MODELING THE RHEOLOGY OF POLYMER DISPERSIONS USING GPU-ACCELERATED DISSIPATIVE PARTICLE DYNAMICS

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Polymer dispersions are in the interest of a large number of applications, such as the pharmaceutical industry, paints or plastics. The macro-scopic flow properties can be influenced by phenomena, which take place on much smaller spatial and time scales (the so-called *meso-scale*) and it is difficult to examine them experimentally.

We model the flow properties of polymer dispersions using Dissipative Particle Dynamics (DPD). It is a stochastic simulation method focused on phenomena, which take place on the meso-scale. DPD uses discrete elements that represent clusters of molecules of the specific matter. These elements then interact with each other to provide soft fluid interactions by conservative, random and dissipative force and the evolution of the element positions is governed by the second Newton´s law. For the evaluation of the viscosity from simulated data we use a stress tensor in a simple shear mode.

For simulations of larger systems we performed the code optimization and based the computing on the graphics processing unit (GPU). GPU provides strong parallelization possibilities to run the model on hundreds or thousands of cores, which leads to a rapid increase of the computation speed.

The model is able to simulate the reorganization of lamellar structures in a two-phase emulsion system and provides the time evolution of viscosity. In agreement with literature experimental data, the shear-thinning behavior was observed in a system containing oligomer molecules. Currently, the work continues on the validation of the results by experimental measurements and on further investigation of the broad spectrum of rheological phenomena occurring in polymer dispersions.