CHEMICAL ENGINEERING TRANSACTIONS
VOL. 57, 2017

A publication of
AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Sauro Pierucci, Jiří Jaromír Klemeš, Laura Piazza, Serafim Bakalis

ISBN 978-88-95608- 48-8; **ISSN** 2283-9216

Electromagnetic Model for Determining the Speed of Absorptive Photonic in a Solar Collector in V (V-Collector)

German Ramos[a], Pablo Velásquez[*a], Paola Acevedo[a], Angélica Santis[a], Johan Rincón[a] , Andrés López[b]

[a]Universidad Cooperativa de Colombia – UCC (Bogotá)
[b]Universidad Libre – (Bogotá)
pablo.velasquez@campusucc.edu.co

The electromagnetic model for determining the speed of absorptive photonic in a V-collector was developed as the function of electrical and magnetic characteristics of a medium, considering both the phase factors and the attenuation of the suspension. For this purpose the six-flux model was used to simulate the photonic absorption and the ray-tracing tool was used to model the rays of incident radiation on the V-collector. The developed model represents a new approach to those reported previously in the literature.

1. Introduction

The heterogeneous photocatalysis based on TiO_2 and modified semiconductors have been recently used for the treatment and purification of slightly contaminated effluents (<1 mg L^{-1}), in self-cleaning of surfaces and as an alternative route in the generation of energy in a sustainable way. By means of the irradiation of the semiconductor with energy of impinging photons higher than its band gap (TiO_2 λ <384 nm) the procedure generates a couple electron/hole capable of initiating reactions of reduction and oxidation. Oxidation reactions generate holes that occur at the surface of TiO_2 in an aqueous medium, through hydroxyl radicals responsible for the degradation of a wide range of pollutants, including organic and inorganic compounds, and inactivation of microorganisms and toxins

The quantum yield of the photocatalytic process can be determined when the spatial and directional distributions of radiation intensities are known in the suspension, thus partially solving the problem of the reaction rate. This ratio is described by the local volumetric rate of photon absorption (LVRPA) representing the spatial distribution or the photon availability in the reactor. The electromagnetic waves (photons) that are responsible for the catalyst activation process when they penetrate into the medium, are dispersed, absorbed and reflected by the suspension. The description of this complex process is performed by means of a physicomathematical model, which is known as the radiative transfer equation (RTE).

Many studies have been developed in this way, because of the complexity of the analytical solution. Both the empirical models for the determination of LVRPA and the estimation of experimental parameters that fit the solution of the RTE result in an of great mathematical complexity that makes it practically impossible to scale up. To pass from the laboratory to the commercial scale implies the inability of controlling parameters such as albedo, solar dispersion in the medium, etc. It is noteworthy that in any controlled photocatalytic process, the kinetics of catalyst activation is always a photochemical act that depends on the local value of the volumetric rate of energy absorption (LVREA).

Most studies have focused on the RTE solution for modeling LVRPA and LVREA in parabolic trough collectors (PTC) and parabolic concentrators (PC). Considering that the overall performance in terms of the accumulated energy by a V-collector is close to obtaining in a PTC (Bandala et al., 2004), it makes interesting the LVRPA determination. Since there are no reports for this type of configuration of V collector. In the same article, it was concluded that "the incidence angle affects the total amount of energy achieved, but it does not greatly reduce the efficiency of the reactors to use this energy in the photocatalytic process"

For the estimation of the speed of local photon absorption (LVRPA) in photocatalytic heterogeneous systems the six-flux approach absorption-scattering model (SFM) was proposed (Brucatto et al., 2006). This approach

is based on the directional dispersion in three axes, combined with the technique based on the ray-tracing for modeling of the incident radiation. A model for the LVRPA in photocatalytic mineralization of pollutant compounds is also presented.
In this research we develope an electromagnetic model of estimation of the absorbed UV energy by the catalyst in a suspension in order to evaluate the absorption of photons in a heterogeneous photocatalytic reactor (v collector) based on electrical and magnetic characteristics of the suspension. The analysis of the electromagnetic characteristics of the medium allow us to estimate the local energy absorption inherent to the medium and to determine the model of the local volumetric speed of absorption of photons.

2. Material and methods

For the elaboration of the proposed model, the electromagnetic model for the LVRPA, the two-flux (TFM) and the six- flux (SFM) approaches were used. Using the electromagnetic theory was presented a way to establish the LVRPA from the characteristics of the medium and the frequency of the incident rays on the aqueous medium, which correspond to the rays reflected by the reflective surface of the V-collector.
In order to delimit the study, as well as to establish an equivalence between the developed models (the two-flux and six-flux), it was assumed the following:
1. Cylindrical coordinate system, it best describes the behavior of the rays reflected by the flat reflectors of the V-collector, on the cylindrical glass tube through which the suspension runs.
2. The direction of incidence of the rays is radial with respect to the cylindrical coordinate system proposed.
3. There are n planes with the same form of particle distribution.
4. The incident rays will be reflected at an angle θ with respect to the radial direction.
5. The catalyst absorbs all the local radiation, because of this it becomes necessary to calculate the attenuation factor of the electromagnetic waves in the medium.
6. There is no emission by the heterogeneous system.

