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Simulation of a Photocatalytic Reactor Using FiniteVolume and Discrete Ordinate Method: A Parametric Study

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ABSTRACT: Advanced oxidation processes for wastewater treatment have received recently a great deal of attention. Photocatalytic oxidation processes decompose water pollutants using nano-structured photocatalyst materials, titanium dioxide, and ultraviolet irradiation. Although there is extensive experimental research in this field, designing a photoreactor is still a challenge. An effectual approach to this issue is the application of computational fluid dynamics. The performance of the catalyst, which is activated by ultraviolet irradiation, is one of the important factors affecting photoreactor efficiency. In the case of poor ultraviolet radiation distribution inside the reactor, the performance decreases due to catalyst inactivity. In this study, a computational fluid dynamics model for the simulation of radiation distribution inside a photoreactor was developed and evaluated against experimental data. Simulations were then carried on different catalyst loading, lamp power and wall reflectivity. The result showed that at a low concentration of catalyst (0.4 g/l), the reaction rate increases by up to 50% by increasing the wall reflectivity to 98%. At the lamp power of 2P and P, the reaction rate increases by up to 12.2 % and 11% respectively, meaning only a 1% increase in reaction rate while increasing lamp power.

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1. INTRODUCTION

In recent years, wastewater treatment has received wide attention due to limited water resources in the world. Advanced Oxidation Processes (AOPs) are one of the promising technologies for wastewater treatment. Photocatalytic oxidation processes involve the use of oxygen and nano-structured photocatalyst materials, predominantly Titanium Dioxide (TiO_2), activated by Ultraviolet (UV) irradiation [1, 2]. Radiation distribution inside the reactor is one of the key factors to achieve the desired performance. Many studies have been carried out to study the Radiative Transfer Equation (RTE) [3, 4]. Chen et. al. [5] showed that in a UV disinfection reactor, the effect of wall reflection is more influential at higher inactivation levels.

In this study, the radiation distribution inside a photocatalytic reactor was studied by means of Computational Fluid Dynamics (CFD) simulation. The outcome of the CFD model was firstly compared with published experimental results for validation of the model, and then the performance of the reactor at different conditions was analyzed.

2. METHODOLOGY

In this research, the simulation of the photocatalytic reactor was done in a three-dimensional computational model by commercial CFD software Ansys Fluent 17.2. Fig.1 shows the computational domain and boundary conditions. The pollutant concentration at the inlet is 0.0011 kg/m^3 and the specific absorption coefficient and scattering are 338 m^2/kg and 964 m^2/kg, respectively.

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The RTE was solved using the Discrete Ordinate Method (DOM). Transport and chemical reaction were modeled by solving mass, momentum, and species conservation equations. To define the reaction rate as a function of absorbed radiation by the medium, a User Defined Function (UDF) code was written for the below equation;

$$r_p = k_1 \times (LVREA)^m C_j^n \tag{1}$$

where *LVREA* is local volumetric rate of energy absorption, and k_1, *m,* and *n* are equal to 7.5e-6, 1 and 0.82, respectively.

3. RESULTS AND DISCUSSION

Mesh independent result obtained at 830000 hexahedral cells. Fig. 2 shows the reaction rate against incident radiation which closely matches the experimental data reported by Puma et al [6].

Fig. 3 shows the reaction rate at two wall reflection values and different catalyst concentrations. As the results show, the reaction rate increases by increasing the catalyst concentration up to 0.4 g/l, although at higher concentrations the absorption coefficient of the medium increases but UV light penetration inside the reactor decreases due to increased turbidity. Fig. 3 shows that by increasing wall reflectivity at low catalyst concentration (<0.4 g/l) the reaction rate increases by up to

