Modelling the viscosity of nanoparticulate suspensions via coupled CFD-DEM simulations

When it comes to the flow of suspensions, especially nanoparticulate suspensions, viscosity is one of the key parameters to characterize the system. It is an important product quality in both consumer goods and intermediate industrial products developed for many fields of applications. In recent years fiber-reinforced composites found increasing application in automotive and wind energy industries since they constitute a promising material for load baring structures at reduced weight compared to conventional materials. In order to improve their mechanical properties, nanoparticles are embedded in the polymer matrix. This however triggers an immense increase in viscosity, which impedes the resin injection into the fiber layers.

Until today, the origin of this viscosity increase is not fully understood. Analytical models derived for micro particle suspension fail to describe the observed viscosity increase and the few nanoparticle-related models developed base on empiric observations with little regard to physical fundamentals. Many researchers consider long ranging surface forces to be the cause of the deviating behavior of nanoparticulate suspensions from microparticulate systems, since the specific surface of nanoparticles is high, the specific number of particles per volume is extremely high and the distances between nanoparticles are already in close proximity to each other at low volume fractions. However, no modelling approach so far fully quantified the influence of surface forces on the suspension viscosity.

Therefore, the aim of this study was to set up a simulation environment that allows the predictive estimation of the viscosity of a nanoparticulate epoxy resin suspension and disclose the origin of the rheological behavior. This is why a contact model was implemented into the DEM code, which accounts for van der Waals forces acting between the particles within an epoxy resin. The open source software package CFDEM was used to run coupled CFD-DEM simulation in order to regard for the interaction of particles and fluid. A cubic unit cell with an edge length of a few micrometres was chosen as a representative volume from a laminar flow field. For the estimation of the suspension viscosity the fluids drag forces acting on the particle surface were considered. It can be shown that they increase proportional to the viscosity measured in shear viscosity experiments with nanoparticulate epoxy suspensions. From this, a model equation could be derived that allows the calculation of the viscosity based on the simulated drag forces and the volume fraction. If simulations were run without van der Waals forces the calculated viscosity resembles the behaviour of micro suspensions rather than nanoparticulate suspensions.