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Ultraviolet photocatalytic oxidation for indoor environment applications: Experimental validation of the model

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ABSTRACT

The development of a reliable and validated model can facilitate the widespread application of ultraviolet photocatalytic oxidation (UV-PCO) for indoor air treatment and purification in building mechanical ventilation systems. This paper reports the development of a time-dependent model for predicting the performance of an in-duct PCO air cleaner under the conditions relevant to the actual applications. The model was developed by integrating light scattering model, reaction kinetic model, mass balance as well as optional ozonation model. The comprehensive model incorporates the influences of properties of light sources and catalyst, reactor geometry, mass transfer parameters, kinetic parameters, operational conditions, as well as ozonation effect. These parameters can be estimated easily from experiments and/or empirical equations. The UV-PCO model and UV-PCO model combined with ozonation model were validated with experimental results for fiberglass fibers coated with TiO_2 (TiO_2/FGFs) air filters under different conditions. There was good agreement between the prediction made by the model and the experiment results. It was also demonstrated that the developed model can be applied to predict the UV-PCO performance for carbon cloth fibers loaded with TiO_2 (TiO_2/CCFs) air filters.

1. Introduction

As an alternative approach to improve the indoor air quality (IAQ) and well-being of occupants, a technology of ultra-violet photocatalytic oxidation (UV-PCO) becomes prevalent with the advocacy of reducing building energy consumption in the recent years [21,22]. Heterogeneous UV-PCO is a series of physico-chemical process designed to remove volatile organic compounds (VOCs) in air by oxidation. To be more specific, the catalytic technology employs UV irradiance absorbed by semiconductor materials to induce negative electron-positive hole pairs separation with formation of hydroxyl radicals (•OH) able to oxidize VOCs.

Photocatalytic degradation of gaseous pollutants is a heterogeneous physical mass transfer process combined with a complex photochemical process and the catalytic reaction rate is an essential gauge of the efficiency of UV-PCO system. Previous studies have demonstrated that the reaction rate of a UV-PCO system depends on light intensity, types and concentration levels of reactants, flow rate, moisture levels and properties of catalyst used. In fact, the computer tool is an important means to qualitatively and quantitatively analyze the impact of these factors on the performance of UV-PCO. Optimal design also closely relies on both validated modeling and reliable simulation results. Hence, to develop a PCO model that can be used for PCO reactor design and optimization plays a necessary role to help widespread applications of PCO technology for air purification.

Although significant literature has been published in the field of heterogeneous photocatalysis for air treatment, the majority of the work has been performed in bench-top scale reactors under ideal reaction conditions [3,8,9,15,18,19]. In consequence, most of the existing PCO models were established based on the small-scale observations and were verified by these test results. Unfortunately, some parameters like photocatalytic reaction rate closely depend on the experimental setup, the experimental conditions as well as the kinetic model since they affect significantly the PCO behavior. The values of kinetic parameters obtained from small experiments could be questionable and may not be scaled up to predict the performance of the full-scale systems. Furthermore, most of PCO models are not intended for mechanical ventilation applications and cannot correctly simulate the behavior of a PCO reactor under the conditions encountered in buildings [21]. Moreover, most of PCO models were validated with one or a few VOCs, and there could be unknown effects if they were challenged with other VOCs.

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Due to these limitations, there is a great need to develop a reliable time-dependent PCO model to simulate an in-duct PCO air cleaner under the conditions relevant to the real applications. Experimental evaluation of UV-PCO technology for air purification has been conducted and the results reveal the effects of the experimental and operational variables on the photocatalytic conversion. In this paper, a mathematical PCO model is developed by integrating light scattering model, reaction kinetic model, mass balance as well as optional ozonation model. The proposed UV-PCO model has applied to predict the PCO performance for eight VOCs removal in a pilot-scale system using TiO_2 as the photocatalyst for the model validation. The validated PCO model would be able to facilitate the design of large-scale UV-PCO air cleaners.

2. Mathematical modeling

2.1. Model assumptions

A schematic representation of UV-PCO reactor with different configurations is shown in Fig. 1. UV-PCO model is developed on the basis of fundamental mechanisms involved in the UV-PCO technology (Fig. 1(a), UVC lamps with TiO_2 air filters): convection, diffusion and boundary transfer of contaminants in the air-phase; inter-phase mass transfer of reactant species; adsorption and photocatalytic oxidation reaction in the solid-phase. Several assumptions are applied in the development of UV-PCO model.

