

A New Electromagnetic Model for Determining the Speed of Photon Absorption in a Photocatalytic Process for Wastewater Treatment

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In the following work a new mode of operation is presented, as a continuation of the research developed on the elaboration of an electromagnetic model for the determination of the speed of photonic absorption in a solar collector in V (V - collector) (Ramos et al. 2017). The electromagnetic characteristics of the fluid in the suspension will be studied, such as electric permittivity, magnetic permeability, electrical conductivity and frequency of incident light. Likewise, the time variable is included as the innovation in the model to obtain the factors of the phase and the attenuation of the electromagnetic wave that penetrates the suspending medium and the photocatalytic process. For the model, an opto-geometric analysis of the V collector was used, which was studied and contrasted with the literature (Bandala et al. 2004).

1. Introduction

Water, a vital resource, has been the main protagonist of the existence of living beings because thanks to it there is the reproduction of life and its sustenance. However, this role has been dramatically affected by anthropogenic activities, where the main component is abuse since man is not aware of the affectation of both the surrounding environment and his existence. The abuse of water has brought the generation of wastewater, which initially was not applied any treatment and was deposited directly to bodies of water. Because this practice not only contaminated the water sources but affected the health of the people, since many diseases spread along the tributaries that provided the resource to the populations, they began to study and implement systems for the treatment of wastewater (Salgot et al. 2018). The wastewater treatment systems have treatment methods, among which we can mention the physical processes, chemical processes and, biological processes. However, given nature and physicochemical properties of the wastewater, the previous methods are not sufficient or inadequate to remove some contaminants (ex: heavy metals, emerging pollutants, among others). If it wants to achieve the water quality conditions that the laws require, the application of other treatments is needed, as is the case of advanced oxidation processes. During the use of this method, contaminants are doing destroyed forming hydroxyl radicals, which will have an oxidizing effect on chemical pollutants since the contaminated water is doing subjected to ultraviolet light in the presence of catalysts. For the construction of the photocatalytic reactor model, some techniques are used to determine the reflected rays in the concentrators (Lary et al. 1991). One of these techniques is ray tracing, which some authors define as a tool for generating images. This technique allows the application of a global lighting model for the calculation of local illumination. The raytracing technique is applied to simulate direct solar radiation. In this technique neglecting the diffuse component of it. Because the random nature of solar radiation does not play a predominant role in the opto-geometric study of collector V. Since the sun's rays can be described as rays of parallel photons that are directed vertically towards the wall of the photoreactor, simulating the solar irradiation at noon and therefore receiving the most significant amount of energy. With this work, a significant contribution

will be made to simulate photocatalytic reactors exposed to solar radiation in a V collector, which makes possible the design and scaling of these reactors for industrial scale application.

2. The solar collector in V

For the realization of the model, was used a solar collector in V. Said collector in V is a solar concentrator constituted of two flat reflecting plates that form an angle of opening θ , and an angle for the horizontal one that reflects the solar light about said angle (see Figure 1). Above the vertex at a height h , the cylindrical glass tube of radius r is located, inside which circulates the suspension of TiO_2 solution, and where the rays reflected by the reflecting plates impinge activating the photocatalytic process.

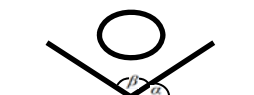


Figure 1. Representation of a V collector

2.1 Formulation of the opto-geometric model of the V collector

1. The coordinate system that adjusted in the best way to the elaboration of the model corresponded to the Cartesian coordinate system was selected. The vertex between planes is taking as the origin of the coordinate system. The product of the high symmetry, the subsequent analysis was performing in the XY plane (See Figures 1 and 2)
2. The equation of the reflecting plane as a function of the angle of inclination of the same for the horizontal (X) was defined. According to this and to step 1, the line representing the reflective plane passes through the origin (vertex) and has a known slope.
3. The tracing of the incident rays was generated using the ray tracing technique. The vertical rays and parallel to each other affected the reflective plane and reflected according to the same angle of incidence concerning the normal.
4. The Normal reflective line was determined, knowing that the slope of the normal line must fulfill the condition that a right angle must exist between the reflecting plane and the normal line.
5. The equation of reflected rays was calculated. The rays reflected by the reflecting plane must have the same incident angle of the incident rays for the normal line. The slope of the reflected rays was obtained.
6. The maximum length of the reflective plates was calculated. Since for each incident ray in the reflecting plane, there will be an incidence point in the glass tube through which the suspension flows. It is essential to find the one that impacts tangentially to the surface of the tube because this is the lower and upper limit that determines the length of the reflecting plane.
7. The involute was calculated since for value is determined by the length of the reflective plane.

