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Mathematical modeling of wastewater decolorization in a trickle-bed bioreactor

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ABSTRACT

This work focuses on mathematical modeling of removal of organic dyes from textile industry waste waters by a white-rot fungus *Irpex lacteus* in a trickle-bed bioreactor. We developed a mathematical model of biomass and decolorization process dynamics. The model comprises mass balances of glucose and the dye in a fungal biofilm and a liquid film. The biofilm is modeled using a spatially two-dimensional domain. The liquid film is considered as homogeneous in the direction normal to the biofilm surface. The biomass growth, decay and the erosion of the biofilm are taken into account. Using experimental data, we identified values of key model parameters: the dye degradation rate constant, biofilm corrugation factor and liquid velocity. Considering the dye degradation rate constant 1×10^{-5} kg m^{-3} s^{-1}, we found optimal values of the corrugation factor 0.853 and 0.59 and values of the liquid velocity 5.23×10^{-3} m s^{-1} and 6.2×10^{-3} m s^{-1} at initial dye concentrations 0.09433 kg m^{-3} and 0.05284 kg m^{-3}, respectively. A good agreement between the simulated and experimental data using estimated values of the model parameters was achieved. The model can be used to simulate the performance of laboratory scale trickle-bed bioreactor operated in a batch regime or to estimate values of principal parameters of the bioreactor system.

1. Introduction

Synthetic dyes are present in effluents of many industries (e.g. textile industry, leather tanning industry or paper production). They exhibit significant structural diversity and can even act as carcinogens or mutagens. Their release into the environment may therefore cause serious ecological problems. Traditional wastewater treatment technologies are not able to degrade highly persistent synthetic dyes (Forgacs et al., 2004). A wide range of new methods for dyes removal has been studied. Among others, adsorption on inorganic or organic materials, photocatalytic or chemical oxidation, and degradation by means of various microorganisms can be mentioned (Forgacs et al., 2004; Robinson et al., 2001). In recent years, the use of white-rot fungi for biological decolorization has been extensively studied. These fungi producing lignin degrading enzymes capable to decompose a wide variety of commercial dyes are a relatively inexpensive and effective alternative to other decolorization technologies (Kaushik and Malik, 2009). Our work is focused on mathematical modeling of the use of a white-rot fungus for degradation of synthetic dyes from aqueous solutions in a trickle-bed bioreactor.

A significant amount of literature dealing with mathematical modeling of biofiltration processes has been published in the past three decades and many reviews summarized the topic (Chaudhary et al., 2003; Devinny and Ramesh, 2005; van Loosdrecht et al., 2002; Wang and Zhang, 2010; Zarook and Shaik, 1997). Generally, models for the simulation of biofilm development can be divided into three categories: cellular automata models (Hermanowicz, 2001; Picioreanu et al., 1999), individual-based models (IbM) or so-called particle-based models (de Bivar Xavier et al., 2005; Kreft et al., 2001; Picioreanu et al., 2004) and continuum models (Duddu et al., 2009; Eberl et al., 2000).

Both the cellular automata models and the individual-based models make use of a combination of deterministic and stochastic rules to simulate the biofilm formation processes. The cellular automata models use the discretization of the biomass along a spatial grid. The state of every grid cell is updated in a course of simulation according to the same set of biological rules (Wang and Zhang, 2010). In IbM, each bacterium (Kreft et al., 2001) or a cluster of bacterial cells (Picioreanu et al., 2004) is considered to be a sphere, which grows and, after fulfilling a prescribed condition, divides.

Mathematical models describing the entire biofilter performance consist of mass balances of a substrate in a biofilm and in an extracellular liquid medium. Models are usually one- or two-dimensional. Biomass growth and the biofilm development are usually described in a simplified way compared to the IbM and cellular automata models. Many authors consider a planar biofilm with the diffusion of dissolved substrates only in the direction perpendicular to the biofilm surface. Some models assume the

