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3D Model for Estimating LVRPA in a solar collector in V (V-Collector)

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This article is the continuation of the investigation on the electromagnetic model to estimate the Local Volumetric Rate of Absorption of Photons in a solar collector in V(Ramos et. al. 2017). A new model for the LVRPA is presented based on the electromagnetic characteristics of the participating medium, electrical permittivity, magnetic permeability, electrical conductivity, from which the propagation factors, phase factors and attenuation of the electromagnetic wave are derived. The article shows the 3D model of the process. The six-flow model was used to simulate photon absorption and the ray tracing technique to describe the type of radiation incident on the V collector. This model is presented as a new alternative for photocatalytic processes and with a view to scalability of the process from laboratory to industry.
The ray tracing technique is applied to simulate direct solar radiation, neglecting its diffuse component (Lary. Et. al 1991), since the random nature of solar radiation does not play a preponderant role in the optogeometric study of collector V since the solar rays can be described as parallel photon rays that are directed vertically towards the wall of the photoreactor, thus simulating the solar irradiation at noon receiving the greatest amount of energy.
Some authors have applied the technique to simulate the incident radiation flux in compound parabolic collectors and tubular photoreactors. The study of the involute geometry allowed generating the data, which coupled with the models that describe the incident rays in the collector, served to obtain the rays reflected in the regions adjacent to the collector.

1. Introduction

Heterogeneous photocatalysis based on TiO2 and modified semiconductors has been used for the treatment and purification of slightly contaminated effluents (<1 mg L-1). By irradiating the semiconductor with energy levels higher than its band gap (TiO2 λ <384 nm), an electron / hole pair is generated capable of initiating reduction and oxidation reactions. Oxidation reactions through the gaps generated, occurs on the surface of TiO2 in aqueous medium through hydroxyl radicals responsible for degradation. Photogenerated electrons can reduce heavy metals and be used to generate photocatalytic hydrogen.
The results obtained in the laboratory have been enough, but they are not successful at an industrial or commercial level since the technique requires, among other factors, the adequate scaling of the photoreactor. Due to the complexity of studying the interaction between the incident photons and the photogenerated electron / hole pairs and their existing relationship between the optics of the photoreactor, many of the commercial applications have been presented by performing approximations due to the complexity of their interpretation and development. Part of this limitation is due to the scaling of the photoreactor is based on the determination of the kinetic parameters, which are a function of the quantum yield in the photoreactor.
The quantum yield can be determined if the spatial and directional distributions of radiation intensities are known in the suspension, partially solving the reaction rate problem. This relationship is described by the Local Volumetric Rate Photonic Absortions (LVRPA) that represents the spatial distribution or photonic availability in the reactor. Electromagnetic waves (photons) that are in charge of the catalyst activation process when they penetrate the medium, are dispersed, absorbed and reflected by the suspension. The description of this complex process is carried out by means of a mathematical physical model, which is known as the radiative transfer equation (ETR).

Most studies have focused on the ETR solution to model LVRPA and LVREA in parabolic trough collectors (CCP) and parabolic concentrators (CP). Considering that the global performance in terms of energy accumulated by a collector in V is close to that obtained in a CCP [8], the determination of the LVRPA becomes interesting, even more when there are no reports for this type of collector configuration in V, in the same article it was concluded in this comparative study that "the angle of incidence affects the total amount of energy obtained, but does not greatly reduce the efficiency of the reactors to use this energy in the photocatalytic process".
In this research, a geometric mathematical analysis of the V collector was carried out to simulate the absorption of the incident radiation, which combined with the electromagnetic model proposed to determine the local volumetric speed of photon absorption. Based on the electrical and magnetic characteristics of the suspension, it was possible to determine the quantum yield of the heterogeneous photocatalytic process (TiO2) in the collector. The analysis of the electromagnetic characteristics of the medium made it possible to estimate the local energy absorption inherent in the medium, in order to obtain a model of the local volumetric rate of photon absorption.

1.1 Materials and Methods

The six Flow Model SFM approach was used to model the proposed LVRPA. Using electromagnetic theory, a way to establish the LVRPA was presented from the electromagnetic characteristics of the medium and the frequency of incident rays in the UV spectrum on the aqueous medium.
The following hypotheses were presented as characteristics of the electromagnetic model developed:
1. Cylindrical coordinate system, best describes the behavior of the rays reflected by the reflector planes of the 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 proposed cylindrical coordinate system.
3. There are n planes with the same shape of particle distribution.
4. The catalyst absorbs all the local radiation, due to this it is necessary to calculate the attenuation factor of the electromagnetic waves in the medium.
5. There is no emission by the heterogeneous system

