Cyprus University of Technology

Faculty of Geotechnical Sciences and Environmental Management

Bachelor's Thesis

COMPUTATIONAL FLUID DYNAMICS AND REACTION MODELLING STUDY OF BIO-OIL CATALYTIC HYDRODEOXYGENATION IN MICROREACTORS

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Limassol, May, 2022

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ABSTRACT

Due to high energy demands and environmental issues that arise from the use of fossil fuels, there is a turn for the use of more sustainable fuels. The utilization of alternative fuels based on biomass have been in development in recent years. Bio-oil is obtained from fast pyrolysis of biomass feedstocks but for its use as a transportation fuel, a method for upgrading it, called catalytic hydrodeoxygenation, needs to be applied. The hydrodeoxygenation reaction of 4-propylguaiacol, a compound derived from lignin and present in bio-oil, is investigated using a computational fluid dynamics model. A 2D packed bed plug flow microreactor was developed with the use of a pre-sulphided $NiMo/Al_2O_3$ catalyst and several operational parameters, such as temperature and pressure, were investigated and compared with experimental results. Phenomena such as internal and external mass transfer limitations were also investigated. It was concluded that there is a good agreement between the results obtained from the CFD model simulation and the experimental results.

Keywords: Biomass, pyrolysis bio-oil, catalytic hydrodeoxygenation, microreactors, CFD simulations