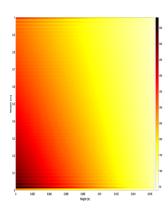
# Modeling the Radiation Transfer in Rectangular Slurry Photocatalytic Using the Six-Flux Model 2-Dimensional (2-D) Approach

Ph.D. Student: N Journal: YES - CEJ

ORAL

**G. Li Puma**<sup>1</sup>, C. Nchikou<sup>2</sup>, J.A. Loredo-Medrano<sup>2</sup>, A. Hernandez-Ramirez<sup>2</sup>, J.A. Colina-Marquez<sup>3</sup>, M.A. Mueses<sup>3</sup>. (1) Environmental Nanocatalysis & Photoreaction Engineering, Department of Engineering, University of Palermo (UNIPA), Viale delle Scienze, Ed. 6, 90128 Palermo, Italy. (2) Facultad de Ciencias Química, Universidad Autónoma de Nuevo León, UANL, Universidad s/n, Cd. Universitaria, C.P. 6645, San Nicolás De Los Garza, Nuevo León, México. (3) Chemical Engineering Department, Universidad de Cartagena, A. A. 1382 - Postal 195, Cartagena, Colombia, Email: mmueses@unicartagena.edu.co



The radiative transfer equation (RTE) in slurry photocatalytic reactors with flat-slab geometries was solved analytically through a new two-dimensional six-flux model approach (SFM-2D) which overcomes the limitations of the SFM and SFM-HG approaches regarding long photon pathways and non-uniform radiation distributions on the front wall of the slab. The model yields an analytical solution of the local volumetric rate of photon absorption (LVRPA). The radiant field of a flat plate photocatalytic reactor using the proposed model was compared with the SFM-HG approach, with variable incident radiation boundary conditions. The LVRPA profiles in a flat-slab showed significant differences in the regions far away from the slab front wall. The SFM-2D provides a more accurate optimization of the radiation field in a flat plate and allows the estimation of the optimum catalyst load and slab thickness facilitating the design of photocatalytic reactors with suspended photocatalysts.

#### Introduction

Photocatalytic reactors are devices that activate photocatalysts with light, which usually enters from a reactor boundary i.e., a free fluid surface or a transparent reactor wall. Typically, they are used for environmental applications such as water or air decontamination, renewable energy applications, such as water splitting, hydrogen production or photo-reforming of chemical species, and also synthesis of chemicals by partial oxidation. The key feature that distinguishes them from chemical rectors is the presence of light, and of an heterogenous radiation field. Essentially reactors utilizing suspended photocatalysts, require the evaluation of the local volumetric rate of photon absorption (LVRPA) to estimate the species reaction rates. This is done by solving the integral-differential radiative transfer equation (RTE). Previous studies have focused on the numerical solution of the RTE, using Monte Carlo (MC) and Discrete Ordinates Method (DOM) and on development of simplified models such as the Six-Flux Model (SFM) yielding an analytical solution of the RTE. Simplified modeling approaches are very attractive since facilitate the design and optimization of photocatalytic reactors avoiding lengthy and costly numerical calculations, particularly with fluctuating radiation sources (e.g., solar light). The SFM facilitates the optimization of solar photocatalytic reactors through the selection of optimal catalyst concentration and reactor geometry based on the concept of optimum optical thickness. The SFM

stipulates that a photon after colliding with a suspended particle can be reflected (or scattered) along the six cartesian coordinates with a welldefined probability. This approach demands significantly less computational time and effort, and returns minor significant discrepancies compared to more complex numerical solution of the RTE such as DOM. Nonetheless, the model is developed considering infinite dimensions along two reactor dimensions and the analytical solution is limited to one dimension (the reactor depth), considering the case where the incoming radiation intensity reaching the slab geometry remains constant. Such assumptions can be limited for the design of practical photocatalytic reactors using suspended photocatalysts.

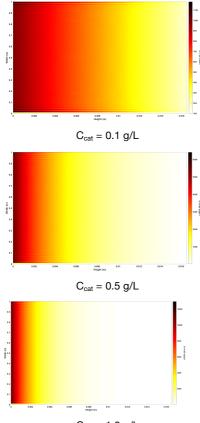
To overcome these limitations, this study proposes a solution of the RTE over two dimensions in rectangular coordinates through the formulation of the SFM-2D which yields an analytical solution of the LVRPA to describe the radiant field in slabs geometries. Overall, the SFM-2D provides a more accurate optimization of the radiation field in a flat plate regarding the optimum catalyst load and slab thickness facilitating the design of photocatalytic reactors with suspended photocatalysts.

## Material and Methods

The radiative transfer equation (RTE) in slurry photocatalytic reactors with flat-slab geometries was solved analytically through a new twodimensional six-flux model approach (SFM-2D) which overcomes the limitations of the SFM and SFM-HG approaches regarding long photon pathways and non-uniform radiation distributions on the front wall of the slab. The model builds a set of partial differential equations of photon balances solved by combining different mathematical methods and suitable boundary conditions and yields an analytical solution of the local volumetric rate of photon absorption (LVRPA). The radiant field of a flat plate photocatalytic reactor using the proposed model was compared with the SFM-HG approach, with both constant and variable incident radiation boundary conditions.

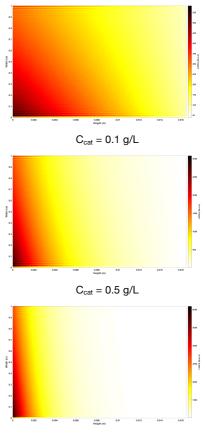
### **Results and Discussion**

The radiation absorption distribution inside a flat slab reactor for several  $TiO_2$ -P25 catalyst loading (0.1, 0.5 and 1 g/L) was determined using constant (Figure 1) and variable (Figure 2) incident radiation. The LVRPA decreases from the reactor wall toward its bottom. Moreover, for the geometry tested at catalyst loading higher than 0.5 g/L, the clouding effect begin to prevent photons reaching the far deeper regions of the reactor.



 $C_{cat} = 1.0 \text{ g/L}$ 

Fig. 1. LVRPA distribution in a flat slab photocatalytic reactor at different catalyst concentrations with constant incident radiation.



 $C_{cat} = 1.0 \text{ g/L}$ 

Fig. 2. LVRPA distribution in a flat slab photocatalytic reactor at different catalyst concentrations with variable incident radiation.

The LVRPA profiles in the flat slab further showed significant differences in the regions far away from the slab front wall (results not shown here). The model definition and further results will be presented at the meeting.

# Conclusions

In this study, the RTE was solved in 2D in rectangular coordinates with the SFM approach considering both constant and variable incident radiation boundary conditions. The SFM-2D provides a more accurate optimization of the radiation field in a flat plate and allows the estimation of the optimum catalyst load and slab thickness facilitating the design of photocatalytic reactors with suspended photocatalysts.

#### Acknowledgments

The authors thank to Universidad Autónoma de Nuevo León and Universidad de Cartagena for supporting this publication. Prof. Mueses thanks Grant 031-2022 (Research Vice-Head) of University of Cartagena. Dr. Clovis Nchikou dedicates this article to the memory of Dr. Juan-Antonio Rojas-Estrada.