

Numerical Analysis of a Simple Mathematical Model to Design Bioremediation System in Rhizosphere

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Abstract

Soil bioremediation, especially in the rhizosphere area, is the result of interaction between plant roots and microorganisms. It can be considered as one of the remarkable ways to eliminate pollutants. Various factors control the process with special relationships in the rhizosphere environment; changing each of them can impress on the system destination. With mathematical modeling, behavior of the process can be predicted and controlled, and improved by appropriate changes in the model. In this study, the effects of different parameters of a simple mathematical model, represented to predict microbial growth and necessary substrate changes in the rhizosphere have been studied using numerical finite difference method. Influences of the parameters on biomass and substrate concentrations were evaluated at different times. A number of variables directly, some negatively, and others neutrally impacted on the biomass and substrate concentrations. Investigating variables differently affecting on a model is important since perfectly tuning them can optimize the system performance, and achieve higher efficiency.

Keywords: Mathematical Model, Numerical Solution, Soil Bioremediation, Rhizosphere

1. Introduction

Soil pollution, one of the environmental crises, must be eliminated. Soil is contaminated with different inorganic and organic materials such as agricultural pesticides, petroleum, and heavy metals which are remediated by the appropriate method to reduce pollution level. A suitable method can be selected on the volume of pollutants, soil type, and environmental conditions. Different methods such as

adsorption, precipitation, complexation, consumption by plants, and microbial removal can efficiently reduce pollutants in the soil [1, 2].

Soil bioremediation in rhizosphere is one of the oldest and most effective methods to treat soil [3, 4]. Rhizosphere is a zone of soil, containing plants roots. The area includes not only plant root and food, but also interaction among soil microorganisms, roots, and root products [5, 6]. Rhizosphere bioremediation

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is a combined technology that is performed with plants and soil microorganisms. Plants can control microbial growth and act as food products for them. Microbes begin to grow based on rhizosphere conditions and plant products; and can reduce pollutants in the soil to a certain extent [7-10].

Each phenomenon requires simulation and modeling to monitor, analyze, and precisely predict. Therefore, various rhizosphere models were derived to identify and predict behavior of the area in the soil [11]. Although many models have been reported in relation to soil, the first mathematical model proposed for rhizosphere was reported by Baker et al. in 1967, who explained that the rhizosphere zone was a cylindrical area with constant radius [12]. Since then, many models have been tested on the rhizosphere. Each of them followed particular purposes. One of the goals was the behavior recognition of soil bioremediation; so far some models have been reported in relation to it [13-15]. Generally, in rhizosphere bioremediation, five processes can be represented, and reduction of soil contamination can be predicted by modeling them. 1 - Changes in organic matter and substrate for microorganisms which are involved in biodegradation of pollutants. Sung et al. have presented a simple model to predict microbial growth on the substrate [16]. 2 - Changes in oxygen demand in the rhizosphere. Hogberg and Sorensen have reported a model for oxygen consumed by microorganisms in the rhizosphere [17]. 3 - Root activities and effectivity on rhizosphere conditions. The simplest model for uptake of soil nutrients by the root have been studied by Roose et al. [18], offered based on previous models. Rhizosphere was provided

in cylinder form that was centered on root, consisting of infinite radius [19, 20]. 4 - Microbial growth and changes in different biomasses concentrations in the rhizosphere. Strigul and Kravchenko have reported models of various microbial lives in the rhizosphere due to the type of microbes, substances in soil, and plant products for microbial growth [21]. 5 - Changes in pollutants on the microbial activities. Kim et al. provided a model to predict contaminant mass changes in the rhizosphere based on the relationship between substances in aqueous phase of the rhizosphere, and materials absorbed and excreted from plant root [22]. In this study, a mathematical model for rhizosphere has been used to predict microbial and substrate changes in soil bioremediation process. Changes in substrate amount and microbial growth rate have been numerically investigated based on the model variables. It was solved with numerical finite difference method using a program written in MATLAB software (R2010a).

2. Mathematical model

The model represents the changes in necessary substrate for microbial activities in the rhizosphere. In the model, the microorganisms in the soil follow Monod model. In equation 1, microbial growth is considered as two substrates model, and also the microbial death is predicted [16].

$$\frac{dC_m}{dt} = \mu_{m,(T)} \left(\frac{c_p}{K_p + C_p} \right) \left(\frac{c_o}{K_o + C_o} \right) - K_d J C_m \quad (1)$$

$\mu_{m,(T)}$ is dependent on temperature. For calculating substrate changes in the rhizosphere, equation 2 is used. According to the release of organic substrates from plant root and penetration in soil, substrate

changes are modeled [16].

$$\frac{dC_p}{dt} = Q_{sp} + Q_{sx} + Q_{si} + Q_{so} \quad (2)$$

Rate of substrate penetration from plant root into the soil can be defined based on the equation 3 [23].

