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A Numerical Model for Adsorption and Bio restoration in a Saturated Porous Media

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Abstract

In this work, we are going to illustrate the effect of adsorption and diffusion phenomena on the rate of biodegradation in a system of a column of the soil. We study the mineralization of phenol as a contaminant substrate by pseudomonas-sp bacteria. We found that the monod kinetics which suppose that all of the substrate is available for bacteria doesn't describe the biodegradation of the phenol in our system. A two-compartment model is so developed to explain the rate of biodegradation of the contaminant in the studied system. The model supposed that the substrate existed in two forms: The first is the adsorbed fraction on the solid phase, which is inaccessible for biodegradation. The second is the rate of substrate in the solution phase, which is accessible for microorganisms. After the mineralization of the contaminant in the aqueous phase, the rate of biodegradation is controlled by the part of substrate, which is diffused from the sites inaccessible for biodegradation to the regions accessible for microorganisms. The numerical simulation is based on a forth runge-kutta method which allows as by a series of comparison between experiment and numerical results to determine the rate of adsorption and biodegradation in our system.

Keywords: Adsorption, Diffusion, Two-Compartment Model, Column of the Soil, Pseudomonas-SP Bacteria, phenol, Least Square Method.

INTRODUCTION

Bioremediation is one of the important techniques for groundwater decontamination. It is a natural process, which can be active by the injection of nutrients such as oxygen (aerobic biodegradation) and nitrate (anaerobic process). However, some factors influence the rate of biodegradation such adsorption and diffusion.

In this study, we are interested by the mineralization of the phenol as a substrate contaminant by a pseudomonas – sp bacteria in a system of a column of the soil. We illustrate that the monod kinetics [2] doesn't describe the biodegradation of the substrate in our system. A two-compartment model is proposed to explain the biodegradation of the substrate in our case.

This model suppose that the substrate existed in a two forms: The first one is the portion of the substrate adsorbed on the solid phase which is protected from microorganisms. The second fraction is the part of the substrate in the solution phase which is available for biodegradation. After the mineralization of the substrate in the aqueous phase, the rate of biodegradation is controlled by the phenomena of desorption or diffusion of the substrate from the inaccessible sites for biodegradation to the regions accessible for microorganisms. The numerical simulation implemented here is based on a forth explicit runge kutta method [1] and the parameters of the simulation (the rate of desorption and the rate of biodegradation) are determinate experimentally [3] in our system of the column of the soil.

A least square method [4] enable us to determinate the rate of mass transfer between the two compartments by a series of comparison between numerical and experimental result.

MATHEMATICAL MODEL

Many authors [3] found that the monod kinetics doesn't describe the biodegradation of the contaminants in the subsurface of the soil because it suppose that all of the substrate is available for microorganisms. The simple model of monod kinetics is given by the following equation:

$$\frac{\partial S}{\partial t} = -kX\frac{S}{S+k_s} \tag{1}$$

Where:

k: The rate maximum utilization of substrate

(M substrate/M cellule.T)

X : The concentration of biomass (M/L^3).

S: The concentration of substrate (M/L^3).

k_s: The substrate half saturation constant (M/L^3).

For low concentration of substate ($S<<k_s$), the kinetics of monod is reduced to a first order kinetics for biodegradation.

$$\frac{\partial S}{\partial t} = -kXS \qquad (2)$$

We describe so a two compartment model [3] to explain the biodegradation of phenol in our system of the column of the soil.

The model supposes that the substrate has a low concentration in order to consider a first order kinetics for mass transfer between the two compartments and for the biodegradation of the contaminant in the liquid phase.

MATHEMATICAL FORMULATION

If k1and k2 are the rate of mass transfer between the two compartment and k3 is the rate of biodegradation in the liquid phase, we obtain the following simplified form of the two compartment model [3]:

S1: The concentration of substrate adsorbed in the solid phase.

S2: The concentration of substrate in the liquid phase.

NUMERICAL SILULATION

The system of equations (3) is simulated by an explicit forth runge kutta method [1]. The parameters of simulation are determinate by a series of experiences in batch system of the considered soil. The experiment data are shown in (table 1).

Components	Value
PH	7.0
Temperature	32 C°
Dissolved oxygen	20% of the maximum solution of oxygen
Final absorbance	1.5 to 500 wt %
Rate of the kinetics k3	0.2
Material	Saturated sand
Porosity	0.44
Column	30cm, 2.54 for diameter
Flux of flow	5ml/min

In a first test, we suppose that all of the substrate is available for microorganisms and the monod kinetics describe the biodegradation of phenol in our system. We also suppose that there are no desorption or diffusion between the two compartment of our model. Figure (1) compares the numerical results to the experimental one.