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Nomenclature

A	actual area of the biofilm domain (m^2)
a_t	carrier surface density (m^{-1})
$c_{b,i\|3}$	concentration of the ith component in the biofilm ($kg\,m^{-3}$)
$c_{i\|3}$	concentration of the ith component in the liquid ($kg\,m^{-3}$)
c_{0i}	concentration of the ith component in the reservoir at the beginning of the reactor operation ($kg\,m^{-3}$)
c_{0ij}	concentration of the ith component in the reservoir at the beginning of the reactor operation in the jth set of experiments ($kg\,m^{-3}$)
$c_{out,i}$	concentration of the ith component in the reservoir ($kg\,m^{-3}$)
$\tilde{c}_{b,i\|3}$	dimensionless concentration of the ith component in the biofilm
$\tilde{c}_{i\|3}$	dimensionless concentration of the ith component in the liquid
$\tilde{c}_{out,i}$	concentration of the ith component in the reservoir ($kg\,m^{-3}$)
d_{car}	diameter of the carrier (m)
d_{chan}	diameter of the channel in the carrier (m)
d_{col}	diameter of the reactor column (m)
D_i	diffusion coefficient if the ith component in water
$D_{b,i}$	diffusion coefficient if the ith component in the biofilm ($m^2\,s^{-1}$)
g	acceleration of gravity ($m\,s^{-2}$)
H	column height (m)
K_S	half-saturation constant for the substrate ($kg\,m^{-3}$)
k_B	zero-order degradation rate constant for the dye ($kg\,m^{-3}\,s^{-1}$)
k'_B	first-order degradation rate constant for the dye ($kg\,m^{-3}\,s^{-1}$)
k_d	biofilm decay constant (s^{-1})
k_e	biofilm erosion constant ($kg\,m^{-4}\,s^{-1}$)
$\tilde{K}_S$	dimensionless half-saturation constant for the substrate
l	coordinate along the biofilm surface (m)
$\tilde{l}$	dimensionless coordinate along the biofilm surface
$\dot{m}_B$	mass rate of the dye degradation in the system at anytime ($kg\,s^{-1}$)
n	coordinate normal to the biofilm surface (m)
$\tilde{n}$	dimensionless coordinate normal to the biofilm surface
r	reaction rate ($kg\,m^{-3}\,s^{-1}$)
$r_{b,n}$	biofilm growth rate ($kg\,m^{-3}\,s^{-1}$)
r_B	actual dye degradation rate in the biofilm ($kg\,m^{-3}\,s^{-1}$)
t	time (s)
V_b	biofilm volume with non-zero dye concentration (m^3)
V_h	liquid hold-up on the biofilm (m^3)
V_{ht}	total liquid hold-up in the reactor (m^3)
V_r	reactor volume (m^3)
V_t	reservoir volume (m^3)
$\dot{V}_f$	liquid volume flow through the reservoir and on the biofilm ($m^3\,s^{-1}$)
v	mean liquid velocity in the laminar velocity profile ($m\,s^{-1}$)
$v_{b,n}$	velocity of the biofilm surface movement ($m\,s^{-1}$)
X_0	biomass density in the biofilm ($kg\,m^{-1}$)
X	dye conversion
x	spatial coordinate (m)
$\tilde{x}$	dimensionless spatial coordinate
Y	mass yield coefficient for the substrate (biomass produced per substrate consumed) ($kg\,kg^{-1}$)
y	spatial coordinate (m)
$\tilde{y}$	dimensionless spatial coordinate

Greek letters

β_i	source term for the ith component in the biofilm ($kg\,m^{-3}\,s^{-1}$)
$\tilde{\beta}_i$	dimensionless source term for the ith component in the biofilm
δ	actual biofilm thickness (m)
δ_f	liquid film thickness (m)
δ_{max}	maximum biofilm thickness (m)
δ_0	thickness of the surface layer of the biofilm that participates on the biofilm growth (m)
θ	corrugation factor (1)
μ^*	maximum specific growth rate of the biomass (s^{-1})
ν	liquid kinematic viscosity ($m^2\,s^{-1}$)
ξ	temperature in the reactor (°C)
τ	dimensionless time

Dimensionless quantities

Pe_i	Peclet number of the ith component, the rate of convective transport in the liquid film, to the rate of the diffusion transport in the liquid film
$Pe_{b,i}$	Peclet number of the ith component, the rate of convective transport in the liquid film, to the rate of the diffusion transport in the biofilm
$Da_{b,i}$	Damköhler number of the ith component, the rate of chemical reaction to the rate of convective transport
γ	ratio of the column height to the maximum biofilm thickness
σ	ratio of the maximum biofilm thickness to thickness of the liquid film

existence of a planar biofilm of a constant thickness within the entire bioreactor and invariant in time (Zarook et al., 1997a,b). More realistic models take into account variations in biomass concentration along the reactor, but assume constant biofilm properties. Thus, the models do not include biofilm growth and biomass accumulation (Baquerizo et al., 2005; Rama Rao et al., 2010; Spigno and De Faveri, 2005). The problem of biofilm growth and biomass accumulation in a bioreactor is considered, for example, by Iliuta and Larachi (2004, 2006) who attempted to describe the processes that may lead to biological clogging and, consequently, to a pressure drop increase and flow channeling in trickle-bed bioreactors.

Our objective is to construct a mathematical model describing a biofiltration process in a trickle-bed reactor for textile wastewater decolorization. The model would enable to predict both the behavior of an experimental bioreactor and the biofilm growth in a simplified but sufficiently exact way. The biofilm is formed by a mycelium of a filamentous fungus. We assume that the biofilm structure can be described as a thin film made of the fungus hyphae surrounded by extracellular polymeric substances. The cellular automata or individual-based approaches dealing with individual cell or cell clusters are not suitable for the description of the fungal biofilms due to their specific filamentous structure. Moreover, our objective is the description of the performance of the entire reactor. Thus, our two-dimensional model is based on the continuum approach using the mass balances of substances in a biofilm and in a trickling liquid film.