AN APPROACH TO BIOREMEDIATION

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Abstract: This paper provides some mathematical models associated with bioremediation processes. Bioremediation is a process in which contaminants in polluted soils are eliminated by bacteria. The initial model is the one given by Keller and Segel. The Keller-Segel model takes into account the movement of bacteria by diffusion and chemotaxis. Starting from this generalized model, we present different forms of diffusion and chemotactic coefficients. All particular cases presented were confirmed experimentally or numerically.

Keywords: bioremediation, bioaugmentation, biostimulation, chemotaxis.

1. A BRIEF HISTORY OF BIOTECHNOLOGY AND BIOREMEDIATION

In the last years, due to industrial activities and/or agriculture, a growing number of chemical compounds are released into the environment with negative impacts on it. In particular, the rapid industrialization of agriculture, the unprecedented development of chemical industry and the increasing need to generate cheap forms of energy, resulting in contamination of soil and groundwater, with a large number of xenobiotic products. They have negative and irreversible effects on the quality and environmental health. Thus, the problem of soil and groundwater contamination by organic pollutants has become a serious and widespread problem of the environment.

Over the past decades, biological methods of cleaning the environment have shown a special interest. These methods, called bioremediation methods, will reduce the risk of organic pollutants in soils and even eliminate the pollutant, restoring chemical balance. These soil bioremediation methods are considered non-aggressive treatment. They are based on spontaneous and/or controlled action of microorganisms that are able to convert pollutants from soil in less toxic or nontoxic chemical compounds, which will involve attenuation or complete elimination of pollution. Unlike other physical or chemical treatments of soil or water, that can transfer the pollutant from one area to another or from one phase to another, with slight improvement, bioremediation offers a final solution. For example, bioremediation is often the preferred method for removing petroleum hydrocarbons, because it turns them into harmless products such as carbon dioxide and water. Bioremediation has a much more convenient price-quality standard compared to other technologies.

Bioremediation is defined by the American Academy of Microbiology as "the use of living organisms to reduce or eliminate environmental hazards resulting from accumulations of toxic chemicals and other hazardous wastes" (Gibson and Sayler, 1992).

The history of bioremediation is short and influenced by economic forces. Interest in the use of microorganisms in the degradation of chemical pollutants dates from 1952 when Gayle has proposed the following theory: for

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any organic compound there exists a microorganism that can destroy it, if the appropriate conditions are met. Otherwise, there may be a strain to destroy it.

2. STRATEGIES FOR BIOREMEDIATION THE POLLUTED SOIL

2.1. Physical model of bioremediation

Soil is a rich but fragile ecosystem, and is defined as the soft and brittle layer which is found in the surface of terrestrial crust, which together with the adjacent atmosphere, represents the living environment of plants and animals. The soil is an environmental factor that must be protected to the same extent as the water and the air. Both soil and groundwater are the preferred drainage places of chemical compounds. As a consequence, many properties of chemical, biological and biochemical properties of soil are altered, and the long-term effect is the loss of support functions of living organisms. In general, when an organic chemical compound penetrates into the soil, one of the following phenomena may occur: the phenomenon of transfer which does not modify the structure of the substance or phenomenon that changes the chemical structure by decomposing it into different substances. The purpose of soil bioremediation "is not only to enhance the degradation, transformation, or detoxification of pollutants, but also to protect the quality and capacity of the soil to function within ecosystem boundaries, to maintain environmental quality and sustain biological productivity" [1]. Soil health has been defined as "the continued capacity of the soil to function as a vital living system, within ecosystem and land-use boundaries, to sustain biological productivity, promote the quality of air and water environments, and maintain plant, animal, and human health" [2]. Remediation techniques, based on physical, chemical or biological methods, suitable for full or partial remediation of soils, can be used in situ, i.e. in the contaminated area, offering advantages for the ex-situ technologies. The best technique will depend on the nature and concentration of the pollutant and on the environmental characteristics.