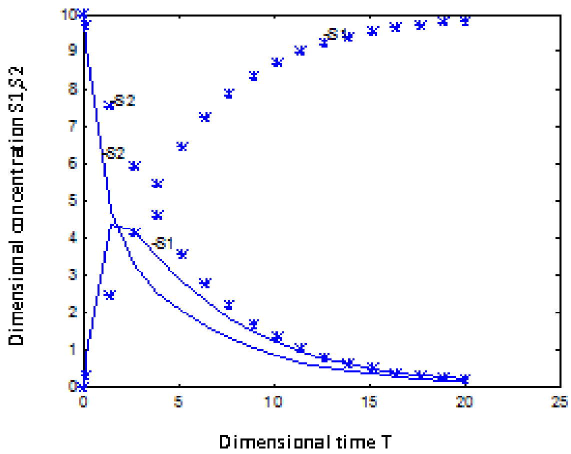

Figure 1: Comparison between experimental result (solid curve) and numerical result (curve with *) using Monod kinetics for biodegradation

Figure (1) show that the Monod kinetics doesn't describe the biodegradation of phenol in our column of the soil. The choice of a two-compartment model is necessary to explain the mineralization of the substrate in our system.

In a second test, we suppose that a two-compartment model (equation 3) describes the biodegradation of substrate. A least square method allows as to determine the rate of mass transfer between the two compartments (k1 and k2) by a series of comparison between experimental data and numerical results. Figure (2) shows a best accord between the experimental data and the numerical results for k1=0.5 and k2=0.3

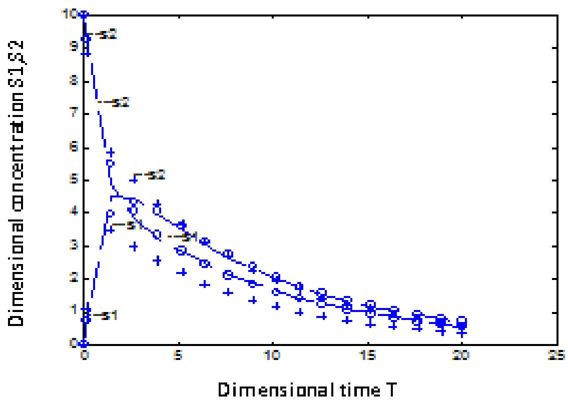

Figure 2: Good agreement between numerical results and experiment data for k1=0.5 and k2=0.3.

Figure (2) show an important rate of desorption of contaminant to the site accessible for biodegradation, which enhanced the rate of biodegradation

If k3 (The rate of biodegradation in the aqueous phase) is great than the difference between k1 and k2, the model show a limitation of the rate of desorption (figure 3).

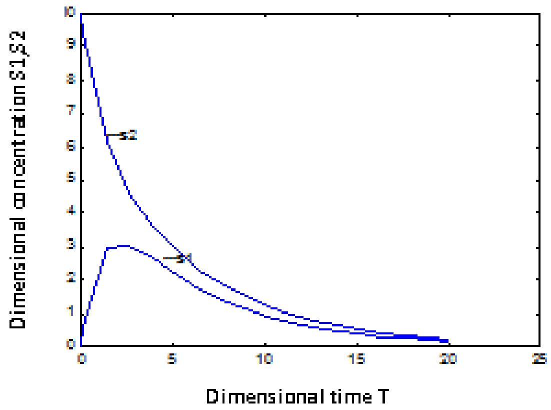

Figure 3: Limitation of the desorption process

In a latest test, we show how diffusion influences the rate of biodegradation. So, we consider a system in which the bacteria of pseudomonas-sp metabolize the phenol (in this system, we can control the volume of the sites inaccessible for biodegradation).

Figure (4) show that augmenting the volume of the regions don't containing the microorganisms diminish the rate of mineralization of the substrate because of the important diffusion of the contaminant to the sites in which it is protected from microorganisms.

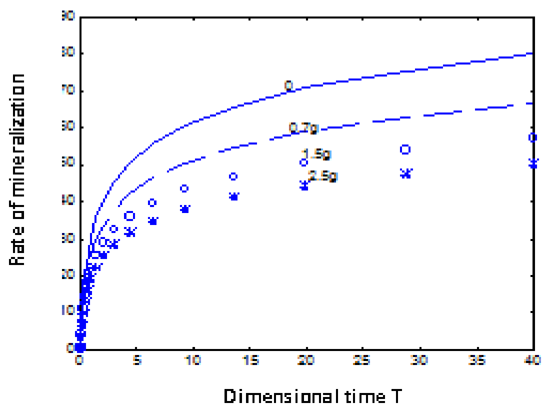

Figure 4: Mineralization of phenol by pseudomonas-sp bacteria. The numbers show the augmenting of the part of the soil inactive for biodegradation

CONCLUSION

In this work, we have illustrated the different factors influencing the rate of biodegradation in a system of a column of the soil such adsorption and diffusion.

We have developed a two- compartment model to explain the mineralization of the phenol by the pseudomonas –sp bacteria. We have shown that the monod kinetics doesn't describe the biodegradation of the substrate in our system because of the diffusion and the desorption of the substrate to the sites accessible for microorganisms. The rate of biodegradation is enhanced by the rate of desorption and he diffusion in the studied system.

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