# Numerical Simulations of Particulate Flows in Industrial Applications

J.A.M. Kuipers

*Department of Science & Technology*
*University of Twente*
*P.O. Box 217, 7500 AE Enschede, The Netherlands*

**Abstract**

*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 problematic and is 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 to a large extent govern the prevailing flow phenomena, 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, we 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 models which can be used to compute the flow structures on a much larger (industrial) scale. Our multi-scale approach (see Figure 1) 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. In this paper we give an overview of the multi-scale modeling strategy, accompanied by illustrative computational results for bubble formation. In addition, areas which need substantial further attention will be highlighted.*

## 1. Introduction

Dense gas-particle flows are frequently encountered in a variety of industrially important gas-solid contactors, of which the gas-fluidized bed can be mentioned as a very important example. Due to their favorable mass and heat transfer characteristics, gas-fluidized beds are often applied in the chemical, petrochemical, metallurgical, environmental and energy industries in large scale operations involving a.o. coating, granulation, drying, and synthesis of fuels and base chemicals (Kunii and Levenspiel, 1991). Lack of understanding of the fundamentals of dense gas-particle flows, and in particular of the effects of gas-particle drag and particle-particle interactions (Kuipers et al., 1998 and Kuipers and van Swaaij, 1998), has led to severe difficulties in the scale-up of these industrially important gas-solid contactors (van Swaaij, 1990). To arrive at a better understanding of these complicated systems in which both gas-particle and particle-particle interactions play a dominant role, computer models have become an indispensable tool. However, the prime difficulty with modeling gas-fluidized beds is the large separation of scales: the largest flow structures can be of the order of meters; yet these structures are found to be directly influenced by details of the particle-particle collisions, which take place on the scale of millimeters or less. Therefore, we have adopted a multi-level modeling strategy (see Figure 1), with the prime goal to i) obtain a fundamental insight in the complex dynamic behavior of dense gas-particle fluidized suspensions; that is, to gain an understanding based on elementary physical principles such as drag, friction and dissipation ii) based on this insight, develop models with predictive capabilities for dense gas-particle flows encountered in engineering scale equipment. To this end, we consider gas-solid flows at four distinctive levels of modeling.

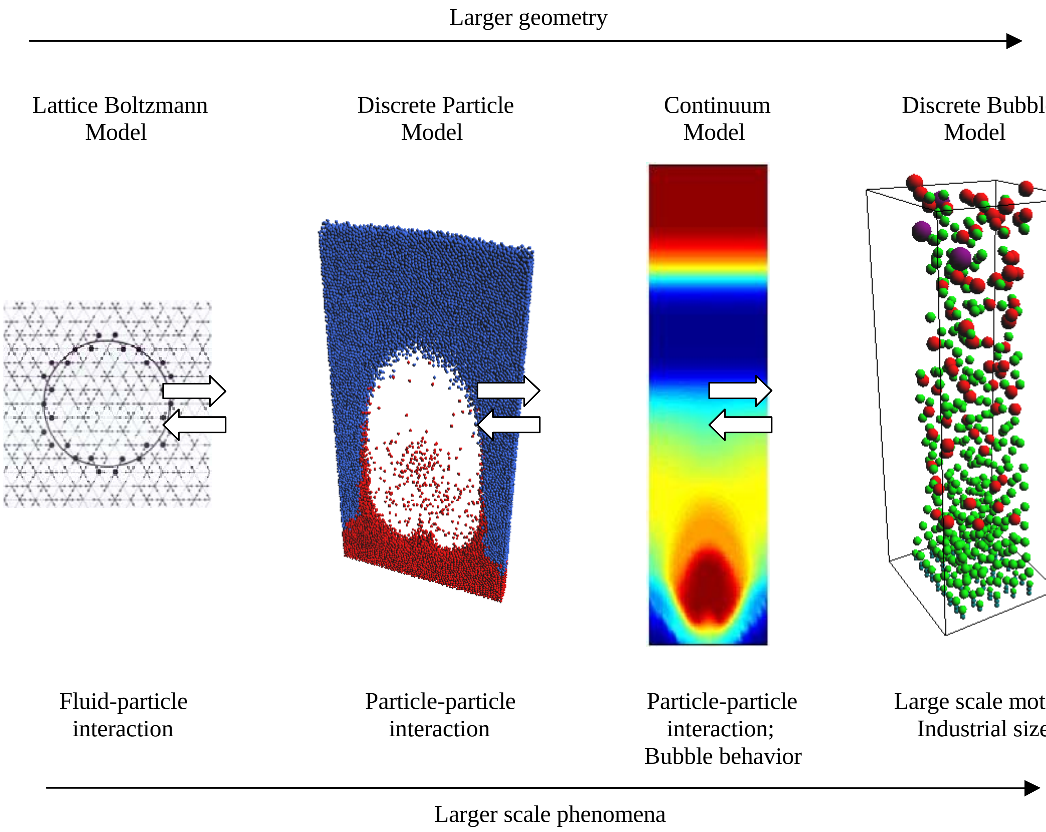


**Figure 1:** Multi-level modeling scheme for dense gas-fluidized beds.

At the most detailed level of description the gas flow field is modeled at scales smaller than the size of the solid particles. The interaction of the gas phase with the solid phase is incorporated by imposing “stick" boundary conditions at the surface of the solid particles. This model thus allows us to measure the effective momentum exchange between the two phases, which can be used in the higher scale models. In our model, the flow field between spherical particles is solved by the lattice Boltzmann model (Succi, 2001 and Ladd and Verberg, 2001) although in principle other methods (such as standard computational fluid dynamics) could be used as well. At the intermediate level of description the flow field is modeled at a scale larger than the size of the particles, where a grid cell typically contains $O(10^2) – O(10^3)$ particles, which are assumed to be perfect spheres (diameter *d*). This model consists of two parts: a Lagrangian code for updating the positions and velocities of the solid particles from Newton’s law, and a Eulerian code for updating the local gas density and velocity from the Navier-Stokes equation (Hoomans et al., 1996). The advantage of this Discrete Particle Model (DPM) is that it can account for particle-wall and particle-particle interactions in a realistic manner, for system sizes of about $O(10^6)$ particles, which is sufficiently large to allow for a direct comparison with laboratory scale experiments. As a logical consequence of this approach a closure law for the effective momentum exchange has to be specified, which can be obtained from the aforementioned lattice Boltzmann simulations. Note that in chemical engineering, to date mainly empirical relations are used for the friction coefficient $\beta$ (defined by (5)), such as the Ergun (1952) correlation for porosities $\varepsilon < 0.8$: