Institut für Chemieingenieurwesen
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Bachelor/Master Thesis, Research Internship (**Chem. Eng.**):

Mass transfer modeling and simulation of soft matter immobilized photocatalytic water splitting in an annular fluidized-bed reactor

Research background:

The main obstacle of scaling up photocatalytic processes is related to designing effective photoreactors. There are two types of reactors based on the type of catalytic particles. One type is a reactor with suspended catalyst particles, while the other one is a reactor with catalyst fixed on some materials, such as glass beads, ceramic foam, etc. Additional need to separate catalyst particles from photocatalytic products is the main flaw of using suspended catalysts [1]. Therefore, focus on immobilized materials has been a growing research interest on photocatalysis.

One of the key influential factors in assessing the photocatalytic effectiveness is the mass transfer rate. In other words, to design an effective photocatalytic process, it is necessary to design a photoreactor which can enhance the mass transfer. For immobilized photocatalyst, both external and internal mass transfer influence the reaction rate [2]. External mass transfer rate determines how fast the reactant reaches the catalyst surface, while internal mass transfer rate controls the diffusion rate of reactant within the porous catalyst film. Consequently, both external and internal transfer need to be considered to study the mass transfer effect and optimize the reaction progress by reaction engineering means [3].

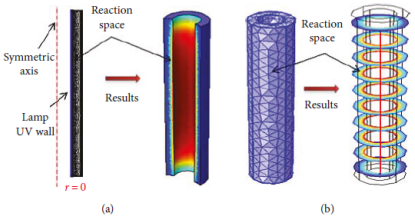

Figure 1: *Graphical representation of an annular photoreactor and geometry in COMSOL Multiphysics: (a) four-flux model, (b) discrete ordinate method [4].*

Current work and possible working packages:

In order to elucidate the influence of reaction engineering parameters, in this study, soft matter immobilized photocatalysts are studied with respect to the interaction with the mass transport phenomena in photocatalytic water splitting process by modelling and simulation. There are many parameters which influence mass transfer rate during the photocatalytic reaction, such as water input flow rate, irradiation rate, photocatalyst load amount, etc.[4] To study the influence of these parameters on mass transfer rate, different operating conditions will be theoretically investigated and the results will be compared to have a better and clearer understanding of mass transport phenomenon.

References

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[2] D. Chen, F. Li and A.K. Ray, *Catal. Today* **2001**, 66, 475-485.

[3] F. Guba, Ü. Tastan, K. Gugeler, M. Buntrock, T. Rommel and D. Ziegenbalg, *Chem. Ing. Tech.* **2019**, 91(1-2), 17-29.

[4] O. Alvarado-Rolon, R. Natividad, R. Romero, L. Hurtado and A. Ramírez, *Int. J. Photoenergy* **2018**, Article ID 1678385.

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