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AN ATTEMPT AT MATHEMATICAL MODELLING OF THE PROCESS OF MICROBIOLOGICAL BIODEGRADATION OF DIESEL OIL

A mathematical model has been created describing the process of biodegradation of diesel oil. Data for model development were obtained from two previously conducted laboratory experiments. The correlation between the measured and calculated of the biodegradation of diesel fuel data indicates the existing connection between them. It was found that the proposed mathematical approach of the biological process showed similar direction and nature of changes occurring in these two data sets.

1. INTRODUCTION

Each day, a number of xenobiotics enters natural environment, including petroleum derived compounds which disturb soil biological balance and metabolism. Decomposition of pollutants of such a character is a long-term process thus it is important to increase the efficiency of processes which accelerate their elimination from environment. Petroleum derived products in environment are subject to transformations of abiotic character (evaporation, leaching, chemical and photochemical oxidation etc.) as well as biotic ones where plants [1, 2] and soil microflora [3, 4] take part in the remediation of soils contaminated with petroleum derived products. A biological method of cleaning the environment contaminated with petroleum derived product is one of the most rapidly developing fields of environmental restoration [5], involving native microbial populations [6] or exogenous microorganisms [7, 8].

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Efficiency of remediation measures is being evaluated based on costly chemical analyses [9] or soil biological activity indicators including determination of the number of microorganisms [10], respiration [11], the biomass of microorganisms [12], the enzyme activity of soils [13], the process of nitrification [14]. In this study an attempt was taken up to predict the progress of biodegradation of diesel oil in soil based on the mathematical model created. Data enabling development of the model were obtained from two laboratory experiments carried out.

2. MATERIALS AND METHODS

Data enabling development of the model were obtained from two laboratory experiments. First, activity of isolated bacterial strains in the process of diesel oil biodegradation in batch culture was evaluated (experiment 1 [15]), then the effect of applied bioremediation measures on the efficiency of diesel oil degradation in soil was assessed (experiment 2 [16]). To elaborate the model, the program "Statistica" has been used. In this work, among others, approximation by the Newton's method and Pearson correlation coefficients were made.

3. RESULTS

While taking into account the results of model experiment 1 for one of the bacterial strains analysed, marked as BS 101, the degree of diesel oil degradation was determined in grams per 1 milliard bacterial cells. Data referring to the quantity of diesel oil degraded by this bacterial strain were subject to approximation by Newton's method, by fitting them to function in the form of third-degree polynomial. It proved to be the most suitable (Fig. 1), the evidence of which can be seen in a high value of coefficient R (0.9915) and the proportion of explained variance (0.9831).

$$y = 0.0261905 + 0.181525x - 0.0072838x^2 + 0.0001271x^3 \quad (1)$$

where: y – quantity of biodegraded diesel oil, g, x – duration of culture, days.

This is also confirmed by high conformity of the results measured experimentally and calculated based on Eq. (1) (Fig. 2).

The next stage was to determine correlation between time in days and the number of cells of bacterial strain BS 101 in culture on liquid medium containing diesel oil. Experimental data were fitted to exponential equation (2), obtaining the value of the coefficient $R = 0.9988$, and the proportion of explained variance 0.9977 (Fig. 3). High conformity of experimental data and the calculated ones is presented in Fig. 4.

$$y = 3.4673230000e^{(0.165564x)} \quad (2)$$

where: y – number of bacterial cells, x – duration of culture, days.

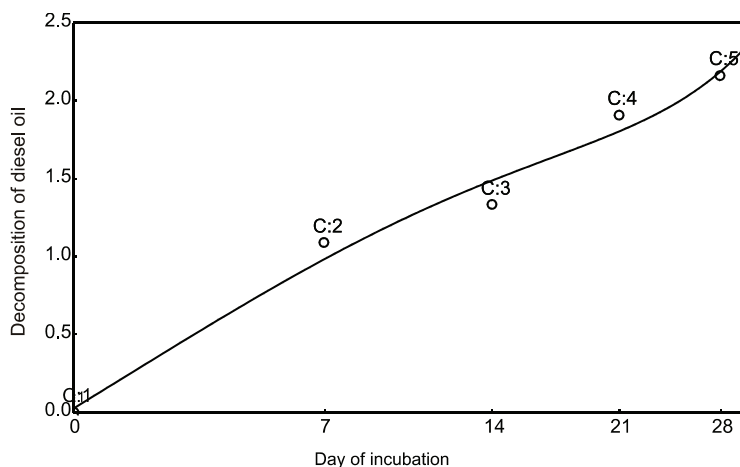


Fig. 1. Quantity of diesel oil degraded in liquid medium by bacterial strain BS 101 during a 30-day incubation and correlation equation curve for time and quantity of diesel oil degraded

