Description of bioremediation of soils using the model of a multistep system of microorganisms

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Abstract. The paper deals with the development of a mathematical model describing the interaction of a multi-step system of microorganisms in soil polluted with oil products. Each step in this system uses products of vital activity of the previous step to feed. Six different models of the multi-step system are considered. The equipping of the models with coefficients was carried out from the condition of minimizing the residual of the calculated and experimental data using an original algorithm based on the Levenberg-Marquardt method in combination with the Monte Carlo method for the initial approximation finding.

1. Introduction

Bioremediation is the most environmentally friendly method of soil purification from oil pollutants based on the ability of microorganisms (MO) to oxidize hydrocarbons. To optimize the scenario of recovery measures, a correct mathematical model of the process is necessary. In this case, the main difficulty is the closing of the model of transport of pollutants by kinetic relationships describing the vital activity of microorganisms. This article is devoted to the selection of the most suitable kinetics of vital activity of the MO based on comparison with experimental data.

Unlike most known models [1, 2], the article deals with the case of a multistep MO system. Each step in this system uses products of vital activity of the previous step to feed. The initial substrate was oil.

Several different models of the kinetics of a multistep system are formulated. The equipping of the models with coefficients is carried out from the conditions for minimizing the calculated and experimental data. For this purpose, an original optimization algorithm [3] was implemented, based on the use of the Levenberg–Marquardt method.

2. Basic equations of models

We consider $N$ different biomasses, metabolism products each of which is a substrate for the biomass growth of next stage of consumption. The equations determining the key processes of vital activity of such a multistep MO system can be written in the form

$$
\frac{dM_i}{dt} = v_i M_i - d_i M_i, \quad i = 1..N;
$$

(1)
where $M_i$ is the concentration of biomass of step $i$ MO in the soil (mg/g); $v$ and $d$ are the growth rate and rate of death of biomass ($s^{-1}$); $t$ is the process time ($s$);

$$\frac{dC_i}{dt} = \begin{cases} -\alpha_i v_i M_i, & i = 1, \\ -\alpha_i v_i M_i + \beta_{i+1} v_{i+1} M_{i+1} + \gamma_{i+1} d_{i+1} M_{i+1}, & 1 < i < N + 1, \\ \beta_{N+1} v_{N+1} M_{N+1} + \gamma_{N+1} d_{N+1} M_{N+1}, & i = N + 1; \end{cases}$$

(2)

where $C_i$ is the concentration of substrate (mg/g); $\alpha$ is the economic coefficient; $\gamma$ and $\beta$ are the coefficients that determine the quantity of metabolite appearing in the decomposition of the death and the growth of new biomass unit.

Initial conditions

$$M_i(t = 0) = M_i^0, \quad i = 1..N,$$

$$C_i(t = 0) = C_i^0, \quad i = 1..N + 1.$$  

(3)

To determine the functions $v$ and $d$, three models were used. They reflect various options for accounting the effect of metabolites on them.

2.1. Model 1
The rate of production growth is determined by the Monod kinetics [4], and the death rate given by [12]:

$$v_i = \alpha_i C_i / (K_i + C_i), \quad i = 1..N,$$

(4)

$$d_i = \delta_i (1 + C_{i+1} / \xi_i), \quad i = 1..N,$$

(5)

where $\alpha_i$ is the maximum growth rate ($s^{-1}$); $K_i$ is the half saturation constant (mg/g). $\xi_i$ is the constant (mg/g).

2.2. Model 2
The growth rate is defined by the formula Monod – Ierusalimskii [5]:

$$v_i = \alpha_i \xi_i C_i / [(K_i + C_i) (\xi_i + C_{i+1})], \quad i = 1..N,$$

(6)

where $\xi_i$, $K_i$ are the half saturation constants (mg/g).

The rate of death $d$ is considered as a constant:

$$d_i = \delta_i, \quad i = 1..N.$$

(7)

2.3. Model 3
In some cases [1] it is possible to improve the description of the production process by the introduction of the inhibition constant into the kinetic equation (4):

$$v_i = \alpha_i C_i / (K_i + C_i) [K_{ii} / (K_{ii} + C_i)],$$

(8)

where $K_i$, $K_{ii}$ are the half saturation constants (mg/g). For the rate of death, we use equation (4).

3. Modification of models
In equation (1), we introduce the control variable $K_m$ (mg/g) [2], which allows us to control the growth rate of the MO

$$\frac{dM_i}{dt} = v_i \left(1 - M_i / K_m\right) M_i - d_i M_i.$$  

(9)

Options for all three models, in which the equation (1) is replaced by equation (9), will be denoted by an additional symbol (a).