$$Q_{sp} = \frac{1}{r} \frac{\partial}{\partial r} (r D_{rm} \frac{\partial C_p}{\partial r}) \quad (3)$$

Substrate consumption rate by microorganisms is calculated with equation 4 [16].

$$Q_{sx} = -\frac{C_m}{Y_p} \left[\mu_{m,(T)} \left(\frac{C_p}{K_p + C_p} \right) \left(\frac{C_o}{K_o + C_o} \right) - K_d \right] \quad (4)$$

This has occurred in combination with equation 1, estimating the microbial growth rate, and efficiency coefficient Y_p which reflects yield of the microbial growth on the substrate consumption rate. When soil loses its moisture and becomes dry, microorganisms die and decompose into organic matter. Consequently, the process causes feeding the new microorganisms. Rate of Changes in endogenous substrate can be defined by the microbial decrease rate [16].

$$Q_{si} = IC_{im} \quad (5)$$

Equation 5 represents the rate of endogenous substrate production based on a first order equation. The rate of exogenous substrate changes Q_{so} varies due to the type of

substances in soil and substances which microorganisms consume as soil contaminants.

Derivatives 1 and 2 are derived with respect to time. Also, partial derivative 3 is derived in relation to radius. Consequently, the main equation, mathematically combining biomass balance and microorganisms required substrate in the rhizosphere, is derived by replacing equations 3 to 5 in equation 2 with respect to time and radius [16].

$$\begin{aligned} \frac{dC_p}{dt} &= \frac{1}{r} \frac{\partial}{\partial r} (r D_{rm} \frac{\partial C_p}{\partial r}) \\ &- \frac{C_m}{Y_p} \left[\mu_{m,(T)} \left(\frac{C_p}{K_p + C_p} \right) \left(\frac{C_o}{K_o + C_o} \right) - K_d \right] \\ &+ IC_{im} + Q_{so} \end{aligned} \quad (6)$$

Solving the equation requires satisfying boundary conditions for the numerical parameters. Due to the type of rhizosphere soil, environmental and geometric conditions, different boundary conditions and various factors can be determined to solve them.

3. Solving mathematical model

To solve the original equations which include equations 1 and 6, the finite difference method is used. Equations 7 and 8 are, respectively, solution of the equations 1 and 6.

$$Cm_{i+1} = Cm_i + \left[\mu_{m,T} \left(\frac{C_{pi}}{K_p + C_{pi}} \right) \left(\frac{C_o}{K_o + C_o} \right) - K_d \right] Cm_i \times \Delta t \quad (7)$$

$$Cp_{i+1} = \frac{Cp_i + \left[\frac{D_{rm}}{r} \left(-\frac{Cp_i}{\Delta r} \right) + D_{rm} \left(\frac{-2Cp_i + Cp_{i-1}}{(\Delta r)^2} \right) - \frac{Cm_i}{Y_p} \times \left[\mu_{m,T} \left(\frac{Cp_i}{K_p + C_{pi}} \right) \left(\frac{Co}{Ko + Co} \right) - K_d \right] + IC_{im} + Q_{so} \right] \Delta t}{1 - \Delta t \left(\frac{D_{rm}}{(\Delta r)^2} \right) - \Delta t \left(\frac{D_{rm}}{(r \Delta r)} \right)} \quad (8)$$

Concentration of biomass in equation 7 is obtained due to the biomass and substrate concentrations in the past, and set parameters for the system. Equation 8 is capable of calculating substrate concentrations in the rhizosphere for each time based on defined system variables, the substrate and biomass concentrations in the past.

4. Parameters and initial conditions

There are a number of variables in the model, affecting the substrate and biomass concentrations in the rhizosphere. To investigate the changes in substrate and biomass, the influence of desired parameters were tested with numerical changes. Others, which were not changed, were replaced based on default values.

In the bioremediation, initial biomass is injected into the rhizosphere. Initial substrate is not artificially prepared; rather, it is produced by microbial activities. Therefore, due to the equations, the initial condition for substrate concentration should be calculated by equation 9.

$$C_{po} = \frac{K_d K_p}{\mu_m \left(\frac{C_o}{C_o + C_o} \right) - K_d} \quad (9)$$

Default values for each parameter, which are supposed independent, are given in Table 1 [16].

