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A Mathematical Model of a Slurry Reactor for the Direct Synthesis of Hydrogen Peroxide

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1. Introduction

Hydrogen peroxide is a key compound in the sustainable chemical industry. This reactant has many applications in textile, pulp/paper, wastewater treatment and chemical industries, or even in soil remediation, disinfection and sterilization processes. It is a powerful, attractive and versatile oxidizing agent due to its "green" nature. Indeed, it decomposes to water and oxygen only, which gives it an exceptional pollution control ability and significantly decreases the end user waste disposal cost [1]. Actually, hydrogen peroxide is produced by the anthraquinone auto-oxidation (AO) process, where it is formed via two-step process on an organic carrier molecule [2]. Although this conventional process is a well-proven and reliable operating technology and it has been the dominant method of H_2O_2 production since the middle of the twentieth century, it has several important drawbacks [3]. A direct synthesis (DS) of hydrogen peroxide in the presence of a catalyst and a solvent seems to be the best option, merely because in theory it is exceptionally easy: by just combining one molecule of hydrogen with one of oxygen and having water as only by-product. The aim of this work is the formulation of a mathematical model for the direct synthesis of hydrogen peroxide in a continuous catalytic three phases reactor. The process is realized with a once-through flow of slurry made up of the solvent, namely water, and the catalyst, e.g. a supported catalyst in which the active element consists of Pt (or Pd).

2. Methods

Fluid dynamic aspects of the system have been studied, along with kinetics and interphase mass exchange. In our conditions, the gas/liquid mass transfer was prevailing, thus the reactor was working in the convective mass transfer regime. Model equations have been written and implemented in order to lead different simulations and obtain a first dimensioning of the reactor. It should be underlined that the definition of a model can constitute a step forward the opening of the industrial world doors to the H_2O_2 direct synthesis, turning this process to an effective industrial production. The reactor in this case study basically consists of two segments. In the first one hydrogen is adsorbed onto the catalyst, while in the second one oxygen is adsorbed.

3. Results and discussion

The number of segments and the length of each of them allow us to determine the space necessary to complete the fueling gas adsorbing process. The length depends only on the mass transfer coefficients, in particular the gas/liquid one. Results for the baseline simulation are illustrate in Figure 1, showing the evolution of the gas hold-up in the different reactor segments. Different boundary conditions have been changed (such as the bubble dimension or the pressure) in order to observe the overall effect on the final results.

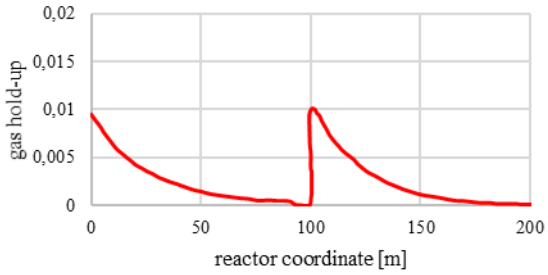

Figure 1. Gas hold up change in the baseline simulation. Two-segment reactor, d_b=1500 μm, P=150 atm.

4. Conclusions

The simulations that have been carried out show the feasibility of a process based on direct synthesis of hydrogen peroxide. If the reactor size is properly designed it is possible to obtain a certain productivity, in particular:

- The length of each segment depends basically on the interphase mass transfer efficiency, being that the stage that kinetically controls the process is the gas/liquid mass transfer.
- The diameter of the reactor depends on the flow dynamics and stability of the bubble motion.
- The number of segments depends on the amount of gas that can be adsorbed by the catalyst, a function basically of the amount of catalyst dispersed and its loading capacity.

References

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