ANNALS OF THE ORADEA UNIVERSITY
Fascicle of Management and Technological Engineering
ISSUE #1, MAY 2015, http://www.imtuoradea.ro/auo.fmte/

APROXIMATION FUNCTION FOR NUTRIENT INJECTION TIME PREDICTION

Ioan MOGA[1], Tiberiu VESSELENYI[2], Ovidiu MOLDOVAN[3], Istvan KISS[4]
[1] University of Oradea, Oradea, Romania, imoga@uoradea.ro
[2]University of Oradea, Oradea, Romania, tvesselenyi@yahoo.co.uk
[3]University of Oradea, Oradea, Romania, ovidiu30@gmail.com
[4]Bay Zoltan Institute, Szeged, Hungary, kissur@baybio.hu

***Abstract*—**In this paper we present results on application of bioremediation technology of oil polluted terrains. The use of bacteria clean the soil is based on three methods: laboratory analysis, mathematical modeling and on-site experiments. Starting from in situ experiments we tested two mathematical functions in order to approximate temperature data obtained after injection of nutrients. The obtained function helps predicting the time for the next injection of nutrients.

***Keywords*—**bioremediation, biological activity temperature monitoring, curve fitting methods.

I. Introduction

Biodegradation is the breakdown of materials that occurs when microorganisms are feeding on a substance which is used as a energy and carbon source of. Bioremediation is the use of microorganism to transform pollutants into materials which will not be harmful for the environment. Bioremediation methods can be in situ or ex situ bioremediation. In situ bioremediation is the treatment of the contaminated soil at the site and in ex situ bioremediation the soil is transported elsewhere to be decontaminated. In-situ bio-remediation is one of the most environmentally friendly methods to eliminate contamination. In order to optimize the bioremediation process the state of the bacteria must be also studied under different conditions.

II. Bioremediation Process Description

In biodegradation temperature is an important variable. Most biodegradation occurs at temperatures between 10 and 35°C. The oxidation of organic substances to carbon dioxide and water is an exothermic (heat releasing) process.

In order to study the bioremediation process a research platform was developed in the framework of cross-border cooperation program CBC-HURO, 0802/155 _AF,acronym “Micromodel” project [1]. The bioremediation laboratory consists of two test recipients with soil through which water flows to obtain a subsurface flow. Then different materials are added together with a solution with bacteria which will degrade the pollutant. In this process the important fact is to study the subsurface flow, as well as pressure and speed of flow for different types of liquids in different soils. The temperature of the process is also measured because it gives good information about the state of the bacteria. Temperature sensors for multipoint measurement system have been tested at Bay Zoltan in Szeged and in the laboratory of the University of Oradea [2], [3].

Another way to study the process is to measure the temperature in the field where the pollutant is treated by injection of bacteria and nutrients. The experiments in the field were conducted by the specialists from Bay Zoltan Institute, collecting temperature data from different points in the field, situated a different distances from the injection point (as it is shown in Fig. 1).

In Fig. 2, the diagram of measured temperatures versus time at point S5 `presented in Fig.1, are shown. These measurements were realized in 91 days. Together with the process temperatures, control temperatures are also measured in order to know the natural outside temperature of the medium in which the process takes place.

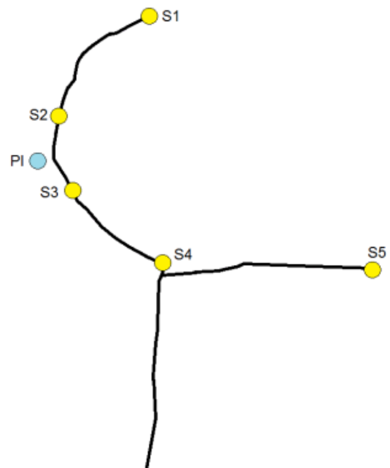

Fig. 1. Position of injection point (PI) and temperature measurement points (S1…S6) in the field