3. Results and Discussion

3.1 Opto-geometric development of the V collector

For this study and in order to simplify the reactors it was considered to be irradiated by the direct component of solar radiation. The diffuse component has not been taken into account in order to avoid complications due to the random nature of its spread through space. It is also assumed that the photon beams are parallel and that they are directed vertically towards the photoreactor to simulate the conditions of solar irradiation at noon. In the subsequent development the geometry of the collector in V will be studied, by defining the angle β (see Figure 2) corresponding to the degree of inclination of the reflective flat plates, constitutive of the collector with respect to the horizontal i.e., $\theta = \pi - 2\beta$, or its equivalent $\beta = ((\pi - \theta)) / 2$.

From Figure 2 the equation of the reflecting plane was obtained (Eq. 1)

$$y = \tan(\beta) x \quad (1)$$

Any point in said plane will have coordinates

$$P(x, y) = l \cos(\beta), l \sin(\beta) \quad 0 < l \leq L, \text{ where } L \text{ is the length of the plane.}$$

For practical purposes it was fundamental to find the equation of the normal line to the reflecting plane, in such a way that the slope of the normal line described in Eq. 2 is calculated.

$$\tan\left(\beta + \frac{\pi}{2}\right) = -\cot(\beta) \quad (2)$$

So known the point P and the slope the equation of the normal line was found

$$-\cot(\beta) = \frac{y - l \sin(\beta)}{x - l \cos(\beta)}$$

Rearranging

$$y = -\cot(\beta) x + l[\cot(\beta)\cos(\beta) + \sin(\beta)]$$

As the angles of incidence and reflection have to be equal with respect to the normal line, the equation of the rays reflected thus was determined,

$$y = -\cot(\beta) x + l \csc(\beta)$$

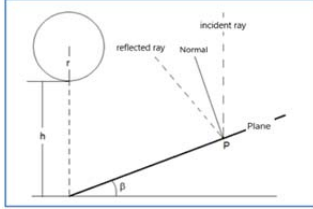


Figure 2. Schematic representation of incident rays, reflected reflector plane, plane angle, vertex height and radius of the cylinder.

Known the slope of the reflected rays

$$m = \tan\left(2\beta + \frac{\pi}{2}\right) = -\cot(2\beta)$$

and point P , the equation of the reflected rays was determined (Eqs 3-5).

$$-\cot(2\beta) = \frac{y - l \sin(\beta)}{x - l \cos(\beta)} \quad (3)$$

$$y = -\cot(2\beta) x + l[\cot(2\beta)\cos(\beta) + \sin(\beta)] \quad (4)$$

$$y = -\cot(2\beta) x + \frac{l}{2 \sin(\beta)} \quad (5)$$

In order to establish the relationships between the height h and the radius r with the angle β , it was necessary to analyze the reflecting plane with the equation of a circle with center in (H, K) through Eq. 6.

$$(x - H)^2 + (y - K)^2 = r^2 \quad (6)$$

Making $H = 0$ and $K = h + r$ (position of the tube axis in the photoreactor), we have the equation

$$x^2 + [y - (h + r)]^2 = r^2$$

so that:

$$x^2 + [y - h - r]^2 = r^2$$

As it wants to find what is the maximum length of the plates (L) about the angle of inclination of the planes and the height h , the slope of the line tangent to the circumference is calculated using Eq. 7.

