University of Stuttgart
Institute for Combustion Technology (ITV)

Bachelor or Master Thesis

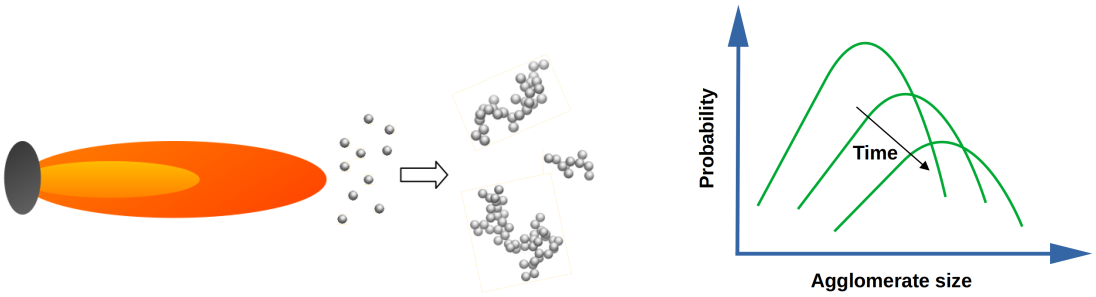
Statistical modelling and simulation of nanoparticle agglomeration

Motivation

Agglomeration of small particles is an important growth mechanism in many industrial and natural processes. It plays an essential role during the formation of soot and the production of flame-made commodities like fumed silica or titania which are used, for example, as agents in the food-processing and pharmaceutical industry. As the shape and size of the forming agglomerates determine the product characteristics, it is desirable to develop suitable models that help predict and control the growth dynamics in these processes.

Project description and research goals

The goal of this project is to conduct detailed particle simulations with the OpenFOAM library. The simulation tool allows the tracking of individual particle trajectories and a collision detection routine is used to identify agglomeration events where approaching particles are connected to form complex, non-spherical clusters over time (see Fig. 1a). As a consequence, a polydisperse size distribution develops as illustrated in Fig. 1b. Modelling the temporal evolution of this agglomerate size distribution and identifying the controlling parameters are the focus of this research project.



(a) (b)

Figure 1: Formation of agglomerates in a flame (left) and evolution of agglomerate size distribution (right)

Tasks

- Perform a literature review on nanoparticle agglomeration and modelling strategies
- Simulate the agglomeration process of monodisperse nanoparticles
- Assess the effect of environmental conditions, material properties and numerical models on agglomeration dynamics
- Evaluate and analyze the simulation results
- Write a thesis and present your results

Prerequisites

- Basic knowledge in fluid dynamics, programming with Matlab, Python or similar
- Beneficial: knowledge in C/C++, experience with computational fluid dynamics (CFD) and molecular dynamics (MD), OpenFOAM

Contact

If you are interested, feel free to contact:

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