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Comparison of CFD simulation and PIV measurement of a new reactor for hybrid catalysis.

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1. Introduction

The use of enzymes in fine chemistry has been the subject of much research in the last decades. Among these works the concept of **hybrid catalysis** has recently emerged: the coupling of conventional chemical catalysis with enzymatic catalysis [1,2]. The aim of the GLYCYBRIDE project, on which this study is based, is to develop a synergy between enzymatic and heterogeneous catalysis in a one-pot reactor with the end-application of transforming glycerol into value-added chemicals.

The feasibility of a model one-pot reaction in three-phase hybrid catalysis, one step being an oxidation has been shown [3]. The model reaction proposed is a two-step reaction: an enzymatic catalyzed isomerization of fructose to glucose followed by a heterogeneously catalyzed oxidation of glucose to gluconic acid.

2. Methods

The hydrodynamics of the reactor has been characterized by physical methods such as: k_La of O_2 measurement (dynamic method with O_2 probe), mixing time measurement and RTD (NaCl used as a tracer). PIV velocity measurements have also been performed to determine the velocity of the flow field in the different areas of the reactor.

A CFD modeling of the hydrodynamics and thermal behavior of the reactor has been carried out with the Fluent© software (Ansys) using the realizable $k-\varepsilon$ turbulence model associated to Multiple Reference Frame model to deal with rotating parts [4].

Particle Image Velocimetry (PIV) experiments have been run at different stirring rates using PCO CMOS Camera synchronised with an acquisition system (Lavision System Davis). A low frequency (10 Hz) Nd Yag Laser was used. Fluorescent particles are used to minimized reflexions in our geometrically complex installation. They have a diameter around 10 µm [7].

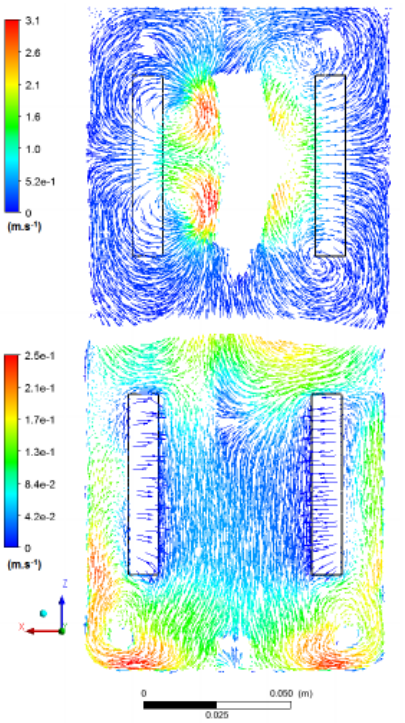
3. Results and discussion

Values of kLa between 0.02 s^{-1} and 0.035 s^{-1} are measured, consistent with values of single basket reactor reported in the literature. Mixing times of 15 to 20 s are observed for stirring rates above 500 rpm, in good agreement with the one calculated by CFD simulation. RTD measurement showed a behavior very close to the one expected for an ideal CSTR.

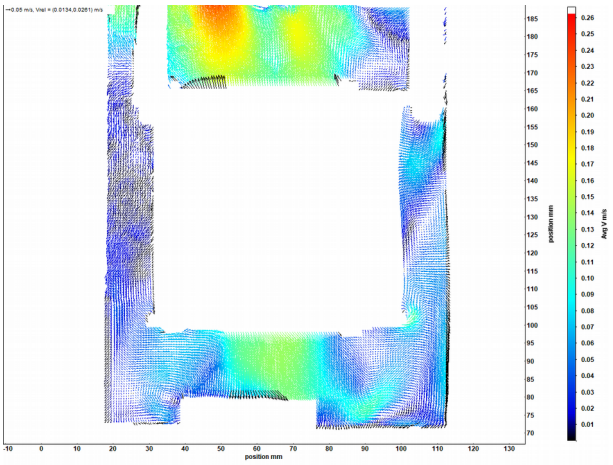
The CFD simulation provided the values of velocities in the different parts of the reactor, with velocities reduced in the basket holding the catalysts as expected (Fig. 1a). These values are discussed in relation with the experimental one derived from PIV measurements (Fig. 1b).

Figure 1. Flow fields on a vertical plane at y = 0 cm. Vector length is normalized. Stirring rates at 1100 rpm for the impeller, 300 rpm for the magnetic bar:

a) CFD simulation



b) PIV measured 2D-velocity field



The measured and predicted velocity were compared. PIV visualisation are restricted to area of interest outside the catalytic basket. Nevertheless flow rates could be evaluated in different zones as the zone between wall tank and basket or zone between upper basket and lower basket.

Computed or measured mean recirculation zones are clearly similar. Some discrepancies exist which could be clearly affected to the difference existing between the real tank and the geometry used for numerical simulation. Location of the lower magnetic barrel is also a possibility of error due to the difficulty to exactly localized the center of the magnetic influence at the exact center of the cylindrical tank. Nevertheless results are surprinsingly very close both for mean and turbulent quantities.

4. Conclusions

A novel double-basket reactor designed for hybrid catalysis has been first characterized for its physical transfer properties such as k_L.a, mixing time and RTD and simulated using CFD. Values of k_L.a measured are consistent with values of single basket reactor reported in the literature. The CFD simulation provided the values of velocities in the different parts of the reactor which have been compared with PIV measurements. The mixing time obtained by simulation are similar to the experimental ones. Interesting analysis could be now conducted comparing the momentum exchanges existing between the different zones of interest where reactive mechanisms have to be specific.

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