$$2x + 2(y - h - r) \frac{dy}{dx} = 0 \quad (7)$$

From where:

$$\frac{dy}{dx} = -\frac{x}{y - h - r}$$

As the slopes of the lines tangent to the circumference must be equal to the slope of the incident rays at the extreme point, it must be fulfilled that:

$$-\frac{x}{y - h - r} = -\cot(2\beta) \quad (8)$$

If in Eq. 8, $x = r \cos(\theta)$ and $y = h + r + r \sin(\theta)$, the equations of the circumference in polar coordinates whose center is in the point $(0, h + r)$ are given by the equivalence relation and determines that:

$$-\frac{r \cos(\theta)}{h + r + r \sin(\theta) - h - r} = -\cot(2\beta)$$

In this way:

$$-\cot(\theta) = -\cot(2\beta) \quad (9)$$

$$\theta = 2\beta$$

Eq. 9 means that the incident ray impacts tangentially to the circumference for an angle $\theta = 2\beta$. This condition is also true for the negative angle in such a way that the region of reflection will be restricted, between $-2\beta \leq \theta \leq 2\beta$.

3.2 Proposed Model For The Calculation Of The LVRPA In The V-Collector

Consider a vector field in \mathbb{R}^3 that is to say

$$U(x, y, z) = u(x, y, z)\hat{e}_1 + v(x, y, z)\hat{e}_2 + w(x, y, z)\hat{e}_3$$

Where the vectors $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$ are a canonical basis in a system of orthogonal curvilinear coordinates (Spiegel et al 2011). Suppose that U is a force field. Suppose further that Ω is a bounded region of \mathbb{R}^3 and additionally the regularity of the U function 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 Taylor's theorem, we have in Eq. 10 that

$$U(\vec{x} + \vec{h}) = U(\vec{x}) + J_{\vec{z}}U(\vec{x})\vec{h} + o(|\vec{h}|^2) \tag{10}$$

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 $\vec{h} \rightarrow 0$ you 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, while $J_{\vec{z}}U(\vec{x})\vec{h}$ is written as

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

Considering the symmetric and antisymmetric part of A that is,

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

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

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

further

$$D = \begin{pmatrix} u_x & \frac{1}{2}(u_y + v_x) & \frac{1}{2}(u_z + w_x) \\ \frac{1}{2}(u_y + v_x) & v_y & \frac{1}{2}(v_z + w_y) \\ \frac{1}{2}(u_z + w_x) & \frac{1}{2}(v_z + w_y) & w_z \end{pmatrix}$$

So

$$Trace(D) = \nabla \cdot U$$

By applying a change of orthogonal curvilinear coordinates, it can change the matrix D in a diagonal matrix \tilde{D} of the form

$$\tilde{D} = \begin{pmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{pmatrix}$$

and we have to $Trace(D) = \nabla \cdot U$, since the Trace is an invariant under the transformation of orthogonal curvilinear coordinates. The values d_i are related to the scale factors of each coordinate system. So, $D\vec{h}$ is interpreted in the following way. Let P_0 be a parallelepiped and $P(t)$ the evolution of P_0 at time t that is, if $\vec{h}(t) = (h_1(t), h_2(t), h_3(t))^t$ are the sides of $P(t)$ $\vec{h}_0 = (h_{01}, h_{02}, h_{03})^t$ the sides of P_0 is verified

$$\begin{cases} \frac{d\vec{h}}{dt}(t) = D\vec{h}(t) \\ \vec{h}(0) = \vec{h}_0 \end{cases}$$

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

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

and therefore,

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

The divergence measures the rate of change of volume associated with the U field. It has been finally established that the substitute suitable for the derivative as the rate of change in \mathbb{R}^1 is the divergence (Peral et al 1995). The field flux is a scalar quantity that expresses the measure of the field that crosses a surface. This field can be speed field, electric field, magnetic field among others. The net field flux is a measure of the net number of field lines emerging from a closed surface. Under the assumption that the appropriate substitute in \mathbb{R}^2 for the derivative is the divergence, it can be expressed that the divergence of the field is proportional to the magnitude thereof, that is, it is a 3D extrapolation to what is commonly known as the absorption law of Lambert in 1D. Under this assumption and those listed in the proposed model (Ramos et al. 2017), these hypotheses lead to the proposed equation.