2. Equations

The geometry of the collector in V will be studied by defining the angle β corresponding to the inclination of the flat reflecting plates, constituting the collector with respect to the horizontal, that is, $\theta = \pi - 2\beta$, or its equivalent $\beta = ((\pi - \theta)) / 2$. The geometry of the collector in V will be studied, by defining the angle β corresponding to the inclination of the flat reflecting plates, constituting the collector with respect to the horizontal, that is, $\theta = \pi - 2\beta$, or its equivalent $\beta = ((\pi - \theta)) / 2$.
The equation of the reflective plane

$$y = \tan(\beta)\, x$$

Any point in said plane will have coordinates $P(x, y) = l\cos(\beta), l\, sen(\beta) \quad 0 < l \leq L$, where L is the length of the plane.
For practical purposes it became essential to find the equation of the normal line to the reflecting plane, in such a way that the slope of the normal line is calculated

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

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

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

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

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

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

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.

$$-cot(2\beta) = \frac{y - l\, sen(\beta)}{x - l\, cos(\beta)}$$

$$y = -cot(2\beta)\, x + l[cot(2\beta)cos(\beta) + sen(\beta)]$$

$$y = -cot(2\beta)\, x + \frac{l}{2\, sen(\beta)}$$

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 at (H, K) using

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

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

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

Since it is desired to find the maximum length of the plates (L) in relation to the angle of inclination of the planes and the height h, the slope of the tangent line to the circumference is calculated using.

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

from where:

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

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

$$-\frac{x}{y - h - r} = -ctg(2\beta)$$

If $x = rCos(\theta)$ y $y = h + r + rSen(\theta)$, the equations of the circumference in polar coordinates whose center is at the point $(0, h + r)$ is given by the equivalence relation and determines that:

$$-\frac{rCos(\theta)}{h + r + rSen(\theta) - h - r} = -Ctg(2\beta)$$

In this way

$$-Ctg(\theta) = -Ctg(2\beta)$$
$$\theta = 2\beta$$

This means that the incident ray hits the circumference tangentially for an angle $\theta = 2\beta$. This is also true for the negative angle such that the region of reflection will be restricted between $-2\beta \leq \theta \leq 2\beta$.

The phenomenon of the transport of energy of light in a medium (such as the incident radiation in a catalyst suspension), can be described by Maxwell's laws. This is the principle by which the quantity of photons that are locally present in a medium radiated with UV radiation can be predicted. This application is very useful for modeling LVRPA in a suspension, since photons are corpuscular representations of electromagnetic waves.

The procedure for obtaining the model is described below:
1) Choice of flow models: The flow model represents a way of describing how photons interact with the suspension. This fact establishes the possibility of having the six-flow model no longer in Cartesian coordinates but in cylindrical coordinates.
2) Substitute for the derivation: A mathematical development was presented to establish the appropriate substitute for the total derivation (rate of change in one dimension). It was established that the appropriate surrogate for the one-dimensional derivative is divergence.
3) Proposed model: The six-flow model represents an approximation of how photons interact with the medium. It was then proposed that the flux of photons per unit area that hit the particle should be proportional to the number of photons that penetrate the suspension.
4) Solution of the proposed equation: Taking the divergence in cylindrical coordinates, the partial differential equation was solved using the Fourier variable separation method, where a constant (dependent on the initial conditions) and an eigenvalue (dependent on the conditions appeared) border), which had to be determined to obtain the proposed electromagnetic model, which clearly represents a new way of dealing with the problem.
5) Determination of the constants: To determine the constants, the concepts of attenuation factor, phase and propagation 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.
Under the assumption that the appropriate substitute in R ^ 2 for the derivative is the divergence, it can be expressed that the divergence of the field is proportional to its magnitude, that is, it is a 3D extrapolation to what is commonly known as the absorption law Lambert in 1D. Under the hypotheses listed in the proposed model, these hypotheses lead to the proposed equation.

$$\vec{\nabla} \cdot \vec{I} = -k|\vec{I}|$$

It is written in cylindrical coordinates as

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

Using the method of separation of Fourier variables, assuming solution of the form

$$I(r, \theta, z) = R(r)\Theta(\theta)Z(z)$$

$$\frac{1}{r}\left\{\frac{\partial}{\partial r}(rR\Theta Z) + \frac{\partial}{\partial \theta}(R\Theta Z) + \frac{\partial}{\partial z}(rR\Theta Z)\right\} = -kR\Theta Z$$

