Development of an advanced three-phase continuous process for bio-compound valorization

Sébastien Leveneur
E-mail: sebastien.leveneur@insa-rouen.fr
Phone : +33 2 32 95 66 54
LSPC-INSA de Rouen

1. Context

The use of renewable feedstock and the development of safe processes are important goals when aiming at sustainable chemical industry. From an academic point of view, it is essential to work on platform molecules and, thereby, using the green chemistry philosophy defined by Paul Anastas and John Warner in 1998. In essence, valorization of lignocellulosic biomass is the future of chemical industries producing fine and specialty chemical as well as modern transportation fuels. One of the main points is to use lignocelluloses, which do not compete with food production.

To achieve economic viability in biorefineries, it is compulsory to develop continuous production processes as traditional batch processes are no longer competitive in many applications. The study of multiphase reaction system in continuous reactors, such as fixed-beds, can be cumbersome due to e.g. mass transfer limitations, changes in viscosity, uneven flow patterns, and the presence of hot spots. Thus, thorough investigation utilizing modern experimental and analytical equipment combined with advanced mathematical modeling of the reaction and reactor performance at both steady state and at transient conditions is a necessity. Catalyst development and application as well as Computational Fluid Dynamics are vital parts of these processes. The successful performance of this work calls inevitably for conducting research in an interdisciplinary environment with experts from several areas. teams research. This modern cross-disciplinary approach in research is not easy, but it is the only efficient way to tackle complex problems presented in modern industry. On the other hand, it gives the possibility to learn multidisciplinary approaches and is very rewarding when successful.

At LSPC laboratory, we have studied different biomass valorization system such as production of polyurethanes [1]; carbonation of vegetable oils [2]; epoxidation of vegetable oils [3] or hydrogenation of levulinic acid [4].

LSPC laboratory (EA 4704) is located at 1.5 hours by train from Paris. There are around 25 researchers of different nationalities (Dominican, Chinese, French, Moroccan,..). Research activities of our laboratory are process intensification and process safety. Process intensification activity is mainly focused on microwave irradiation and CO_2 capture and valorization. Further, process safety is focused on thermal and calorimetric measurements thus addressing the safety assessment. This project will benefit from the expertise of these two research activities. Furthermore, our laboratory is close to an analytical laboratory, essential to the success of this effort.

This work will be done in close collaboration with Åbo Akademi University (Finland) and particularly with Professor Grenman, who's research team is part of the well known Johan Gadolin Process Chemistry Centre. Grénman is also part of the Laboratory of Industrial Chemistry and Reaction Engineering, which also belongs to this Centre of excellence.

The Johan Gadolin Process Chemistry Centre (PCC) is one of the centres of excellence for scientific research, appointed by the Åbo Akademi University. The PCC comprises of the laboratories in Analytical Chemistry, Industrial Chemistry and Reaction Engineering, Inorganic Chemistry, Wood and Paper Chemistry, and Organic Chemistry. The PCC has collaborated very actively since the year 2000 in cross disciplinary research, of which the majority is devoted to biomass conversion. During the year 2016, 166 peer-review journal articles were published in high-ranking international journals. The Centre combines expertise from hydrocarbon and wood chemistry, reaction mechanisms, detailed analytics, extraction, mathematical modelling and reactor design. The laboratories have a combined experience covering several hundred of high-ranking publications concerning biomass extraction and utilization. The Centre possesses the necessary facilities and knowhow for the proposed research, except for the expertise obtained by collaboration described in the research plan.

The Laboratory of Industrial Chemistry and Reaction Engineering, which is a partner in the current project, focuses on three main areas: catalysis, kinetics and reaction engineering aiming to maintain and develop the knowledge in catalyst development and characterization, in the kinetics and mechanisms of catalytic reactions, in the kinetic analysis of complex chemical reaction networks and in the modeling and optimization of chemical reactors. Thus, the research areas form a logical path from laboratory synthesis to full scale production. The know-how has been applied in several fields ranging from environmental protection to the synthesis of fine and specialty chemicals.

The Laboratory of Industrial Chemistry and Reaction Engineering is currently very active in the field of biomass valorization. Research concerns valorization of chemicals derived from biomass and focuses on catalytic hydrogenation and oxidation of several types of mono-, di and oligosaccharides, heterogeneous catalytic isomerization of linoleic acid, hydrogenolysis of hydroxymatairesinol, catalytic pyrolysis of wood and upgrading of pyrolysis products, i.e. levoglucosan, aqueous phase reforming of sugars and sugar alcohols for production of fuel like hydrocarbons and hydrogen, deoxygenation of fatty acids to name a few projects. Besides development of new active and selective catalysts, various aspects of reaction engineering, e.g. catalyst deactivation and reaction kinetics are considered.