3. Results and discussion

The Maxwell's equations are a set of physical-mathematical descriptions that represent any classical phenomena of nature either electric, magnetic or electromagnetic character. The phenomenon of light energy transport in a medium (as in the case of radiation incident in a catalyst slurry) can be described by Maxwell's equations. They offer a way how to predict the amount of photons that are present locally in a medium radiated with UV radiation. This application is very useful to model the LVRPA in suspension since the photons are corpuscular representations of electromagnetic waves.

The procedure for obtaining the model is described below:

1) Choosing the flow models: The flow model represents a way of describing how photons interact with the suspension. The photon flux was modeled assuming the photons interact with the medium and had only two possible directions of dispersion (forward-back) (Brucato and Rizzuti, 1997). The six-flux model represents the two-flux model carried to three rectangular coordinates such that there would be six possible dispersion directions (six-flux). This fact establishes the possibility of having the six-flux model not in Cartesian coordinates but in cylindrical coordinates.
2) Substitute for derivation: a mathematical development to establish the appropriate substitute for total derivation (rate of change in one dimension) was presented. It was established that the adequate substitute for the one-dimensional derivative is the divergence.
3) Proposed model: Two-flux and six-flux models represent approximations of how photons interact with the medium. It was then proposed that the photon flux per unit area impacting the particle should be proportional to the number of photons that penetrate the suspension.
4) The proposed equation solution: Taking the divergence in cylindrical coordinates, the partial differential equation was solved using the Fourier variable separation method. Where appeared a constant (dependent on the initial conditions) and an own value (dependent on the boundary conditions), which should be determined to obtain the proposed electromagnetic model, which clearly represents a new way of dealing with the problem.
5) Determination of constants: In order to determine the constants, the concepts of attenuation, phase and propagation factor were applied in a medium where the density or distribution of charges is not significant. The attenuation and phase factors are related to the constants.

Consider a vector field in $\mathbb{R}^3$,

$$U(x,y,z) = u(x,y,z)\hat{e_1} + v(x,y,z)\hat{e_2} + w(x,y,z)\hat{e_3} \tag{1}$$

Where the vectors $\{\hat{e_1}, \hat{e_2}, \hat{e_3}\}$ are a canonical basis in an orthogonal curvilinear coordinate system (Spiegel, 1959).
In addition, assume that Ω is a bounded region of $\mathbb{R}^3$ and additionally the regularity of the function U of $\mathbb{R}^3$ in $\mathbb{R}^3$ that defines the field. This means that $U \in C^1(\mathbb{R}^3)$, which means that U and its first-order derivatives are continuous.

Applying the Taylor theorem, we have in Equation. 1

$$U(\vec{x} + \vec{h}) = U(\vec{x}) + J_{\vec{z}}U(\vec{x})\vec{h} + o\left(\left|\vec{h}\right|^2\right) \tag{2}$$

Where $\vec{x} = (x,y,z)$, $\vec{h} = (h_1, h_2, h_3)$ and $J_{\vec{z}}U(\vec{x})$ is the Jacobian of U at the point $\vec{x}$. If $\vec{h} \to 0$ we can take $U(\vec{x}) + J_{\vec{z}}U(\vec{x})\vec{h}$ as the approximate value of $U(\vec{x} + \vec{h})$.

$U(\vec{x})$ represents a translation, whereas $J_{\vec{z}}U(\vec{x})\vec{h}$ is written as

$$J_{\vec{z}}U(\vec{x})\vec{h} = \begin{pmatrix} u_x & u_y & u_z \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{pmatrix}\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} \equiv A\vec{h} \tag{3}$$

Considering the symmetric and antisymmetric part of A that is,

$$D = \frac{1}{2}(A + A^t) \quad y \quad R = \frac{1}{2}(A - A^t) \tag{4}$$

The approximate value of $U(\vec{x} + \vec{h})$ can be expressed as

$$U(\vec{x}) = D\vec{h} + R\vec{h} \tag{5}$$

Therefore

$$Trace(D) = \nabla \cdot U \tag{6}$$

When applying an orthogonal curvilinear coordinate change, the matrix D can be changed into a diagonal matrix D of the form

$$\widetilde{D} = \begin{pmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{pmatrix} \tag{7}$$