5. Results and discussion

According to the results computed by MATLAB, the changes in substrate and biomass have been achieved depending on the time. Many changes can not be observed the first time. Discussion and conclusions are presented based on a longer time. Although

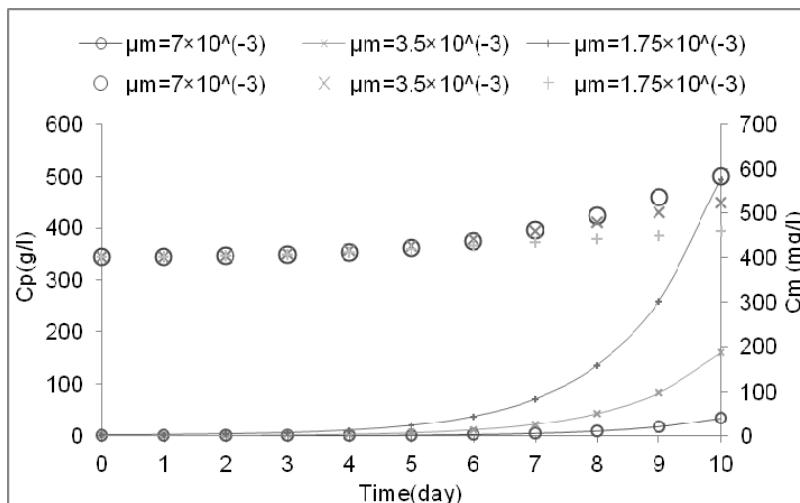
the results are based on the model and its parameters, other variables can also be effective. Factors such as sources of carbon and nitrogen in the soil determine activity or inactivity of microorganisms [24]. Also, chemical and physical conditions in the soil affect the rate of degradation and root affect leakage [25].

5-1. Influence of apparent maximum microbial growth rate (μ_m)

According to Fig. 1, whenever μ_m is lower, substrate concentrations in the environment get higher. Microbial growth rate is high, and ultimately more biomass is associated with a reduction of substrate, if the value of μ_m becomes higher. On the other hand, during the first 5 days, substrate production and biomass concentration have changed very little. So the rate of substrate changes has happened quickly so that with doubling the μ_m value, the substrate has reduced after several times. Unlike the substrate production, the biomass production continues slowly, and does not have the increasing production of the substrate; so by doubling the μ_m value, the biomass amount is multiplied after some time. Sung et al. have also reported rapid changing of substrate and slow growth of biomass after a time [16]. Consequently, to design a bioremediation system in the rhizosphere, substances in the environment should be controlled, and tuning based on available time, since changes in the substrate are much more effective than changes in the type of microorganisms. Besides, various microbial species can be used because of the low impact of microorganisms in this process. Also, the results can be implemented to mixed

Table 1. Default parameters in the mathematical model

$\mu_m (h^{-1})$	3.5×10^{-3}	$K_d (h^{-1})$	3.5×10^{-4}	$IC_{im} (mg\ cm^{-3}\ h^{-1})$	0.011
$K_p (mg\ cm^{-3})$	2.02	$D_{rm} (cm^2\ h^{-1})$	3.6×10^{-5}	$Q_{so} (mg\ cm^{-3}\ h^{-1})$	1
$K_o (g\ cm^{-3})$	4×10^{-6}	$r(cm)$	0.02	$C_{m0} (\mu g\ cm^{-3})$	403
$C_o (g\ cm^{-3})$	8×10^{-6}	$Y_p (mg\ g^{-1})$	400		

**Figure 1.** Changes in substrate (line style) and biomass (dot style) based on apparent maximum microbial growth rate (μ_m)

microbial systems. The results presented in the model are satisfactorily flexible in relation to the microbial parameter to alter the type of microorganism. Therefore, the ability to approximately predict a process with processes studied by other microorganisms exists.

5-2. Influence of microbial death coefficient (K_d)

Fig. 2 is depicted as if K_d gets more, the production of substrate and biomass increase. The substrate production rate is much higher than the biomass production rate. K_d is very influential on substrate production in such a way that with doubling it over time, the substrate becomes multiplied. It seldom

affects increasing biomass. In high values of death coefficient changes it obtains similar results about the biomass production. Time takes increasing substrate and biomass. The impact of time on substrate production is much more. Increase of this parameter causes the microbial death to increase in raising the endogenous substrate production. On the other hand, it causes a decrease in microbial growth rate. Therefore, low microbial growth consumes the substrate slowly, and substrate production rises. Design of bioremediation systems in the rhizosphere requires considering the microbial death rate to control materials. However, changing this parameter does not affect the biomass production rate. To predict the microbial

concentrations, other results can be used which can be obtained based on various K_d parameters for the new system. According to the model, prediction of the microbial growth rate is practical for various systems, and control of substrate concentration is determined by the microbial death coefficient.

5-3. Influence of microbial growth yield coefficient (Y_p)

As Fig. 3 represents, changing the yield coefficient does not cause any significant changes in the biomass and substrate production. Strigul and Kravchenko have reported the variations of the coefficient that have no effect on the biomass increasing in rhizosphere after 3 days [21]. Time can serve as an effective parameter so that substrate and biomass production increase. Role of time on the biomass growth rate is less influential. Consequently, the influence of the term can be surrendered in the design since it can not control and tune bioremediation efficiency. It is a neutral parameter in the model. Putting each value instead of it does not cause evolution in the

ultimate behavior of the model to the microbial concentration and growth.

