Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Monte Carlo simulation of the light distribution in an annular slurry bubble column photocatalytic reactor

*John Akach**, *Aoyi Ochieng*

Centre for Renewable Energy and Water, Vaal University of Technology, Vanderbijlpark 1900, South Africa

ARTICLE INFO

Article history:
Received 29 September 2016
Received in revised form 12 October 2017
Accepted 13 November 2017
Available online 21 November 2017

Keywords:
Photocatalysis
Slurry bubble column reactor
Light distribution
Monte Carlo
LVREA

ABSTRACT

Slurry bubble column photocatalytic reactors have been used for photocatalytic wastewater treatment. In order to design and optimize these reactors, the light distribution needs to be determined. In this work, the light distribution in a slurry bubble column photocatalytic reactor was simulated using the Monte Carlo model. The model was validated using total transmitted radiation (TTR) measurements. The validated model was then used to determine the local volumetric rate of energy absorption (LVREA) and volumetric rate of energy (VREA) profiles. Very good agreement was achieved between experimental and simulated TTR values at different catalyst loadings using a Henyey-Greenstein scattering parameter of 0.84. The Monte Carlo model was more accurate than the six-flux model. From an analysis of the LVREA profiles, the light distribution along the radial coordinate was found to be highly non-uniform. Using the VREA, the optimum catalyst loading was estimated to be 0.4 g/L. Bubbles were observed to slightly decrease the TTR while slightly increasing the light absorption especially at low catalyst loadings; therefore, bubble simulation could be neglected without significant loss of accuracy. This work highlights the accuracy and utility of Monte Carlo simulation for determining the light distribution in an annular slurry bubble column photocatalytic reactor.

1. Introduction

The increase in recalcitrant chemicals in wastewater streams is a concern since these chemicals cannot be eliminated by conventional wastewater treatment plants (Klavarioti et al., 2009). As a result, a concerted research effort has been targeted towards the development of cost effective, efficient and scalable treatment methods capable of removing recalcitrant chemicals from wastewater. One of the most promising method for treating recalcitrant chemicals has been photocatalysis. This is due to its relatively low cost, non-toxicity and its ability to degrade pollutants instead of merely transferring them to another phase (Malato et al., 2009). Photocatalysis is based on the absorption of photons of appropriate energy by a semiconductor catalyst resulting in the generation of highly reactive electron-hole pairs. These electron-hole pairs then participate in a series of redox reactions with water and dissolved organic pollutants which degrade the pollutants successively into simpler chemicals (Gaya and Abdullah, 2008). The most popular photocatalyst has been P25 TiO_2 due to its balanced properties of high reactivity, chemical resistance, non-toxicity and resistance to photo-corrosion (Malato et al., 2009).

Photocatalysis is normally carried out in reactors which bring pollutants, catalyst particles and light photons into contact (Braham and Harris, 2009). The catalyst in these reactors can be applied in slurry form or immobilized on supports (Apollo et al., 2014). While catalyst separation is less costly with supported catalysts, they tend to have lower rates of reaction as compared to suspended catalysts due to mass transfer limitations (Chong et al., 2010). Several light sources have also been investigated for illuminating the catalyst such as mercury ultraviolet (UV) lamps (Apollo and Aoyi, 2016), light emitting diodes (Jo and Tayade, 2014) and sunlight (Malato et al., 2009). Mercury UV lamps remain the

* *Corresponding author.*
E-mail address: johna@vut.ac.za (J. Akach).
https://doi.org/10.1016/j.cherd.2017.11.021

most attractive light source since the other alternatives are unreliable or inefficient.

Currently, the most efficient reactors have the UV lamp installed inside a column and the catalyst applied in suspended form (Chong et al., 2010). In these reactors, the suspended catalysts can be fluidized with the wastewater or compressed air (Apollo and Aoyi, 2016). The use of compressed air for fluidization is especially attractive since it is less costly and has the additional advantage of supplying oxygen as an electron acceptor directly into the reactor (Gaya and Abdullah, 2008). This was demonstrated by Matsumura et al. (2007) and Chong et al. (2009) who reported an increase in the rate of photocatalysis with an increase in the air flow rate in their bubble column photoreactors. In the design, analysis and scale up of a slurry bubble column reactor, all the factors that could affect the rate of photocatalysis namely catalyst, bubble, pollutant and light distribution should be accounted for. Very good mixing is possible in a slurry bubble column reactor; therefore, an assumption of homogeneous catalyst, pollutant and bubble distribution in the reactor can be made (Boyjoo et al., 2014a). Such an assumption is not valid for light distribution which is always inhomogeneous (Camera-Roda et al., 2016). As a result, most photocatalytic reactor models have focused on light distribution.

Light distribution is crucial as it is the basis of such important photocatalytic reactor design parameters such as the local volumetric rate of energy absorption (LVREA), photocatalysis intrinsic kinetics and efficiency parameters (Moreira et al., 2010). Experimental determination of the light distribution in a reactor is not feasible; instead, light distribution has been established using simulation. The most rigorous light distribution simulations have been carried out by solving the radiation transport equation (RTE) (Eq. (1)). For photocatalysis systems, the scattering terms on the right-hand side of the RTE renders an analytical solution to the RTE impossible. Therefore, numerical methods have been developed for solving the RTE. The most rigorous of these numerical methods are the deterministic discrete ordinates method (Boyjoo et al., 2013) and the stochastic Monte Carlo method (Moreira et al., 2010; Valadés-Pelayo et al., 2014). Methods with several simplifying assumptions such as the six-flux method (Li Puma et al., 2010) and P1 method (Orozco et al., 2009) have also been used to solve the RTE.

