catalysts

Supplementary material.

1. Reactor Modelling:

Radiation absorption and scattering is described by the Radiative Transfer Equation (RTE) as follows:

$$\frac{dI_\lambda(S,\Omega)}{dS} = -\kappa_\lambda I_\lambda(S,\Omega) - \sigma_\lambda I_\lambda(S,\Omega) + \frac{\sigma_\lambda}{4\pi}\int_{\Omega=4\pi} p(\Omega' \to \Omega) I_\lambda(S,\Omega') d\Omega' \quad \text{(S1)}$$

ABSORPTION OUT-SCATTERING IN-SCATTERING

Where I_λ is the photon incident irradiance at λ is the wavelength, $\kappa_\lambda$and σ_λ are the absorption and scattering coefficients respectively, S is a spatial coordinate and Ω is the directional solid angle [1]. The main difficulty in the application of RTE is to define the term $p(\Omega' \to \Omega)$ which is the scattering phase function representing the probability of a photon to be redirected by scattering from the direction Ω', around position S, into the direction Ω [2]. In the last few decades, some authors had focused their efforts to solve the RTE using several approaches, such as the Discrete Ordinary Method (DOM) and the Monte Carlo (MC) stochastic method [3].

The Six Flux Absorption-Scattering Model (SFM) has been proposed as a practical and simplified approach for solving Equation (S1) [1]. The principal assumptions of this model are [2]:

1. The photocatalyst particles are distributed in the reaction volume in a uniformly way.
2. The fluid photon absorption is negligible.
3. The photons with lower energy than the photocatalyst band-gap are not considered.
4. The photons are either absorbed or scattered upon colliding with catalyst particles and scattering follows the route of one of the six directions of the Cartesian coordinates.
5. The optical properties are described considering geometric coordinates.

First, the directions of Cartesian coordinates were assigned with scattering probabilities related to a photon balance proposed by Brucato et al. [3] in order to define the phase function. Afterwards, the phase function was estimated by the Henyey-Greenstein scattering phase function (SFM-HG) based on the assumption that in a heterogeneous photocatalytic reactor the scattering of photons occurs only along the six cartesian directions. These directions were assigned with scattering probabilities: "sideward probability" (p_s), "backward probability" (p_b) and "forward probability" (p_f) and in this work were P_b=0.133, P_f=0.754, and P_s=0.028 obtained for commercial TiO_2 P25 Aeroxide catalyst from literature [1]. In this work, the SFM-HG was used to estimate de Local Volumetric Rate Photon Absorption (LVRPA) in any point on the reactor. This model is applied for planar geometry. Since the light distribution around our reactor was homogeneous, it was considered that the light behavior is the same in a plane that at any point of the reactor height. So that, the spatial Cartesian coordinate was adapted to polar coordinates in order to describe the reactor geometry. Thus, the equation system employed to for LVRPA evaluation is shown in (S2).

$$\mathrm{LVRPA} = \frac{\mathrm{I_0}}{\lambda_{\mathrm{Rcorr}} \times \mathrm{R_{corr}} \times (1-\Upsilon)} \times \left[\left(\mathrm{R_{corr}} - 1 + \sqrt{1-\mathrm{R_{corr}^2}}\right) \times e^{\frac{-\mathrm{Rp}}{\lambda_{\mathrm{Rcorr}}}} + \Upsilon \right.$$
$$\left. \times \left(\mathrm{R_{corr}} - 1 - \sqrt{1-\mathrm{R_{corr}^2}}\right) \times e^{\frac{\mathrm{Rp}}{\lambda_{\mathrm{Rcorr}}}} \right] \quad \text{(S2)}$$

Equation (S2)has been explained in section 3.4. Before solution of S2, S3-S10 should be solved:

$$\mathrm{R_{corr}} = \frac{\mathrm{b}}{\mathrm{a}} \quad \text{(S3)}$$

$$a = 1 - R \times p_f - \frac{4 \times R^2 \times p_s^2}{1 - R \times p_f - R \times p_b - 2 \times R \times p_s} \quad \text{(S4)}$$

$$b = R \times p_b + \frac{4 \times R^2 \times p_s^2}{1 - R \times p_f - R \times p_b - 2 \times R \times p_s} \quad \text{(S5)}$$

$$R = \frac{\sigma}{\beta} = \frac{\sigma}{\sigma + \kappa} \quad \text{(S6)}$$

$$\lambda_{Rcorr} = \frac{1}{a \times \beta \times \sqrt{1 - R_{corr}^2}} \quad \text{(S7)}$$

$$\gamma = Gamma = \frac{1 - \sqrt{1 - R_{corr}^2}}{1 + \sqrt{1 - R_{corr}^2}} \times e^{-2 \times TaoApp} \quad \text{(S8)}$$

$$TaoApp = a \times Tao \times \sqrt{1 - R_{corr}^2} \quad \text{(S9)}$$

$$Tao = L \times \beta \times Ccat \quad \text{(S10)}$$

Equation S3 defines the corrected Albedo number (R_{corr}) and refers to the probability of photon collision with a catalyst particle inside the reactor. S4 and S5 were used to calculate the corrected Albedo number based on the probabilities calculated for the commercial titanium dioxide and already published in literature [1]. S6 refers also to the Albedo number (R), and it was calculated based on the specific extinction (β), absorption (κ) and scattering (σ) coefficients. The parameter λ_{Rcorr} (S7) relates the probabilities of scattering (p_s, p_b, p_f), the specific extinction coefficient (β) and the corrected Albedo number (R_{corr}). S8 includes the TaoApp parameter, which involves the apparent optical thickness (Tao) (S9) and is related to the catalyst concentration (S10). Thus, the influence of the catalyst concentration on the radiation field distribution can be evaluated and optimized with the Overall Volumetric Rate Photon Absorption (OVRPA) calculation (S11)

$$OVRPA = \int_0^V LVRPA \, dV \quad \text{(S11)}$$

2. High-Performance Liquid Chromatography:

The calibration curve used in the High-Performance Liquid Chromatography (HPLC) was added to the Supplementary Material as Figure S1. The R^2 for the correlation is 0.994. The limit of quantification (LOQ) is 0.5 mg/L.

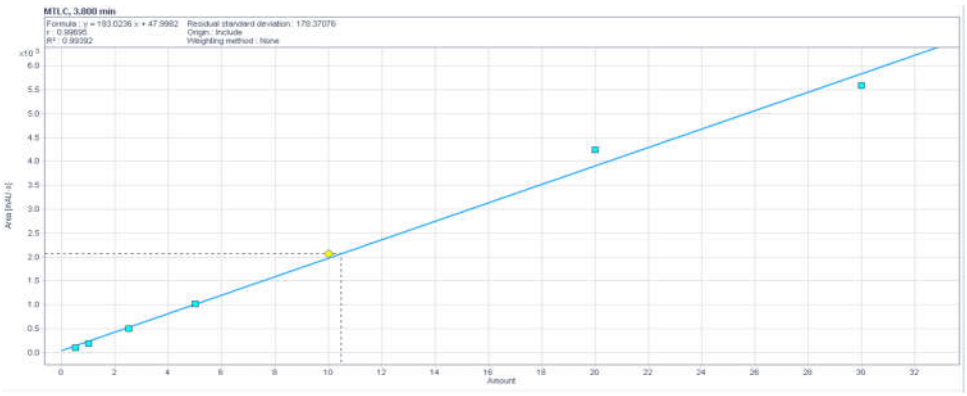

Figure S1. Calibration Curve for the S-Metolachlor using in the HPLC.

Bibliography

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