PORE SCALE CFD SIMULATION TO INVESTIGATE TRANSPORT PHENOMENA IN MULTIPHASE CATALYTIC PACKED-BED REACTORS

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Designing chemical reactors in chemical engineering typically involves extensive lab-scale experimentation, often with significant consumption of catalysts and reagents. To reduce these costs, experimental setups are miniaturized. However, smaller systems amplify the influence of transport phenomena, particularly in packed beds when the ratio of reactor diameter to particle size is small, thus intensifying deviations from laboratory to industrial scale.

To better capture the interplay of transport and reaction, computational fluid dynamics (CFD) at the pore scale enable simulation of actual geometries. A practical application is aqueous phase reforming (APR), which generates hydrogen from wastewater at moderate temperatures (220–270 °C) and employs a fixed-bed reactor containing catalytic particles. The goal of this work is to use CFD to investigate how catalyst geometry influences reactive transport and reactor performance.

A 3D representation of the catalyst packing was created using Blender, based on real catalyst fragments. Initial simulations focused on the dispersion of an inert species in a single-phase flow to highlight geometry-induced flow anomalies such as bypasses and stagnant zones. OpenFOAM was used to solve the mean age transport , that represents residence time in the domain.

Subsequently, experimental tests were carried out in a perfectly mixed batch system, where the absence of transport resistance is ensured. From this data, a kinetic model for glycerol APR was developed by fitting the experimental data as shown in Figure 1 a).

The kinetic model thus developed was implemented in OpenFOAM to simulate, through reactive pore scale CFD, the performance of a packed-bed reactor as shown in Figure 1 b) and c). The reactions were implemented as a boundary condition in the catalytic external surface, and fluid flow is considered only outside the catalyst. This methodology was then also compared to a more accurate model that resolves also the species transport inside the catalyst, increasing the accuracy of the simulation, at the cost of increasing computational expense and numerical instability.

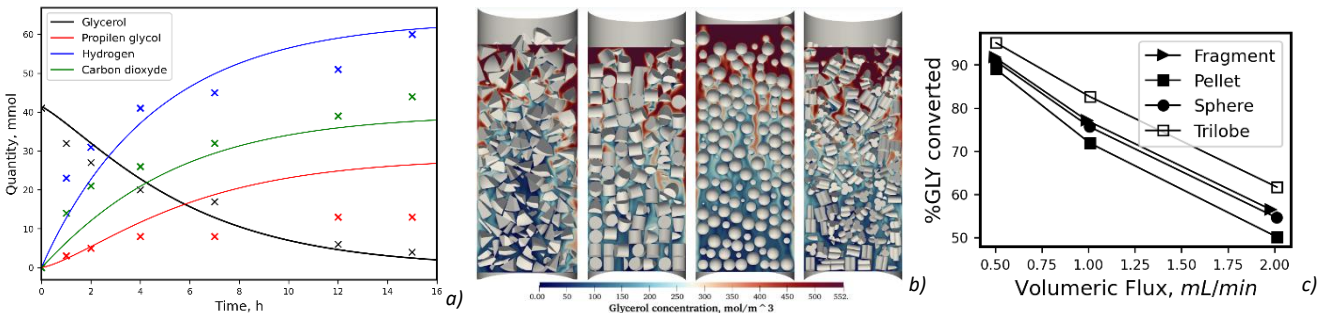

Figure 1: a) Experimental fitting to obtain the kinetic model. b) Contour plot of the glycerol concentration. c) Glycerol conversion at different condition

Keywords: Computational Fluid Dynamics, Aqueous phase reforming, catalytic Packed-bed reactor.

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