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R2Chem: Structure Optimization of Renewables-to-Chemicals Production Systems

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For CO2 reduction in the chemical industries, the massive use of renewable energies and the substitution of fossil feedstock by implementation of Renewables-to-Chemicals (R2Chem) production systems are of key importance. Due to the multitude of alternative feedstock sources and possible process technologies a large number of rivalling chemical pathways are possible for converting renewables to valuable target products. In our work [1,2] we propose a method for the identification of the optimal R2Chem process structure under consideration of an economic objective function. By use of process extent variables it is possible to avoid binary decision variables, resulting in a purely continuous optimization problem. The derived cost function includes operational cost as well as capital cost. Furthermore, a penalty term for carbon dioxide emissions is considered. It is shown that an acceptable trade-off between cost and emissions is realizable by using natural gas as the main feedstock, especially if the required energy is supplied from renewable sources (wind/solar). A net consumption of CO2 of the overall production system is only possible if renewable energies sources are exploited while using CO2 as feedstock source at the same time. In case of using fossil energy sources, a negative carbon footprint is unavoidable due to high indirect CO2 emissions due to the energy supply (electricity, heat). Thus, in addition to economic challenges of using CO2 as feedstock also the ecologic impact strongly depends on the energy source used. The main advantage of the proposed methodology is the fast identification of an optimal process system within a superstructure containing many alternative configurations. The method is exemplified for the production of methanol from different feedstock and energy supply sources.

References

[1] Schack, D., Rihko-Struckmann, L. and Sundmacher, K.: Linear Programming Approach for Structure Optimization of Renewable-to-Chemicals (R2Chem) Production Networks. *Industrial & Engineering Chemistry Research* 57 (2018) 9889-9902.

[2] Schack, D., Liesche, G. and Sundmacher, K.: The FluxMax Approach: Simultaneous Flux Optimization and Heat Integration by Discretization of Thermodynamic State Space Illustrated on the Methanol Synthesis Process. *Computers & Chemical Engineering* (2019), under review.

Bio: Prof. Dr. Kai Sundmacher :

2017-2018 : Managing Director of the Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
Since 2010 : Guest Professor at East China University of Science and Technology, China
Since 2001 : Director and Scientific Member of the Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
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1997-1998 : Postdoctoral researcher at Department of Chemical and Process Engineering, University of Newcastle, U.K.
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