The resulting equations are:

$$\frac{1}{Z}\frac{dZ}{dz} = -\eta$$

It has as a solution

$$Z = Z_0 e^{-\eta z}$$
There Z_0 is a constant. Now the equation
$$\frac{1}{rR}\frac{d}{dr}(rR) + \frac{1}{r\Theta}\frac{d\Theta}{d\theta} + k = \eta$$
Separating the variables we have the equations:
$$\frac{1}{\Theta}\frac{d\Theta}{d\theta} = -\lambda$$
Whose solution is
$$\Theta = \Theta_0 e^{-\lambda\theta}$$
And finally
$$\frac{1}{R}\frac{d}{dr}(rR) + kr - \eta r = \lambda$$
What is the solution
$$R = R_0 e^{-(k-\eta)r + (\lambda-1)Ln\, r}$$
The general solution is
$$I = I_0 e^{-(k-\eta)r + (\lambda-1)Ln\, r} e^{-\lambda\theta} e^{-\eta z}$$
Where $I_0 = R_0\Theta_0 Z_0$ constant, besidese λ, η constants (Eigen Values).
To determine the constants we refer to electromagnetism. Maxwell's laws in phasor form are
$$\vec{\nabla}\cdot\vec{E} = \frac{\rho}{\varepsilon}, \quad \vec{\nabla}\cdot\vec{H} = 0, \quad \vec{\nabla}\times\vec{H} = \sigma\vec{E} + j\omega\varepsilon\vec{E}, \quad \vec{\nabla}\times\vec{E} = -j\omega\mu\vec{H}$$
Applying the vector identity to Maxwell's laws with which mathematical expressions are derived.
$$\vec{\nabla}\times\vec{\nabla}\times\vec{A} = \vec{\nabla}(\vec{\nabla}\cdot\vec{A}) - \nabla^2\vec{A}$$
The equations of Electromagnetic Waves are arrived at
$$\nabla^2 E = \gamma^2 E, \quad \nabla^2 H = \gamma^2 H$$
The factor γ is known as the propagation factor of the electromagnetic wave and is related to the characteristics of the medium, that is, to the electrical permittivity (ε) expressed in the S.I. in Farad / meter, magnetic permeability (μ) in Tesla-meter / Ampere and electrical conductivity (σ) in Siemens / meter. Since the propagation factor is a complex number, it can be written
$$\gamma = \alpha + j\beta$$
Where:

- α: electromagnetic wave attenuation factor.
- β: phase factor of the electromagnetic wave.

Having as results
$$\alpha = \omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2} - 1\right]}$$
and
$$\beta = \omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2} + 1\right]}$$
If we say that κ = (k-η) and raising the time dependence of the process, the solution of the model takes the form
$$I = I_0 e^{-\kappa r + (\lambda-1)Ln\, r} e^{-\lambda\theta} e^{-\eta z} e^{j\omega t}$$
$$(\lambda-1)Ln\, r - \kappa r = \alpha r = \omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2} - 1\right]}\, r$$
you get that
$$\lambda = 1$$
Now the condition that $\lambda\theta = \beta\theta$ must be fulfilled, bearing in mind that β is the imaginary part of the γ complex. If $\lambda = 1$, then $\theta = -j\beta$ 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:
$$I(r,\theta,z,t) = I_0 e^{-\omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2}-1\right]}\cdot r} e^{-j\left(\omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2}-1\right]}\right)\theta} e^{-\eta z} e^{j\omega t}$$
Or in another way
$$I(r,\theta,z,t) = I_0 e^{-\left[\omega\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2}-1\right]}\cdot r + \eta z\right]} e^{-j\omega\left[t + \left(\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2}-1\right]}\right)\theta\right]}$$
The Equation corresponds to the analytical solution of the proposed model with the conditions established in the development where:
ω represents the average frequency of 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.
Whose first factor

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

It corresponds to a loss of power in the electromagnetic wave produced by the depth of penetration of the wave in the participating medium and by the characteristics of the contaminated medium, together with the movement of the medium.

$$e^{-j\omega\left[t+\left(\sqrt{\frac{\mu\varepsilon}{2}\left[\sqrt{1-\left(\frac{\sigma}{\omega\varepsilon}\right)^2}-1\right]}\right)\theta\right]}$$

This factor corresponds to changes in the frequency of the incident electromagnetic wave dependent on these changes in the characteristics of the polluted medium and the time of exposure to UV radiation.

