Predictive Model for UV Light Irradiation and PCO Reaction Kinetics in a Photocatalytic Reactor

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Abstract

A novel type of photocatalytic reactor, i.e. parallel flow tube reactor (PFTR) is presented for the degradation of indoor air pollution with UV-light. A Multiphysics model was developed in COMSOL Multiphysics® to predict the steady-state behavior under different inlet concentrations and incident irradiation intensity, with acetaldehyde as a model compound for the organic fraction of the indoor air pollutants. The 3D-model couples the Ray Optics Module for UV-light intensity predictions within the reactor, with the Laminar Flow and Transport of Diluted Species physics interfaces in order to simulate the transport of the pollutant as it progresses through the reactor. Finally the Optimization Module was used to fit the model predictions with experimental measurements.

An alternative approach to determine the layer thickness and refractive index of a P25-powder modified sol-gel coating, was proposed, using the Ray Optics module to estimate these parameters based on light intensity measurements. The optical model was able to accurately predict the light intensity distribution on the catalytic surface within the reactor.

Consequently, the optical model was used to define a light intensity dependent reaction rate constant in a coupling with the Laminar Flow and Transport of Diluted Species physics interfaces. A Nelder-Mead algorithm (Optimization Module) was deployed to estimate the intrinsic parameters of adsorption, desorption and reaction on the TiO2-surface, using experimentally determined steady-state outlet concentrations of acetaldehyde. The Multiphysics model showed excellent agreement with the experimental data, as evidenced by a coefficient of determination of 0.998. The Multiphysics model showed excellent agreement with the experimental data, as evidenced by a coefficient of determination of 0.998. Additionally, a validation test was performed under conditions of lower UV-light intensities (only one UV-lamp) to emphasize the reliability and accuracy of the intrinsic parameters for adsorption, desorption and reaction. The Multiphysics model is a useful tool to predict reactor performance and to optimize the reactor design.

Figures used in the abstract

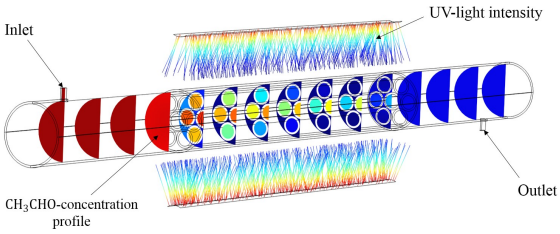

Figure 1: Visual representation of the concentration profile in a photocatalytic Parallel Flow Tube Reactor.