5-4. Influence of substrate half-saturation coefficient (K_p)

Fig. 4 shows that the K_p parameter can be very effective on the substrate concentration, but not efficiently change biomass production. Increasing K_p causes a quick increase in substrate production while it does not appreciably change the biomass production. Biomass and substrate concentrations go up with time. In higher K_p , there are major changes for the substrate. In Monod model, increasing the parameter causes a reduction in change rate for the substrate which leads to increasing the substrate concentration. The model is not sensitive to tuning the coefficient for variation in the microbial growth rate. To design a system on the model, only the optimum efficiency of the substrate concentrations can be provided by determining different values for the parameter, however, microbial growth is almost identical.

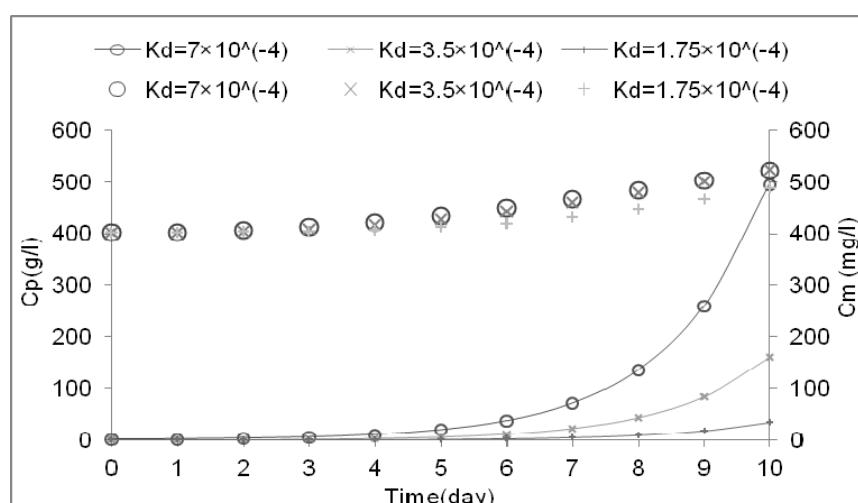


Figure 2. Changes in substrate (line style) and biomass (dot style) based on microbial death coefficient (K_d)

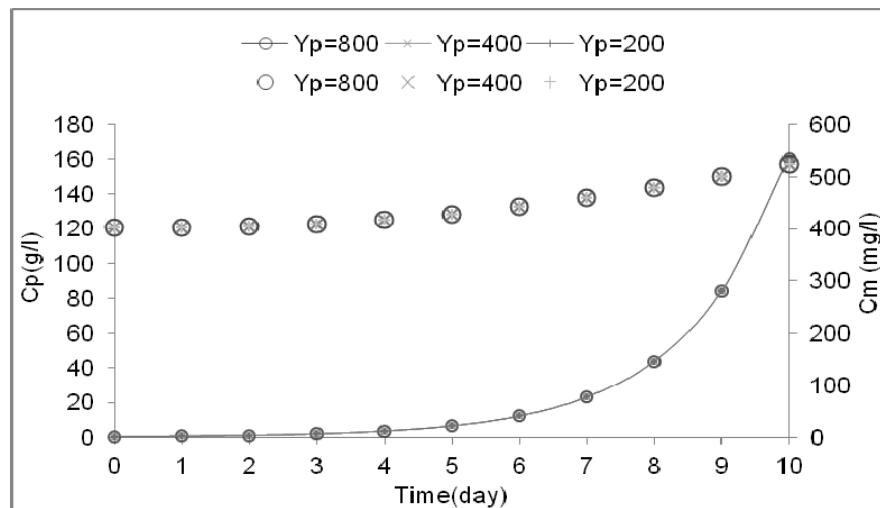


Figure 3. Changes in substrate (line style) and biomass (dot style) based on microbial growth yield coefficient (Y_p)

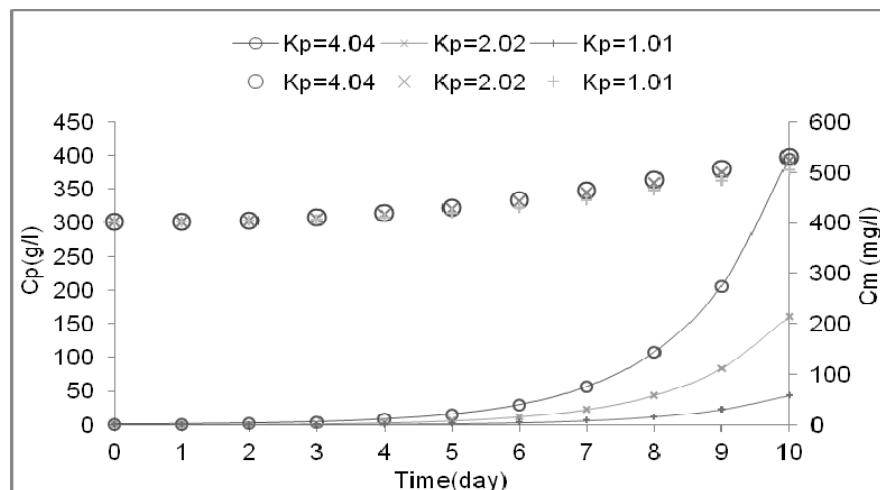


Figure 4. Changes in substrate (line style) and biomass (dot style) based on substrate half-saturation coefficient (K_p)

