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Production and purification of hydrogen in Catalytic Micro reactor with Aspen plus software and optimization of reactor temperature with genetic algorithms in Matlab software

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Abstract : In this project was simulated the conversion reaction of methanol/steam in the reactor catalyst bed, the simulation was performed with two different kinetics. In the following simulation results were compared with experimental results. The difference between simulation and experimental results between 0.5% to 0.7%. Then, produced was the effect of temperature, feed composition, feed rate and the size of the reactor on the amount of hydrogen. Also, With data changes length of reactor, the reactor outlet temperature and the temperature inside the reactor of moles of hydrogen emission output optimization and the attainment of hydrogen, using genetic algorithms in Matlab. According to the simulation results has decreased of mol fraction of methanol and water in the reactor and The mole fraction carbon dioxide and hydrogen increase during the process. Retention time for the reaction in the reactor with a length of 12 cm was 3.83 seconds. By reducing the input feed rate increases methanol conversion and hydrogen production rate. According to the results of genetic algorithms was equal to optimize the reactor to 44.61 cm. This is the highest amount of hydrogen production will be achieved with the lowest temperature. In this case, the temperature inside (the last point of the tube reactor) reactor will be 140 C. By selecting the optimum condition was simulation of the software Aspen and Matlab. Mole fraction of hydrogen to simulate optimum 59.94, present Of hydrogen production by over 99%, and The percent of Consumption for methanol consumption was 100%, After optimization and achieve optimal profile, the process was simulated with two different kinetic parameters, The results showed. Simulations of the kinetics is first better than the second kinetics. The first kinetic less residence time is about 1 second and The percent of hydrogen is good. The kinetics of hydrogen production at a rate of 0.24% more than the second kinetics.

Key words: Hydrogen, the reaction of methanol / water vapor, catalysts, catalytic bed reactor, GA.

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