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

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

$$\frac{dI}{dr} = -\alpha I \quad (11)$$

In orthogonal curvilinear coordinates, the Lambert equation in \mathbb{R}^3 , is represented in Eq. 12.

$$\vec{\nabla} \cdot \vec{I} + k|\vec{I}| = \frac{1}{J} \sum_{i=1}^3 \frac{\partial}{\partial q_i} \left(\frac{J I_i}{h_i} \right) + kI \quad (12)$$

The h_i are the scale factors in the coordinate transformation. The values corresponding to the cylindrical coordinates (Ramos et al. 2017), are $h_r = 1$; $h_\theta = r$; $h_z = 1$ whereby Eq. 12 takes the form

$$\frac{1}{r} \left\{ \frac{\partial}{\partial r} (rI) + \frac{\partial}{\partial \theta} (I) + \frac{\partial}{\partial z} (I) \right\} + kI = 0 \quad (13)$$

Due to the conditions described in the model (Ramos et al. 2017), Eq.13 does not depend on z , so the proposed equation can be written as:

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

which represents a radial variation of the flow dependent on the factor k that is related to the electromagnetic characteristics of the medium. To find the solution of the partial differential equation (Eq.14) the solution was proposed by the method of separation of Fourier variables (Kaplan et al. 1998) assuming the solution of the equation of the form

$$I(r, \theta) = R(r)\Theta(\theta) \quad (15)$$

The solution of Eq.14 is:

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

and how $r^{\lambda-1} = e^{Ln r^{\lambda-1}} = e^{(\lambda-1)Ln r}$

it can be written as:

$$I(r, \theta) = I_0 e^{(\lambda-1)Ln r - kr} e^{-\lambda\theta} \quad (16)$$

The values of λ and k correspond to the eigenvalues of Eq.16 related to the boundary conditions and the electromagnetic characteristics of the suspension respectively. These are the electrical conductivity, the magnetic permeability and the electric permittivity, which are typical of the environment where the electromagnetic wave (suspension) propagates. Because light is an electromagnetic wave, it is subjected to the phenomenon of attenuation (loss of power when penetrating the medium). This loss of power is related to the depth of penetration of the wave and its attenuation factor 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 beam in the Eq.11 medium. The α factor represents the attenuation that is specific to each medium and is related to its properties. It can be established that part of said loss is related to the absorption of the radiation by the semiconductor in order to participate in the process of photodegradation of the contaminants. This factor is related to λ of the solution of the proposed model (Eq. 14).

As

$$(\lambda - 1)Ln r - kr = ar = \omega \sqrt{\frac{\mu\epsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega\epsilon}\right)^2} - 1 \right]} r$$

you get that

$$\lambda = 1$$

Now the condition must be fulfilled that $\lambda\theta = \beta\theta$ keeping in mind that β is the imaginary part of the complex γ . If $\lambda = 1$, we have that $\theta = -j\beta$ or $\theta = 0$. For either of the two cases, the solution of the equation is independent of the angle variation (it is constant). Thus, the proposed model takes the form:

$$I(r, \theta) = I_0 e^{-\omega \sqrt{\frac{\mu\epsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega\epsilon}\right)^2} - 1 \right]} r} e^{-j \left(\omega \sqrt{\frac{\mu\epsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega\epsilon}\right)^2} - 1 \right]} \right) t} e^{j\omega t} \quad (17)$$

$$I(r, \theta) = I_0 e^{-\omega \sqrt{\frac{\mu\epsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega\epsilon}\right)^2} - 1 \right]} r} e^{j \left\{ \omega \left[t - \sqrt{\frac{\mu\epsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega\epsilon}\right)^2} - 1 \right]} \right] \right\}}$$

$$I(r, \theta) = I_0 e^{-\omega \sqrt{\frac{\mu\epsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega\epsilon}\right)^2} - 1 \right]} r} \cos \left\{ \omega \left[t - \sqrt{\frac{\mu\epsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega\epsilon}\right)^2} - 1 \right]} \right] \right\}$$

Eq. 17 corresponds to the analytical solution of the proposed model (Eq. 14) 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 electric permittivity of the suspension.