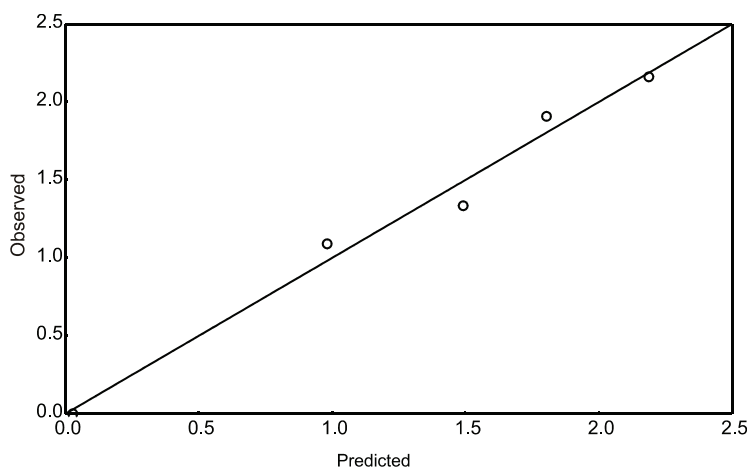


Fig. 2. Comparison of experimental data and calculated quantities of diesel oil being biodegraded in bacterial strain BS 101 culture on liquid medium

Based on Equations (1) and (2), it was possible to calculate the number of bacteria as well as the quantity of degraded diesel oil for any day of culture. These data can be then substituted to Eq. (3) as m_x , $m_{(x-1)}$, l_x and $l_{(x-1)}$:

$$y = \frac{(m_x - m_{(x-1)}) \times 10^9}{(l_x - l_{(x-1)})} \quad (3)$$

where: y = twenty-four-hour degradation of diesel oil in grams per 10^9 cells in day x , m_x – mass of diesel oil being biodegraded to day x of culture, $m_{(x-1)}$ – mass of diesel oil

being biodegraded to day $(x - 1)$ of culture, l_x – number of bacteria in culture in day x , $l_{(x-1)}$ – number of bacteria in culture in day $(x - 1)$, x – duration of culture, day.

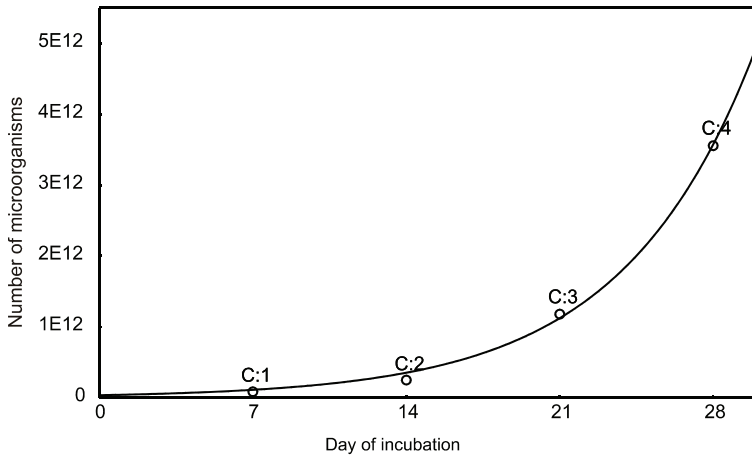


Fig. 3. Correlation equation curve for time in days and the number of cells of bacterial strain BS 101 in culture on liquid medium containing diesel oil

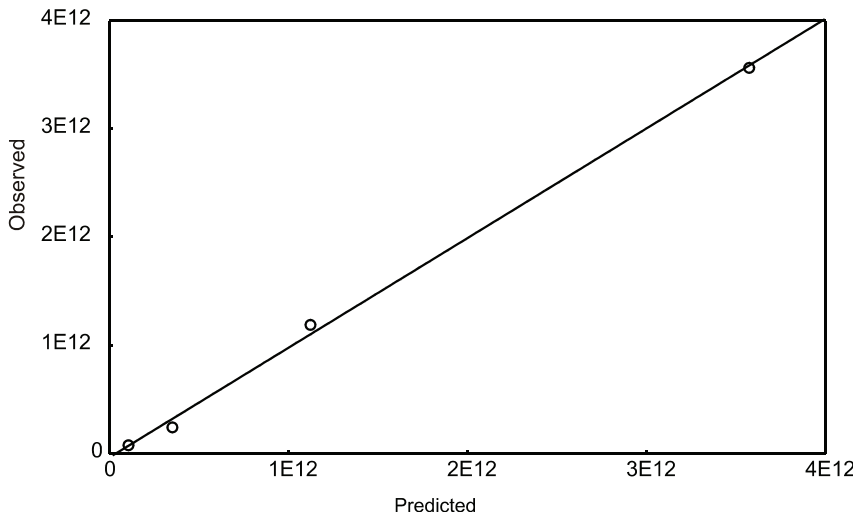


Fig. 4. Comparison of experimental data and calculated numbers of cells of bacterial strain BS 101 in culture on liquid medium

Equation (3) allows calculation of twenty-four-hour degradation of diesel oil in grams per 10^9 bacterial cells in any day of culture. This value for the bacterial strain analysed is the largest in the initial period of culture and decreases during it. Some

data of the twenty-four-hour degradation of diesel oil by bacterial strain BS 101 is presented in Table 1.

