Modelling of microreactors for ethoxylation reactions using a laminar flow approach

M. Di Serio, [1]V. Russo, [2]W. Hreczuch
[1]Università di Napoli Federico II, via Cintia 4. IT-80126 Napoli, tel +39081674414, e-mail: diserio@unina.it;
[2]MEXEO, PL-47-200 Kędzierzyn-Koźle

The ethoxylation of fatty alcohol is an important process to produce non-ionic surfactants. Ethylene oxide reacts rapidly with long chain alcohols, reaction promoted by strong base catalyst, reaching almost full selectivity to the desired products, as no-side reactions are favoured in the presence of base catalysts. The alkoxylation reactions are generally performed in semibatch reactors [1], also in series, in which the catalyst and the substrate (alkyl phenols, fatty alcohols or acids) are initially charged while epoxide (ethylene or propylene oxide) is added during the reaction course. The use of semibatch reactors, however, surely have drawbacks that can be solved using continuous reactors (e.g. safety, productivity). In the scientific and patent literature both traditional tubular reactors and more innovative reactor configurations, like microreactors, have been proposed for the alkoxylation reactions. These last are particularly suitable for exothermic and multiphase reactions, thanks to the high heat and mass transfer exchange, showing good performances in terms of reaction conversion and thermal control, allowing to work at relatively high temperatures (240°C) [2,3]. Even though in the adopted experimental conditions it was demonstrated that the flow-pattern is laminar [4], the collected data are normally simulated with a plug-flow model approach [2,3]. At this purpose, in the present work a laminar-flow model was applied to the description of the experimental data collected in the literature.

A laminar-flow reactor model was tested to determine the kinetic and equilibrium parameters for octanol ethoxylation data reported in the literature [2,3]. The developed model was firstly applied to conduct a sensitivity study, showing high flexibility of the model, simulating for a very exothermic reaction temperature gradients along the radial coordinate. Them, the model was applied to describe the experiments conducted at different temperatures (from 180 to 240°C) taken from the literature [2,3]. In every case, a good fit was obtained (Figure 1).

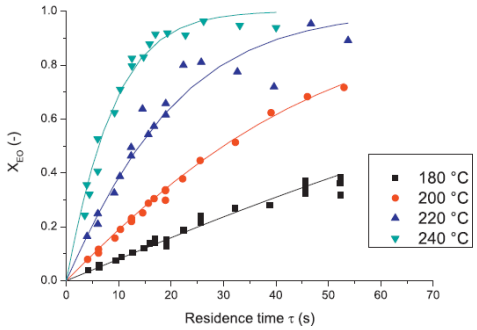

Figure 1. Ethylene oxide conversion along the residence time of the microreactor. Experiments conducted at different temperatures, taken from the literature [2,3].

The kinetic parameters shown a deviation from the ones obtained using a plug flow-approach (30% deviation), demonstrating the validity of the present model.

References

[1] M. Di Serio, R. Tesser, E. Santacesaria. I&ECR 44 (2005) 9482-9489.
[2] M. Rupp, W. Ruback, E. Klemm. ChemEngProcess: Process Intensification 74 (2013) 19-26.
[3] M. Rupp, W. Ruback, E. Klemm. ChemEngProcess: Process Intensification 74 (2013) 187-192.
[4] P.D. Hermann, T. Cents, E. Klemm, D. Ziegenbalg. I&ECR 55 (2016) 12675-12686.