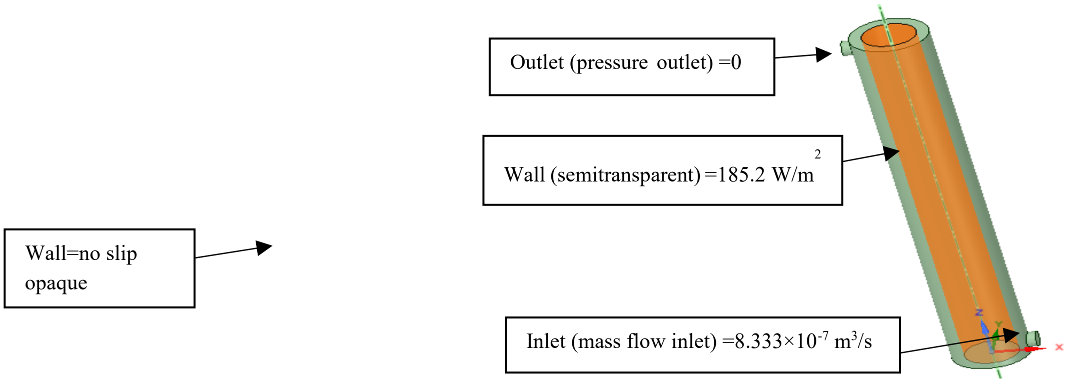

Fig. 1. Schematic of the photoreactor and boundary conditions

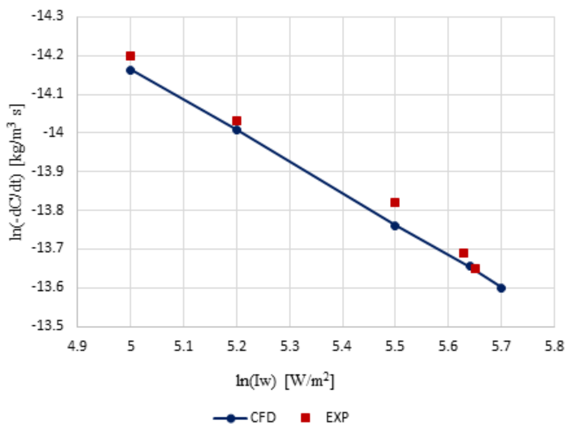

Fig. 2. Validation of the simulation results against experimental data

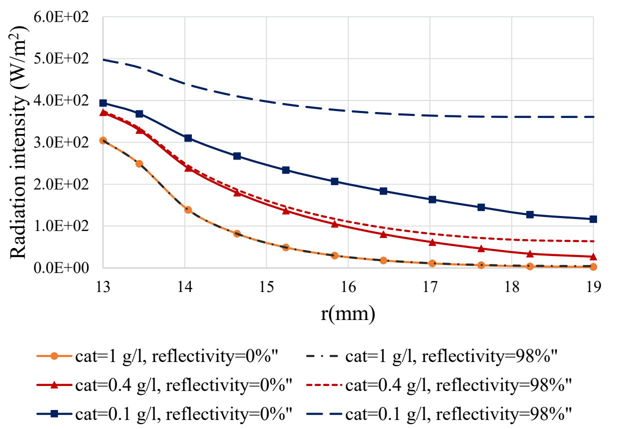

Fig. 4. Radial distribution of radiation intensity at different catalyst concentration and wall reflection

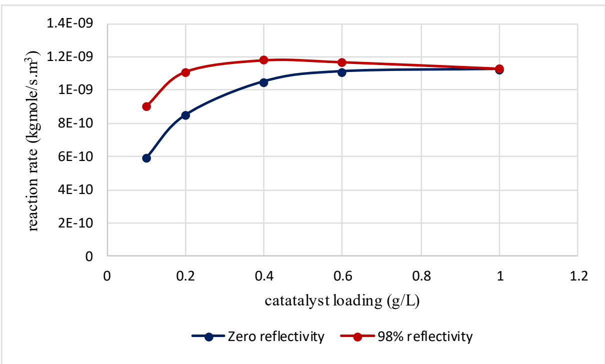

Fig. 3 Effect of wall reflectivity on the reaction rate

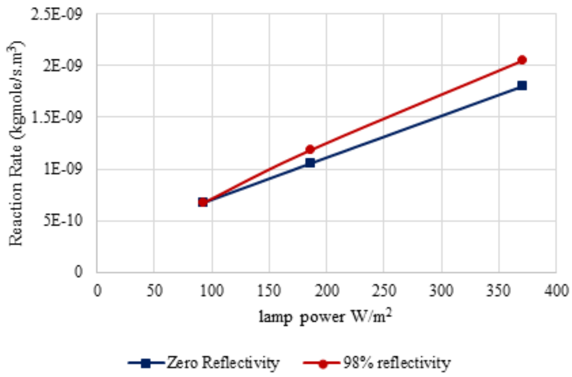

Fig. 5. Reaction rate profile at different lamp power and wall reflection of zero and 98%

50% while the increase of reaction rate for higher catalyst concentrations is only 5%. That is due to the fact that lower catalyst concentration yields a lower absorption coefficient and hence a considerable amount of radiation intensity reaches the photoreactor outer wall. This is shown in Fig. 4.

Radial distribution of radiation intensity at different catalyst concentrations and wall reflection is shown in Fig. 4. As discussed earlier, at low concentrations the photoreactor outer walls get a higher amount of radiation.

Fig. 5 shows that increasing the lamp power from *P* (initial value) to 2*P* increases reaction rate to 100% and decreasing lamp power to 0.5*P* reduces reaction rate to 50% of the initial value. To investigate the effect of wall reflection, the reaction rate at the wall reflection of 98% at different lamp powers is also plotted. Results show that increasing wall reflection increases the reaction rate 12.2% at initial lamp power (*P*). The increase of the reaction rate at the lamp power of 2*P* is 11%. This means that the effectiveness of wall reflectivity is negligibly enhanced by increasing the lamp power.

4. CONCLUSIONS

In the present research work, a slurry photocatalytic reactor was simulated using computational fluid dynamics. Firstly, the model is validated by experimental data reported in the literature. Second, the validated model was used to study the reactor performance at different conditions including catalyst concentration, wall reflectivity, and lamp power.

The results show that the higher wall reflectivity is more effective in lower catalyst concentrations (below 0.4 g/l in this work). At the catalyst concentration of 0.4 and 0.6 g/l, the increase of reaction rate is 50% and 5% when the wall reflection is 98%. Increasing lamp power to 2P increases the reaction rate up to 100% but it has a negligible effect on the received amount of radiation near the outer wall of the photoreactor. Although at low catalyst concentration, increasing lamp power enhances the effectiveness of wall reflectivity.

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