Modeling Hydrogen Production From Methane Pyrolysis Using Machine Learning

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In the pursuit of sustainable energy, converting methane to hydrogen presents a vital pathway for mitigating greenhouse gas emissions. While methane is a potent feedstock, traditional reforming processes are carbon intensive. This study investigates methane pyrolysis—an emerging technology that thermally decomposes methane into gaseous hydrogen and solid carbon, effectively bypassing carbon dioxide production. A review of current literature identifies the primary challenge as optimizing operating conditions to maximize hydrogen yield while minimizing energy input. To address this, we integrate experimental data from literature with in-house kinetic modeling. Initial analysis utilized baseline machine learning methods (linear and logistic regression) to assess the impact of temperature, pressure, and methane concentration. To capture complex nonlinearities, a neural network incorporating gated recurrent units was developed to predict the temporal evolution of hydrogen yield under diverse operating conditions. The findings elucidate the intricate interactions between process parameters, and provide a scalable framework for cost-effective hydrogen production, underscoring the synergy between renewable biogas, advanced thermal conversion technologies, and artificial intelligence in enabling a hydrogen-based energy future.

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