



Advanced Prediction and Identification to Crystallization Enhancement

APICE

Project Initiator(s)

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Project context

The aim of the project is the prediction of the crystallization performances by using historical data available in chemical industry. The project aims to design the crystallization operation for a novel molecule utilizing artificial intelligence technique. The model will be able to predict crucial parameters for the process (e.g. the maximum amount of impurities allowed and the shape of the crystal in the various scenarios).

Innovation goal

The goal of the project is the design of a crystallization process of a novel molecule by minimizing the amount of the experiments required in the lab. Furthermore, the same model will be able to predict the performances of the crystallization process executed on the production line. This will be executed utilizing artificial intelligence techniques, such as graph neural networks. Nowadays, the predictions of the crystallization performances are executed utilizing kinetic rate equation and population balance. However, these techniques are poorly scalable to the plant due to the presence of reality-gap. In addition, they require high amount of experiment for the investigation of the process, and they poorly utilize historical data about previous molecules. We propose the integration of these techniques with artificial intelligence for the creation of a hybrid model able to reduce the amount of experiments during the design phase and able to be utilized in real-life production as operative tool.

Requested expertise

We are looking for two main partners. The first one is a chemical or pharmaceutical company with a large availability of historical data about production and previous molecule crystallization. The ideal scenario is the case where this company is developing a new process for a new molecule. This will be the case study. The other partner is a knowledge institution with expertise in process control utilizing AI techniques (e.g. reinforcement learning). In this way we can integrate the model to create an optimal control for the operation in the various scenario.