World Academy of Science, Engineering and Technology
International Journal of Energy and Power Engineering
Vol:18, No:06, 2024

Theoretical and Experimental Study on the NO Reduction by H_2 over Char Decorated with Ni at low Temperatures

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Abstract : In this study, we propose a reaction system for the low-temperature reduction of NO by H_2 on carbon-based materials decorated with 5%wt. Ni. This cost-effective catalyst system efficiently utilizes pyrolysis carbon-based materials and waste hydrogen. Additionally, it yields environmentally friendly products without requiring extra heat sources in practical SCR devices. Density functional theory elucidates the mechanism of NO heterogeneous reduction by H_2 on Ni-decorated char surfaces. Two distinct reaction paths were identified, one involving the intermediate product N_2O and the other not. These pathways exhibit different rate-determination steps and activation energies. Kinetic analysis indicates that the N_2O byproduct pathway has a lower activation energy. Experimental results corroborate the theoretical findings. Thus, this research enhances our mechanistic understanding of the NO-H_2 reaction over char and offers insights for optimizing catalyst design in low-temperature NO reduction.

Keywords : char-based catalysis, NO reduction, DFT study, heterogeneous reaction, low-temperature H_2-reduction
Conference Title : ICCEUT 2024 : International Conference on Combustion, Energy Utilisation and Thermodynamics
Conference Location : Montreal, Canada
Conference Dates : June 13-14, 2024