The accuracy of the Monte Carlo method for light distribution simulation has been highlighted by several researchers (Moreira et al., 2010; Valadés-Pelayo et al., 2014). The Monte Carlo method solves the RTE stochastically by tracking a statistically adequate number of photons from the lamp until they are absorbed in the slurry or lost in the reactor wall. Several studies have employed the Monte Carlo method to determine the light distribution in photocatalytic reactors. Singh et al. (2007) simulated the light distribution in a monolith reactor for air treatment using the Monte Carlo method. Imoberdorf et al. (2008) used the Monte Carlo method to determine the light distribution in a fluidized bed reactor with TiO_2 coated spheres. Moreira et al. (2010) and Valadés-Pelayo et al. (2014) developed a Monte Carlo algorithm for establishing the light distribution in a slurry photocatalytic reactor with nanosized TiO_2 catalysts. All these previous studies were carried out in a slurry photocatalytic reactor with no air bubbles. According to the authors' knowledge, the Monte Carlo method has never been applied to determine the light distribution in a slurry bubble column reactor.

A few studies have reported the light distribution in a slurry bubble column reactor using other simulation methods. Boyjoo et al. (2013) simulated the light distribution in a multi-lamp bubble column reactor using the discrete ordinates method. They found that bubble scattering was negligible as compared to the catalyst scattering. Motegh et al. (2013) utilized a bi-directional scattering model to study the effect of bubbles in a theoretical three-phase reactor with suspended catalysts. They concluded that bubbles at typical sizes and gas flow rates have no significant effect on the light absorption. Trujillo et al. (2007) used the discrete ordinates method to model the light distribution on catalysts immobilized on flat plates which were immersed in a bubble column. They found that bubble scattering improved the light distribution on the flat plates. The effect of bubbles on gas-phase photocatalytic reactors was investigated by Iatridis et al. (1990) and Brucato et al. (1992). In these reactors, an increase in gas flow rate was observed to increase the light transmission through the reactor.

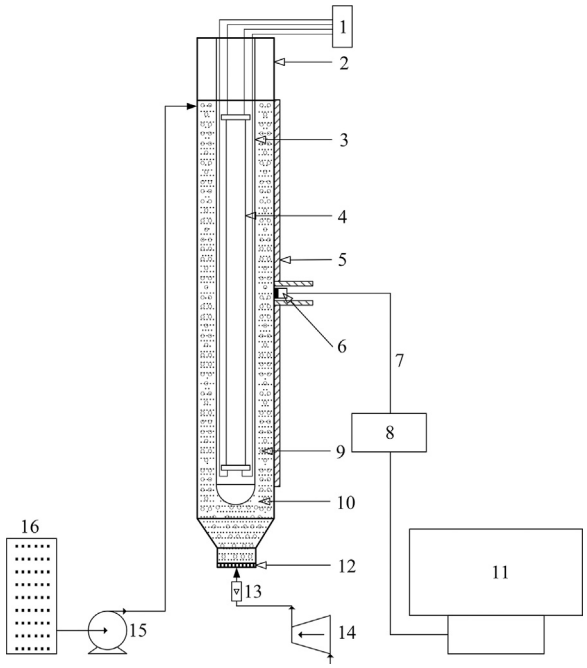

Fig. 1 – Radiation field measurement setup. (1) Power supply, (2) reactor wall, (3) lamp sleeve, (4) black light lamp, (5) radiation sensor support, (6) radiometric sensor, (7) fibre optic cable, (8) spectroradiometer, (9) air bubble, (10) catalyst slurry, (11) computer, (12) porous distributor, (13) rotameter, (14) air compressor, (15) peristaltic pump, (16) feed tank.

An important question in a slurry bubble column reactor is if bubbles affect light absorption and if it is necessary to include bubble simulation in the light distribution model (Motegh et al., 2013). The only study which attempted to answer this question, Motegh et al. (2013), concluded that bubbles have a negligible effect on light absorption by the catalysts. However, they modelled a theoretical reactor using a highly simplified model which was not validated. Clearly more work needs to be carried out in this area using rigorous validated models in order to establish the conclusions made by other authors. In the present study, a rigorous model based on the Monte Carlo method was validated and then used to simulate the light distribution in a slurry bubble column photocatalytic reactor. The aim of this work was to investigate the effect of catalyst and bubbles on the light distribution in a slurry bubble column photocatalytic reactor.

2. Methodology

2.1. *Reactor set up*

The slurry bubble column photocatalytic reactor (Fig. 1) consisted of a 2.2 mm thick reactor wall and a 1.4 mm thick glass sleeve made of clear borosilicate glass. The reactor wall outer diameter and the glass sleeve outer diameter were 65 and 34 mm, respectively. Air was supplied to the reactor from an oil free compressor (Jun-Air) through a borosilicate glass porous distributor with a pore size of 10–16 μm. A rotameter was provided to control the flow rate of the air entering the reactor.

The total height of the reactor was 900 mm with a working height of 600 mm and a liquid capacity of 1.25 L. The reactor was operated in continuous mode for the air and batch mode for the liquid and catalyst. Reactor illumination was provided by an 18 W low pressure black light blue lamp (Philips) installed inside the glass sleeve. The lamp had a diameter of 26 mm, arc length of 515 mm and a photon emission rate of 2.1×10^{-5} Einsteins/s. The light passing through the reactor