Laboratoire
d'automatique,
de génie des procédés
et de génie pharmaceutique

Université Claude Bernard Lyon 1 – UMR CNRS 5007 – ESCPE Lyon

Postdoctoral offer – 1 year - LAGEPP
Modelling of membrane crystallization process: Coupling of Hydrodynamics and Population balance

Keywords: modelling, CFD-Population Balance coupling, membrane crystallization process.

Context of the research: This study is a part of an ANR JCJC Project named ICARE. It follows experimental results obtained during a PhD study.

Scientific context:
Crystallization/precipitation of a compound occurs under a modification of temperature and/or composition (solvent evaporation, add of an antisolvent, seeding…) of a supersaturated solution. Hence, the fine control of the heat and/or mass transfer is a key parameter of the process.
Membrane processes are considered as one of the most promising technology to develop an intensified process (decrease of size/cost, increase of the production/purity…), continuous and easy to extrapolate, allowing a fine control of the hydrodynamic and the heat/mass transfer. The use of a dense membrane (non-porous) could mitigate membrane fouling while keeping the advantages of membranes-based technology. Nevertheless, this process remains relatively unexplored and tackles a major scientific challenge: predict crystallization mechanisms, location in/on the dense polymer material used in continue.
One of the main challenges of the modelling strategy is to predict the crystal size distribution as a function of the operating conditions. Population balance-based models are already developed in LAGEPP for a batch reactor but they consider mean hydrodynamic properties. The challenge is here to consider the spatial heterogeneity of the hydrodynamic properties of the process.

Purpose of the study: The aim of the study is the development of a mathematical model which takes into account the local interaction between hydrodynamics and the dispersed phase in order to predict the final properties of the crystals.

Work program:

- Population balance model development in the case of a crystallization process (using e.g. Matlab).
- Computational Fluid Dynamics of the process (using e.g. Comsol Multiphysics®).
- Population balance model-hydrodynamics coupling.
- Comparison between the numerical predictions and the experimental available results.

Place and duration of the study: Lyon 1 University, Laboratory of Automatic Control, Chemical and Pharmaceutical Engineering (LAGEPP), Doua Campus, Villeurbanne – 1 year.

Gross salary: 2380 € /month. Position to be filled quickly (at most in January 2021).

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Profile required: PhD in Process Engineering or Fluid dynamics. Profile in simulation and modelling.

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