5-5. Influence of substrate penetration coefficient (D_{rm})

As Fig. 5 represents, raising the substrate penetration coefficient in the soil can increase the substrate production rate. Substrate production rate can not be changed by tuning the parameter in their high values;

however, it is changed with tuning the coefficient values from low to high. The substrate production can be quite various. Biomass concentrations increase as time increases, but increasing or decreasing the penetration coefficient does not have much

impact on it. Increase in penetration coefficient in the soil causes substrates that have been produced by the roots to be transmitted into the soil, rapidly enter to the rhizosphere and substrate concentrations in the environment rise up. Besides, due to the production rate by plant roots that is constant, the final substrate amount produced by the roots is constant. Also, whenever the D_{rm} coefficient becomes more, it can not transfer into the environment more than the amount produced. Therefore, the model has simulated the behavior of penetration well, and shown that raising the penetration coefficient causes an increase of the substrate in the environment. Due to the limited and constant plant production rate and substrate concentration, penetrating the concentration into the environment eventually reaches a constant value, and further increasing the penetration coefficient has no effect. In the design, soil should be chosen to desire aims based on the required penetration coefficient.

Soil type should be selected on the substrate, required time for the bioremediation, and satisfying penetration coefficient. Soil type does not impress on microbial growth. Therefore, changing the parameter can only tune the substrate concentration of the system.

5-6. Influence of production rate of endogenous substrate (IC_{im})

Fig. 6 states that the production rate of endogenous substrate in the rhizosphere can not directly impact the increase or decrease of the biomass and substrate. Thus, changing the parameter is ineffective; however, the time parameter can be effective. The model offered does not respond to changing the variable, which causes changes in the amount of endogenous substrate which does not damage the system balance. Hence, there is no need to control the parameter, difficultly measured, that reduces the cost of operation of bioremediation system.

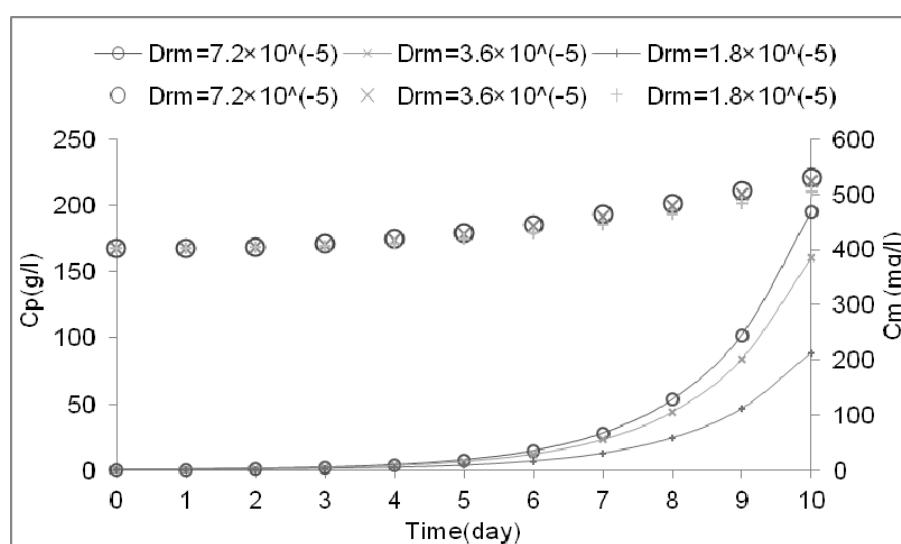


Figure 5. Changes in substrate (line style) and biomass (dot style) based on substrate penetration coefficient (D_{rm})

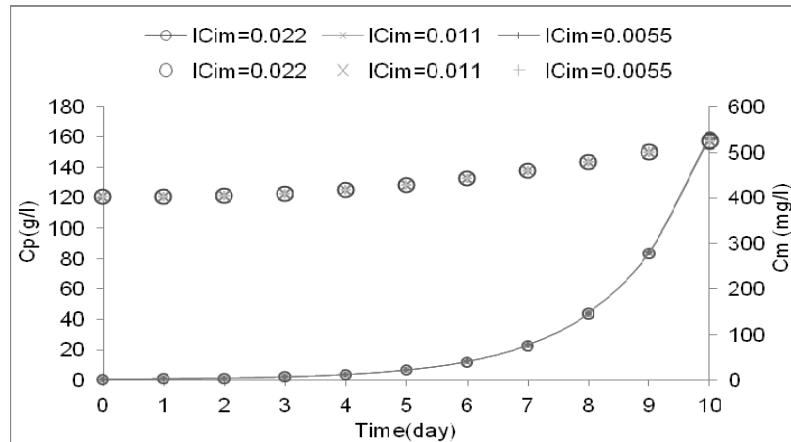


Figure 6. Changes in substrate (line style) and biomass (dot style) based on production rate of endogenous substrate (IC_{im})