Table 1
Twenty-four-hour degradation of diesel oil
with bacterial strain BS 101

Culture day	Daily decomposition [g]
7	$24.5038 \cdot 10^{-4}$
14	$3.4488 \cdot 10^{-4}$
21	$0.6614 \cdot 10^{-4}$
28	$0.2452 \cdot 10^{-4}$

Verification of the presented model was carried out using the results of experiment 2. For calculations, the value of twenty-four-hour degradation computed as a mean from maximum and minimum values calculated for the initial and the final periods of culture ($12.375 \times 10^{-4} \text{ g} \cdot \text{day}^{-1} \cdot 10^9 \text{ cells}^{-1}$) was assumed. The number of bacteria capable of degrading diesel oil in soil was calculated separately for each day of incubation. Since analyses of bacteria number were performed in 30-day intervals, it was calculated in each of these 30-day intervals according to equation:

$$y = l_p + x(l_k - l_p)x \quad (4)$$

where: y – number of bacteria capable of degrading diesel oil in soil in day x , l_p – number of bacteria at the beginning of 30-day period between analyses, l_k – number of bacteria at the end of 30-day period between analyses, x – successive day of the period between performed determinations of the bacteria number.

Table 2
Comparison of experimental data
and those calculated according to the model

Days	Measured values [g]	Calculated values [g]
0	0.052705	0.000136
30	0.772117	0.005617
60	1.569402	0.132065
90	1.613678	1.150958
120	1.630988	2.030526
150	1.913550	2.080094

The number of bacteria capable of degrading diesel oil present in soil in respective days of incubation was then employed to determine the quantity of diesel oil being biodegraded during each of these days. This was obtained by multiplying the number

of bacteria by the value of twenty-four-hour degradation in grams per one milliard bacteria. After adding up the quantity being degraded in successive days, the total quantity of diesel oil being degraded since the beginning of soil incubation period was obtained. Execution of the above calculations allowed obtaining prediction of the value of diesel oil biodegradation in soil (Table 2).

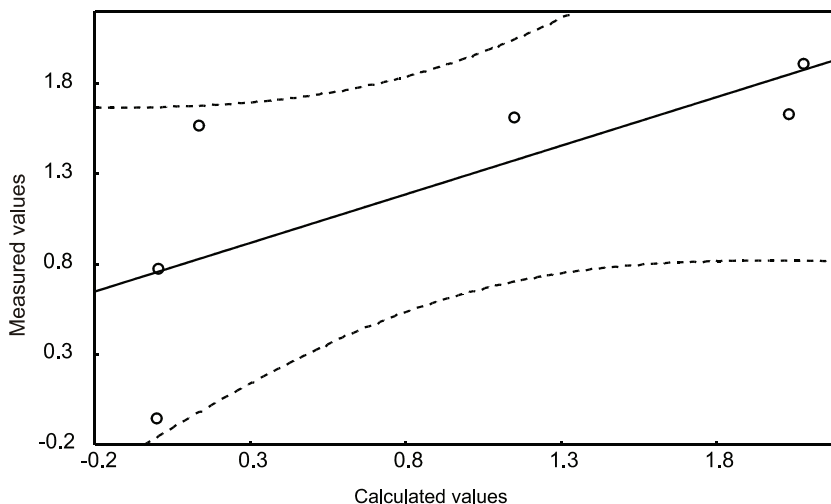


Fig. 5. Comparison of experimental data and calculated quantities of diesel oil being biodegraded in the model experiment

The evidence of the conformity of experimental data and calculated ones is significant and a high value of the coefficient of correlation between them ($r = 0.7227$). The fitting of these data is presented in Fig. 5. This attempt at mathematical modelling of the process of diesel oil biodegradation may be the basis for taking up further studies that aim at development of the methods for predicting and forecasting the course of degradation of petroleum derived compounds in soil being useful in practical applications.

4. CONCLUSIONS

Undoubtedly, the progress of biodegradation depends on the number of cells of bacteria capable of metabolising diesel oil as well as their activity [17]. Out of these two parameters, determination of the number of bacteria – changes in which may be precisely determined – is much simpler. The activity of bacteria depends on many factors and differs for young and old cells. During the growth of bacteria population in soil, bacterial cells of different age are being found in it, hence it is purposeful to employ averaged, mean values. Such an approach is being met after all in different at-

tempts to determine aggregate effects of metabolic transformations being a result of the activity of mixed populations of microorganisms in soil, like decomposition of pesticides or gas exchange resulting from metabolism.

Execution of some measurements and analyses in nature is not always possible and there is frequently a necessity to determine correlations and regularities, which may be next used for explaining the course of *in vivo* phenomena, under model conditions or in experiments on artificial mediums. An attempt at mathematical modelling of the process of diesel oil biodegradation taken up in this study may be the basis for development of the methods for predicting and forecasting the course of biodegradation of petroleum derived compounds in soil being useful in practical applications.

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