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General method of simulating radiation fields using measured boundary values

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ABSTRACT

A general methodology integrating the Fresnell, Snell, and Beer-Lambert laws for modeling the radiant distribution in a medium is presented. The model considers refraction/reflection through/from the body of the UV lamp and sleeve, as well as the reflections from other sources, such as the reactor body. The measured boundary conditions are applied to realistically simulate the fluence/irradiance rate around the radiant source, in particular, in the zone closest to the radiant source. Different low-pressure UV lamps were tested under different operating conditions using photodiodes and a radiometer. The experimentally measured irradiance rate was in a very good agreement with the simulation results of the presented model.

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1. Introduction

UV radiant energy promotes the production of radicals (e.g. hydroxyl and oxide radicals) that can cause photodegradation, photosynthesis, or photolysis in gases, liquids, or on photocatalytic surfaces without the addition of any other chemicals. The application of UV photoreactors to drinking water is a well-established technology (e.g. Lyn et al., 1999; Lawryshyn and Cairns, 2003; Ducoste et al., 2005), but other applications of this clean technology are becoming popular. For example, there is growing interest in using UV photoreactors for food preservation (e.g. Kucuk et al., 2003; Beltran and Barbosa-Cánovas, 2004; Mahmoud and Ghaly, 2004). In addition, a number of researchers have demonstrated the possibility of converting methane to methanol using UV radiation under the mild conditions of near ambient temperature and pressure (e.g., Noceti et al., 1997; Taylor and Noceti, 2000; Gondal et al., 2003, 2004).

The modeling of UV photoreactors requires simultaneous solution of the mass and momentum conservation equations, along with the radiation field equation, all of which affect the rate of photochemical reactions. The governing equations of a photoreactive system can be combined and solved simultaneously by applying computational fluid dynamics (CFD). In order to achieve a better understanding of photoreactors for design and optimization purposes, it is essential to have a reliable model for the radiant energy distribution that is capable of simulating the behavior of any UV source. A mathematical representation of the radiant energy can be obtained by solving the radiation transfer equation (RTE).

The photon balance equation and the RTE can both be solved analytically for simple geometries. For more complicated geometries, several researchers have used the finite volume numerical method (Chui and Raithby, 1993; Cassano et al., 1995; Romero et al., 1997; Raithby, 1999). Romero et al. (1997) presented a detailed description of radiation field modeling for an annular photocatalytic reactor adapted from the general transport theory and, particularly, from neutron transport applications. Although the finite volume model yields a general solution to the RTE, it has some limitations, such as spatial and directional discretional errors investigated by Raithby (1999). The discretization of the control volume and solid angle should be carefully selected in order to minimize those errors. In addition, this method needs considerable computational resources, particularly when the number of solid angle discretization is increased. These limitations make the utilization of this method problematic, although it has been employed to simulate the radiant field in photoreactors (Pareek et al., 2003).

This work attempts to present a simple, general method of modeling radiant energy distribution for any type of radiant source through consideration of the medium properties and the UV source geometry. It simplifies the RTE to the Beer-Lambert formula, which is easily solvable for all rays from any complex UV source using numerical methods. This method considers refraction/reflection through/from the body of the UV lamp and sleeve

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of the UV source. In addition, it resolves the reflections from other sources, such as the reactor body. Using an iterative numerical technique, this method can also handle the scattering effect of particulates and optical variations in the medium. The presented modeling approach uses radiation power measurement close to the lamp for setting the boundary condition of the differential equations describing radiation transport. This technique produces more realistic results with minimum error by taking into consideration any non-uniformity in the radiant emission from the source, as a result of special lamp operating conditions. Using radiation measurement at boundaries integrates reflections from all interfaces and Fresnel's law (reflections) can be ignored in the model, resulting in a simpler modeling approach.

2. Radiation modeling

Before presenting the general radiation model, certain standard optical radiation terms are provided below:

Solid angle, Ω, is defined as the surface area of a section of a sphere divided by r^2, where r is the radius of the sphere. The solid angle has units of steradians and the maximum solid angle is 4π steradians.

Radiant power, P, is the rate of radiant energy emitted in all directions by a light source. In general, radiant power includes all spectral waves emitted by the source. For UV photochemistry or disinfection, P is usually specified only for the effective spectral wave range.

Radiant intensity, I, is the total radiant power emitted by a source in a given direction per solid angle Ω. Note that, in a non-absorbing medium, the radiant intensity does not decay with distance. For a sphere, $I=P/4\pi$; for a flat plane, $I=P/2\pi$.

Although radiant energy is naturally a scalar parameter, emitted radiation is described by its spectral wavelength range and directional distribution. Radiation transfer is defined as the transmission of electromagnetic radiation through space under the influence of the medium. The chemicals and particles in the medium can absorb, scatter, or re-emit the incident rays. Fig. 1 shows a photon balance within a control volume of the medium for a specific direction.