5-7. Influence of oxygen half-saturation coefficient (K_o)

Fig. 7 shows that increasing the oxygen half-saturation coefficient raises the substrate but decreases the production of biomass. The influence of the factor on the substrate production is much more. In fact, biomass concentration decreases with increasing K_o , but this reduction is not very noticeable. Also, time increases biomass and substrate concentrations. Due to the microbes need for oxygen for continuing life, the oxygen supply rate and oxygen consumption rate

should be high. Rate of changes in oxygen as a vital substrate, reduces with the increase in the oxygen half-saturation coefficient. It means the rate of oxygen consumption by microbial cells has decreased which decreases biomass in the rhizosphere. Loss of biomass rapidly increases the substrate because if there is not enough oxygen for microbial growth, microbial consumption reduces and substrate concentrations increases. Whenever the amount of oxygen is less, the microbial growth becomes less too,

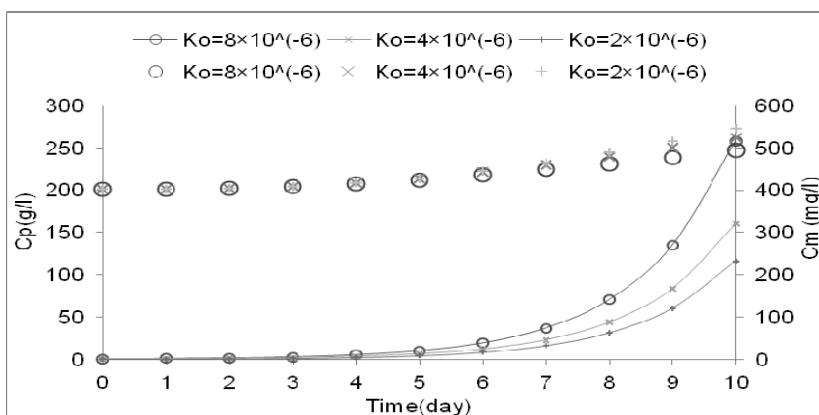


Figure 7. Changes in substrate (line style) and biomass (dot style) based on oxygen half-saturation coefficient (K_o)

and eventually substrate increases. The parameter changes are not so effective compared to the amount of microbial cells, and the cell growth does not significantly vary by changing it. Microbial growth rate can be raised by adjusting the oxygen amount, conditions of oxygen acceding to the rhizosphere, and reducing K_o . Thus, generally, it increases the efficiency of bioremediation system in the soil.

5-8. Influence of rhizosphere radius (r)

As Fig. 8 indicates, increasing the radius of the rhizosphere, which is the centrality of plant roots, has led to an increase in the substrate concentration. Microbial concentration has no variation, whereas the passage of time can increase the biomass. Sung et al. also showed time naturally causes development of the rhizosphere radius [16]. At large distances from the plant root, it is expected that the effect of increasing radius has been reduced [16]. In the short radius, multiplying the radius can increase substrate production. The distance increases over a long time may accomplish a higher concentration of the substrate. The main reason to increase substrate concentration

based on increasing radius is an assumption about the steadiness of production rate by the plant roots. The constant rate of plant production stabilizes the rate of substrate penetration in the rhizosphere. Fick's first law represents the constant penetration rate and the penetration coefficient, supposedly fixed, cause changes in substrate concentration and become constant to rhizosphere radius. Thus, with the rhizosphere radius becoming longer, the substrate concentration necessarily increases. Besides, the radius can not directly affect the microbial concentrations. Consequently, microbial concentrations remain unchanged with increasing the rhizosphere radius [16]. In general, to set up a proper bioremediation system based on the model, the appropriate changes in the size of the selected zone in a rhizosphere and its scale can be helpful. Nevertheless, the impact of the rhizosphere on the substrate is limited by a specific scale, more than this is useless. Also, increasing the rhizosphere radius is associated with increased costs. Therefore, the choice of an optimal size should be considered in the design.

