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Non-linear Regression and Simulation of the Effect of Thermal Treatment and Reaction Temperature on Pd-Ni/AC Catalyst for the Thermo Catalytic Decomposition of Methane

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Abstract: The effects of the thermal treatment and reaction temperatures on 5% (wt/wt) 1:1 (mol:mol) *Pd-Ni* on activated carbon (AC-ITDI) catalyst acquired from the Industrial Technology Development Institute (ITDI) of the Department of Science and Technology (DOST) of the Philippines (*Pd-Ni*/AC) for the thermocatalytic decomposition of CH_4 were determined in this study. The thermal treatment parameters investigated were the carbonization temperature and calcination temperature; the effect of reduction temperature was not investigated. AC carbonization was done at 700°C, 800°C and 900°C in argon and catalyst calcination was done at 500°C, 600°C and 800°C. The thermal decomposition reaction temperatures were 750°C, 850°C and 950°C for the catalyst that exhibited the best initial activity. Catalyst pre-characterization showed that the catalyst pore size increased with carbonization temperature but decreased with calcination temperature. Pd particle dispersion was better also at lower calcination temperatures. Catalytic activity test results show that *Pd-Ni*/AC carbonized at 700°C and calcined at 500°C had the highest initial H_2 yield (0.4056 mol H_2/mol CH_4), an H_2 yield of (0.0276 mol H_2/mol CH_4) after 24 hours and a 7-hour average H_2 yield of 0.007371. The developed non-linear regression model indicated that H_2 yield is mainly affected by carbonization temperature with a total parameter significance value of 94.5776% due to its effect on catalyst pore size and by calcination temperature with a parameter significance value of 5.4224% due to its effect on *Pd* particle dispersion. The predicted maximum H_2 yield value of 0.00689 was found at a carbonization temperature of 900°C and a calcination temperature of 600°C. H_2 yield values are expected to increase at higher reaction temperatures (>950°C).

Key Words: activated carbon (ITDI), methane decomposition, non-linear regression, simulation, thermal treatment