And we have that $Trace(D) = \nabla \cdot U$ since the *Trace* is an invariant under the transformation of orthogonal curvilinear coordinates. The values d_i are related to the scale factors characteristic of each coordinate system.
Thus, $D\vec{h}$ is interpreted as follows. Let P_o be a parallelepiped and *P(t)* the evolution of P_o at time *t* i.e., If $\vec{h}(t) = \left(h_1(t), h_2(t), h_3(t)\right)^t$ are sides of *P(t)* y $\vec{h}_0 = (h_{01}, h_{02}, h_{03})^t$ the sides of P_o is verified

$$\begin{cases} \dfrac{d\vec{h}}{dt}(t) & = D\vec{h}(t) \\ \vec{h}(0) & = \vec{h}_0 \end{cases} \tag{8}$$

The $\tilde{h}_i, i = 1,2,3$ the transformations of the h_i scale factors of the transformation of orthogonal curvilinear coordinates.

$$\frac{d\tilde{h}_i(t)}{dt} = d_i\tilde{h}_i(t), \quad i = 1,2,3 \tag{9}$$

And therefore,

$$\frac{d}{dt}Vol\big(P(t)\big) = \frac{d}{dt}\left(\tilde{h}_1(t), \tilde{h}_2(t), \tilde{h}_3(t)\right) = \left(\sum_{i=1}^{3} d_i\right)\left(\tilde{h}_1(t), \tilde{h}_2(t), \tilde{h}_3(t)\right) = (\nabla \cdot U)Vol\big(P(t)\big) \tag{10}$$

The divergence measures the rate of change of volume associated with the field *U*. It has been finally possible to establish that substitute adequate to the derivative such as rate of change in $\mathbb{R}^1$, is the divergence (Peral-Alonso, 1995).
The flux field is a scalar quantity that expresses the measurement of the field that crosses to a surface. Such field can be the field of speeds, electric field, and magnetic field among others. The net field flux is a measure of the net number of field lines that come out of a closed surface
Under the assumption that the adequate substitute in $\mathbb{R}^2$ for the derivative in the divergence, it can be expressed that the divergence of the field is proportional to the magnitude of the same i.e. it is a 3D

extrapolation to what is commonly known as Lambert law of Absorption. Under this assumption and those listed in the proposed model, these assumptions lead to the proposed equation.

$$\vec{\nabla} \cdot \vec{I} + k|\vec{I}| = 0 \tag{11}$$

The principle of Lambert (Equation 11) states that when a ray of light passes through a substance, the ratio with which its intensity decreases *I* is proportional to *I(r)*, where r represents the thickness of the medium.

$$\frac{dI}{dr} = -\alpha I \tag{12}$$

In orthogonal curvilinear coordinates, Lambert's equation in $\mathbb{R}^3$ is represented

$$\vec{\nabla} \cdot \vec{I} + k|\vec{I}| = \frac{1}{J}\sum_{i=1}^{3} \frac{\partial}{\partial q_i}\left(\frac{JI_i}{h_i}\right) + kI \tag{13}$$

The h_i are the scaling factors in the coordinate transformation. The values corresponding to the cylindrical coordinates (condition 1) are $h_r = 1;\ h_\theta = r;\ h_z = 1$ whereby Eq. 13 takes the form

$$\frac{1}{r}\left\{\frac{\partial}{\partial r}(rI) + \frac{\partial}{\partial \theta}(I) + \frac{\partial}{\partial z}(I)\right\} + kI = 0 \tag{14}$$

By the conditions exposed in the model (condition 3), Eq. 14 does not depend on z whereby the proposed equation can be written as

$$\frac{1}{r}\left\{\frac{\partial}{\partial r}(rI) + \frac{\partial}{\partial \theta}(I)\right\} + kI = 0 \tag{15}$$

Which represents a radial variation of the flux dependent on the k factor that is related to the electromagnetic characteristics of the medium

In order to find the solution of the partial differential equation (Eq. 15), the solution was proposed by the method of separating Fourier variables (Tessè, and Lamet, 2011), assuming the solution of the equation of the form

$$I(r,\theta) = R(r)\Theta(\theta) \tag{16}$$

The ordinary differential equations are obtained

$$R + r\frac{dR}{dr} + krR = \lambda R \tag{17}$$

$$\frac{d\Theta}{d\theta} = -\lambda\Theta \tag{18}$$

Whose solutions are in Eq. 19 and 20.

$$R(r) = R_o r^{(\lambda-1)} e^{-kr} \tag{19}$$

$$\Theta(\theta) = \Theta_0 e^{-\lambda\theta} \tag{20}$$

The solution to Eq.15 is:

$$I(r,\theta) = I_0 r^{(\lambda-1)} e^{-(kr+\lambda\theta)} \tag{21}$$

Can be written as

$$I(r,\theta) = I_0 e^{(\lambda-1)Ln\, r - kr} e^{-\lambda\theta} \tag{22}$$

The values of λ and k correspond to the eigenvalues of Eq.15 related to the boundary conditions and the electromagnetic characteristics of the suspension respectively.