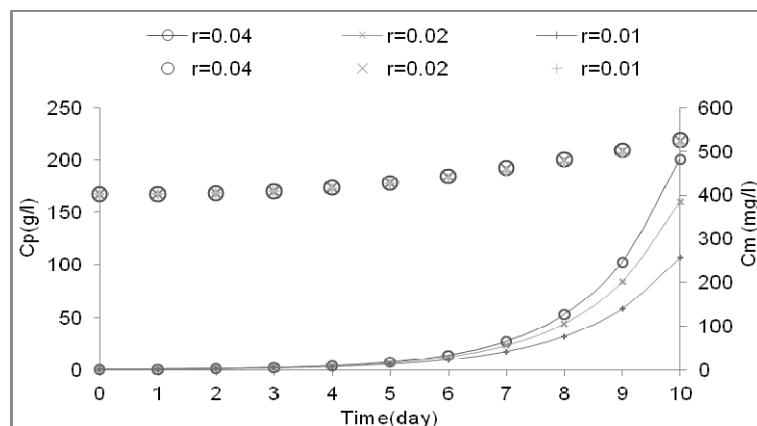


Figure 8. Changes in substrate (line style) and biomass (dot style) based on rhizosphere radius (r)

5-9. Influence of production rate of exogenous substrate (Q_{so})

According to Fig. 9, it is observed that if production rate of the exogenous substrate is higher, the substrate concentration decreases, and the biomass concentration is not changed. Time affects the concentrations. At longer times, it is expected that reducing Q_{so} increases substrate concentration. However, the effects of Q_{so} at high values are similar, and changing them can not help to further increase the substrate concentration. One of the main reasons for decreasing the substrate concentration is that, whenever the amount of substrate increases, the driving force for transferring substrate mass from the roots to the rhizosphere reduces. The driving force is directly linked to substrate concentration difference. Whenever the environment is poorer about substrate, the substrate can transfer further from the root to the rhizosphere. With increasing concentrations of exogenous substrates in the rhizosphere, the penetration of substrate produced by the roots reduces; ultimately, the overall substrate concentrations in the environment reduce. Due to the results, it is supposed decreasing exogenous substrates can increase the microbial mass in addition to conducting

the plant substrates into the process, and optimum efficiency is obtained based on the defined purpose for the system.

5-10. Influence of oxygen substrate (C_o)

Fig. 10 indicates that concentration of dissolved oxygen in the soil reduces substrate and increases microbial growth. The model is used for aerobic microorganisms. Increasing oxygen as a vital matter is essential for microbial growth and increasing the biomass. Naturally, the microbial increment increases substrate consumption, and reduces substrate concentrations in the environment. Although changes in oxygen concentration can not make significant changes in microbial growth [21], the substrate transformation rate is very tangible. Over long periods of time, reducing the oxygen concentration can make more substrates in the rhizosphere. According to the essential and available facilities, the system designer can set conditions by increasing or lessening oxygen in the environment. Although taking up the oxygen in the rhizosphere requires facilities and investment, economical gain and efficiency of bioremediation system determine the oxygen concentration.

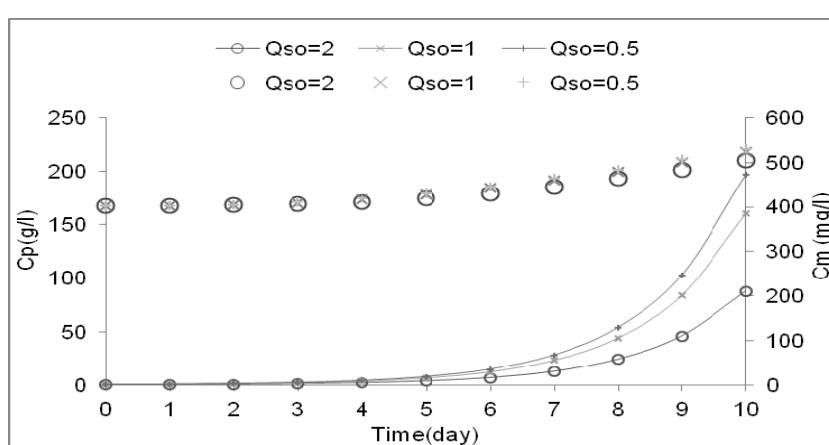


Figure 9. Changes in substrate (line style) and biomass (dot style) based on production rate of exogenous substrate (Q_{so})

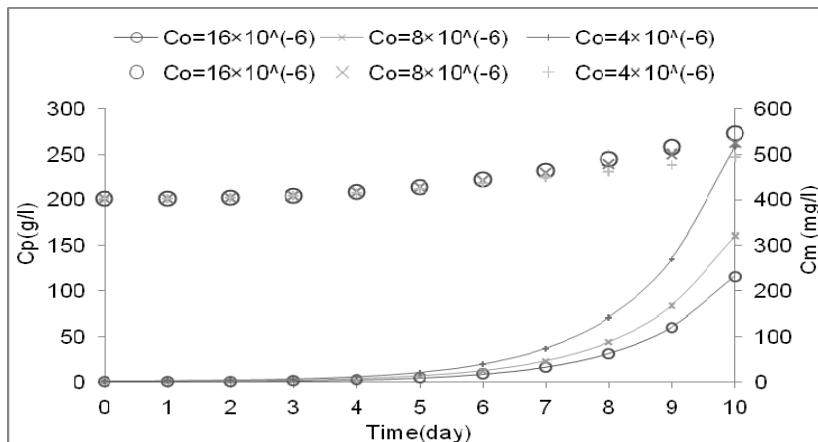


Figure 10. Changes in substrate (line style) and biomass (dot style) based on oxygen substrate (C_o)

