Modelling the Hydrochlorination of Glycerol - Applying a detailed kinetic model to an industrial plant

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Highlights

- The hydrochlorination of glycerol in an industrial bubble column reactor was investigated.
- Based on detailed reaction kinetics seven reactor concepts were modelled and evaluated.
- A tube bundle reactor with ideal solution of HCl could replicate the bubble column reactor.

1. Introduction

Valorization of cheap and abundant renewable glycerol can be achieved by hydrochlorination. It is the first step of Epichlorohydrin production. The economically most important products are epoxy resins. In this contribution, the hydrochlorination of glycerol in an industrial bubble column reactor was model based studied. Process data were provided by a company. Detailed reaction kinetics from the literature were used to compare seven potential reactor designs with the existing process.

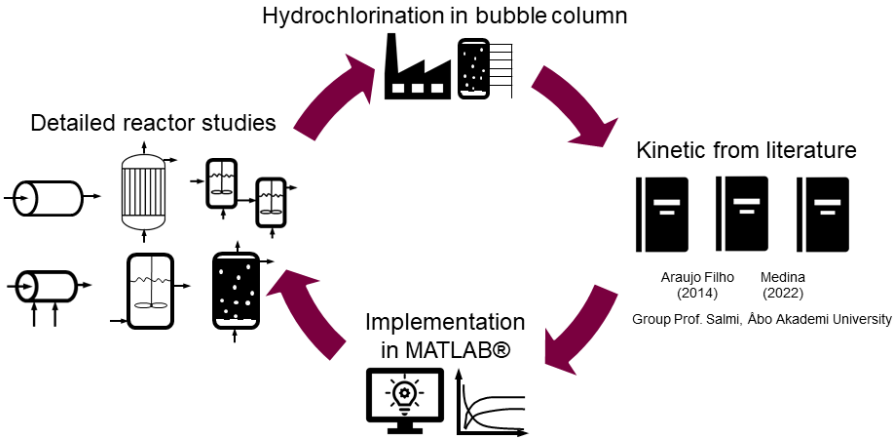

Figure 1. Workflow in this contribution.

2. Methods

The study was conducted with MATLAB® simulations based on a mechanistic kinetic model by Araujo Filho et al. [1]. Preliminary, the model was validated with experimental data of lab-scale experiments provided by Medina et al. [2]. The model predicts the experimental data very well, the mass transport being the only shortcoming of the model. Applying models of PFTR, CSTR and dispersion model, the most relevant states of homogenization have been considered [3]. Additionally, CSTR-Cascades and discreet continuous dosing concepts were compared with real industrial plant data (Figure 1).

3. Results and discussion

Of those models, a tubular bundle reactor replicates the product distribution of the industrial bubble column reactor best (Figure 2). Therefore, such a model could be used to represent the bubble column reactor to describe the total production process in a steady state including separation and recycle streams.

In the hydrochlorination gaseous HCl is fed into the liquid reaction medium including glycerol and recycle streams. Those streams include high amounts of unknown substances that accumulate during

the production process. Therefore, the unknown amount of active catalyst species was estimated by parameter optimization. The simulations strongly suggest the presence of major amounts of catalyst in the reaction mixture. The mass transfer was analyzed and estimated by parameter optimization, respectively. In fact, the best similarity between the industrial production plant and simulation was obtained by assuming an instant ideal solution of HCl in the reaction mixture (Figure 2).

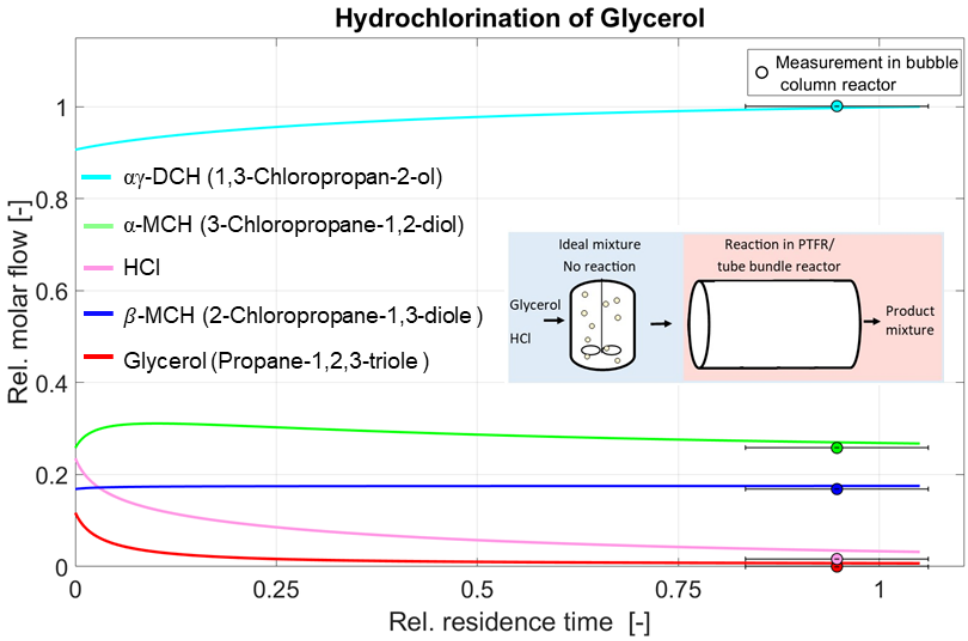

Figure 2. Hydrochlorination in the bubble column reactor could be modeled by assuming ideal solution of HCl in reaction mixture and reaction in a tube bundle reactor.

4. Conclusions

The yields of the industrial bubble column reactor could be replicated using a tube bundle reactor model. Due to the complex feed mixture catalyst content and mass transfer were estimated by parameter optimization. The results provide the basis for future process intensification and further investigations into optimal reactor design. In future works, the heat balance will be investigated and unknown components in the reaction mixture will be analyzed concerning unwanted side products. Those will have to be implemented in the reaction network and mechanistic kinetic modelling of the present multi-phase systems [4].

References

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Keywords

"Hydrochlorination", "Column reactor", "Reactor modelling", "Kinetics"