EVALUATION OF PHOTON ABSORPTION PARAMETERS IN AN AQUEOUS PHOTOCATALYTIC SLURRY REACTOR USING MONTE CARLO SIMULATIONS AND MACROSCOPIC BALANCES

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Summary

The radiation field for an annular photocatalytic reactor is simulated using a modified Monte Carlo method (MC) for two different TiO_2 suspensions in water. Two models are studied: Model A considers that the black-light (BL) lamp absorbs all the photons back-scattered by the annular region, whereas model B assumes that the BL lamp reflect them. Experimental evaluation of photon absorption and forward-scattering rates are determined by a Macroscopic Radiation Balance (MRB). The MC simulations with Model B agreed closely with experimental observations. The optimal TiO_2 DP25 concentration calculated by MC was 0.14 g/*l*, is comparable to the experimentally observed optimum value in photocatalytic phenol degradation.

Keywords

Annular photoreactor, Monte Carlo simulation, radiation field

Introduction

Heterogeneous photocatalysis is a promising alternative method for the removal of organic and inorganic pollutants in water.[1] Photocatalytic reactions are the result of the interaction of light with the semiconductor generating e^-/h^+ pairs which are responsible for the degradation of organic compounds. Efficiency factor determination, case of the Photochemical Thermodynamic Efficiency Factor[1], involves a common variable, the rate of photons absorbed by the photocatalyst. An accurate estimation of local volumetric rate of energy absorption (LVREA) is therefore necessary in rating of photoreactors.[2] LVREA can be found from the solution of the radiative transfer equation (RTE). A numerical solution seems however to be a best approach in solving the RTE. Moreover, stochastic simulation methods, such as MC method, can be implemented with advantage over deterministic methods in finding the LVREA for complicated geometries.[3] Furthermore, experimental macroscopic radiation balance (MRB) can be conducted combining radiometric measurements with a radiation balance to determine the radiation absorbed by the photocatalyst.[4]

Modeling Approach Adopted

In the present study, MC simulations were performed to determine the LVREA inside the Photo-CREC Water-II reactor. The scattering and absorption coefficients used for the simulations were the ones reported in the literature. The experimental LVREA was found from the MRB applied to a control volume in the photoreactor with boundaries containing the slurried TiO_2 catalyst.[2] Parameters such as extinction coefficient, the probability of photon absorption by the catalyst and the probability of radiation absorption by the internal Pyrex glass tube and, isotropic scattering mode were assumed. Two models were considered in the simulation: Model A which considers that the BL lamp absorbs all the back-scattered photons, whereas Model B assumes that the BL lamp reflect them.

Comparison of light absorption and forward-scattering radiation from MRB and MC simulation showed a satisfactory agreement when the spectral distribution for the absorption and scattering coefficients were used in the case of the more phenomenologically sound Model B.

In the MC simulation, the RTE is solved by tracing trajectories and fates of all the photons emitted by the lamp which are found by using random numbers.[3] The model assumptions made in this study include the following:

i. Photon emission from the lamp surface is assumed to be uniform and directional dependent.
ii. Photon emission from the lamp surface is considered to be a stochastic process.
iii. Emitted photons have a 6% probability to be absorbed by the Pyrex glass before entering the reacting medium. Furthermore, reflected photos by the slurry medium are

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absorbed with the same probability. Photons reaching the lamp are absorbed with Model A, while Model B assumes that they are elastically reflected at the same with different angular and equatorial angles. Photon scattering by the reacting medium is assumed to be elastic and perfectly diffuse (isotropic scattering).

iv. Photons reaching the outer polyethylene reactor wall, are considered absorbed. These photons are counted as a transmitted photon only.

Results and Conclusions

Figure 1 reports the comparison of experimental LVREA and transmitted radiation through the reactor compared

