Determination of mass transfer resistances in trickle bed reactors

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Highlights

- Predictions of mass transfer resistances in 3-phase mechanically agitated reactors using a genetic algorithm.
- Modelling of 3-phase mechanically agitated reactor.
- Determination of mass transfer resistances in trickle bed reactor.

1. Introduction

Gas-liquid-solid three-phase reactors are of great importance in pharmaceutical and fine chemical industry. Although hydrogenation reactions in presence of metal catalyst would benefit in terms of the required reaction time, hydrogen and solvent amounts [1], the mechanically agitated slurry reactors are still the most common type of three phase reactors which are used within these industries [2]. During the three-phase reactions a number of mass transfer processes need to take place before the surface catalytic reaction. Each of the mass transfer processes and the intrinsic reaction rate affect the overall process rate in different extent. The objective of this article is to present a methodology of determining the mass transfer coefficients in TBR combining experimental results from batch and continuous flow.

2. Methods

We develop a genetic algorithm to determine the mass transfer resistances of a batch mechanically agitated reactor based on the concentration profile of styrene during its hydrogenation over Pd/C. Given, the results from the genetic algorithm, we tune the experimental variables (i.e. agitation speed, hydrogen pressure, catalyst loading and temperature) in such a way to be in reaction limited regime. Once we have tuned the variables and the process is limited by the intrinsic reaction rate, we feed the genetic algorithm with the concentration profile of styrene obtained under reaction limited experimental conditions in order to determine the mass transfer resistances and the intrinsic reaction rate constant.

To determine experimentally the mass transfer resistances and compare with the algorithm predictions we use the proposed methodology of Stamatiou and Muller [3]. Briefly, this methodology consists of two sets of experiments; at the first set, we conduct several reactions by changing each time the catalyst loading in the reaction mixture while we keep the same the hydrogen pressure and the agitation speed. At the second set of experiments, we conduct several reactions by changing the hydrogen pressure while we keep constant the catalyst loading and the agitation speed. We make two plots; at the first, we plot the overall resistance with respect to catalyst loading reciprocal to determine the resistance related to gas-liquid mass transfer. At the second, we plot the overall resistance with respect to the square root of hydrogen concentration to determine the resistance related to the intrinsic reaction kinetics.

$$\Omega_{tot,BR} = \frac{1}{k_L \cdot \alpha} + \frac{1}{k_s \cdot \alpha_s} \cdot \frac{V_L}{W_c} + \frac{1}{\varepsilon \cdot k'_o} \cdot \frac{V_L}{W_c} \cdot \frac{1}{\sqrt{\beta \cdot C_{H_2,i}}} \qquad \text{Equation 1}$$

Once, we have determined the intrinsic reaction rate constant, we transfer the process to a trickle bed reactor. To characterize the trickle bed reactor, we need to determine the gas-liquid and liquid-solid mass transfer resistances. To achieve that, we conduct several reactions by changing the loading of active pellets in the

reactor bed to separate the gas-liquid mass transfer resistance from the combined resistances of liquid-solid mass transfer and intrinsic reaction kinetics.

$$\Omega_{tot,TBR} = \frac{1}{k_L \cdot \alpha} + \frac{1}{k_s \cdot \alpha_s} \cdot \frac{W_{bed}}{W_{act}} + \frac{1}{\varepsilon \cdot k'_o} \cdot \frac{W_{bed}}{W_{act}} \cdot \frac{1}{\sqrt{\beta \cdot C_{H_2,i}}} \qquad \text{Equation 2}$$

3. Results and discussion

The experimental results for the batch mechanically agitated reactor and the experimental and simulated styrene concentration profiles are depicted in Figure 1. Table 1 summarizes the calculated values for $k_L \cdot \alpha$, $k_s \cdot \alpha_s$ based on the experimental method and the predicted values of the coefficients using the genetic algorithm.

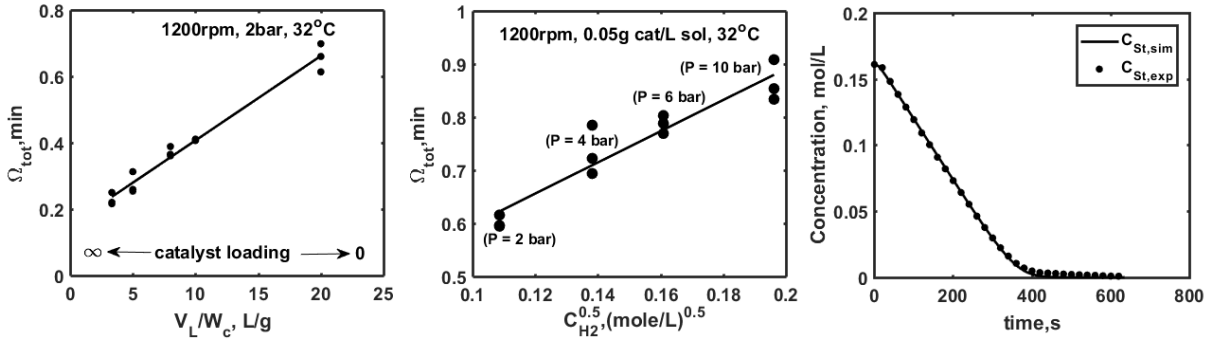

Figure 1: From the left to the right: Overall mass transfer resistance against the reciprocal of catalyst concentration and square root of H_2 concentration, experimental simulated concentration profile of styrene.

Table 1: Results of mass transfer coefficients based on experimental method and predictions from ga

	Experimental	Predictions
$\mathbf{k_L \cdot \alpha}, \frac{1}{s}$	0.087	0.092
$\mathbf{k_s \cdot \alpha_s}, \frac{L}{g \cdot s}$	2.35	1.021

4. Conclusions

The mass transfer resistances of a 3-phase reaction were calculated based on experimental methodology. A model of the batch mechanically three-phase reactor was built and it was used to the developed genetic algorithm for predicting the mass transfer resistances. The mass transfer resistances in trickle bed reactor were also calculated based on experimental methodology.

References

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Keywords
3-phase reactors; mass transfer; modelling; genetic algorithm.