Research Internship

Compartmental-based approach for the modelling of oxalic precipitation

Location: UCBL1 https://www.univ-lyon1.fr/
Host laboratory: LAGEPP (https://lagepp.univ-lyon1.fr)/ Département de Recherche sur les Procédés pour la Mine et le Recyclage du Combustible - CEA (https://www.cea.fr/marcoule)

Supervisor(s): Camilo RUIZ (PhD candidate), Denis MANGIN (Prof.), Noureddine LEBAZ (Ass. Prof.) Murielle BERTRAND (CEA researcher)

Scientific Domains: Applied mathematics (numerical analysis), Chemical Engineering (crystallization), Process Engineering (unit operations modelling).

Research project

Nuclear fuel cycle includes a recycling step: spent fuel undergoes physicochemical and mechanical treatments in order to recover remaining fissile materials and send them back to the exploitation step. A critical unit operation in the used fuel treatment is the separation and purification of unreacted actinides. At industrial scale, this is achieved by oxalic precipitation.

During crystallization/precipitation, the solid phase properties evolve both in time and space depending on operating conditions and the local environment characteristics. The modelling of this dynamic process is generally achieved through the population balance framework which consists of a set of partial differential equations. However, because of the spatial heterogeneities occurring in the reactor, a spatial discretization is further needed to get access to the local hydrodynamic properties. This is achieved through Computational Fluid Dynamics (CFD). Coupling the population balance equation with CFD is computationally expensive and numerically tricky. Hence, an alternative to this approach is the use of a coarse spatial discretization consisting of few homogeneous interconnected compartments which reproduce the global flow characteristics. The population balance equation is then solved in each compartment and transported through the different zones.

The general objective of such modelling approach is the prediction of the particle size distribution (PSD) of the crystals at the outlet of the reactor depending on the operating conditions. For this, in a first step, the modelling of one homogenous compartment (referred to, in industrial crystallization, as Mixed Solution Mixed Product Removal crystallizer) will be carried out. This will take into account different phenomena such as nucleation, crystals growth and aggregation with respect to the principles of chemical reactions, solid-liquid equilibria and population/mass balances. In a second step, the model will be implemented in a more complex configuration: the interconnected compartments grid. Optimization procedures as well as convergence analysis will be studied in order to test the robustness of the modelling approach. The model prediction capabilities will be compared to experimental results already available.

Duration and remuneration: 5 to 6 months with an allowance of 546 € net per month. It has to be made during the year 2021.

Required profile: Master degree or equivalent in Process Engineering, Numerical Analysis or Applied Mathematics. Advanced skills in programming are required (e.g. Matlab, Python)**.** Proficient level on one of the following languages: French and/or English.

To apply: Send CV and cover letter to camilo.ruiz@etu.univ-lyon1.fr