results on an overall process simulation using population balance equations was studied. In the second part of this study the effect of the drag coefficient and the fracture processes of aggregates with various fractal dimension and solid bond properties are discussed numerically.

1. Introduction

Stirred media mills are very common in the chemical, pharmaceutical, mining or paint industry for fine wet grinding and dispersing of product particles down to a target particle size of few microns or less. Apart from fragmentation of particles, agglomerates and aggregates (e.g. [1,2]) followed by a stabilization process, emulsification processes [3], disruption of single-celled microorganisms [4–6], particle synthesis [7] or chemical reactions are potential applications for stirred media mills. The grinding chamber volumes of stirred media mills vary from a few millilitres in the pharmaceutical industry up to 20 cubic meters with a power consumption of several megawatts in the mining industry. The mill chamber is filled with grinding media (grinding beads) and a suspension with product particles (aggregates or primary particles that shall be milled or dispersed). A rotating stirrer, which exists in various designs e.g. disc, pin or screw stirrers, moves the grinding beads and the suspension. Semi-empirical models are used to rationalize the choice of process parameters such as grinding media size and material, the grinding media filling degree, the stirrer speed and the solid content of the suspension [8–10]. The characteristic stressing energy and stressing frequency numbers properly show with simple proportionalities the influence of process parameters on the grinding result [10]. However, due to the simplified assumptions, the values do not represent quantitatively the actual stressing conditions. This makes it difficult to compare these characteristic numbers to material data. In an advanced approach Breitung-Faes et al. [9] include material data and geometrical aspects of different stirred media mills in the stressing energy model to predict optimal process conditions for several inorganic materials and mill designs based on few experiments. Based on a microhydrodynamic view of the particle stressing in stirred media mills, [11] Afolabi et al. [8] define a process parameter depending milling intensity factor that correlates with the breakage kinetics of drug nanoparticles.

CFD-DEM simulations of stirred media mills help to get an understanding of the grinding media movement and the influence of the process parameters on the media collisions (e.g. [12]). Important outcomes of the simulations are collision energy, collision frequency and distribution of grinding media in the chamber. Recently, Beinert et al. [13] presented a detailed evaluation of grinding media contacts in stirred media mills. For fine grinding,

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simulations on the mill level are usually limited to grinding media and liquid while product particles are not simulated due to high computational costs. More detailed simulations on the microscopic level are an approach to understand the capturing and stressing of particles and aggregates between grinding beads. Multiscale modeling is an approach to close the gap between the scales. With increasing computer performance multiscale modelling has been applied to other solid processes [14–16]. It becomes apparent, that different simulation scales and techniques cannot be generically applied to different processes. The multiscale simulation approach needs process specific submodels to gain the critical process model information. For ball mills impact energy distributions gained via DEM simulations of the charge motion are used to predict the influence of process parameters on the material breakage rate for population balance models (e.g. [17–19]). For wet stirred media milling we propose the following multiscale simulation approach that includes simulations from micro to process scale (Fig. 1). Important model parameters and findings from different scales are transferred to other scales (Fig. 2).

- The micro scale model (particle/aggregate scale) allows the prediction of the influence of different materials, particle sizes and morphologies on the grinding and dispersing process. The fracture processes on the micro scale can be investigated numerically and experimentally as function of the particle/aggregate material, structure, size distribution and solid bond properties. The resulting fracture force/energy distribution depends on the acting fluid and compression forces and the stressing/capture probability provided by the meso scale model. Moreover, the drag coefficient as function of the fractal dimension of the aggregates can be derived on the micro scale simulation level.
- The meso scale model (grinding media scale) links the interaction between macro-scale flow conditions and micro-scale aggregate and particle dynamics. Based on the experimental and numerical study of the behavior of two grinding beads in a product suspension and the product particles in-between various aspects can be considered for model optimization, e.g. single or multiple grinding media stressing, damping due to the fluid displacement effecting the grinding bead velocities, displacement of particles due to fluid flow, effect of fluid rheology, relative velocities and eccentric stress events. Functions for stress and fracture probability, frequency and intensity as well as the coefficient of restitution should be derived.
- The macro scale model (mill scale) provides information of the stressing energy distribution of the mill based on the numerical calculation of the relative velocity distribution between grinding beads or, as determined in former times, experimental determination of the velocity distribution. The coefficient of restitution is an input parameter from the meso scale model. Based on this values a product related stressing energy distribution can be calculated, which is necessary for the prediction of the grinding or dispersing efficiency. The relative velocities of the grinding media are required as input parameters for the meso scale model.
- On the process scale, the information of the other scales are used to calculate process relevant data. For example, the change of the particle size distribution over time can be calculated by a population balance model. The parameter specific breakage rate and breakage distribution function depend on the machine stressing conditions and the material answer to this stressing [20], which can be derived from macro scale (stressing energy distribution), meso scale (capture probability) and micro scale (fracture energy distribution).