Henrik Grénman is an Associate Professor (tenure track) in molecular process and materials technology at Åbo Akademi University. The field is one of the strategic profiling areas of the university funded by the Academy of Finland. His research interests include applied aspects of inorganic and organic solid-liquid reactions covering a broad range of applications, with the focus on chemical kinetics and reaction engineering supported by mathematical modeling. He has been intensively involved in biomass valorization especially in selective fractionation and catalytic valorization of hemicellulose fractions and alcohols. He is currently a work package leader at the Johan Gadolin Process Chemistry Centre at ÅAU. Moreover, he is the Principal Investigator in a 4 year project granted by the prestigious Academy of Finland (September 2017-), which is related to selective fractionation and valorization of wood derived polysaccharides and a 2 year project (September 2017-) financed by Tekes and 3 companies, which is directly related to developing the APR process concept and reactor setup for sugar alcohols (not directly sugars). Grénman is active in supervising doctoral theses (holds several grants at the moment for the purpose) and has been involved in teaching in the fields of combined reaction and separation in green process technology, non-ideal reactor systems, industrial reactors, computer-aided chemical reaction engineering, and chemical reaction engineering. Industrial collaboration has always been an essential part of his research and he collaborates very actively with academic research groups in the Netherlands, Spain, Italy and France. He has conducted research at the Ian Wark Research Institute, University of South Australia and at the Delft University of Technology.

The CFD part will be done in close collaboration with Professor Abdellah Hadjadj & Associate-Professor Mostafa Safdari Shadloo who are specialist in this field.

In essence, the objective of this project is to develop and study a safe and continuous process to yield a green chemical product from lignocellulosic biomass. Different three phase system will be studied in a continuous reactor.

Dr. Sébastien Leveneur will supervise the PhD thesis. On the 20th of February 2015, he has defended his *Habilitation à Diriger des Recherches* at INSA de Rouen (France). In November 2014, he has passed with honor the lecture test to the appointment as a *docent* at the Åbo Akademi University (Finland). Dr. Henrik Grénman (with the assistance of colleagues) will participate in the supervision of the doctoral thesis.

The candidate should have a solid background in chemical engineering (chemical reaction engineering, catalyst, kinetics, thermodynamics,..). She/He should have some experience in numerical methods and in CFD (OpenFoam,...). Some knowledge in analytical method will be appreciated. The candidate will work in collaboration with different research laboratories, thus she/he should speak and write English fluently. We promise and inspiring research environment, challenging and interesting research opportunities and the possibility for genuine interdisciplinary work, which is both demanding, but also rewarding.

References

1. X. Cai, J.-L. Zheng, J. Wärnå, T. Salmi, B. Taouk, S. Leveneur, Influence of gas-liquid mass transfer on kinetic modeling: Carbonation of epoxidized vegetable oils, Chemical Engineering Journal, 313 (2017) 1168-1183.
2. W. Y. Pérez-Sena, X. Cai, N. Kebir, L. Vernières-Hassimi, C. Serra, T. Salmi, S. Leveneur, Aminolysis of cyclic-carbonate vegetable oils as a non-isocyanate route for the synthesis of polyurethane: a kinetic and thermal study, Chemical Engineering Journal, 346 (2018) 271-280.
3. J.-L. Zheng, J. Wärnå, F. Burel, T. Salmi, B. Taouk, S. Leveneur, Kinetic modeling strategy for an exothermic multiphase reactor system: application to vegetable oils epoxidation by using Prileschajew method, AIChE Journal, 62(3) (2016) 726-741.
4. B. Huang, S. Leveneur, T. Zamar, J.-P. Mikkola, B. Taouk, Towards production of γ-valerolactone via hydrogenation of aqueous levulinic acid, International Journal of Chemical Reactor Engineering, 13(1) (2015) 119–127.
5. Grénman, Henrik; Eränen, Kari; Krogell, Jens; Willför, Stefan; Salmi, Tapio; Murzin, Dmitry Yu. The Kinetics of Aqueous Extraction of Hemicelluloses from Spruce in an Intensified Reactor System. *Industrial and Engineering Chemistry Research* 2011, 50, 3818–3828.
6. Rissanen, Jussi V.; Murzin, Dmitry Yu.; Salmi, Tapio; Grénman, Henrik. Aqueous extraction of hemicelluloses from spruce – from hot to warm, *Bioresource Technolog*y 2016, 199, 279-282
7. Rissanen, Jussi; Grénman, Henrik; Xu, Chunlin; Willför, Stefan; Murzin, Dmitry; Salmi, Tapio. Obtaining spruce hemicelluloses of desired molar mass by using pressurized hot water extraction, *ChemSusChem* 2014, 7, 2947-2953
8. Perez Nebreda, Andrea; Salmi, Tapio; Murzin, Dmitry Yu; Grenman, Henrik. High purity fructose from inulin with heterogeneous catalysis - kinetics and modelling, *Journal of Chemical Technology and Biotechnology,* 93 (1), 224-232