Cyprus University of Technology

Faculty of Geotechnical Sciences and Environmental Management

Bachelor's Thesis

COMPUTATIONAL STUDIES ON BATCH REACTORS FOR HYDROGEN PRODUCTION VIA THE DECOMPOSITION OF HYDROUS HYDRAZINE USING HETEROGENEOUS CATALYSTS

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Limassol, May 2024

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ABSTRACT

The main concern of the world and especially the scientific community is the emissions coming from the burning of fossil fuels to produce energy. Thus, greener energy methods should be developed like this work's objective, the decomposition of hydrous hydrazine (HH) for emission-free hydrogen production. The HH stands out as a highly promising compound since it has a large hydrogen content and favorable decomposition kinetics. Since hydrogen faces a wide range of challenges, such as storage and transportation due to its different characteristics, more efficient ways were developed. It is preferable to produce H_2 on-site by other chemicals such as HH.

The H_2 generation in this study was executed by using a commercial 0.5 wt% Rh/Al_2O_3 catalyst with optimized conditions in a batch reactor. The use of heterogeneous catalysts has a crucial role in the acceleration of the decomposition of HH and therefore to the rates of hydrogen generation and selectivity. The importance of using heterogeneous monometallic catalysts and the batch reactor was also explained in this work. Moreover, a data comparison throughout computational validation was conducted between Rh and Ir-based catalysts supported on alumina (Al_2O_3) and nickel oxide and titanium oxide (NiO-TiO_2) respectively, with the best results, which were rhodium's, being tested further in a 2D study. Furthermore, computational fluid dynamics (CFD) simulations were conducted to correctly validate the experimental simulations using the rhodium's results. CFDs were also performed to study the uniformity of the system through the velocity and concentration distributions in the reactor. In order to achieve this hydrogen production, COMSOL Multiphysics 5.5, a modeling simulation software for finite element analysis, such as heat transfer, fluid flow, and mass transport, has been used in 0D and 2D experimental modeling. These computational simulations helped in the conduction of the experimental results and to a better understanding of the reaction kinetics and provided useful information about new ways of hydrogen generation and possible applications of it.

Keywords: Hydrogen; hydrous hydrazine; batch reactor; heterogeneous catalyst; CFD

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