Transient CFD Investigation of a Photocatalytic Multi-tube Reactor

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Abstract

In industrial countries, people spend most of their time indoors. Stringent heat-insulation measures in combination with deficient ventilation have a negative impact on indoor air quality [1]. Integration or retrofitting of a photocatalytic oxidation or PCO reactor into continuous flow systems like HVAC (Heating, Ventilation and Air Conditioning) equipment is an interesting approach for abating indoor air pollution [2]. The PCO purification method exposes a catalyst like titanium dioxide (TiO2), to ultraviolet (UV) light to produce hydroxyl radicals and superoxide anions. These radicals are extremely reactive and are able to oxidize harmful volatile organic compounds (VOCs) into H20 and CO2. PCO technology is very cost-effective, efficient and it does not produce any waste streams.

Determining the kinetic parameters describing the PCO reactions is an important step in the development of efficient air purification units for integration in HVAC systems. Calculation of PCO kinetic parameters is amply discussed and relatively 'straightforward' for batch processes [3]. It is somewhat more difficult for continuous flow systems, unless steady state conditions are attained. An efficient PCO reactor should have a high degradation efficiency, high photon utilization and low pressure drop and power consumption, in a physically compact vessel [4]. In this work, we estimated the 'intrinsic' PCO related kinetic parameters (adsorption, desorption and photocatalytic rate constants as well as the total number of active sites), by comparing results from a COMSOL Multiphysics® model including kinetic rate expressions with experimental results using an optimization approach. Acetaldehyde was chosen as a model VOC. Contrary to analytical methods, which often oversimplify the physical and chemical phenomena, CFD and a Multiphysics approach can take into account the geometric design of the reactor and all relevant characteristics of the air flow [5]. Figure 1 shows the velocity profile in our reactor geometry to demonstrate local differences in a lab-scale reactor.

COMSOL® software proved to be a versatile and accurate tool to extract all relevant acetaldehyde adsorption and photocatalytic parameters, even for situations in which analytical estimations would otherwise fail. Our model is able to simulate the transient adsorption/desorption (Figure 2) and photocatalytic removal (Figure 3) of acetaldehyde with good agreement to experimental data as evidenced by high coefficients of determination. The kinetic parameters can be used as useful design variables for the future development of air purifiers based on PCO reactors integrated in continuous flow systems. A validation test which includes simultaneous adsorption/desorption and photocatalytic reaction showed that the model is able to accurately simulate the transient

phenomena occurring during the operation of a PCO reactor.
Two methods to automatically calculate the view factors with LiveLink™ for MATLAB® are presented and results of the simulation regarding performance and thermal comfort are presented and discussed.

Reference

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Figures used in the abstract

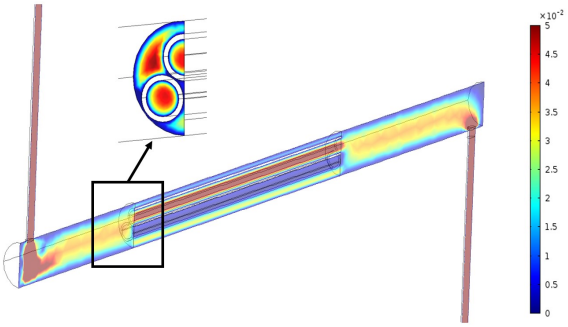

Figure 1: CFD velocity profile in a lab-scale reactor.

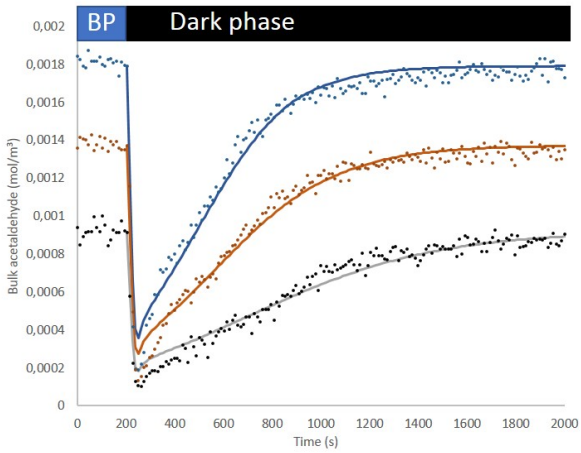

Figure 2: Adsorption phase: COMSOL simulations (lines) versus experimental data.

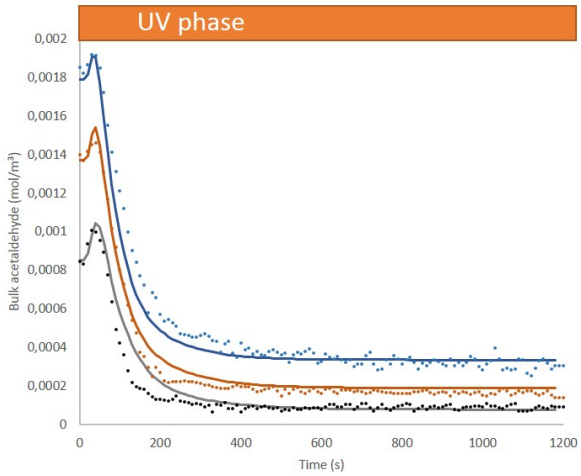

Figure 3: Photocatalytic phase: COMSOL simulation (lines) versus the experimental data (dots).