The vector identity applied to the equations of Maxwell (Moreira et. al. 2011) which mathematical expressions are deduced is described in Eq. 23.

$$\vec{\nabla} \times \vec{\nabla} \times \vec{A} = \vec{\nabla}(\vec{\nabla} \cdot \vec{A}) - \nabla^2\vec{A} \tag{23}$$

Where $\vec{A}$ is a vector field

Applying the rotational to the law of Ampere-Maxwell and to the law of Faraday, we have following equations:

$$-\nabla^2 H = -j\omega\mu(\sigma + j\omega\varepsilon)H \tag{24}$$

$$-\nabla^2 E = -j\omega\mu(\sigma + j\omega\varepsilon)E \tag{25}$$

Defining

$$\gamma^2 = j\omega\mu(\sigma + j\omega\varepsilon) \tag{26}$$

Equations 24 and 25 take the form

$$\nabla^2 E = \gamma^2 E \tag{27}$$

$$\nabla^2 H = \gamma^2 H \tag{28}$$

Which are known as electromagnetic wave equations [8].

The γ factor is known as the propagation factor of the electromagnetic wave and is related to the characteristics of the medium i.e. with the electrical permittivity (ε) expressed in the S.I. In Farad/meter, magnetic permeability (μ) in Tesla-meter / Ampere and the electrical conductivity (σ) in Siemens/meter. Since the propagation factor is a complex number, it can be written by Eq.11.

$$\gamma = \alpha + j\beta \tag{29}$$

Where:

- α: The attenuation factor of the electromagnetic wave.
- β: Phase factor of the electromagnetic wave.

The focus is then on determining the wave attenuation factor since it indicates the power loss of the wave as it penetrates the medium. For practical purposes, it would correspond to determine the power loss in the suspension.
The relationship between attenuation and phase factors with the electromagnetic characteristics of the medium$(\varepsilon, \mu, \sigma)$, and the frequency of the electromagnetic wave(ω) can be determined

Eq.28 is a function of a complex variable that can be written as:

$$\gamma^2 = j\omega\mu(\sigma + j\omega\varepsilon) = (\alpha + j\beta)^2 \tag{30}$$

Replacing according to the electromagnetic characteristics of the medium and separating real and imaginary parts it is concluded that:

$$\alpha = \omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2} - 1\right]} \tag{31}$$

This factor clearly depends on the frequency of the electromagnetic wave (ω).

The values of the properties of the medium, such as the frequency of the electromagnetic waves, must be determined experimentally.

In the same way, the phase factor of the electromagnetic wave can be calculated and results in:

$$\beta = \omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2} + 1\right]} \tag{32}$$

Because the light is an electromagnetic wave, it is subject to the phenomenon of attenuation (the power loss when penetrating the medium). This power loss is related to the depth of penetration of the wave and the attenuation factor of the wave in the medium.
As mentioned above, when the electromagnetic wave passes through a substance, the ratio with which its intensity *I* decreases is proportional to *I(r)*, where r represents the penetration length of the light ray in the medium

$$\frac{dI}{dr} = -\alpha I \tag{33}$$

The factor *α* represents the attenuation that is typical for each medium and it is related to the properties of the sample.
Clearly, a part of this loss is related to the absorption of radiation by the semiconductor in order to participate in the process of photodegradation of the pollutants (condition 5 and 6).
As

$$(\lambda - 1)Ln\, r - kr = \alpha r = \omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2} - 1\right]}\, r \tag{34}$$

It is obtained that the solution to Eq. 15 is:

$$I_0 e^{-\omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2}-1\right]}\cdot r}\; e^{-\left(\omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2}-1\right]}\right)} \tag{35}$$

The Eq. 35 corresponds to the analytical solution of the proposed model, with the conditions established in the development where:

ω represents the average frequency of the incident rays (average frequency of UV radiation).
μ is the magnetic permeability of the suspension.
ε is the electrical permittivity of the suspension.
σ is the electrical conductivity of the suspension.

The first factor of Eq. 35 represents the energy loss of the incident electromagnetic waves by penetrating the suspension a distance r with respect to the incident energy wave I_0.
The electromagnetic waves at the reactor surface ($r = 0$) have an energy I_0. This decreases in relation to the depth of penetration r and the second factor represents the characteristic of the suspension that is inherent to the electromagnetic properties of the medium. Then, which by means of the assumption 3, are assumed constant, i.e., proper of each analyzed medium.

4. Conclusions

The proposed model places emphasis on the electromagnetic characteristics of the suspension, such as the permittivity, conductivity, and permeability. We also studied how chemical properties of the sample are related to variations of these electromagnetic characteristics.

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