Intensified Production of 5-hydroxymethylfurfural and Furfural from Biomass in Multiphase Systems

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Abstract

The valorization of lignocellulosic biomass derived sugars has gained more interest for the production of chemicals. 5-hydroxymethylfurfural (HMF) and furfural are highly valued building blocks that can be obtained by the dehydration of glucose, fructose and xylose. To prevent the formation of undesired humins and other by-products that occur in monophasic systems, a multiphase approach can be followed, whereby a reaction with *in situ* extraction takes place. With regard to Green Chemistry, the choice of solvents is a matter of interest. Therefore, environmental, health and safety (EHS) as well as the performance of the chosen solvent have to be considered. Several solvent selection guides have been established taking the EHS parameters into account. To assess the performance, the Conductor-like Screening MOdel for Real Solvents (COSMO-RS) is a proven tool for screening different candidates based on structural information of the molecules. COSMO-RS screenings among a pool of selected solvent candidates gave methyl propionate and ethyl acetate as best performing extraction phases. In addition, methyl isobutylketone (MIBK) also showed a promising performance with the advantage of not undergoing hydrolysis under the typical acidic conditions of the reaction. Dehydration reactions were conducted in a biphasic system with MIBK as extracting phase, with ethylene diaminetetraaceticacid (EDTA) as a catalyst due to its thermomorphic behaviour at temperatures above 140 to 170 °C. In addition, autocatalytic reactions are very promising although they are less productive, since catalyst removal is no longer needed as a further workup step. Furthermore, highly advantageous partition coefficients for furfural in MIBK and water can be observed, emphasizing the suitability of MIBK for this reaction setup.