Applied Mathematical Modelling 40 (2016) 4812–4821

Contents lists available at ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

Modeling of a falling-film photocatalytic reactor: Fluid dynamics for turbulent regime

Jose Colina-Marquez [a,*], Deyler Castilla-Caballero [b], Fiderman Machuca-Martinez [b]

[a] Chemical Engineering Department, Programa de Ingeniería Química, Universidad de Cartagena, Sede Piedra de Bolívar, Avenida del Consulado 48-152, Cartagena, Colombia
[b] Chemical Engineering School, Universidad del Valle, Cali, Colombia

ARTICLE INFO

Article history:
Received 5 July 2012
Revised 13 November 2015
Accepted 7 December 2015
Available online 17 December 2015

Keywords:
Flat plate
Eddy viscosity
LVRPA
Six-flux model
Film thickness
Photocatalyst

ABSTRACT

The falling-film photocatalytic reactor is a photochemical device used for several environmental applications due to its simple buildup and its high solar radiation usage. As most of photocatalytic reactors, modeling the falling film photoreactor can be a challenging task. The most difficult aspect of modeling is the photon absorption by the solid catalyst. Nonetheless, modeling the fluid dynamics in turbulent regime of a falling film reactor can also be very demanding. In this work, the eddy viscosity approach was applied for estimating the average velocity profile and the film thickness for turbulent regime. Also, a sensitivity analysis was made for determining how different variables like: flow rate, tilting angle and fluid viscosity, affect to the average velocity profile and the film thickness. As remarkable results, it was found that the flow rate was the most significant operating variable and affects both considered parameters. The model was validated with experimental measurements of the film thickness at three different flow rates. The relative errors between the experimental values and the film thickness values estimated with the model can be considered as plausible, since the maximum was 13.06%. However, regarding to the local volumetric rate of photon absorption (LVRPA) estimation from the calculated and experimental values of the film thickness, the errors were negligible. According to previous works, high flow rates ensure the turbulent regime and therefore, the mass-transfer limitations due to catalyst settling can be avoided; but also with larger film thicknesses can reduce the photon absorption because of longer optical paths. So, the optimization of the photon absorption, based on the film thickness and restricted to the turbulent regime, is a necessary study that can be developed in a future work.

1. Introduction

Falling film reactors are known by their application for processes that imply mass transfer in a liquid–gas interphase. In addition, they can be used for photochemical reactions, which need a deep interaction of the light. Photocatalysis is considered as one of the most promissory emergent photochemical technologies aimed to remove non-biodegradable substances in industrial wastewaters [1]. Nevertheless, its applicability has faced important challenges regarding to design, simulation and scaling up of reactors. Although there are several types of photocatalytic reactors, falling-film reactors have been studied at pilot scale in previous works [2–4]. Despite the simple geometry of this reactor, its modeling can be a complicated task. Apart from the photon

* Corresponding author. Tel./fax: +575 6752040.
E-mail address: jcolinam@unicartagena.edu.co (J. Colina-Marquez).

http://dx.doi.org/10.1016/j.apm.2015.12.007

Nomenclature

A_t	Eddy viscosity, kg/m s
C_{cat}	Catalyst load
f	Damping factor, dimensionless
g	Gravitational constant, 9.8 m/s^2
I_0	Photon flux, W/m^2
L	Reactor length, m
LVRPA	Local volumetric rate of photon absorption, W/m^3
OVRPA	Overall volumetric rate of photon absorption, W/m^3
Q	Flow rate, m^3/s
V	Velocity, m/s
W	Reactor width, m
y	Distance from the reactor wall through the film thickness, m
Greek letters	
δ	Film thickness, m
ε_t	Dynamic eddy viscosity, m^2/s
φ	Tilt angle, °
σ	Specific scattering coefficient, m^2/kg
κ	Specific absorption coefficient, m^2/kg
Γ	Surface mass flow, kg/m^2 s
γ	SFM parameter
λ	Extinction length, m
μ	Fluid viscosity, kg/m s
ν	Kinematic viscosity, m^2/s
ρ	Fluid density, kg/m^3
ω	Scattering albedo
τ_{yz}	Shear stress, N/m^2
Subscripts	
avg	Average
cat	Catalyst
corr	Corrected
w	Relative to reactor wall
z	Relative to *z*-axis

absorption estimations, the fluid dynamics of a falling film in turbulent regime is an important issue to be solved. Whereas the laminar flow regime for falling films has been the most studied [5], the turbulent flow regime requires more rigorous expressions which can describe the viscous sub-layers along the limit layer. These features, besides to the random nature of the behavior for the turbulent flow, require a demanding mathematical work. Because of this, most of the reported studies of photocatalytic applications have been aimed to semi-empiric or simplified approaches, which consider laminar flow regime, in order to obtain a practical model [2,3,6,7].

Several approaches of fluid dynamics for turbulent flow regime in falling films have been reported. The characteristics and modeling of the waves formed at turbulent Reynolds number have been studied in previous works [8–11]. A wavy flow implies a variable film thickness; therefore, a statistical study of the waves is needed [12]. For avoiding large computational times, necessary to estimate film thickness profiles, the eddy viscosity concept was introduced to obtain average film thickness which simplified the calculations and agreed satisfactorily with experimental data [13–15]. Despite the numerous studies developed for fluid dynamics of falling films under turbulent regime, works with photocatalytic reactors under this regime are very scarce. It is known that for slurry photoreactors, the turbulent flow is strongly recommended for avoiding mass transfer limitations. It has been reported that a Reynolds number greater than 15,000, it is necessary for not allowing catalyst sedimentation in tubular reactors [16].

In this work, a set of mathematical equations was developed for obtaining a model able to describe the velocity profile and to estimate the film thickness in a falling-film photocatalytic reactor under the turbulent flow regime. These two parameters are very important for modeling and simulating these reactors, since the film thickness defines the optical thickness of the reactor. The film thickness is a parameter that is relevant in the photon absorption models [17,18] and the velocity profile is necessary for estimating the reactor mass balance. In addition, a sensitivity analysis was made varying the flow rate, the tilt angle and the fluid viscosity. The obtained results showed that the flow rate affected to the film thickness and the velocity profile significantly. Experimental measures of the film thickness under turbulent regime were carried out in order to validate