The following steps are necessary for a good program of soil bioremediation:

- understanding the past history of the polluted area and the activities that led to the site's pollution;
- the examination and the quantification of severity of the pollution;
- the development of a specific remediation program for that pollutant;
- the development of a specific remediation program for that site;
- monitoring the efficiency of adopted bioremediation program.

It was shown that most chemical pollutants can be transformed by microorganisms. Intrinsic bioremediation is a natural phenomenon of mitigation which appears in the polluted soils and contribute to their rehabilitation. Intrinsic bioremediation is of great importance because it is realized with an minimal cost, avoids disturbing the environment and the human exposure. The main factors influencing it are the concentration, the pH and the temperature of the pollutant and the availability of acceptor electrons. The disadvantage is that this natural process is slow. Thus, we need to use techniques to accelerate the intrinsic bioremediation. They are: bioaugmentation, i.e. the increasing number of microorganisms with degradation capabilities, and biostimulation, which means supplementation of carbon sources or other nutrients that stimulate the activity of existing microorganisms. Despite bioaugmentation is a controversial method in environmental microbiology, it is used to increase the genetic capacity of a given site. The usefulness of bioaugmentation is demonstrated by studies showing the inability of microorganisms in some cases to destroy the pollutant and the obvious increase of bioremediation rate with microorganisms supplementation [3].

Once a bioremediation program has been implemented, its effectiveness will be demonstrated through a continuous monitoring of chemical and biological indicators of the environment, but also of the pollutant. These indicators should determine if the site's cleaning was successful and if the pollutant was completely eliminated. Chemical and analytical tests will be made in order to ascertain whether the target objectives of cleaning have been achieved or not. The presence of microorganisms and the diversity of microbial populations will demonstrate the biological nature of bioremediation processes. The toxicity tests will determine if the pollutant was completely removed and if the bioremediation involved any environmental risk.

The goal of bioremediation is to reduce the concentration of organic pollutants to undetectable levels, or at least below the limits set by regulatory agencies. In order to consider the bioremediation a practical method of treatment, several criteria must be satisfied:

- the presence of microorganisms and their catabolic activity;

- the micro-organisms' ability to transform the pollutant and to decrease the concentration of the standard values;
- not occur compounds which are toxic for concentrations that are likely to be achieved;
- not produce chemicals that inhibit the bioremediation process;
- the targeted pollutant must be bio-available;
- the properties of the site must support the work of microorganisms;
- the bioremediation must have a lower cost or at most equal to other decontamination techniques.

None of these criteria should be neglected. If one of them is not taken into consideration, the method of bioremediation can be rejected, or may work but not to reach target audiences cleaning. Once the bioremediation program has been developed, its feasibility is assessed by the following criteria:

- applicability is strictly related to soil and pollutant properties;
- the studies to determine the potential of bioremediation, to define operating conditions, for development and implementation of bioremediation plan and an adequate and effective monitoring program;
- possible disadvantages and limitations of the program;
- advantages related to its potential to exploit the bio-geo-chemical natural processes, immobilize or destroy, partially or completely, the agent of pollution.

When all these criteria will be covered, we will have successful bioremediation process, which does not affect soil quality.

2.2. The mathematical models of soils bioremediation

In this paper we consider a one-dimensional polluted soil, homogeneous, occupying the layer $0 < x < L$. We consider in this soil the propagation of a single pollutant and one single type of bacteria able to destroy it. During bioremediation, bacteria migrate by diffusion and chemotaxis. Diffusion is the movement of molecules within the meaning of decreasing concentration of bacterial population (in an area with a higher concentration to an area with a lower concentration). Chemotaxis phenomenon is particular sensitivity of some microorganisms (bacteria in our case) to the attraction of a chemical (in our case the pollutant). Such movement was for the first time reported in the nineteenth century [4-6]. Consider also that the soil contains adequate nutrients for maintenance of the bacteria, at a temperature that is convenient and does not contain other chemicals that could inhibit the bioremediation process.

