AUTOMATING THE ASSESSMENT OF RENEWABLE FEEDSTOCK CONVERSION KINETICS

Joris W. Thybaut

Ghent University, Laboratory for Chemical Technology,
Tech Lane Ghent Science Park 914,
B-9052 Ghent, Belgium
Joris.Thybaut@UGent.be

Chemical kinetics constitute the key-essential property in the transformation of reactants into products. Dedicated catalyst development as well as (industrial) reactor design require precise knowledge of these kinetics, on top of an assessment of transport and hydrodynamics phenomena, to propose economically viable process lay-outs. Efficiently dealing with complex mixtures involving hundreds, if not thousands of species and even more reactions interconverting them, comes within reach when these species and reactions can be classified in a limited number of types and families. Yet, one would not reach far without software tools allowing the automation of the microkinetic assessment of such a complex mixture's conversion. An identical challenge has already been addressed for conventional hydrocarbon conversion [1]. The developed methodology now needs to be extended to renewable resources conversion aiming at a future, sustainable supply of liquid fuels and chemicals. Specific challenges to be addressed in this respect are:

- accounting for the presence of heteroatoms such as oxygen in the considered species,

- on top of complementary reaction families related to these new functionalities.

The extent of the latter may increase such that reaction network size control will be essential in order to limit the required computational effort and simultaneously assure that the network focuses on the most relevant elementary steps. Glycerol hydrogenolysis has been selected as a model reaction [2]. The significantly enhanced biodiesel production in the first decade of this century has led to an oversupply of the by-product glycerol. Hydrogenolysis of biomass-derived glycerol has been investigated as an alternative route for the production of green, value-added chemicals, such as 1,2-propanediol, commonly denoted as propylene glycol [3,4]. The same reaction has been selected for a proof-of-concept illustrating the potential for automation in kinetic modelling.

References

[1] J.W. Thybaut, G.B. Marin, J. Catal. 308 (2013) 352–362.
[2] S. Sato, M. Akiyama, R. Takahashi, T. Hara, K. Inui, M. Yokota, Appl. Catal. Gen. 347 (2008) 186–191.
[3] E.S. Vasiliadou, A.A. Lemonidou, Chem. Eng. J. 231 (2013) 103–112.
[4] Z. Zhou, X. Li, T. Zeng, W. Hong, Z. Cheng, W. Yuan, Chin. J. Chem. Eng. 18 (2010) 384–390.