Cyprus University of Technology

Faculty of Geotechnical Sciences and Environmental Management

Bachelor's Thesis

COMPUTATIONAL STUDIES ON MICROREACTORS FOR HYDROGEN PRODUCTION FROM FORMIC ACID DECOMPOSITION USING HETEROGENEOUS CATALYSTS

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Limassol, May 2024

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ABSTRACT

Hydrogen, as a clean and efficient energy carrier, holds significant promise for addressing the challenges posed by climate change and dwindling fossil fuel resources. A method for producing hydrogen on demand is formic acid decomposition, which benefits both storage and transportation. The kinetics of the reaction are enhanced using heterogeneous catalysts, which makes it suitable for more practical applications. The objective of the thesis focuses on computational studies aimed at optimizing microreactors, in order to improve their performance and efficiency of hydrogen production through formic acid decomposition using heterogeneous catalysts. Computational studies are executed using advanced modeling techniques, such as computational fluid dynamics (CFD). 0D and 2D microreactor configurations were solved using COMSOL Multiphysics. Key parameters such as fluid flow rate, temperature, concentration, bed porosity, and porosity of catalyst were studied in the simulation. The selection of boundary layers for the simulation of the 2D model was chosen after the initial boundary layer of the inflow until the boundary condition for the outflow of the materials. According to the base case conditions, the maximum conversion was found at 82.38% after 27.3 minutes of the initial feed of formic acid. From the 28th minute up until the 38th minute, there was a sharp decrease in the conversion rate due to the production of carbon monoxide and its poisoning of the catalyst of the study. Furthermore, until the end of the study, the rate of deactivation decreased and the conversion rate decreased at a slower rate reaching a conversion rate of 32.22%.

Keywords: Hydrogen, decomposition, formic acid, microreactor, modeling

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