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Optimizing methanol synthesis from CO_2 using graphene-based heterogeneous photocatalyst under RSM and ANN-driven parametric optimization for achieving better suitability

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Assessment of the performance of linear and nonlinear regression-based methods for estimating *in situ* catalytic CO_2 transformations employing TiO_2/Cu coupled with hydrogen exfoliation graphene (HEG) has been investigated. The yield of methanol was thoroughly optimized and predicted using response surface methodology (RSM) and artificial neural network (ANN) model after rigorous experimentation and comparison. Amongst the different types of HEG loading from 10 to 40 wt%, the 30 wt% in the HEG-TiO_2/Cu assisted photosynthetic catalyst was found to be successful in providing the highest conversion efficiency of methanol from CO_2. The most influencing parameters, HEG dosing and inflow rate of CO_2, were found to affect the conversion rate in the acidic reaction regime (at pH of 3). According to RSM and ANN, the optimum methanol yields were 36.3 mg g^{-1} of catalyst and 37.3 mg g^{-1} of catalyst, respectively. Through the comparison of performances using the least squared error analysis, the nonlinear regression-based ANN showed a better determination coefficient (overall R^2 > 0.985) than the linear regression-based RSM model (overall R^2 ∼ 0.97). Even though both models performed well, ANN, consisting of 9 neurons in the input and 1 hidden layer, could predict optimum results closer to RSM in terms of agreement with the experimental outcome.

1. Introduction

Amidst the worldwide growing energy crisis, fixed and dwindling stock of fossil fuels, and extreme pollution, finding acceptable means to produce alternative fuels is a significant breakthrough.[1,2] According to experts, the exponential growth in atmospheric CO_2 concentration caused by human activity is the most severe threat biotic societies face nowadays. Human population expansion, a modern luxurious lifestyle, and significant industrial development have all increased CO_2 emissions, making this an increasingly serious issue.[3] There is no better method for addressing the energy and environmental crises than by utilizing cutting-edge photocatalytic technology to convert ambient CO_2 into useable fuel hydrocarbons (such as methanol or ethanol) under solar excitation.[4,5] Next-generation biomimetic technologies look promising because they reduce potential pollutants while also converting to low-cost hydrocarbon-based fuels, *viz.*, methanol, by using solar energy and atmospheric CO_2 as raw materials.[6] The development of appropriate photocatalysts for the effective redox photosynthesis of CO_2 to hydrocarbons under UV/visible light, on the other hand, remains a considerable challenge.[7,8]

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