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Optimization of the concentration field in a suspended photocatalytic reactor

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ABSTRACT

In the present study, the photon absorption in a suspended photocatalytic reactor was simulated by adopting Monte Carlo method and the six-flux radiation absorption-scattering model. Different photocatalyst concentrations, i.e. uniform concentrations, linearly increasing concentration gradients and linearly decreasing concentration gradients, were taken into account. Simulation results indicated that increasing the photocatalyst concentration would cause higher photon absorption in the front layer but faster attenuation along the photon transfer direction. To the dilute solutions, the top layer photon loss was linearly influenced by the photocatalyst concentration. And the increasing concentration gradient resulted in higher photon absorption than the decreasing concentration gradient. The present work is expected to be of effective value for obtaining the optimal operating parameters for industrial photocatalytic applications.

1. Introduction

Photocatalytic reactors are used in wastewater degradation [1], water splitting for hydrogen production [2] and air purification [3]. Main concerns on the photocatalytic reactors are the mass transfer limitation between the photocatalyst and the solution, and the concentration or radiation distribution in the photoreactors. In order to reduce the limitation between the photocatalyst and the solution, many kinds of photoreactors are designed, i.e. the parabolic trough reactors [4], the flat-plate reactors [5], the rotating disk reactors [6], the optical fiber reactors [7] and the suspended reactors [8]. The suspended photoreactor holds high photocatalyst surface areas and mass-transfer rates, and thus has received much attention [8–11]. From the radiation transport point of view, photoreactors with suspended photocatalyst particles are different from homogeneous photoreactors because radiation scattering cannot be neglected. Fig. 1 shows a random geometry channel in a suspended photoreactor. According to Fig. 1, the RTE (radiation transport equation) in slurry photoreactors can be represented as:

$$\frac{\mathrm{d}I_{\lambda,\Omega}(s,t)}{\mathrm{d}s}+\underbrace{\kappa_\lambda(s,t)I_{\lambda,\Omega}(s,t)}_{\text{absorption}}+\underbrace{\sigma_\lambda(s,t)I_{\lambda,\Omega}(s,t)}_{\text{out-scattering}} = \underbrace{j^{\mathrm{e}}_\lambda(s,t)}_{\text{emission}}+\underbrace{\frac{\sigma_\lambda(s,t)}{4\pi}\int p(\Omega'\rightarrow\Omega)I_{\lambda,\Omega'}(s,t)\mathrm{d}\Omega'}_{\text{in-scattering}} \quad (1)$$

According to Fig. 1 and Eq. (1), the radiation at a point dA in space, with a direction of propagation Ω, traveling along distances measured by the spatial parameter "s", may be changed by: 1) a gain of photons by emission; 2) a loss of photons by absorption; 3) a loss of photons by out-scattering; and 4) a gain of photons by in-scattering resulting from multiple scattering phenomena occurring in the space surrounding point dA_0 or dA'. In order to solve the RTE, several solutions have been proposed, including Monte Carlo Method [12,13], Discrete Ordinate Method [14], Finite Volume Method [15], Ray Tracing Nodal Analytical Method [16], etc. The Monte Carlo Method is widely utilized because of its characteristics of accuracy, high-efficiency and little computation resource requirement. When the photons reaching

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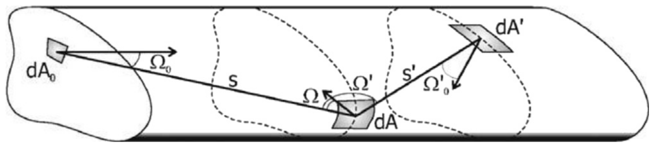

Fig. 1. Schematic of the photon transfer in the solution.

the photocatalyst, two models are mainly used in the literature, i.e. the two-flux radiation absorption model [17] and the six-flux absorption-scattering model [18]. The two-flux absorption model only takes the reflection and absorption into account whereas the six-flux absorption-scattering model considers the photon transmission, absorption, reflection and scattering.

