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On a free boundary problem for biosorption in biofilms

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ABSTRACT

The work presents the qualitative analysis of the free boundary value problem related to the biosorption process in multispecies biofilms. In the framework of continuum biofilm modeling, the mathematical problem consists of a system of nonlinear hyperbolic partial differential equations for microbial species growth and spreading, a system of semilinear parabolic partial differential equations describing the substrate trends and a system of semilinear parabolic partial differential equations accounting for the diffusion, reaction and biosorption of different agents on the various biofilm constituents. Two systems of nonlinear hyperbolic partial differential equations have been considered as well for modeling the dynamics of the free and bounded sorption sites. The free boundary evolution is regulated by a nonlinear ordinary differential equation. Overall, this leads to a free boundary value problem essentially hyperbolic. The main result is the existence and uniqueness of the solutions to the stated free boundary value problem, which have been derived by converting the partial differential equations to Volterra integral equations and then using the fixed point theorem. Moreover, the work is completed with numerical simulations for a real case examining the growth of a heterotrophic–autotrophic biofilm devoted to wastewater treatment and acting as a sorbing material for heavy metal biosorption.

1. Introduction

Over the years, biofilms have been recognized as the most prevalent form of microbial life in various habitats with medical, industrial, and ecological relevance [1]. Biofilms are mainly constituted by bacterial cells of a single or multiple different species in proximity one to another, associated to a solid surface or phase inter-phase and embedded in a self-produced primarily polysaccharide matrix [2]. The interspecies interactions [3,4], the presence of a multitasking matrix [5] and the structure itself, provide to the biofilm several capabilities, such as increased tolerance against antimicrobial agents [6] and protozoan grazing [7],

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improved degradation of organic compounds, high sorption properties for a variety of recalcitrant or slow-degrading compounds, e.g. toxic metal ions and xenobiotics, which are mainly exploited in the field of bioremediation and wastewater treatment [8]. The use of biomass as sorbents for the removal and recovery of organic and inorganic substances in gaseous, soluble or insoluble forms is known as *biosorption* [9]. The term traditionally refers to the passive physico-chemical metabolism-independent process, involving a solid phase (biosorbent) and a liquid phase containing the dissolved or suspended species to be sorbed (sorbate) (e.g. metals, dyes, fluoride, pharmaceuticals, phenols) and resulting in an accumulation at the sorbate–sorbent interface [10]. This relatively new process has become during the last years one of the most promising and cost-effective alternative technologies for the removal and recovery of a wide range of organic and inorganic compounds from industrial effluents and natural waters as it is characterized by a low cost, high removal efficiency, reduced chemical use, reuse potential of biomaterials and nutrients, and possibility of metal recovery [11]. Various materials of biological origin can be used as biosorbents, including plant biomass, bacteria, fungi, and algae, etc. [12]. Dead biomass has been preferred in most of experimental studies due to the following advantages: absence of toxicity limitations; easy absorbance and recovery of biosorbed metals; easy regeneration and reuse of biomass; possibility of easy immobilization of dead cells; easier mathematical modeling of metal uptake [10]. However, additional benefits might result from the metabolic activities (respiration, nutrient uptake, EPS, metabolite release and oxido-reductive transformations) of living organisms which might alter the microenvironment around the cells and contribute to the overall removal process. Biofilms have drawn particular interest in this context due to the abundant binding site concentration in both microbial cell walls and extracellular polymeric substances and the natural absence of toxicity limitations. The binding mechanism of the sorbate onto the biomass surface can be performed by many mechanisms occurring under different operating and environmental conditions, including electrostatic interactions, covalent binding, ions exchange, microprecipitation, chelation and complexation [13]. Biosorption efficiency is affected by various environmental factors, such as pH, which rules metal mobility and speciation, temperature, with an optimal value ranging between 20 and 35 C, and the co-presence of multiple heavy metals. Besides the factors above mentioned, the amount of sorbent used significantly affects process efficiency and stability as a higher sorbent concentration increases the availability of active sites that can effectively bind metal ions [13]. Although the high number of experimental studies on biosorption developed during the last decays, several aspects still need to be clarified for the scale-up of the process at the industrial scale.

In this context, mathematical modeling appears as a support to gain essential information for the identification of the key factors affecting biosorption efficiency and stability [14]. Due to process similarities to adsorption, conventional equilibrium and kinetics models have been adapted to the needs of the mathematical description of biosorption and applied to a wide range of batch experimental situations (see [13,15,16] for a recent overview). For single-metal solutions, the most widely used isotherm models are the two-parameter models of Langmuir and Freundlich, which correlate the sorbed and solute sorbate concentration in the liquid phase at equilibrium for constant environmental parameters. These models were originally derived for non-biological systems and are based on assumptions that are quite simplistic for such complex systems. They are not able to reproduce the mechanisms of solute uptake, but they have been widely recognized as efficient tools to provide a suitable description of the experimental behavior. Kinetic models are usually aimed at describing the behavior of the sorption system on time [17] and have been commonly applied to study the contribution of the main rate controlling steps (i.e. bulk diffusion; film diffusion; intraparticle diffusion; chemical reaction) invariably involved in the sorption process [13]. They usually come in the form of generally highly simplified pseudo-first and second order kinetic equations. The most used kinetic model is the Weber–Morris intraparticle diffusion model which describes well the kinetics of biosorption for the first 10 min of the process [10]. Mathematical models for continuous biosorption systems have been developed as well: they usually refer to a flow-through fixed-bed bioreactor configuration and have been originally derived