Qualitative analysis of the moving boundary problem for a biofilm reactor model

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A B S T R A C T

The work presents the qualitative analysis of the free boundary value problem related to a biofilm reactor model. In the framework of continuum approach to mathematical modelling of biofilm growth, the problem consists of a system of nonlinear hyperbolic partial differential equations governing the microbial species growth, a system of semilinear elliptic partial differential equations describing the substrate trends, and a system of nonlinear differential equations for the mass balance in the reactor. The free boundary evolution is governed by a differential equation that also accounts for detachment and attachment. The main result is a uniqueness and existence theorem. By using the method of characteristics, the original differential system is converted to Volterra integral equations and then the fixed point theorem is used. The work is completed with numerical simulations describing the free boundary evolution and mainly focused on attachment/detachment process.

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1. Introduction

The term *biofilm* refers to a form of microbial ecosystem constituted by accumulations of microorganisms, associated to a solid surface or phase inter-phase and embedded in a self-produced primarily polysaccharide matrix [10]. The importance and attractiveness of biofilm systems is undisputed. Biofilms are found in extremely varied environments and are characterized by an inherent robustness and flexibility which have been exploited for many applications, such as bioremediation, water purification and wastewater treatment, biofuels and electricity production. Nearly all biofilm communities in nature comprise a variety of microbial species, which function as a cooperative consortium in a relatively complex and coordinate fashion [9,20]. Generally, the metabolic activities of microorganisms constituting the biofilm determine the formation of various ecological niches due to the local variations in the biofilm environment [11]. Each species fills in

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a specific ecological niche depending on its metabolism and morphology [17]. It is precisely the presence of multiple species within the biofilm that makes it particularly suitable for the treatment of wastewaters, usually diverse in composition and fluctuate in component concentration.

Biofilms have long been considered as a valid alternative technology for wastewater treatment. Over the last decades, their application has considerably increased due to the need of meeting the more stringent requirements for clean water sources and mainly to the significant expansion in the understanding of biofilm properties and formation mechanism [14,15]. Biofilm reactors are characterized by some unique properties when compared to suspended growth systems: bacterial cells in biofilms are more resistant to antimicrobial substances and heavy metals [21]; their residence time is independent of the fluid phase flow rate so they are not subject to washout; biofilm reactors operate at higher biomass density, volumetric productivity and performance stability. Biofilm structure, composition and activity are crucial parameters for the success in operating biofilm reactors [4]. For example, biofilm density and thickness directly affect the efficiency of conversion processes as they define the achievable biomass in the reactor. In addition, microbial diversity is directly related to substrate uptake and to the feasibility of treating contemporary in the same reactor various wastewater constituents.

Mathematical modelling represents a valuable tool in understanding the biofilm microenvironment and ultimately elucidate the macroscale process performance. In the context of engineering practice, biofilm reactor models should account for the multiple physical, chemical and biological processes occurring at different time scales within the biofilm and should be able to describe the fate of wastewater constituents. Specific attention should be paid to the evaluation of biofilm composition in terms of relative mass proportion due to microbial competition; concentration of the particulate components in the bulk liquid with respect to impact on system performance and sludge production; spatial profiles of any number of dissolved components in the biofilm; removal rates and effluent concentrations of the dissolved components; biofilm development in terms of thickness. Specifically, the mathematical modelling of a biofilm reactor usually takes into account two different compartments: the bulk liquid where the dissolved component concentrations vary according to the inlet and outlet flow and the flux into/from the biofilm, and the biofilm itself which grows and consumes the substrates provided by the bulk liquid. The two compartments are interconnected through a flux [12,13]. The biofilm growth can be modeled by using a continuum or discrete approach [22,1,23,16]. 1D continuum models have been widely used to predict the whole process dynamics of biofilm reactors as they have been recognized as suitable tools for most engineering applications [3,2]. Indeed, nowadays many wastewater treatment plant simulators include a mathematical biofilm module typically based on a 1D approach for biofilm representation (see Boltz et al. [3] for a review).

In this work, we refer to the mathematical model derived by coupling the reactor mass balance for substrates with a full one-dimensional Wanner & Gujer type biofilm model as presented in [12,13]. The resulting mathematical problem is constituted by a system of nonlinear hyperbolic partial differential equations which describes biomass dynamics, a system of semi-linear parabolic partial differential equations for substrate distribution in biofilm, a nonlinear ordinary differential equation for biofilm thickness and a system of nonlinear ordinary differential equations for what concerns the bulk liquid phase. All equations are mutually connected and give rise to a free boundary value problem which is essentially hyperbolic. As for the majority of 1D biofilm models, the previous model has been extensively studied through numerical simulations as a rigorous analysis of the dynamic behavior is usually not easily accessible due to the complexity of the system, [13]. Indeed, even when the equations governing the reactor dynamics are not considered, there are only few contributions on the analysis of the Wanner & Gujer type biofilm model, e.g. [18,19].

In this context, a qualitative analysis of the dynamic behavior of the system biofilm-reactor is presented. We assume that the number n of species into the biofilm is arbitrary as well as the number m of substrates. In addition, also the number of dissolved components in the bulk compartment is arbitrary. We use the characteristic-lines to convert all equations, both partial and ordinary differential equations, to integral equations, mainly of Volterra type. Then, the fixed point theorem is used to obtain uniqueness and existence