σ is the electrical conductivity of the suspension.

As the phasor equations, our starting point, the model made in the time domain, must also contain the temporal dependence, this leads to the developed model

$$I(r, t) = I_0 e^{-\omega \sqrt{\frac{\mu \varepsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega \varepsilon} \right)^2} - 1 \right]} \cdot r} e^{-\left(\omega \sqrt{\frac{\mu \varepsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega \varepsilon} \right)^2} - 1 \right]} \right)} e^{j\omega t}$$

$$I(r, \theta) = I_0 e^{-\omega \sqrt{\frac{\mu \varepsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega \varepsilon} \right)^2} - 1 \right]} \cdot r} e^{-\left(\omega \sqrt{\frac{\mu \varepsilon}{2} \left[\sqrt{1 - \left(\frac{\sigma}{\omega \varepsilon} \right)^2} - 1 \right]} \right)} \cos(\omega t)$$

The first factor of Eq. 17 represents the loss of energy of the incident electromagnetic waves when a distance r , about the incident wave of energy I_0 , enters the suspension. The electromagnetic waves on the surface of the reactor ($r = 0$) have an energy I_0 , said energy decreases about the penetration depth r and the second factor represents the characteristic of the suspension inherent the electromagnetic properties of the medium. That using assumption 3 (Ramos et al 2017) constants are assumed, that is to say, typical of each medium analyzed.

4. Conclusions

The replacement of optical variables with electromagnetic characteristics could facilitate the experimental measurement, making the proposed model technologically available. The proposed model could predict the phase and attenuation factors of the electromagnetic wave that penetrate the suspended medium that activate the photocatalytic process in a solar. It is possible to predict the photodegradation time of the suspension to be treated, based on the electromagnetic characteristics of the suspending fluid. Also, in this way to be able to estimate the time required for the photocatalytic process.

References

- Bandala. E, Arancibia-Bulnes. C, Orozco. Z, Estrada. C, 2004, Solar photoreactors comparison based on oxalic acid photocatalytic degradation, *Solar Energy* 77, 503-512.
- Colina. J, Machuca. F., Lipuma. G. 2010, radiation absorption and optimization of solar photocatalytic reactors for environmental applications. *Environmental Science & Technology*. es-2010-00130h
- Hayt. W., Buck. J. 2001 (Ed) *Engineering electromagnetic*. Michigan. McGraw Hill. 119-200.
- Kaplan. W. 1998, (Ed) *Advanced Calculus*. Michigan. Addison-Wesley. 1998. 500-660.
- Kraus. J. *Electromagnetismo*. 2010 (Ed) U.S.A. McGraw Hill. 1986. 125-300
- Lary. D. Pyle. J. 1991, Diffuse Radiative, bought, and Photochemistry – I. *Journal of Atmospheric Chemistry* 13. 373-392
- Lary. D. Pyle. J. 1991, Diffuse Radiative, bought, and Photochemistry – II. *Journal of Atmospheric Chemistry* 13. 1991. .393-406
- Ramos. G., Velazquez. P., Santis. A., Acevedo. P., Rincon. J., 2017, Electromagnetic Model for Determining the Speed of Absorptive Photonic in a Solar Collector in V (V-Collector) *Chemical Engineering Transactions* Vol 57, 1609 – 1614.
- Spiegel. M. 2011, *Vector Analysis*. New York. McGraw Hill. 1959. 200-260.
- Peral, A., 1995, (Ed), *Primer curso de ecuaciones diferenciales parciales*. Madrid. Addison-Wesley/Universidad Autónoma de Madrid. 17-40.
- Salgot. M, Folch. M. 2018, Wastewater treatment and water reuse. *Current Opinion in Environmental Science & Health*. Volume 2, 64-74, ISSN 2468-5844.
- Sears F., Zemansky M., Young H., Freedman R., 2002. *Fisica Universitaria*. California. Pearson Addison-Wesley. 350