Dense gas-particle flows are encountered in a variety of industrially important processes for large-scale production of fuels, fertilizers and base chemicals. The scale-up of these processes is often still problematic, which can be related to the intrinsic complexities of these flows, which are unfortunately not yet fully understood despite significant efforts made in both academic and industrial research laboratories. In dense gas-particle flows both (effective) fluid-particle and (dissipative) particle-particle interactions need to be accounted for, because these phenomena govern the prevailing flow phenomena to a large extent, i.e. the formation and evolution of heterogeneous structures. These structures have significant impact on the quality of the gas-solid contact and as a direct consequence thereof strongly affect the performance of the process.

Due to the inherent complexity of dense gas-particles flows the authors have adopted a multi-scale modeling approach in which both fluid-particle and particle-particle interactions can be properly accounted for. The idea is essentially that fundamental models, taking into account the relevant details of fluid-particle (lattice Boltzmann model) and particle-particle (discrete particle model) interactions, are used to develop closure laws to feed continuum and discrete bubble models, which can be used to compute the flow structures on a much larger and industrial scale.

Our multi-scale approach (see figure below) involves the lattice Boltzmann model, the discrete particle model, the continuum model based on the kinetic theory of granular flow and the discrete bubble model. New improved closure laws for the fluid-particle interaction derived from lattice Boltzmann simulations have been assessed with the discrete particle model. The new closure laws have significant impact on the bubble shape and raining of solids through the roof of the bubble, and yield a much better correspondence to experimental results. Furthermore, the individual calculation of each particle-particle collision according to a detailed collision model in the discrete particle model allows a critical evaluation of the model assumptions used in the kinetic theory of granular flow, which is the basis of all continuum models. With the discrete particle model the local transport, consumption and production of granular energy can be studied in detail, which can help elucidating for example the cause of the over-prediction in the rates of particle segregation in bi- or multi-disperse systems by continuum models. With the continuum models based on the kinetic theory of granular flow, bubble formation, growth, coalescence and break-up can be studied on a larger scale. Finally, using the continuum models closure equations for the bubble behavior and average properties of the emulsion phase can be derived, which can be implemented in discrete bubble models, where the motion of individual bubbles through the emulsion phase is tracked. With the discrete bubble model the large-scale circulation patterns (e.g. how these patterns may be effected by internals) in industrial scale dense fluidized beds can be studied.
In this presentation the emphasis will be on Discrete Particle Models (DPM) for dense gas-particle flows. These models are ideally suited to assess the impact of fluid-particle and particle-particle closures on the macroscopic behaviour of the system. Illustrative examples obtained from detailed DPM simulations will be presented with emphasis on pressure effects and solids mixing. Areas which require substantial future research efforts will also be indicated.