Fachbereich 4 Produktionstechnik Maschinenbau & Verfahrenstechnik





Master thesis: Influence of sample flow on the agglomeration behavior of nanoparticles in microgravity

Nanoparticle agglomeration is a fundamental process in material science, which can be employed as a bottom-up production approach to produce materials with well-defined structural properties. The morphology of agglomerates depends not only on specific interactions between the nanoparticles, but also on gravity. In previous microgravity experiments performed at ZARM, it was found that the mean hydrodynamic diameters of the agglomerates in microgravity are 3 to 5 times larger than on the ground (A. Pyttlik et al., Small 2022, 18, 2204621), which can be explained by a reaction-limited agglomeration process on the ground and a diffusion-limited agglomeration process in microgravity. However, the results may have been influenced by sample flow, resulting from the mechanism used to induce agglomeration.



In this master thesis, numerical simulations of fluid flow will be used to determine how gravitydependent sample flow influences nanoparticle trajectories and agglomeration. The Navier— Stokes equations will be solved together with an appropriate description, possibly Lagrangian, of the particle motions.

Requirements:

- Basic knowledge in computational fluid dynamics (CFD)
- Interest in material science

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Technical details:

Gravity can strongly affect the agglomeration of nanoparticles, for example by changing convection and sedimentation. In experiments, inducing the agglomeration process may involve sample flow, which adds an additional factor that influences the interaction between particles.

In previous experiments, the agglomeration of gold nanoparticles (core diameter of 7.8 nm coated with hexadecanethiol ligands) at a gold concentration of ~1 and ~3 mg mL⁻¹ in tetradecane was investigated under normal gravity conditions (1 g) and under microgravity ($\sim 10^{-6}$ g). The measurements were performed after a rapid temperature drop. For this, directly prior to the start of the experiments, a preheated sample (70 °C) with a volume of 3 mL was injected at a rate of 1 mL s⁻¹ into a pre-cooled cuvette (10 °C) from the top opening of the plug attached to the cuvette (see sketch). A dead volume of approximately 1 mL remained in the tubing, so that the final sample volume was 2 mL. The agglomerate size was measured at the position of the blue dot. More details on the setup are given in A. Pyttlik et al., Microgravity Sci. Technol. 2022, 34, 13. It was found that the mean hydrodynamic diameters of the agglomerates formed after 8 s in microgravity are 3 times (for ~1 mg ml-1) to 5 times (for ~3 mg ml-1) larger than on the ground (A. Pyttlik et al., Small 2022, 18, 2204621). The observations point to a reaction-limited agglomeration process on the ground and a diffusion-limited agglomeration process in microgravity.

This master thesis will focus on the question how gravity-dependent sample flow, caused by inserting the sample into the cuvette, influences nanoparticle agglomeration, investigate by means of simulations.



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