(1) PCO reaction occurs at the surface of catalyst fibers exposed to UV lights. The function of UV-PCO banks is to extend the PCO reaction surface and the concentration difference between banks is not considered.
(2) Photons reaching to the TiO_2 are totally adsorbed by the catalyst. Irradiance does not pass through the air filter and the average irradiance is considered for each bank.
(3) TiO_2 catalysts are uniformly coated at the fiberglass.
(4) Airflow in duct is deemed as ideal plug flow.
(5) UV light is assumed to be monochromatic since approximately 95% of the UV energy emitted from germicidal lamps is at the mercury resonance wavelength of 254 nm.

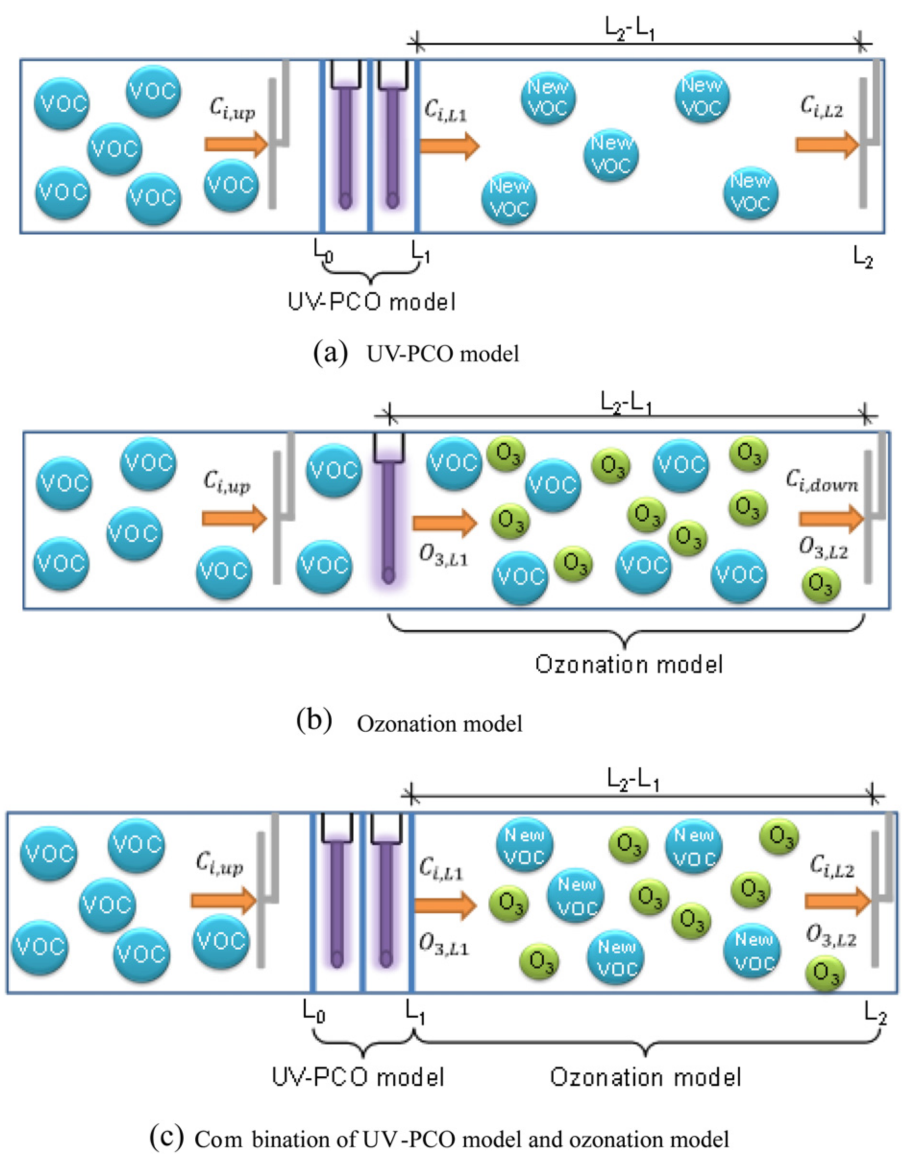

Fig. 1. Schematic diagrams of UV-PCO system for various scenarios: (a) UVC lamps with TiO_2 air filters (b) VUV lamps in the absence of TiO_2 air filters (c) VUV lamps with TiO_2 air filters.