2.2.1. The Keller- Segel model of chemotaxis

We denote the concentration of the pollutant with $c(t,x)$ and the concentration of bacteria with $b(t,x)$, at spatial position x and time t. Bioremediation process starts at $t = 0$. We note with $c_0(x)$ the concentration of the pollutant, respectively with $b_0(x)$ the concentration of bacteria at baseline. Concerning the diffusion process, we introduce the bacterial diffusion coefficient $D(c)$, the diffusion coefficient of the pollutant δ, the chemotactic coefficient $K(c)$. We have the following generalized Keller- Segel (K-S) model on the form:

$$\frac{\partial b}{\partial t} = \nabla \cdot (D(c)\nabla b) - \nabla \cdot (K(c) b \nabla c) + g(b,c) - h(b,c) \tag{1}$$

$$b(0,x) = b_0(x) \tag{2}$$

$$c(0,x) = c_0(x) \tag{3}$$

$$\frac{\partial c}{\partial t} = \delta \Delta c - \varphi(b,c) \tag{4}$$

Where: $g(b,c)$ and $h(b,c)$ are functions describing cell growth and death, respectively, $\varphi(b,c)$ is the function describing pollutant degradation. Generally, the bacterial diffusion coefficient $D(c) = D$ is assumed constant. Boundary conditions are dependent upon the assay being modelled. In general, the limits conditions are

Neumann type. In the generalized K-S model, we include any model which assumes bacteria move by diffusion and chemotaxis. In this model, the pollutant is described by an equation in the form of (4).

Using the model described by the equations (1)-(4), Keller and Segel assumed that the bacteria did not reproduce in the time interval $(0,T)$ and the bacteria responded to a single substrate of attractant which did not diffuse [7]. They assumed that the chemotactic coefficient has the form:

$$K(c)=\begin{cases}\dfrac{K}{c}\ , & c>0\\ K_{\max}\ , & c=0.\end{cases} \tag{5}$$

Keller and Segel noted this form of the chemotactic coefficient allows the model to predict bacterial behaviour when a continuum description for the concentration of the pollutant is no longer adequate, the only condition being $\frac{K}{D}>1$. This model was experimentally verified and confirmed by Holz and Chen [8].

Later, in 1974, Scribner suggested new forms for $\varphi(b,c)$, $K(c)$, $D(c)$. Motivation was that more biologically realistic forms of the pollutant consumption rate, chemotactic and diffusion coefficients should depend upon a critical pollutant concentration level a, such that

$$\varphi(b,c)=\varphi_0(ac)^m,\ c\le\frac{1}{a};\qquad \varphi(b,c)=\varphi_0,\ c>\frac{1}{a};$$

$$K(c)=\frac{K(ac)^i}{c},\ c\le\frac{1}{a};\qquad K(c)=\frac{K}{c},\ c>\frac{1}{a}; \tag{6}$$

$$D(c)=D_0(ac)^n,\ c\le\frac{1}{a};\qquad D(c)=D_0,\ c>\frac{1}{a};$$

Where: i, m, n are all positive real numbers. Scribner assumed that the attractant was free to diffuse through the spatially confined region of interest [9].

Another form for the chemotactic coefficient was suggested by Lapidus and Schiller in 1976:

$$K(c)=\frac{KK_d}{\left(K_d+c\right)^2} \tag{7}$$

Where: K_d is the receptor- ligand binding dissociation constant. By calculating the average number of bacteria which move into the central region of the assay, Lapidus and Schiller were able to determine values for the chemotactic coefficient, K and K_d. Model comparison with experiment showed good agreement [10].

