# Chapter 5 Mathematical Modeling of Microbial Bioremediation: A Key Step in Process Scale-Up

## Mihaela Rosca

Inttps://orcid.org/0000-0002-1405-0848
Ion Ionescu de la Brad Iasi University of Life Sciences, Romania & Gheorghe Asachi Technical University of Iasi, Romania

### Petronela Cozma

b https://orcid.org/0000-0002-9237-3423 Gheorghe Asachi Technical University of Iasi, Romania

#### Maria Gavrilescu

Gheorghe Asachi Technical University of Iasi, Romania & Academy of Romanian Scientists, Bucharest, Romania

## ABSTRACT

Biosorption is a method that holds great promise for environmental bioremediation. However, the process mechanism is not yet fully comprehended as it relies heavily on the characteristics of the biosorbent, properties of the pollutants, and operational conditions. The knowledge and understanding of sorption kinetics and mechanisms are critical for the design and scaling up of biosorption. Applying the proper models and methods in the evaluation of heavy metals biosorption can elucidate mechanisms, analyze experimental data, predict outcomes, and optimize processes. After a brief analysis of the literature in the field of biosorption, it has been found that the most valuable models provide information about process kinetics, maximum biosorption capacity and thermodynamics. Additionally, the preferred methods for studying the interactive effects of process variables and creating a precise mathematical model that describes the process accurately are highly sought after. Thus, the main purpose of the chapter consists in exposing the available mathematical models and methods that can be applied for the evaluation of all factors that could affect the biosorption of heavy metals. The isotherms, kinetic and thermodynamic models, as well as the statistical tools suitable for evaluating biosorption were presented, with a special emphasis on their application, advantages, as well as disadvantages.

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## INTRODUCTION

Bioremediation, a powerful approach in environmental science, leverages the capabilities of microorganisms to mitigate the impact of pollutants on ecosystems. Notably, biosorption and bioaccumulation find preeminent application in the remediation of heavy metals, demonstrating their effectiveness in addressing the challenges posed by the presence of these toxic elements in natural ecosystems (Filote et al., 2022; Gavrilescu, 2004; Rosca et al., 2015). Heavy metals are persistent inorganic pollutants, the concentrations of which often exceed the limits allowed in legislative regulations for water, air, and soil. Research conducted at both laboratory and large scales has demonstrated that biological methods exhibit a high potential for removing heavy metals from wastewaters compared to conventional, physico-chemical methods (Gavrilescu, 2004; Rosca et al., 2019). This symbiotic relationship between microbes and pollutant removal processes underscores the significance of bioremediation in fostering environmental sustainability.

Over the last two decades, numerous studies have focused on biosorption and bioaccumulation processes, and advances in this field have increased interests in these techniques for addressing pollution issues. Most notably, microbial-driven mechanisms play a key role in the removal of pollutants from the environment. Bioaccumulation in microorganisms involves the gradual buildup of heavy metals from their surroundings. Microorganisms, for instance bacteria and fungi, absorb these metals from the water or other environments they inhabit. Over time, the metals accumulate within the living microorganisms' cells or on their surfaces, contributing to the concentration of heavy metals within the microbial biomass (Filote et al., 2021; Limcharoensuk et al., 2015). Bioaccumulation, unlike biosorption, is characterized by a more extended duration, often requiring long periods for the gradual buildup of heavy metals by living microorganisms. The efficiency of bioaccumulation is notably influenced by specific environmental conditions that play a crucial role in shaping the rate and extent of metal accumulation within microbial biomass (Rosca et al., 2015; Sedlakova-Kadukova et al., 2019). Biosorption is a process involving the ability of various biomasses, especially non-living microorganisms like bacteria, fungi, and yeasts, to retain metal ions. This occurs due to the presence of specific sites on the surface of these microorganisms known as active sites or functional groups. These active sites have a chemical affinity for metal ions, meaning they attract and hold onto them. When metal ions come into contact with the microorganisms, these active sites interact with the metal ions, forming a bond (e.g. by electrostatic attraction, ion-exchange processes). This bonding mechanism allows the microorganisms to capture and hold the metal ions, effectively removing them from the surrounding water or solution (Ciobanu et al., 2023; Gavrilescu, 2004; Tinega et al., 2023; Uysal et al., 2022). As non-living microbial biomass is a cost-effective source with a high pollutant retention capacity, biosorption is considered an environmentally friendly and economical option with high efficiency in removing heavy metals from wastewater (Beni & Esmaeili, 2020; Filote et al., 2021; Volesky, 2007).

The study of this process is essential for understanding how to optimize biosorption for the efficient removal of metals in various environmental applications. Moreover, scaling-up of bioremediation processes from the laboratory to an industrial scale remains a challenging task due to the complex interactions between pollutants and biosorbents and the diversity of factors that could affect the process (Rosca et al., 2021). The transfer of data from the laboratory to pilot and industrial scales is typically slow, and optimal conditions may change due to the influence of factors related to bioreactor construction and operation. Therefore, in the exploitation of biosorption, it is essential to study the influence of process-related factors (such as pH, biosorbent dose, initial concentration of the metal in solution, temperature

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