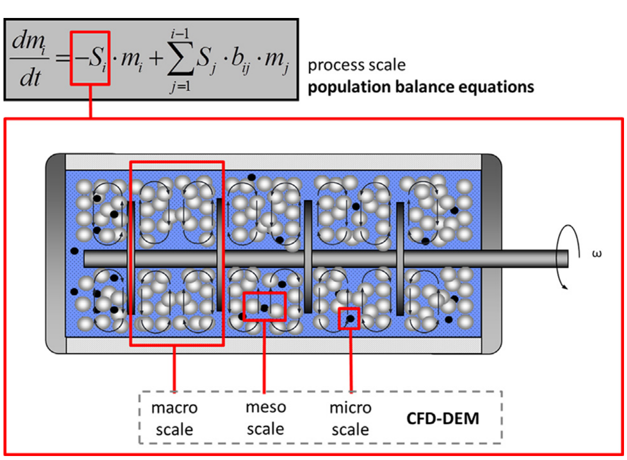

Fig. 1. Multi-scale simulation of fine grinding and dispersing processes in wet operated stirred media mills here represented in batch-operation mode.

We show examples of simulations on these different scales in a study divided into two articles. In the first part of this study (this article), the meso, macro and process scale simulation strategies and some exemplary results are discussed. The acting forces, stressing probability, grinding media motion and the stressing energy distribution of a stirred media mill is taken into account. Moreover, the transfer of the results on an overall process simulation using population balance equations is discussed. The here shown multiscale approach allows to investigate process parameters (e.g. stirrer speed, grinding bead size and filling level), machine parameters (e.g. stirrer geometry) and material parameters (e.g. material laws, agglomerate structure, viscosity). In this study, the influence of stirrer speed and material law is exemplarily shown. In the second part of the study, the processes required for the investigation of grinding and dispersing processes in stirred media mills on the micro scale simulation level, i.e. the strength and drag coefficient of fractal aggregates will be shown.

2. Submodels and simulation methods for the different scales

2.1. Macro scale

For the study of the motion of bulk solids in various machines, DEM has been proved to be a valuable tool. This method is based on the solution of Newton's laws to calculate the position and velocity of every particle. Contact models are necessary to estimate the acting forces while single particles are in contact. Due to limited computational power, it is not possible yet to calculate an entire mill including grinding media and also the product particles in μm-size. However, the calculation of the bead movement and resulting distributions of impact velocities can be used to improve or validate analytical models. Regarding the simulation of dry grinding processes in stirred media mills (or tumbling mills, planetary ball mills, e.g. Rosenkranz et al. [21]) several investigations were published which describe the grinding media distributions (e.g. Kim and Choi [22], Sinnott et al. [23]), flow fields (e.g. Cleary et al. and Sinnott et al. [23,24]), power input [23], resultant wear (e.g. Jayasundara et al. [25] and Cleary et al. [24]) and effect of mill geometries.

As a wet operated mill includes both, grinding media and fluid, the bead motion is strongly coupled to the motion of fluid. On a modelling level this can be realized by coupling the DEM code to a general purpose computational fluid dynamics code in a resolved or non-resolved fashion [26] or by SPH (smooth particle hydrodynamics) modelling [27]. If a coupling between CFD and DEM is required, two different methods are common: a one-way or a two-way coupling. If the influence of the particles on the fluid flow

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