## DECOMPOSITION OF HYDROUS HYDRAZINE ON COMMERCIAL RHODIUM CATALYST: EXPERIMENTAL AND CFD STUDIES.

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### ABSTRACT

Extensive use of fossil fuels has spurred interest in alternative, cleaner energy sources to reduce greenhouse gas emissions and combat climate change. Hydrogen (H<sub>2</sub>) emerges as a promising clean energy carrier, offering high energy content compared to conventional fuels <sup>[1]</sup>. Hydrous hydrazine (N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O) can be decomposed following two paths: hydrogen generation and ammonia (NH<sub>3</sub>) formation, which must be avoided thus, achieving high H<sub>2</sub> selectivity is critical for the development of efficient catalytic systems <sup>[2]</sup>. This study investigates the catalytic decomposition of hydrous hydrazine, employing a commercial 0.5 wt% rhodium (Rh) catalyst supported on alumina (Al<sub>2</sub>O<sub>3</sub>). The experiments were conducted in a batch system, varying parameters such as stirring rate, temperature, catalyst mass, N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O and NaOH concentration. Computational fluid dynamics (CFD) studies were also conducted with the use of COMSOL Multiphysics, for the validation of the experimental results. The optimal conditions determined both by experiments and computational simulations were: stirring rate of 1400 rpm, temperature of 70 °C, a substrate to metal molar ratio of 1000:1 and a NaOH of 0.5 M with H<sub>2</sub> selectivity over 90% in each case. Concentrations of N<sub>2</sub>H<sub>4</sub> as low as 0.05 M had a selectivity over 80% but all the experiments were conducted with 3.3 M as the standard reactant concentration. CFD simulations of a 2D system were also performed to investigate the uniformity of the system, showcasing velocity and temperature distribution over time, where the uniformity of the system was achieved after 0.75s and 30 min respectively. The dispersion of N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O solution and catalytic particles were also simulated, exhibiting evenly distributed particles and reactant solution on the reactor, emphasizing on the importance of efficient mixing for optimal catalytic performance. In conclusion, this work provides valuables insights into optimizing the catalytic decomposition of hydrous hydrazine for hydrogen generation, combining experimental results with CFD simulations to understand and enhance system performance in pursuit of sustainable energy solutions.

KEYWORDS: hydrous hydrazine, batch, hydrogen generation

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