For each directional unit vector (Ω) at a specific wavelength (λ), the radiation transfer equation (RTE) can be obtained from the following photon balance equation (Fig. 1):

(outgoing intensity − incoming intensity)+absorbed intensity =(incoming emission − outgoing emission)+(incoming scattered− outgoing scattered)

$$\nabla[\Omega\, I_\lambda(s,\Omega,t)]+\left[k_\lambda(s,\Omega,t)I_\lambda(s,\Omega,t)+\sigma_\lambda(s,\Omega,t)I_\lambda(s,\Omega,t)\right] = j_\lambda(s,t)+\frac{1}{4\pi}\sigma_\lambda(s,t)\int_{\Omega'=4\pi}\Psi(\Omega'\Omega)I_\lambda(s,\Omega',t)d\Omega' \quad (1)$$

where s, Ω, t, $I_\lambda(s,\Omega,t)$, k_λ, σ_λ, j_λ, and $\Psi(\Omega'\Omega)$ are position vector, directional unit vector, time, radiant intensity for specific solid angle Ω and specific direction s, absorption coefficient of the medium, scattering coefficient of the particulates in the medium, radiation emission, and phase function, respectively. The photon energy equation generally assumes that scattering is multiple, but independent.

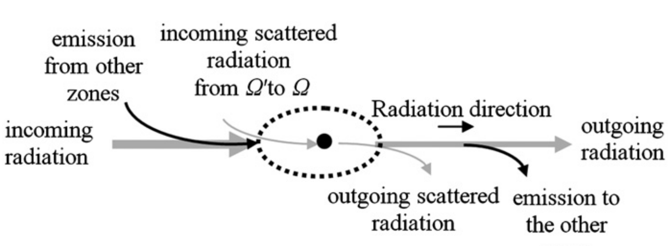

Fig. 1. Conservation of radiant energy.

In many engineering applications, including drinking water treatment, the medium is transparent without solid particulates, or scattering is non-elastic and can be integrated into the absorption coefficient. Thus, the in/out scattering to/from the control volume is negligible. In the majority of photolysis and photocatalytic processes, which are normally carried out at near ambient temperatures, internal emissions can also be neglected. In addition, most such processes operate at steady state. Thus, the above RTE can be simplified for the average spectrum of the light for a specific solid angle. The simplified equation is

$$\frac{dI(s,\Omega)}{ds}+k(s,\Omega)I(s,\Omega)=0 \quad (2)$$

This is referred to as the Beer-Lambert equation for steady-state conditions. Written in integral form, Eq. (2) becomes

$$I(\Omega)=I_0(\Omega)\exp\left(-\int_0^L k(s,\Omega)ds\right) \quad (3)$$

where $I(\Omega)$ is the radiant intensity at distance L from the source for an average spectrum wavelength, and $I_0(\Omega)$ is the radiant intensity at the source.

Irradiation is normally measured in terms of the irradiance rate or power flux (W/m^2) for each wavelength band (Bolton, 1999). The irradiance rate yields the amount of total energy per unit area, per unit time, from all directions. Using the definition of intensity, the following equation for the irradiance rate can be derived for an infinitesimal circular area, A, centered at the measurement location in the medium:

$$Ir(\Omega)=\frac{I(\Omega)\Omega}{A} \quad (4)$$

where $Ir(\Omega)$ is the irradiance rate for one specific direction.

If the area is shrunk to a point, the solid angle, Ω, calculated based on its definition, is equal to $(A/L^2)\cos(\theta)$, where L is the distance between the source of radiation and the center of the area, and θ is the angle between the ray and the normal vector of the area. Thus, Eq. (4) can be simplified as

$$Ir(\Omega)=\frac{I_0(\Omega)}{L^2}\exp\left[-\int_L k(s,\Omega)ds\right]\cos(\theta) \quad (5)$$

Considering refraction and reflection of the rays through and from different media, Eq. (5) can be generalized as

$$Ir(\Omega)=\frac{1}{\left(\sum_{i=1}^{n}L_i\right)^2}I_0(\Omega)\cos(\theta_{Ln})\exp\left[-\sum_{i=1}^{n}\int_{overL_i}k_i(s,\Omega)ds\right]\prod_{i=1}^{m}T_i \quad (6)$$

where L_i, θ_{Ln}, k_i, and T_i, are the path length of the ray through the ith medium, the angle between the normal vector of the studied area and the incident ray the absorption coefficient of the ith medium, and the fraction of the transmitted portion of the ray from one medium to another, respectively. Removing the cosine of the angle term from Eq. (6) yields the fluence rate, which is a crucial parameter in photoreaction rate correlations. Fig. 2 represents the traveling pathway of a ray.

Considering the refraction index of each medium, Fresnel, and Snell's laws can be applied to calculate the refracted ray and the fraction of the ray that passes through the interface between two different media. If the reflector (3 in Fig. 2) is a transparent medium (e.g., the body of UV lamps in the medium), Fresnel's law can be applied to that surface too. Applying this procedure, called

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