Rosen and colleagues analyzed a number of K-S models, in which were considered variations of the attractant degradation term $\varphi(b,c)$. Rosen noted that if $\varphi(b,c)=kbc$ with $\delta=0$ means the K-S model does not admit banded solitary wave solutions, and thus the authors considered:

$$\frac{\partial c}{\partial t}=-kbc^p,\ p\ge 0. \tag{8}$$

This form was found to admit solitary wave solutions for $(1-(K/D)) < p < 1$. Travelling wave analysis of the resultant governing equations allowed the speed of the bands to be determined. Rosen further justified this choice by noting that it may be associated with possible physio-chemical and biological mechanisms.

Rosen and Baloga (1975, 1976) worked with the model given by equations (1) and (8) which admits stable chemotactic solutions. There were obtained approximate analytical solutions for the whole system, solutions have been considered an alternative to numerical solutions obtained by Scribner. To write equations (1) and (4) into a single one, witch admit the wave equation solutions, they considered a transformation of the form $\theta = \left(\frac{c}{c_\infty}\right)^{1-p}$. The aim was to demonstrate that the K-S model where the pollutant concentration decreases exponentially admits the wave equation solution [11].

2.2.2. The Fasano- Giorni model of chemotaxis

The model proposed by A. Fasano and D. Giorni (the F-G model) in [12] is a special case of the K-S model. In this model, the bacteria also migrate by diffusion and chemoattraction. They assumed that the function describing the degradation of pollutant is expressed as $\varphi(b,c) = -\frac{\beta_1 c}{1+\beta_2 c} b$, where $\beta_1 > 0$ and $\beta_2 \geq 0$ are constants. Thus, in the F-G model, for the kinetic term we have the expression:

$$\frac{\partial c}{\partial t} = \delta \Delta c - \frac{\beta_1 c}{1+\beta_2 c} b \tag{9}$$

and $\delta = 0$. Please note also that in the F-G model $f(b,c) = g(b,c) - h(b,c)$.

Consider an isotropic soil, while non-deformable, homogeneous with constant porosity, consisting of a single layer $x \in (0, L)$. Suppose that in this environment a single agent of pollution is acting and one type of bacteria is able to destroy it and that the bioremediation phenomenon is not influenced by any other fluid flow. Let $\Omega = (0, L)$ be an open subset of $\Re$ with the boundary $\Gamma = \partial\Omega = \{x \in \Re : x = 0 and x = L\}$. We denote $Q = \Omega \times (0,T)$ şi $\Sigma = \Gamma \times (0,T)$. The mathematical model is given by a nonlinear boundary problem with initial conditions given by:

$$\frac{\partial b}{\partial t} - D\frac{\partial^2 b}{\partial x^2} + \frac{\partial}{\partial x}\left[bK(b,c)\frac{\partial c}{\partial x}\right] = f(b,c) \text{ for } (t,x) \in Q, \tag{10}$$

$$\frac{\partial c}{\partial t} = -\frac{\beta_1 c}{1+\beta_2 c} b \text{ for } (t,x) \in Q, \tag{11}$$

$$c(0,x) = c_0(x) \ ; \ b(0,x) = b_0(x) \text{ for } x \in \Omega, \tag{12}$$

$$-D\frac{\partial b}{\partial x} + bK(b,c)\frac{\partial c}{\partial x} = 0 \text{ for } (t,x) \in \Sigma. \tag{13}$$

The problem given by (10)-(13) can be treated within the framework of the theory of accretive operators.

3. CONCLUSIONS

We presented the generalized model of Keller- Segel along the time. All particular cases presented were confirmed experimentally or numerically. Starting from the K-S model, an important case is the model given by Fassano and Giorni. The F-G model shows us that the resulting problem is a boundary value problem with initial conditions for a parabolic equation, which can be treated within the theory of nonlinear accretive operators. Although this model is an oversimplification of the real process (for example the bioremediation phenomenon is not influenced by any other fluid flow, the soil is one-dimensional), the resulting mathematical problem is far from being trivial.

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