The radiation distribution in a cylindrical photoreactor, in which the photocatalysis is uniformly distributed, is simulated in Ref. [11]. The radiation field in photocatalytic channels with different sectional configurations is simulated using the Monte Carlo method [12]. The radiation transfer model in the homogeneous photocatalytic reactors is analyzed by Cabrera et al. [19]. They proposed a series of equations for designing photocatalytic reactors based on the heat transfer theories. The two-flux radiation absorption model is proposed by assuming the bubbles uniformly distributed in the solution [17]. The two-flux radiation absorption model is used in the solid–gas photocatalytic system by neglecting the effect of continuous phase to the photons [20]. The random moving model is proposed based on the Monte Carlo method in order to explain the scattering phenomenon in a catalyst-liquid system [21]. It is found from the published literature that most researches concentrated their research under uniform photocatalysis concentration field [11,17,19–21]. There is limited research considering variable catalysis concentrations. In the present study, the photon absorption in a suspended photocatalytic reactor was simulated under different photocatalysis concentration fields. Main contributions in this study could be summarized as:

1) A simplified model is first built to simulate the photon absorption in a suspended photocatalytic reactor.
2) The built mathematical model is then validated through experimental measurement.
3) The photon absorption in the solution, the photon loss on the top surface and the effect of the concentration gradients to the photon absorption are finally analyzed.

2. Mathematical model

2.1. Methodology

There are four assumptions in order to simplify the mathematical model:

1) The photocatalyst particles are assumed to be uniform and in the configuration of ideal ball;
2) The photocatalyst particles are layer-distributing in the solution, and the particle distribution in each layer is uniform;
3) The solution is assumed not to absorb or scatter the photons;
4) During the simulation process, the system is chemically and physically in balance.

The Monte Carlo method and six-flux absorption-scattering model are used in cooperation to solve Eq. (1) in this study. The Monte Carlo method first judges whether the photon would be absorbed, reflected, transmitted or scattered. Then, the six-flux absorption-scattering model controls the photon transfer pathway. In Fig. 2, the six-flux radiation absorption-scattering model is described as the scattered photons following the route of the six directions in the Cartesian coordinate. When photons enter the solution, four phenomena may occur on the surface of the photocatalyst particle, which are absorption, reflection, transmission and scattering. The radiation absorption, reflection and scattering are under the control of certain probability, which are determined by the photocatalyst characteristics. On the other hand, the radiation transmission is the function of the photocatalyst concentration, which could be controlled manually in the present study.

The flowchart of the Monte Carlo method is presented in Fig. 3, where F_{rand} is a random number between 0 and 1, f_{tra}, f_{abs}, f_{ref} are the transmittance, absorptance and reflectance threshold value.

2.2. Configuration of the photoreactor

The configuration of the photoreactor in this study is shown in Fig. 4(a)–(c). A cylindrical photoreactor is used for the following reasons: 1) this kind of photoreactor is commonly used in industry; 2) some simulation results are available in literature for this kind of photoreactor [11]; and 3) not too heavy computer resources are needed while using Monte Carlo method. The titanium dioxide is adopted here as the photocatalyst. And the radiation is normally incident onto the top surface of the photoreactor. Detailed parameters of the photocatalyst and the photoreactor are shown in Table 1.

The boundary conditions of the photoreactor are shown in Fig. 4 (d). The side wall and the undersurface are wrapped by tinfoil in order to reflect the photons, while the top surface of the photoreactor is open without a cover. Light could enter into the photoreactor with no reflection or absorption until reaches the solution top surface.

2.3. Photon transmittance in the solution

The mass of one photocatalyst particle M_0 is:

$$M_0 = P_0 \times \frac{\pi D_0^3}{6} \tag{2}$$

where P_0 is the density of the photocatalyst and D_0 is the diameter of photocatalyst particle.

The total number of photocatalyst particles in the photoreactor N is:

$$N = \frac{M}{M_0} = \frac{P \times V}{P_0 \times \frac{\pi D_0^3}{6}} \tag{3}$$

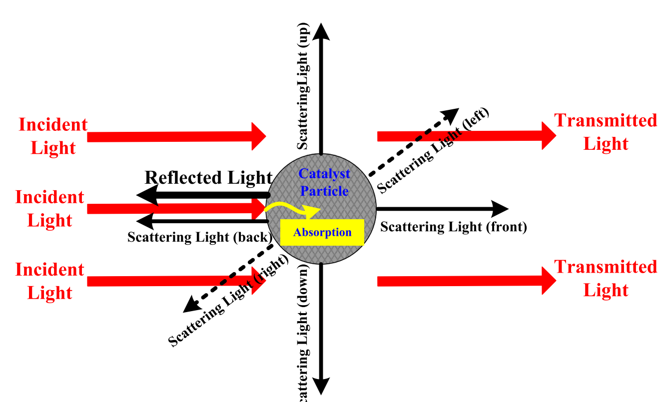

Fig. 2. Schematic of the six-flux radiation absorption-scattering model.