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Numerical simulation of radiation distribution in a slurry reactor: The effect of distribution of catalyst particles

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HIGHLIGHTS

- The radiation distribution in a slurry reactor is studied.
- The absorption coefficient is related to the local catalyst loading.
- There exists an optimal inlet catalyst loading for the photocatalytic reaction.

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ABSTRACT

The multiphase flow leads a non-uniform distribution of catalyst particles in a slurry reactor. The previous studies used the inlet catalyst loading to compute the absorption coefficient and the scattering coefficient in the slurry reactor, which did not consider the non-uniform distribution of catalyst particle. The present study numerically studies the effect of multiphase flow on the radiation distribution in a slurry reactor. Herein, the absorption coefficient and the scattering coefficient are related to the local volume fraction of catalyst. The volume fraction of catalyst is obtained using the Eulerian-Eulerian method. The radiative transfer equation is solved using the DO model. Results show that the local catalyst loading are non-uniform in the slurry reactor. The reactor-averaged catalyst loading is always less than the inlet catalyst loading. It may leads to the underestimation of the incident radiation as well as UV disinfection and the overestimation of LVREA and as well as photocatalytic reaction rate. It is more reasonable to compute the absorption coefficient and the scattering coefficient using the local catalyst loading. A large diameter and a large inlet catalyst loading can lead to a large catalyst loading in the reactor, the large absorption coefficient and scattering coefficient, meaning a low radiation intensity in the reactor. There exists an optimal inlet catalyst loading for the photocatalytic reaction.

1. Introduction

In recent years, photocatalytic oxidation has gained a lot of attention owing to its strong oxidization ability degrading pollutants to carbon dioxide and water under common conditions [1,2]. Photocatalytic oxidation is usually motivated by UV light. When UV light is absorbed by the catalyst, the electron-hole pairs are excited within the catalyst and further hydroxyl radicals are generated on the surface of catalyst. In general, hydroxyl radicals play an important role in the photocatalytic oxidation. The generation rate of hydroxyl radicals depends on the radiation intensity in the reactor. In a slurry reactor, it is difficult to maintain a uniform distribution of radiation intensity, which can be affected by the local hydrodynamics [3,4]. Therefore, it is significant to investigate the distribution of radiation intensity in the slurry reactor.

Due to the difficulty measuring the distribution of radiation intensity, it is popular to obtain the radiation intensity in the reactor through solving the radiative transfer equation (RTE), which is an integro-differential equation describing the radiation propagation, the absorption and the scattering in space. A widely used solution strategy is to solve the RTE using the discrete ordinates (DO) method [5–10]. In the DO model, the RTE is transformed into a number of coupled equations of the discrete directions. After obtaining the distribution of radiation intensity, the incident radiation, which appears in the reaction rate kinetic equation, can be evaluated through the integration of the radiation intensity with respect to spherical coordinate. Another solution strategy is to directly obtain the distribution of incident radiation in the reactor using the P1 model [8,11–15]. The P1 model transforms the original RTE into a single diffusion equation based on the spherical harmonic expansion of radiation intensity. Compared to

