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Aqueous phase reactions of pentoses in the presence of nanocrystalline zeolite beta: Identification of by-products and kinetic modelling

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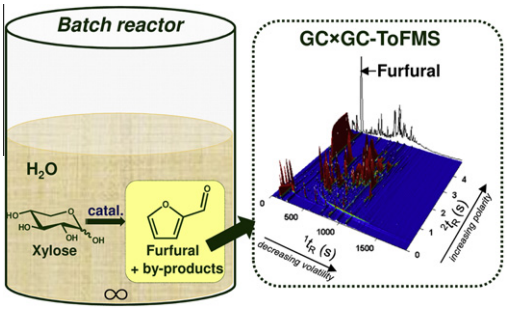
HIGHLIGHTS

- Mechanistic insights into the reaction of xylose in the presence of zeolite beta.
- Pentoses xylulose and lyxose, identified by NMR spectroscopy, are intermediates.
- Identification of by-products by comprehensive SPME/GC × GC–ToFMS analyses.
- Pseudo-homogeneous kinetic model fitted well the experimental data.

GRAPHICAL ABSTRACT



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ABSTRACT

Furfural, a valuable platform chemical that has the potential to replace a variety of oil/coal/gas derived materials and chemical products, is produced by the dehydration of D-xylose, which in turn is obtained from lignocellulosic biomass. Herein, the conversion of xylose in the presence of nanocrystalline zeolite beta in the H^+-form, using water as solvent, was investigated. Detailed batch kinetic studies and products identifications techniques (^1H, ^{13}C NMR and comprehensive two-dimensional gas chromatography (GC × GC) combined with time-of-flight mass spectrometry (ToFMS)) provided mechanistic insights into the overall reaction process. The conversion of xylose to furfural is accompanied by several side reactions, forming complex reaction mixtures. A pseudo-homogeneous kinetic model was proposed that fitted quite well the experimental data.

1. Introduction

Concerns about the depletion of fossil fuel reserves, increasing energy demands and the impact of anthropogenic carbon dioxide emissions, have encouraged the use of renewable biomass as feedstock for supplying fuels, chemicals and materials produced through sustainable process chains. Furfural is possibly the most important platform product derived from the hemicellulose component of biomass, with a wide applications profile (e.g. polymeric, pharmaceutical and agrochemical products), and has been produced industrially for decades [1–3]. Furfural has also been identified as an attractive intermediate for producing additives for biofuels [4–6]. The conversion of hemicelluloses to furfural involves the acid-catalysed hydrolysis of the polysaccharides into the constituent monosaccharides, mainly the pentose D-xylose, and the dehydration of the latter into furfural. The theoretical carbon atom efficiency of this reaction is 100%, i.e. all the carbon atoms going into the reaction end up in the target product. The most common

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