

14.03.2014 12:50

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Numerical study of the packing density of powders using the Discrete Element Method*Eric Parteli (FAU), Jochen Schmidt (FAU), Christina Blümel (FAU), Karl-Ernst Wirth (FAU), Wolfgang Peukert (FAU), Thorsten Pöschel (FAU)*

Numerical simulations by means of the Discrete Element Method (DEM) can provide a helpful tool in the investigation of the packing behavior of powders. In this type of numerical simulations, the Newton's equations of motion for every single particle in the system are solved by taking into account all forces and torques acting on it, both due to external fields and due to interactions with other particles in the system. However, in order to make reliable predictions of the behavior of the bulk from DEM simulations, an accurate physical modeling of the relevant forces governing the interactions between the particles is required. In the present work, we perform DEM simulations of polydisperse packings of glass beads using several particle size distributions, with average particle diameter $\langle d \rangle$ varying within the range between $6.5 \mu\text{m}$ and $56 \mu\text{m}$. The Open-Source DEM solver LIGGGHTS, which is widely used for simulating granular systems of viscoelastic particles, is extended in order to account for adhesive forces between the particles using the model of Johnson-Kendall-Roberts (JKR) as well as for non-bonded attractive inter-particle forces due to van der Waals interactions. We compare the values of packing density obtained in simulations with experimental data where packings of glass beads were generated using the same particle size distributions as considered in the simulations. We find that using only viscoelastic forces in the numerical simulations leads to a bulk density ϕ around 0.62 for all particle size distributions, while by further including adhesive forces, a smaller value of ϕ is obtained, which is around 0.5 and depends slightly on $\langle d \rangle$. This value of ϕ closely matches the packing density obtained in the experiments with average particle size larger than $20 \mu\text{m}$. Moreover, for this range of large particle sizes, the experimental values of packing density show a negligible dependence on $\langle d \rangle$, which is also in agreement with the simulation results. However, the experiments show that, in the range of particle sizes smaller than $20 \mu\text{m}$, the packing density becomes rapidly smaller for decreasing values of $\langle d \rangle$ — the packing produced in the experiment with $\langle d \rangle = 6.5 \mu\text{m}$ has a density of about 0.29. This behavior can be successfully reproduced in the simulations by further including van der Waals interactions between the particles. In this case remarkably good agreement between simulations and experimental data is obtained. We find that, while the inclusion of non-bonded attractive interactions has a negligible effect on ϕ for the samples with $\langle d \rangle > 20 \mu\text{m}$, the formation of large agglomerates within the packings with particle size below this range leads to a strong decrease in the value of ϕ as $\langle d \rangle$ becomes smaller, which is the situation observed in the experiments. Our numerical simulations can provide valuable insights into the relative significance of the different inter-particle forces governing the density of polydisperse packings of powder particles. In the future our simulations will be applied to investigate the packing density of powders made of particles of other materials, in particular of polymeric and metallic powders, as well as to study the effect of the particle shape on the density and structure of the resulting packings.