PROJECT IN MODELING OF CRYSTALLIZATION

Start: Autumn 2019 (HS19)
Due date: To be defined (6 months)
Breakdown: 100% modeling
Deliverable: Semester project report or Master thesis, two oral presentations
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Title: Development and implementation of models for crystallization phenomena

PROJECT DESCRIPTION

Crystallization is the outcome of complex interplay of several mechanisms, namely, growth and dissolution due to size dependent solubility, nucleation, particle agglomeration, and breakage. All the fundamental crystallization phenomena can be described with a complex model, in which the crystal population is mathematically described by a particle size distribution (PSD) [1].

Population balances, i.e. systems of partial integro-differential equations (PDE), are widely used to simulate crystallization processes, as they track the change in the PSD in a control unit [2]. In most cases, the analytical solution of the PDE is intractable. For this reason, on the one hand, several studies and research activities focus on the method to solve and on the solution of the population balance equations to describe processes in which the most common mechanisms are present [3].

On the other hand, when multiple crystal populations are present in the system, and in some cases even interaction is possible between them, the solution of the resulting system of equations becomes complicated. Industrially relevant examples dealing with multiple populations are polymorphic [4] or enantiomeric transformations [5], where only one of the two populations is desired. Solid-state deracemization is a novel technique that converts mixed racemic crystals into enantiomerically pure crystals with the aid of a racemizing agent, and its mathematical model has been recently developed in our group [5, 6].

The goal of the project is to develop a complete overview of crystallization models. In particular, novel, physically consistent mathematical expressions have to be derived and implemented for problems like solid-state transformations, nucleation, breakage, and agglomeration. The starting point will be the existing models developed in the group, and a deep understanding of the mechanisms is necessary to improve and further develop them. The student will be asked to suggest and develop physically sound models for the above mentioned
phenomena and he/she should also be able to implement a numerical method, or a set of numerical methods, to be able to solve the PDEs.

In this context, the student’s task may comprise of:

- Literature review on the different numerical methods adopted to model crystallization
- Familiarize with the models developed in the group
- Model development, based on physical principles, to simulate specific crystallization phenomena
- Selection of numerical methods (or a combination of techniques) to model the chosen crystallization process.

We are looking for highly motivated students, who are able to work independently, and have great interest for process modeling and technology.

Please, send your CV and transcripts of records to bodak@ipe.mavt.ethz.ch or bosettil@ipe.mavt.ethz.ch

REFERENCES


