Growth rate of silica particle in a continuous reactor with Computational Fluid Dynamics and Population Balance Modelling

A. Finzi, S. Calvo and D. Toye
1. University of Liège, Department of Chemical Engineering – PEPs, Belgium
Quartier Agrara - B6C, Allée du Six Août - 15, 4000 Liège, Belgium
*Contact: amirhossein.finzi@uliege.be

Introduction

FLOWSOIL is a collaborative project within the framework of the ERDF program (Project portfolio INTENSE4CHEM), which aims to intensify the synthesis and manufacturing of Alumino-Silicate materials (e.g. Zeolites). The project globally looks on the whole process from synthesis to crystal formation, crystal growth and drying (Figure 1). Three research units are involved in this project: 1. Cerctech defines the optimal conditions (concentration, pH, temperature,...) of synthesis and formation of first crystals; 2. At UULiege – group PEPs, the study focuses on the innovative design of a continuous reactor in which the crystal growth will occurred; 3. The operations related to the shaping and drying of the crystals are intensified at UCL - IMAP.

Currently, soluble production is based on hydrothermal processes performed under controlled condition (temperature and pressure). The crystal properties are adjusted by adjusting crystallization parameters including reaction duration and reactant concentrations [2].

Crystalisation process of zeolites is most often carried out in batch stirred tank reactors which causes many limitations in term of productivity and operating cost. Thus, a way to overcome these drawbacks, is to switch the process from batch to continuous which has several advantages including more reliable reaction control, saving energy and reducing the impact on the environment.

In the present work, the growth of silica nanoparticles (as a particle model for zeolites) is analysed in a continuous 2D reactor with the objective of optimizing the process via the coupling between all major phenomena occurring within the reactor.

Process Description & Case Study

- A typical crystallisation process consists in two steps: the first step is nucleation, during which a crystalline phase (i.e. nuclei) is formed from a supersaturated suspension of dissolved molecules. In the second step, the crystal size in the suspension is further increased to a desired value (i.e. growth step) [2]. Although it is not possible to completely separate the nucleation and growth processes, it is possible to choose operating conditions such that one of the reacting steps is favoured, such that the 2 steps may be successively conducted in two distinct reactors; in the first reactor crystals are produced (Figure 2-a) and then they are supplied to the second reactor for the further growth (Figure 2-b).

- Particle Size Distribution (PSD) is an important property of crystallization quality and is aimed to be controlled in this process. Therefore, Population Balance Model (PBM) is applied to predict the PSD subject to particle growth and various hydrodynamic conditions found in continuous reactor.

RESULTS

II. Hydrodynamic: Laminar Flow

- The influence of hydrodynamics on the PSD was investigated in laminar flow conditions and different inlet flow rates (i.e. different average residence times).

- The final PSD for two different residence times under the laminar flow conditions were simulated and compared (Figure 5), logically the average particle diameter got bigger and the PSD became larger when the residence time increased.

- Figure 6 illustrates the effect of pseudo plastic viscosity on velocity profile (a) as well as on PSD (b).

CONCLUSIONS & PROSPECTS

CONCLUSIONS

- A continuous crystallization process in a 2D configuration was simulated using CFD-PBE model which enables us to successfully follow the evolution of particle size through the reactor under different conditions.

- Numerical investigations were carried out and results were compared to theoretical values.

- The effect of non-Newtonian viscosity was investigated and its impact on the velocity profile and on PSD was analyzed and presented.

- Despite the need for more details on process, this important feature helps to understand the particle distribution and growth as a function of residence time and viscosity.

PROSPECTS

As future investigations, it is planned to account for more phenomena in numerical simulations to complete the model and improve the results:

- Apply crystal growth depending on supersaturation level and temperature.

- Establish the coupling between particle growth, hydrodynamics and fluid rheological behavior.

Acknowledgement

The authors gratefully acknowledge the support of Wallonia region and European Regional Development Fund (ERDF).