CFD investigation on 3D printed reactor for hydrothermal synthesis of Beta zeolite

S. Calvo[1*], A. Firozi[1], P. Eliaers[2], J.-C. Lemaire[2], F. Collignon[2] and D. Toye[1]

1 University of Liège - Dpt. Of Chemical Engineering - PEPs group, Liège, Belgium; 2 Certech, Seneffe, Belgium

**Sébastien Calvo: scalvo@ulg.ac.be*

Highlights

- Continuous hydrothermal synthesis of Beta zeolite.
- CFD characterization of hydrodynamics and heat transfer.

1. Introduction

Hydrothermal synthesis or treatment of solid particles is a process widely used by chemical, pharmaceutical and agrifood industries. This process is carried out most of the time in a mechanically stirred batch reactor. Operating such large batch reactors causes limitations in terms of working pressure and processing time, particularly during the feeding, heating, cooling and discharging steps. In addition, the extrapolation of this type of system at large scales leads to significant investment costs (double envelope thickness). Recently, some research has shown the potential of continuous processing to overcome these drawbacks [1-3]. These processes are mostly carried out in tubular reactors, well adapted to high pressure and high temperature. Pressure may be maintained while working in flow thanks to a back pressure regulator. The dead times referred above can thus be avoided. However, slurry flow is observed in these apparatus. Providing sufficient mixing to ensure homogeneous distribution of solid particles that settle easily in the liquid medium is thus not straightforward. In fact, while efficient mixing is obtained through the motion of the impeller in batch reactor, mixing in continuous reactors comes either from the turbulence of the flow itself or from the use of static mixers or oscillatory flow reactors. The turbulence of the flow could also be increased by raising the flow rate, but to the detriment of the residence time in the reactor. Drawing the reactor geometry in order to create sufficient turbulence may be a good way to ensure particles homogeneity through the reactor. Recent advances in 3D printing allow creating complex geometries in a wide range of materials. Nevertheless, in order to perform high temperature and pressure hydrothermal synthesis, such devices may be characterized not only in term of hydrodynamic and heat-transfer but also in term of robustness to ensure its rigidity when processing at high temperature and pressure. The Use of CFD may allow to fully characterize the hydrodynamic and thermal transfer through the geometry [1] and allow to compute pressure endured by the device during the process.

2. Methods

A schematic view of the hydrothermal synthesis of Beta zeolite is shown on Fig. 1. In this study, the 3D printed reactor (Fig. 1) developed by Certech is numerically characterized using CFD. This reactor consists of 44 superposed horizontal channels (22-22 stages) and works as a plate reactor, i.e., slurry is fed at the bottom and flows one out every two stages when oil with a controlled temperature is flowing from the top (counter-current) through the other stages to ensure the heat transfer (Fig. 2).

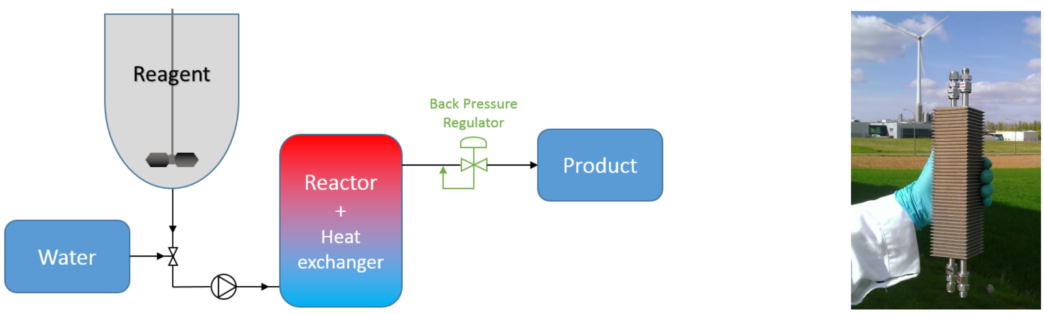
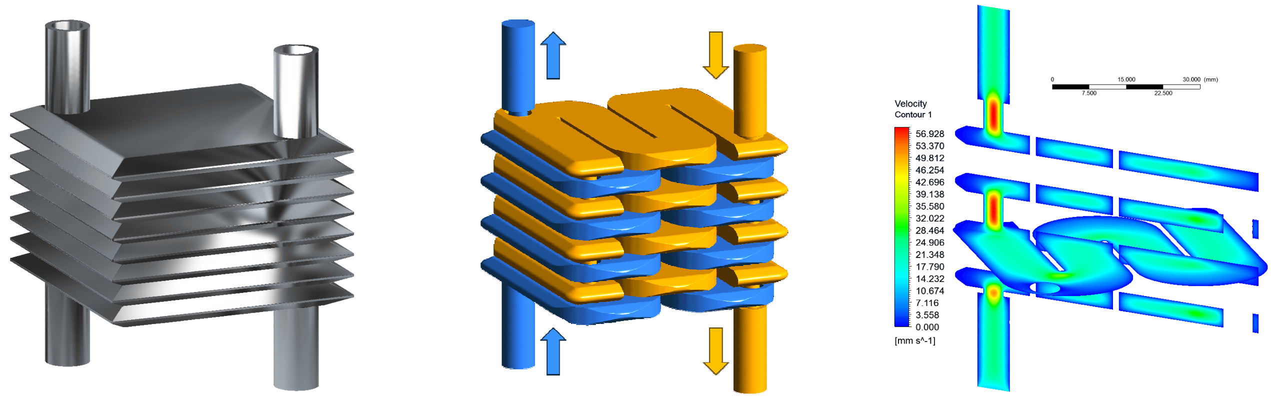


Figure 1. Beta Zeolite process; 3D printed reactor (22-22 stages).

A simplified geometry (4-4 stages reactor) has been modeled (Fig. 2) using Design modeler from ANSYS in order to save computational time. A first set of simulations has been performed through the reactor considering the slurry as water in order to validate the model against experimental data obtained in the same conditions. Thermal properties of the slurry (water), the oil and stainless steel have been taken into account in order to compute heat transfer through the reactor. The simulation has been carried on Fluent (18.2). Laminar flow has been considered with no slip boundary condition.

Then the properties of the slurry have been modeled to performed simulations with process operating conditions.



(a) (b) (c)

Figure 2. CFD geometry/results: (a) stainless steel reactor; (b) reactor internals: blue: slurry channels, yellow: oil channels; (c) contour of velocity of the slurry phase

3. Results and discussion

The results of the first simulations were compared with the experimental data in order to validate the model. The obtained results in process condition were analyzed to quantify the efficiency of the 3D reactor in terms of mixing and heat transfer. The pressure drop has also been quantified to account for the mechanical stresses undergone by the system.

4. Conclusions

CFD simulations showed the potential of the 3D printed reactor. Further simulations must be carried out taking into account the solid phase in order to evaluate the performance of the system as regards the distribution of the suspension.

The coupling of 3D printing with CFD appears to be a useful tool for designing and optimizing continuous reactors used in the intensification of hydrothermal synthesis processes.

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Keywords
Hydrothermal Synthesis; 3D printed reactor; CFD

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