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Review

Some aspects of photocatalytic reactor modeling using computational fluid dynamics

Yash Boyjoo, Ming Ang, Vishnu Pareek*

Department of Chemical Engineering, Curtin University, Perth, WA 6102, Australia

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ABSTRACT

Design and analysis of photoreactors is significantly more challenging than conventional reactors due to participation of radiation in chemical reactions. This problem is further compounded in case of photocatalytic reactors because of presence of photocatalytic particles, which not only produce complex light scattering effects but, in case of slurry systems, also act as an additional phase, the hydrodynamics of which is essential to characterize for evaluating the phase distribution of photocatalyst particles without which it is not possible to calculate the light intensity distribution. This then necessitates the use of a computational fluid dynamics (CFD)-based simulation approach which can simultaneously take into account the hydrodynamics of multiple phases, light intensity distribution and reaction kinetics. This paper presents a sequential review of all steps for CFD simulations of photocatalytic reactors. The hydrodynamic modeling has been considered first with an emphasis on the Eulerian–Eulerian model because of its ability to handle large-scale photocatalytic reactor systems with only relatively moderate computational resources. This has been followed by a review of lamp emission models, which in CFD models are used as boundary conditions for solving the radiation transport equation (RTE). Before discussing the kinetics of photocatalytic reactors, a review of numerical models for solving the RTE has also been presented for both slurry and immobilized reactor systems. Finally, the paper discusses important factors for setting up the boundary conditions for CFD modeling of photocatalytic reactors.

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* Corresponding author. Tel.: +61 8 9266 4687; fax: +61 8 9266 2681.
E-mail address: V.Pareek@exchange.curtin.edu.au (V. Pareek).

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1. Introduction

Photocatalysis is an advanced oxidation process (AOP) that uses a catalyst (often TiO_2), UV light and oxygen to completely decompose organic pollutants found in liquids (e.g. dyes, organic pesticides and surfactants) or gases (such as air toxics coming from paintings and building materials) into carbon dioxide, water and a mineral acid. Alternatively, a parallel AOP can be included with the use of stronger oxidizing agents such as ozone or hydrogen peroxide instead of oxygen. However, for low pollutant concentrations (ppm or mmol L^{-1}), photocatalysis have been found to work best.

The basis of photocatalysis lies in the fact that the catalyst, upon absorption of UV light, generates electron/hole pairs on its surface. These holes can then create the very reactive hydroxyl radicals (*OH.*) via a series of reactions, for example,

$$h^+ + OH^- \rightarrow OH^{\cdot} \quad (R1)$$

The hydroxyl radical assists with the decomposition of the organic compound on the catalyst surface. The role of the oxidant is to prevent the recombination of the electron/hole pairs by reacting with the electron as per the following reaction:

$$e^- + O_2 \rightarrow O_2^- \quad (R2)$$

More details regarding the mechanisms of photocatalytic oxidation can be found elsewhere (Agustina et al., 2005; Turchi and Ollis, 1990). In summary, the photocatalytic oxidation reaction can be described by the following reaction:

$$\text{Organic pollutants} + O_2 \xrightarrow{\text{Catalyst+UV Light}} CO_2 + H_2O + \text{Mineral acid} \quad (R3)$$

Photocatalytic reactors can either be in immobilized form (with the catalyst attached to a surface) or in suspended form (where the catalyst is dispersed in the wastewater). As a result, several designs of photocatalytic reactors have been investigated. Some of the types of immobilized reactors are corrugated plate (Passalia et al., 2011a), optical fiber (Denny et al., 2009), falling film closed loop step (Stephan et al., 2011), tubular (Dijkstra et al., 2003), flat plate (Salvado-Estivill et al., 2007b), monolith (Chong et al., 2011), annular venturi (Romero-Vargas Castrillon et al., 2006), packed bed (Vella et al., 2010), fixed bed (Alexiadis et al., 2001), parallel plate mesh (Esterkin et al., 2005), multi-annular (Imoberdorf et al., 2007b), parallel flat plates (Esterkin et al., 2002) and Taylor vortex (Dutta and Ray, 2004). Slurry reactors can take several forms such as thin film slurry (TFS) (Puma and Yue, 2003), annular recirculating (Pareek et al., 2003b), moving beds (Cassano and Alfano, 2000), fluidized beds (Chiovetta et al., 2001), trickle beds (Cassano and Alfano, 2000) and externally illuminated aerated rectangular tank (Trujillo et al., 2010) reactors. Figs. 1 and 2 show some examples of immobilized and slurry reactors respectively.

Immobilized reactors do not require post-treatment for nano- to micro-sized catalyst recovery, which can end up being costly. On the other hand, slurry reactors ensure better catalyst particle light exposure and high mass transfer coefficients and generally perform better than immobilized systems (Mehrotra et al., 2005; Pozzo et al., 1999). As a result, researchers have been working towards the new design of immobilized systems to account for their limitations, leading to the development of above-mentioned reactors.

Since the generation of UV light is expensive in terms of lamp manufacturing as well as electricity consumption, researchers have taken the advantage of the UV portion of solar light (Alfano et al., 2000; Bahnemann, 2004; Goslich et al., 1997; Romero et al., 1999) by designing solar photocatalytic reactors (Fig. 3). Solar photocatalytic reactors can be in either slurry or immobilized form, and can use either direct sunlight or concentrated sunlight via the means of reflectors. Furthermore, since pure TiO_2 is activated by UV light only, investigations are being carried out for developing catalysts that can be activated by visible light (Chatterjee and Dasgupta, 2005; Rehman et al., 2009).

With all the development arising in the field of photocatalysis, the proper design and optimization of photocatalytic reactors will be of paramount importance. This paper presents a detailed literature review of the pertinent information required for modeling of photocatalytic reactors using Computational Fluid Dynamics (CFD), which is fast emerging as an efficient tool for reactor modeling. As shown in Fig. 4, this paper has been divided into four sequential steps that are required for photocatalytic reactor