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

The participating medium can be examined, at the electromagnetic level, by analyzing electrical conductivity, which involves exploring the electromagnetic characteristics of the medium such as magnetic permeability, electrical permittivity, electrical conductivity, and frequency of the incident electromagnetic wave.
The propagation factor of an electromagnetic wave in any medium, with negligible charge density, is given by:

$$\gamma = [j\omega\mu(\sigma + j\omega\epsilon)]^{1/2}$$

In a medium without conductivity , $\sigma = 0$ la Eq. 14, take the form

$$\gamma = [j\omega\mu(j\omega\epsilon)]^{1/2} = j\omega\sqrt{\mu\epsilon}$$

This indicates that the electromagnetic wave does not present attenuation and therefore Eq. 11 takes the form

$$I = I_0 e^{-j(\omega\sqrt{\mu\epsilon})} e^{j\omega t - \eta z}$$

In a low conductivity material $\sigma < \omega\epsilon$, rewriting 14

$$\gamma = \sqrt{-\omega^2\mu\epsilon\left[1 - j\,\frac{\sigma}{\omega\epsilon}\right]}$$

Or what is the same

$$\gamma = \sqrt{-\omega^2\mu\epsilon\left[1 + \frac{\sigma}{j\omega\epsilon}\right]}$$

Performing a Newton's Binomial Expansion

$$(a+b)^{1/2} = a^{1/2} + \frac{1}{2}a^{-1/2}b - \frac{1}{8}a^{-\frac{3}{2}}b^2 + \frac{1}{16}a^{-\frac{5}{2}}b^3 + \cdots$$

Apply in 14

$$\gamma = j\omega\sqrt{\mu\epsilon}\left[1 + \frac{1}{2}\left(\frac{\sigma}{j\omega\epsilon}\right) - \frac{1}{8}\left(\frac{\sigma}{j\omega\epsilon}\right)^2 + \frac{1}{16}\left(\frac{\sigma}{j\omega\epsilon}\right)^3 + \cdots\right]$$

Then

$$\gamma = j\omega\sqrt{\mu\epsilon} + \frac{1}{2}\sqrt{\frac{\mu}{\epsilon}}\sigma + j\frac{\sqrt{\mu\epsilon}\sigma^2}{8\omega\epsilon^2} - \frac{\sqrt{\mu\epsilon}\sigma^3}{16\omega\epsilon^3}$$

Thus, the propagation factor will have the form

$$\gamma = \frac{1}{2}\sqrt{\frac{\mu}{\epsilon}}\sigma\left[1 - \frac{1}{8}\left(\frac{\sigma}{\omega\epsilon}\right)^2\right] + j\omega\sqrt{\mu\epsilon}\left[1 + \left(\frac{\sigma}{\omega\epsilon}\right)^2\right]$$

And the electromagnetic wave in the middle, it will propagate like

$$I = I_0 e^{-\omega\frac{1}{2}\sqrt{\frac{\mu}{\epsilon}}\sigma\left[1-\frac{1}{8}\left(\frac{\sigma}{\omega\epsilon}\right)^2\right]\cdot r} e^{j\omega\sqrt{\mu\epsilon}\left[1+\left(\frac{\sigma}{\omega\epsilon}\right)^2\right]} e^{j\omega t - \eta z}$$

And the electromagnetic wave in the medium in which the conductivity is high will propagate as

$$I = I_0 e^{\pm\omega(r+1)\sqrt{\frac{\mu\varepsilon}{2}}\sqrt{\frac{\left(\frac{\sigma}{\omega\varepsilon}\right)-1}{2}}} e^{\mp j\omega(r+1)\sqrt{\frac{\mu\varepsilon}{2}}\sqrt{\frac{\left(\frac{\sigma}{\omega\varepsilon}\right)+1}{2}}} e^{j\omega t - \eta z}$$

The contaminated medium will have certain measurable particularities in relation to electromagnetic characteristics such as magnetic permeability, conductivity and electrical permittivity, because these characteristics change, it must be established which characteristics we want in the contaminated water, for example, if water is desired for consumption. water for irrigation or, in general, treated water for practical purposes, from which you can know the electromagnetic conditions and thus know the photodegradation time of the water.

3. Conclusions

When presenting this new model for the absorption of photons, the change of approach was continued for the estimation of the rate of photon absorption in the photocatalytic reactor, as a function of the electrical and magnetic properties of the fluid, such as permeability, permittivity and conductivity, associated with the medium together with the frequency of UV radiation, present an interesting alternative to obtain the LVRPA, clearly important in the molding of photoreactors.

The approximations carried out are intended to be able to estimate the scalability of the photocatalytic process at an industrial level. You can establish the types of water that are required or estimate the type of contamination allowed to obtain a type of water needed. Segment the type of water, for example into three types: Irrigation water, drinking water, pure water, each of these types will have their own permittivity, permeability and conductivity characteristics, in such a way that analyzing the initial conditions of the contaminated water You can obtain the time required to have the water at any of the required levels (Irrigation, consumption, pure).

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