EXPERIMENTAL AND MODELLING STUDIES ON THE PHOTOCATALYTIC GENERATION OF HYDROGEN DURING WATER-SPLITTING OVER A COMMERCIAL TiO_2 PHOTOCATALYST P25

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Photocatalytic generation of hydrogen from aqueous solutions offers potential ways for supplying, increasing fossil energy demand and decreasing global warming problems. However, the limit of efficiency for the photocatalytic hydrogen generation still stays unclear. Here, a phenomenological model of photocatalytic hydrogen generation is established to quantitatively predict the behavior of an experimental photoreactor. The model takes into account the light distribution in the photoreactor, the concentration of photocatalysts, and mass transfer limitations between liquid and gas phases. The main explored parameters of the system were the photocatalyst loading and irradiation. A polynomial function describing the spatial distribution of light irradiation was suggested. Further, it has been found that the mass transfer of hydrogen from the liquid to gas phase significantly affects the hydrogen yield. The initial accumulation of hydrogen in the liquid phase and its delayed transport to the gas phase result in a nonlinear time-dependence of the hydrogen concentration in the gas phase. Regarding the photocatalyst concentration effect on the reaction rate, the theoretical average reaction rate presents a maximum for a photocatalyst concentration of 0.23 g/L, which is very close to the one experimentally observed (0.25 g/L). Moreover, the photonic efficiency, that is, the ratio of the average reaction rate to the average light intensity, reaches a maximum value at 0.25g/L of catalyst and remains constant for higher TiO_2 loads. The results of this investigation can be beneficial in future studies on the effects of interfacial mass transfer of hydrogen or other reaction products in photocatalytic reactors.

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