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Abstract

The design and operation of reactors for photocatalytic degradation of organic pollutants remains challenging due to the complex interplay of photon, mass, and heat transfer. An integrated process model including a radiation field, reaction kinetics, and material balances of an annular LED-based photocatalytic reactor for photocatalytic degradation of toluene is validated using experimental data from a mini-pilot plant. A particular emphasis is on the effect of water on reaction kinetics, toluene conversion, mineralization, and catalyst deactivation, which is currently not well understood. The results from parameter estimation demonstrate that a competitive reaction rate model describes the experimental data with varying water concentration best. Furthermore, experimental trends demonstrate that toluene conversion is highest at low water concentrations, however, mineralization and catalyst lifetime are enhanced by the presence of water. The validation of the integrated process model and understanding of the role of water allow for improved design and operation of future photocatalytic reactors.

Keywords: photocatalysis, light emitting diodes, volatile organic compounds, parameter estimation, model validation, toluene oxidation.