Catalytic conversion of glucose using nano-anatase TiO$_2$ catalyst: kinetic studies

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Abstract
Glucose can be transformed into important chemicals such as fructose and HMF. In this work, nano-structured anatase TiO$_2$ catalyst was synthesized and applied to glucose conversion, investigating its kinetic model. However, the reduced number of identified products avoided a good correlation between the experimental data and kinetic model.

Key words: TiO$_2$ catalyst, glucose conversion, hydroxymethylfurfural (HMF), kinetic model.

Introduction
The catalytic conversion of glucose to biofuels and other value-added chemicals is one of the most promising routes for the future. However, the challenge of developing green chemical methods based on heterogeneous catalysis relies on a deep investigation of the physical and chemical properties of the catalyst as well as the kinetics mechanism of the catalytic reaction. Glucose, obtained from the residual cellulose hydrolysis, can be converted into fructose and hydroxymethylfurfural (HMF) via titania due to acid and basic properties. Thus, this project aims to synthesize TiO$_2$ catalyst to apply in the glucose conversion reactions and to study the reaction mechanism and its kinetic model, performing a numerical regression.

Results and Discussion
The nano-anatase titania was prepared by hydrothermal synthesis using TiCl$_4$ as precursor. The physisorption of nitrogen analysis using BET showed a specific superficial area of the 376 m$^2$/g. The X-ray diffraction analysis (XRD) confirmed the anatase structure and broad diffraction peaks, which indicates nanosized particles.

The catalyst was applied in the glucose conversion reaction using a batch reactor and water as solvent. Reactions were carried out at three different temperatures and samples of the liquid phase were taken during the reaction. Conversion and products were used to determine the reaction model using the maximum-likelihood method. It was observed that the data diverge from the model for long reaction times. This might be related to the unknown reaction paths, since the products identified with HPLC analysis were $\approx$ 50% of the total organic compounds formed. HMF was the major product formed in the three reactions temperatures studied in this work.

Conclusions
The nano-anatase titania synthesized hydrothermally presented promising results on glucose conversion to obtain HMF. However, further analysis for a larger selection of products and improvements on the kinetics model are needed to investigate its performance and future applications.

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