Thus, there are 6 models. The models 1 and 2 contain $L = 7N$ unknown coefficients, the model 3 contains $8N$, the models 1(a), 2(a) contain $8N$, and the model 3(a) contains $9N$ coefficients.
After normalization using characteristic scales 
\[ t' = 1 \text{ day}, \quad M' = M_1^0, \quad C' = C_1^0, \quad \alpha', \quad \beta', \quad \gamma' = C_1^0/M_1^0 \]
the form of the equations remains the same, and the initial conditions take on the form 
\[ M_i(t = 0) = 1, \quad M_i(t = 0) = M_i^0, \quad i = 2..N, \]
\[ C_i(t = 0) = 1, \quad C_i(t = 0) = C_i^0, \quad i = 2..N + 1. \]

4. Results and discussion

Model coefficients were obtained from the conditions of minimizing the residual

\[ R^2 = R_B^2 + R_C^2 + R_{C_{\text{sum}}}^2 \rightarrow \min, \quad R_p^2 = \sum_{k=0}^{N_p} \left( \Delta t_p^k/T_p \right) \left( p^k - p(t_p^k) \right)^2, \quad (10) \]

where \( N_p, T_p \) \((p = B, C, C_{\text{sum}})\) are the numbers of instants of time and the last time moment of the experimental measurements \( p^k \) of the indicator \( p \); \( B \) is the value of the total respiration of all steps MO; \( C_{\text{sum}} = \sum_{i=1}^{N} C_i \) is the total concentration of substrates; \( t_p^k \) is the time moment \( k \) of the indicator \( p \) measurement; \( p(t_p^k) \) is the model value of the indicator \( p \) at the moment \( t_p^k \); \( \Delta t_p^k \) is the local interval of “time of action” \( p^k \) :

\[ \Delta t_p^k = 0.5 \left( t_m - t_m \right); \quad n = \min \left( N_p, k + 1 \right), \quad m = \max \left( 0, k - 1 \right). \]

The measurements of the total respiration were normalized by the initial value. To calculate the model values \( B(t) \), we used equation

\[ B(t) = \theta \sum_{i=1}^{N} M_i(t), \quad \theta = 1/\sum_{i=1}^{N} M_i^0. \quad (11) \]

To solve problem (10), an original technique [3] was used. It is based on the use of the Levenberg-Marquardt method [6] with application of the Monte Carlo principle [7]. This technique operates according to the following scheme:

- the set of random points in which the residual (10) is calculated is "pounced" on the region of the sought coefficients;
- \( L \) points with the least value of a residual are selected of them;
- the problems of minimizing the functional (10) by the Levenberg-Marquardt method are solved using each selected point as the initial approximation; the model coefficients delivering the best approximation of the experimental data are chosen.

It is shown that the one-step system model is not capable to qualitatively describe the experimental values (figure 1), especially the non-monotonic behavior of the dynamics of the total concentration of substrates \( C_{\text{sum}} \), since in the one-step system growth of it is impossible. At the same time its growth is possible in the two-step model, which leads to an improvement in the quality of the approximation of the experimental data (figure 2). Further quality improvement of the model can be achieved due to the control variable. Taking the inhibition constant into account improves the model 1 (a) (table 1). The model 1 (a) and 3 (a) were chosen as the best ones.
Figure 1. Results for a one-tier system (markers – experimental values, lines – model values).
Figure 2. Results for a two-step system (markers – experimental values, lines – model values).
### Table 1. The values of the residuals $R$.

| System  | 1     | 1(a)  | 2     | 2(a)  | 3     | 3(a)  |
|---------|-------|-------|-------|-------|-------|-------|
| One-step| 0.13236 | 0.12906 | 0.13232 | 0.12904 | 0.12947 | 0.17311 |
| Two-step| 0.06466 | 0.03437 | 0.05083 | 0.04057 | 0.05173 | 0.03384 |

### Table 2. Optimal values of model coefficients.

| Model | Step | $\alpha$ | $\beta$ | $\delta$ | $\varepsilon$ | $\zeta$ | $K$ | $K_1$ | $K_m$ | $\omega$ | $\gamma$ |
|-------|------|----------|---------|----------|---------------|---------|-----|-------|-------|----------|---------|
| 1(a)  | 1    | 0.1731   | 0.196   | 0.0279   | 1.303         | -       | 0.4895 | -     | 0.0999 | 0.0609   | 1.1351   |
|       | 2    | 0.1134   | 0.0005  | 0.0001   | 1.7929        | -       | 0.1374 | -     | 0.845  | 0.3315   | 0.0001   |
| 3(a)  | 1    | 0.0587   | 0.189   | 0.1      | 3.2232        | -       | 0.7785 | 0.7785 | 0.0001 | 0.4448   | 0.2263   |
|       | 2    | 0.5      | 0.0039  | 0.0001   | 10            | -       | 0.3802 | 0.3802 | 0.8065 | 0.2243   | 0.0001   |

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