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Field synergy analysis and optimization of the convective mass transfer in photocatalytic oxidation reactors

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Abstract

A convective mass transfer field synergy equation with a specific boundary condition for photocatalytic oxidation reactors developed based on the extremum principle of mass transfer potential capacity dissipation can be used to increase the field synergy between the velocity and contaminant concentration gradient fields over the entire fluid flow domain to enhance the convective mass transfer and increase the contaminant removal effectiveness of photocatalytic oxidation reactors. The solution of the field synergy equation gives the optimal flow field, having the best field synergy for a given viscous dissipation, which maximize the contaminant removal effectiveness. As an illustrative example, the field synergy analysis for laminar mass transfer in plate type reactors is presented. The analysis shows that generating multiple longitudinal vortex flow in the plate type reactor effectively enhances the laminar mass transfer. With the guide of the optimal velocity pattern, the discrete double-inclined ribs can be introduced in actual applications to generate the desired multi-longitudinal vortex flow, so as to enhance the laminar mass transfer, and consequently, improve the contaminant removal performance. The experimental result shows that the contaminant removal effectiveness for the discrete double-inclined ribs plate reactor is increased by 22% compared to the smooth plate reactor.

Keywords: Convective mass transfer; Field synergy equation; Mass transfer potential capacity dissipation; Photocatalytic oxidation reactors; Optimization

1. Introduction

Indoor air quality, which is mostly a function of the contaminant concentration, is very important to people's health and comfort [1–3]. In recent era of energy shortages, buildings have been sealed tightly and fresh air flow rate in air conditioning systems has been decreased sharply to reduce energy consumption. Meanwhile, volatile ornamental materials, household appliances and office equipment (e.g. computers, televisions and printers) that emit volatile organic compounds (VOCs) have become much more widely used. These factors have resulted in increased indoor contaminant concentrations, which are often associated with adverse healthy effects including headache, dry cough and nausea. Therefore, it has fueled huge interest in new effective approaches to reduce VOC concentration.

Photocatalytic oxidation (PCO) by employing ultraviolet (UV) radiation, which offers several environmental and practical advantages over conventional biological or physical disinfection processes include eliminating the contaminant sources and diluting the contaminant concentration with fresh air, is an innovative and promising technology to remove VOCs [4–11]. However, a commercial competitive full-scale photocatalytic oxidation system has not yet been widely accepted in practice. One of the major barriers is its low energy efficiency due, among other factors, to the limited capacity to deliver reactants to catalyst surfaces [12]. And it is found that for many cases, the mass transfer ability of the PCO reactors are the bottleneck factors of improving their VOC removal effectiveness [13].

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Nomenclature

C	contaminant concentration, kg m^{-3}
D	mass diffusion coefficient, m^2 s^{-1}
F	additional volume force per unit volume, N m^{-3}
Fs	field synergy number
J^*	Lagrange function
K	Langmuir adsorption equilibrium constant, m^3 mg^{-1}
k	reaction constant, mol m^{-2} s^{-1}
$\vec{n}$	outward normal unit vector
P	pressure, Pa
r	photocatalytic reaction rate, mol m^{-2} s^{-1}
Re	Reynolds number
S	surface area, m^2
Sc	Schmidt number
Sh	Sherwood number
u, v, w	velocity component in x-, y- and z-directions, m s^{-1}
$\vec{U}$	velocity vector
V	volume, m^3
x, y, z	Cartesian coordinates, m
Y	mass fraction
Z_m	mass transfer potential capacity dissipation function, kg s^{-1} m^{-3}
ε	contaminant removal effectiveness
ρ	air density, kg m^{-3}
μ	dynamic viscosity, kg m^{-1} s^{-1}
Φ	viscous dissipation function, W m^{-3}
∇	divergence operator
Ω	flow domain
Γ	flow domain boundary
A, C_1, C_Φ, E_1, E_2, F_1	Lagrange multiplier

Subscripts

c	constant
s	catalyst surface
in	inlet
out	outlet

In the last several decades of the twentieth century, a large number of novel geometry of the PCO reactors had been developed including plate type reactors, corrugated plate reactors [14], light-in-tube reactor, and honeycomb type reactors [15], to improve the capacity of delivering contaminants. However, most techniques were developed empirically or semi-empirically.

Guo et al. [16] introduced the field synergy concept to improve convective heat transfer performance based on the synergy between the velocity and temperature gradient fields in the fluid flow domain, and then developed the field synergy principle, which states that the overall heat transfer rate depends not only on the velocity and the temperature gradient field, but also on their synergy. For a given set of constraints, an optimal velocity field exists, which improves the synergy between the velocity and temperature gradient fields to maximize the heat transfer rate. This principle has been validated numerically and experimentally [17,18]. Furthermore, Meng et al. [18] then deduced the laminar heat transfer field synergy equation based on the extremum entransy dissipation principle [19], which was originally referred to as the heat transfer potential capacity dissipation extremum principle. The solution of the laminar field synergy equation gave the optimal velocity field, which has a significantly larger heat transfer rate for a given pumping power, for optimizing heat transfer processes.

Delivering reactants to catalyst surfaces is a convective mass transfer process essentially, which is analog to a convective heat transfer process. Mo et al. [13] used the field synergy concept to analyses the influence of the included angle between the velocity and the contaminant concentration gradient vectors to the convective mass transfer rate in the reactor. Chen et al. [20] introduced the convective mass transfer field synergy principle, which states that the overall mass transfer rate depends not only on the velocity and concentration gradient fields, but also on their synergy. Furthermore, Chen et al. [20] also deduced the laminar mass transfer field synergy equation and found a universal method for optimizing indoor decontamination ventilation designs. However, the boundary conditions of photocatalytic oxidation reactors are different from the ones of indoor contaminant sources, and the universal method for optimizing the mass transfer process in photocatalytic oxidation reactors has not been obtained.

This paper first deduces a mass transfer field synergy equation with a specific boundary condition for optimizing the processes of delivering reactants to catalyst surfaces in photocatalytic oxidation reactors. Then the optimal velocity field, which has a large mass transfer rate for a given pumping power, can be obtained by solving the field synergy equation to provide a framework for guiding the photocatalytic oxidation reactors designs. Finally, as an illustrative example, the field synergy analysis is used to optimize the convective mass transfer in plate type reactors to verify the applicability of the convective mass transfer field synergy equation.

2. Theoretical model of photocatalytic oxidation reactors

There are several types of PCO reactors such as plate type reactors, light-in-tube reactors, and honeycomb type reactors. The theoretical schematic of these reactors are summarized in Fig. 1. The upper surface is a UV lamp, which emits ultraviolet photos. The lower is a catalyst surface coated with semiconductor materials such as titanium dioxide (TiO_2). When semiconductor materials are illumi-