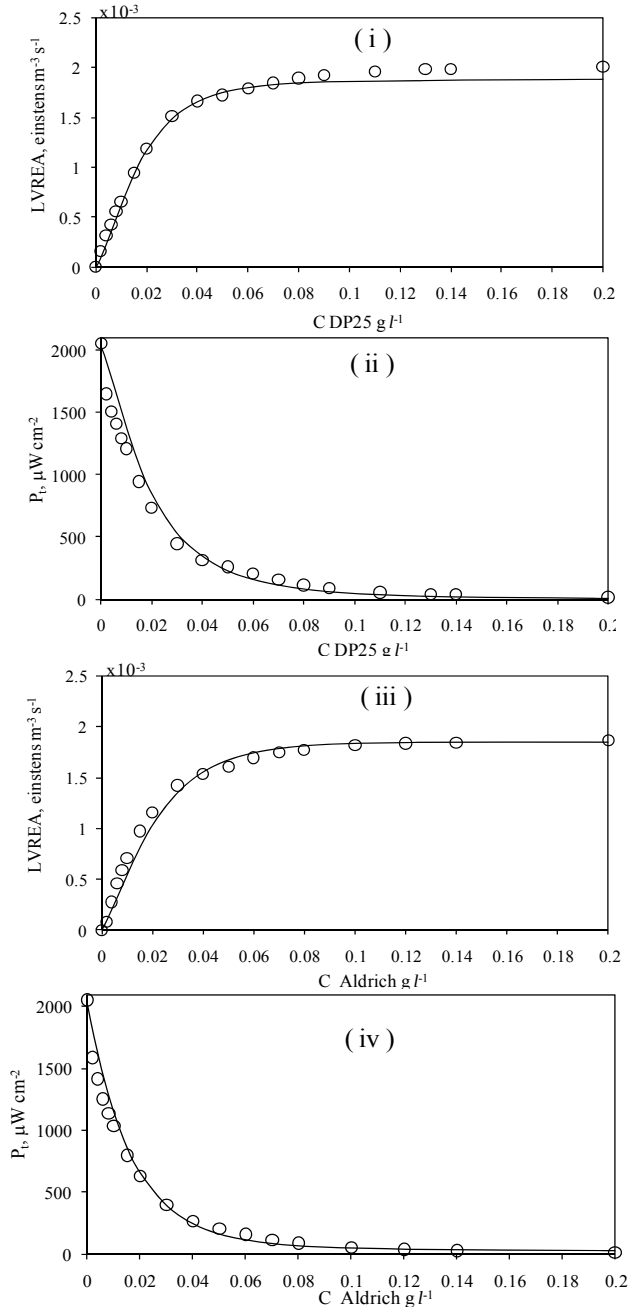

Figure 1. Transmitted radiation and the LVREA for Model B when the spectral distribution for the scattering and absorption coefficients is considered. (○) experimental results, (—) MC simulation. (i) LVREA for DP25, (ii) transmitted radiation for DP25, (iii) LVREA for Aldrich and (iv) transmitted radiation for Aldrich. Experimental results taken from 5 measurements (SD = 2.39%).

with the MC simulation for Model B, when the spectral distribution for the absorption and scattering coefficients were used. A good agreement with experimental results is found for Model B. On the other hand results for Model A (not shown here) demonstrate that when the BL full absorption of back-scattered photons assumption is adopted, a poor prediction for the LVREA and the transmitted radiation is obtained. Furthermore, the MC simulation for different DP25 concentrations revealed that there is an optimum catalyst concentration of 0.14 g/*l*. This optimum photocatalyst concentration is comparable to the experimentally observed optimum in the photocatalytic phenol degradation (Figure 2).[1] On the basis of the above, it can be concluded that,

(a) LVREA can be predicted with Model B. This is confirmed via the excellent agreement of LVREA observed from MRB. Thus, Model B can be considered as an effective tool in finding the LVREA for concentric photocatalytic reactors.

(b) LVREA reaches a maximum value for DP25 at the "optimum concentration" of 0.14 g l^{-1}. This optimum agrees with the optimum found from phenol photocatalytic degradation.

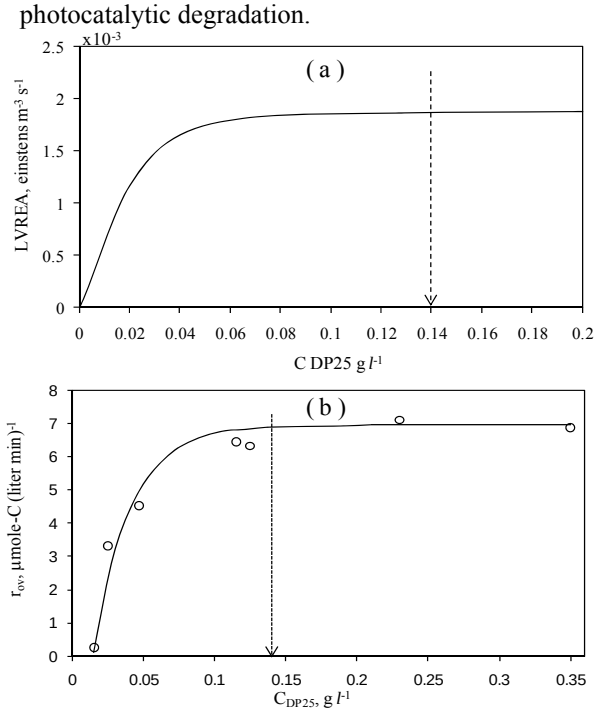

Figure 2. (a) LVREA as a function of DP25 loading. (b) Overall reaction rate for phenol degradation versus DP25 concentration.[1]

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