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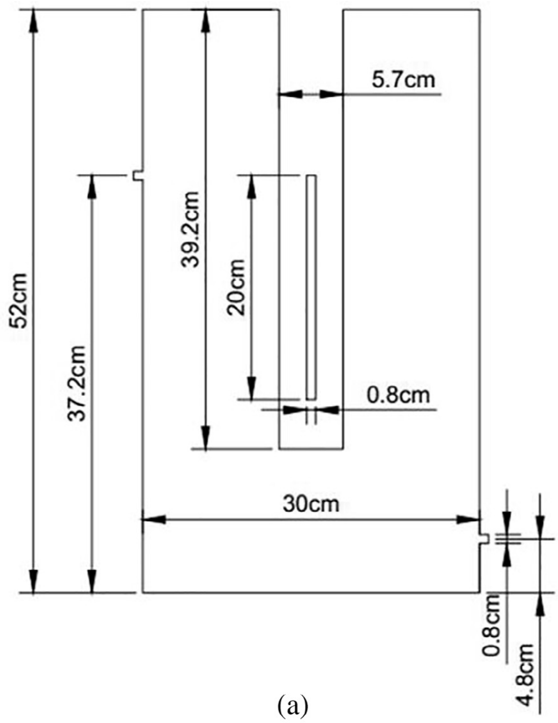
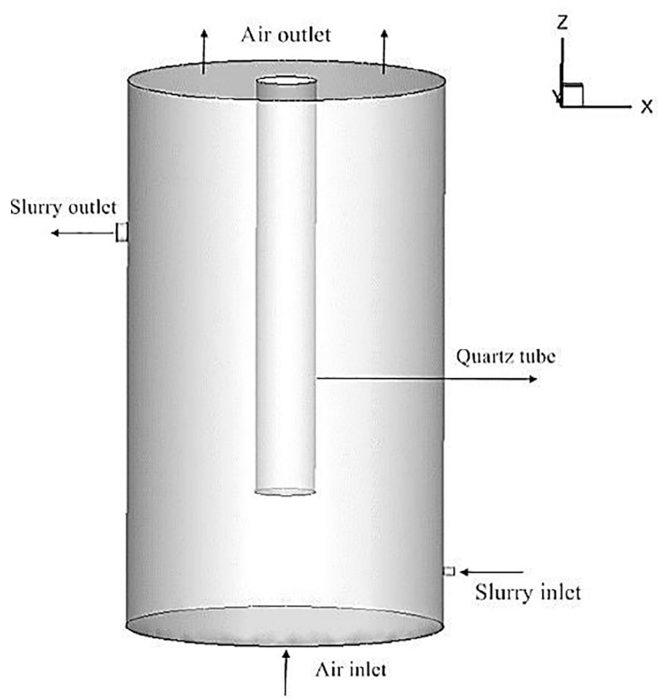


(a)



(b)

Fig. 1. Schematic of a slurry reactor: (a) planner structure and (b) stereogram structure.

the DO method, the computational effort of the P1 model can be reduced.

The key to the solution of the RTE is to determine the absorption coefficient and the scattering coefficient of UV light. For a reactor concerning only a single medium such as water, the absorption coefficient and the scattering coefficient of UV light in the reactor can be easily determined. However, it is somewhat complex in a slurry reactor since there exist multiple mediums such as water, air and catalyst particles. It is essential to have the information of the distribution of catalyst. Due to the interaction of water and catalyst particles, the flow in the slurry reactor should be simulated under the multiphase framework. The Eulerian-Eulerian method has been widely used to simulate the flow in a slurry reactor and the distribution of catalyst particles [3,6,16–18]. Those studies showed that the distribution of catalyst particles was non-uniform in the slurry reactor, which may depend on the density of the solid particles, the position of injection of the solid particles and the diameter of the particles etc. However, when modeling the radiation field in the slurry reactor, the absorption coefficient and the scattering coefficient were just related to the inlet catalyst loading in those studies instead of the local distribution of catalyst particles in the reactor. In other words, the absorption coefficient and the scattering coefficient were still assumed independent from the distribution of catalyst particles.

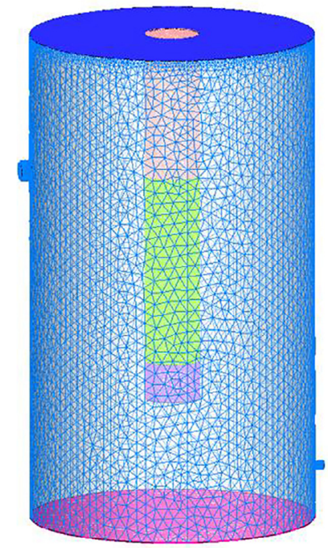


Fig. 2. Grid in the reactor.

The multiphase flow in a slurry reactor leads a non-uniform distribution of local catalyst loading, which is not equivalent to the inlet catalyst loading. Therefore, the absorption and the scattering of UV light in the slurry reactor are not likely to be uniform and cannot be simply calculated by using the inlet catalyst loading. To the best of the authors' knowledge, this non-uniformity from the multiphase flow has not been investigated in literature. The present paper aims to investigate numerically the effect of the multiphase flow on the distribution of radiation in a slurry reactor. The Eulerian-Eulerian method is used to solve the multiphase flow in the slurry reactor. Variables of catalyst particle diameters and inlet catalyst loading are investigated in detail. The absorption coefficient and the scattering coefficient are related to the local catalyst loading by using a formula in literature derived for a single catalyst loading, as shown in the Section 2.3, which may require a more precise expression.

2. Description of CFD model

2.1. Eulerian-Eulerian multiphase model

In a photocatalytic slurry reactor, there may exist water, air and catalyst particles. Under the effect of drag force due to water movement, catalyst particles show a behavior similar to fluid. The multiphase model is a good alternative to describe the flow in the