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Supplementary Materials

Kinetic Study on CO-Selective Methanation over Nickel-Based Catalysts for Deep Removal of CO from Hydrogen-Rich Reformate

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Abstract: The CO-selective methanation process is considered as a promising CO removal process for compact fuel processors producing hydrogen, since the process selectively converts the trace of CO in the hydrogen-rich gas into methane without additional reactants. Two different types of efficient nickel-based catalysts, showing high activity and selectivity to the CO methanation reaction, were developed in our previous works; therefore, the kinetic models of the reactions over these nickel-based catalysts have been investigated adopting the mechanistic kinetic models based on the Langmuir chemisorption theory. In the methanation process, the product species can react with the reactant and also affect the adsorption/desorption of the molecules at the active sites. Thus, the kinetic parameter study should be carried out by global optimization handling all the rate equations for the plausible reactions at once. To estimate the kinetic parameters, an effective optimization algorithm combining both heuristic and deterministic methods is used due to the large solution space and the nonlinearity of the objective function. As a result, 14 kinetic parameters for each catalyst have been determined and the parameter sets for the catalysts have been compared to understand the catalytic characteristics.

Keywords: CO-selective methanation; nickel catalysts; kinetic parameters; genetic algorithm; parameter estimation

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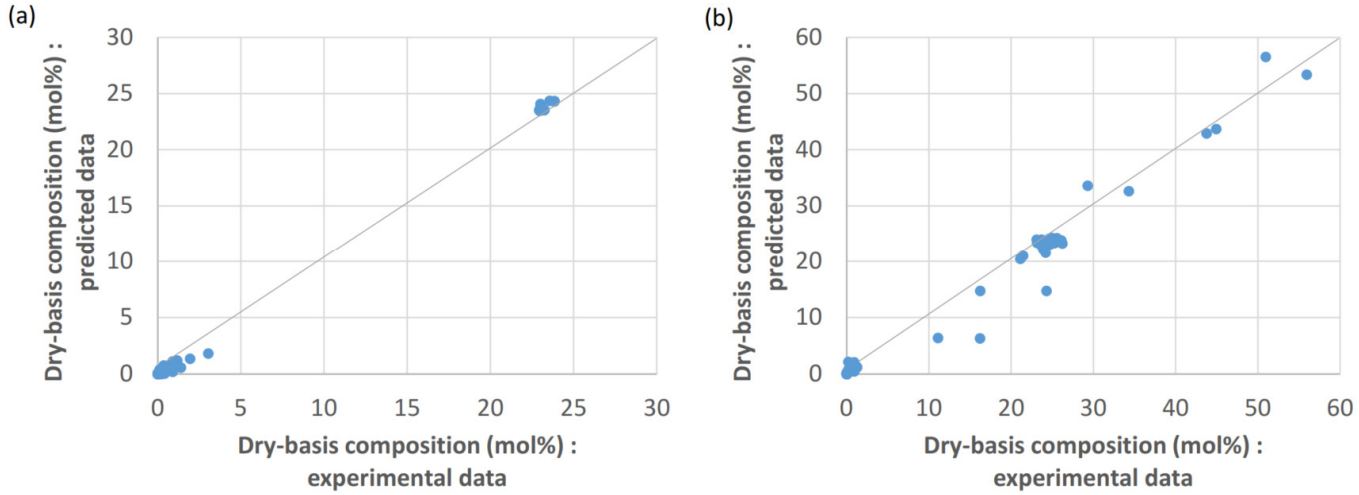

Figure S1. Parity plots and objective function values for both catalysts (**a**) Ir/Ni-MgO/γ-alumina and (**b**) $Ni_{0.5}Zr_{0.5}O_{2}$.