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CFD study on hydrogen peroxide production in a gas – liquid vortex reactor

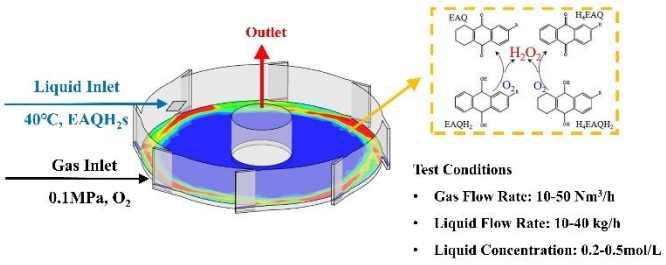
Aim

This thesis aims to investigate the feasibility of using a vortex reactor[1] (VR) to intensify hydrogen peroxide (H_2O_2) production via computational fluid dynamics (CFD) simulations. This work will identify the optimal operating conditions to achieve higher transfer–reaction efficiency and provide guidance for industrial scale–up.

Justification

Hydrogen peroxide (H_2O_2) is an important oxidant and oxygen carrier with wide applications across various industries. In the industrial anthraquinone (AQ) process for hydrogen peroxide production, the oxidation of alkyl anthrahydroquinones ($EAQH_2$ and H_4EAQH_2) with O_2 is a key step that is strongly limited by mass transfer, due to the low solubility of O_2 in the organic solution[2]. Therefore, the selection of a gas-liquid mass transfer intensified reactor is crucial. Conventional stirred tank reactors (STRs) are inefficient for such transfer–reaction systems, and while rotating packed beds (RPBs) can enhance interfacial area under high–gravity conditions, their reliance on high–speed mechanical rotation poses challenges for operational stability and scale–up[3].

In recent years, VRs have attracted attention as intensified contactors for gas–liquid systems[4]. By generating strong swirling flows through static geometries, VRs can enhance turbulence and interfacial area without mechanical rotation, indicating advantages for gas–liquid mass transfer process. This thesis employs CFD to validate the feasibility of applying VR to the H_2O_2 oxidation process. First, a CFD model that takes hydrodynamics, mass transfer, and reaction kinetics into account will be validated. Then, the resulting framework will then be used to assess reactor performance under different operating conditions and to identify an optimal operating window, thereby providing guidance for industrial scale–up.



Vortex Reactor for H_2O_2 Production

Program

- A literature study on H_2O_2 production and possible process intensification approaches.
- Gain proficiency in commercial software ANSYS Fluent
- Develop a CFD model for transfer–reactive process of H_2O_2 in the VR
- Feasibility assessment of the application of VR in H_2O_2oxidation process
- Optimize operating conditions and reactor design for efficient mass transfer and reaction

1. Yi Ouyang et al. WO/2025/003397.
2. Wang, et al. Chemical Engineering Journal. 2022, 428:132066.
3. Wang, et al. Reaction Chemistry & Engineering, 2025, 10(7):1473–1486.
4. Ouyang; et al. AIChE Journal. 2022, 68:e17608.

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