5-11. Influence of initial microbial concentration (C_{m0})

Fig. 11 shows that with increasing initial microbial concentration, particular change in the substrate concentration does not happen, whereas the substrate concentration increases with time. Biomass production can additionally be increased by increasing the initial concentration of microorganisms so that during time and increasing C_{m0} , the biomass production increases sharply. If C_{m0} is more, biomass production rate would also be higher. One of possible reasons for not changing the substrate is that, increasing the initial microbial cells brings about increasing

biomass during the process, and also reduces the substrate. Besides, the death of the microbes causes endogenous substrate to be produced, which can compensate the substrate decreased by microbial consumption. Therefore, the lack of alternation and uniformity in the substrate occur based on initial microbial change. Although the interactions are more complex, the model is able to predict the events simply. As a result, bioremediation systems can follow the process based on the specified aims by adding appropriate initial microbial concentrations.

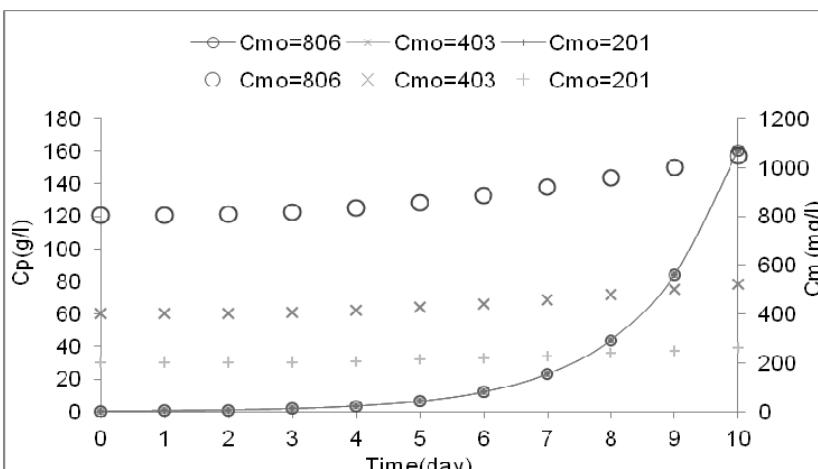


Figure 11. Changes in substrate (line style) and biomass (dot style) based on initial microbial concentration (C_{m0})

6. Conclusions

The results show that generally, the substrate concentration and biomass are increased in the rhizosphere over time. It is noted that in the early days, the concentrations do not show significant changes, and after 5 days, the concentrations usually increase. According to the results of modeling on the rhizosphere, a number of parameters directly, some reversely, and others neutrally influence the concentrations. Increasing K_d , K_p , K_o , r , and D_{rm} respectively perform quick changes in the substrate increasing in rhizosphere. Among the parameters, the effect of K_d is the most, and the influence of D_{rm} is the least. Each parameter can be changed based on facilities, and also desired conditions and aims. Besides, decreasing μ_m , Q_{so} , and C_o respectively, helps greatly in increasing the substrate. Changing Y_p , IC_{im} , and C_{m0} has no results in the substrate changes. To increase biomass concentration and microbial growth rate, C_{m0} and μ_m are raised respectively. Influence of C_{m0} varies for its concentration, but it can be more effective than μ_m . Changing the other parameters also has no affect on the microbial concentration in the rhizosphere. According to the behavior of each parameter in the model, in general, it can be claimed the bioremediation systems, which behave based on the model, can efficiently be run by correctly changing the parameters.

Nomenclature

C_{im}	Endogenous substrate concentration (mg cm ⁻³)
C_m	Microbial concentration (μg cm ⁻³)
C_o	Concentration of electron acceptor

	(oxygen) (g cm ⁻³)
C_p	Solved substrate concentration (mg cm ⁻³)
D_{rm}	Substrate effective penetration coefficient in soil (cm ² h ⁻¹)
I	Rate of endogenous substrates changes (h ⁻¹)
K_d	Negative growth rate constant or microbial death constant (h ⁻¹)
K_o	Half-saturation constants for electron acceptor (g cm ⁻³)
K_p	Half-saturation constants for solved substrate (mg cm ⁻³)
Q_{si}	Rate of endogenous substrate changes (mg cm ⁻³ h ⁻¹)
Q_{so}	Rate of exogenous substrate changes (mg cm ⁻³ h ⁻¹)
Q_{sp}	Rate of substrate changes that release from root (mg cm ⁻³ h ⁻¹)
Q_{sx}	Rate of substrate changes based on the microorganism consumption (mg cm ⁻³ h ⁻¹)
r	Radial distance from root (cm)
t	Time (h)
Y_p	Efficiency coefficient (mg g ⁻¹)

Greek symbols

$\mu_{m,T}$	Apparent maximum microbial growth rate (h ⁻¹)
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