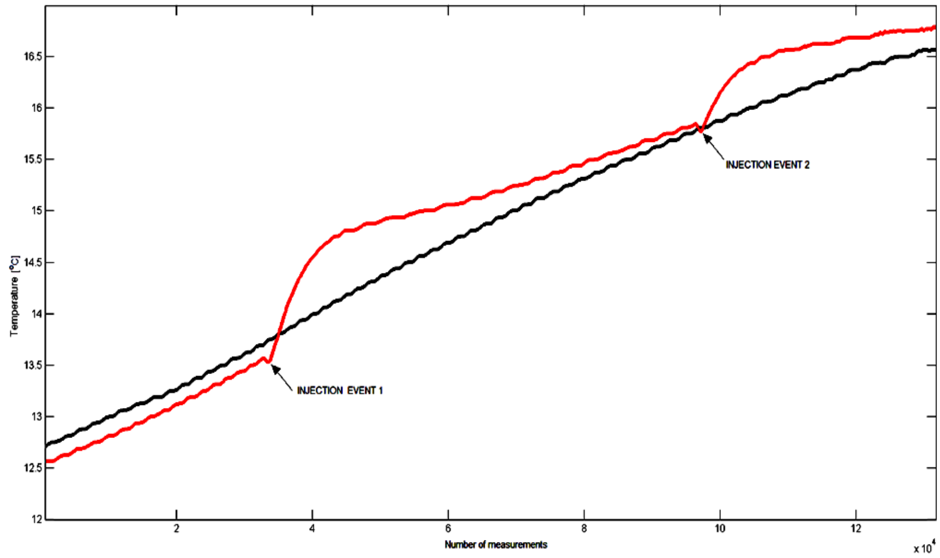

Fig. 2. Diagram of temperature versus number of measurements, measured at point S5 (red) and of the environment unaffected by the process (black).

As it can be observed from the diagram a sudden rise of temperature is registered after each injection of nutrients, reflecting the fact that the bacteria are becoming more active in this period. After reaching a peak value the temperature is starting to decrease slowly till it reaches the outside temperature value. An identical pattern of behavior can be observed at each measured point, during the experiments. It is very important to estimate when the next injection event has to be made in order to prepare the injection works. For this, an approximation function has to be found on the basis of which the next injection event can be scheduled [4], [5], [6].

III. Approximation Function For Experimental Temperature

In order to fit curve to the measured data approximation function had been searched using CFTOOL module of the MATLAB programming environment [7]. Studying the shape of the curve two candidate functions had been proposed, a rational and an exponential function

The curve fitting function is presented in figure 2. The candidate functions were fitted to process data by nonlinear regression using a Marquardt algorithm.

The first candidate function is a rational function and has the following expression and fit characteristics

$$\mathbf{y} = \frac{\mathbf{ax}}{(\mathbf{x}-\mathbf{b})^2+\mathbf{1}} \qquad (1)$$

This has been rewritten in the more general form of:

$$\mathbf{y} = \frac{\mathbf{ax+b}}{\mathbf{x^2+cx+d}} \qquad (2)$$

where x is normalized by a mean value of 2094 and a standard deviation of 1209.

Coefficients with 95% confidence bounds are:
a = 0.399; b = 0.668; c = 3.008; d = 2.452;

The rational fit function is presented in Fig. 3, and it's errors are presented in Fig. 4.

The second candidate is an exponential function given by the equation:

$$\mathbf{y=Ae^{-\alpha x}+Be^{-\beta x}} \qquad (3)$$

Coefficients with 95% confidence bounds: A =1.282; α= -0.0007046; B= -1.577; β = -0.003244.

In order to estimate the error of the candidate functions, three parameters had been taken into consideration [8].

The exponential fit function is presented in Fig. 5, and it's errors are presented in Fig. 6.

A.SSE

This statistic measures is called the summed square of residuals and is usually labeled as SSE.

$$\mathbf{SSE=Sum_{(i=1\ to\ n)}\{w_i(y_i\text{-}f_i)^2\}} \qquad (4)$$

Here y_i is the observed data value and f_i is the predicted value from the fit. w_i is the weighting applied to each data point, usually w_i = 1.

B. R-Square

The fitness parameter *R-square* is defined as:

$$\boldsymbol{R_{square}}\mathbf{=1\text{-}}\frac{[\mathrm{Sum}_{(i=1\ to\ n)}\{w_i(y_i\text{-}f_i)^2\}]}{[\mathrm{Sum}_{(i=1\ to\ n)}\{w_i(y_i\text{-}y_{av})^2\}]}\mathbf{=1\text{-}}\frac{\mathrm{SSE}}{\mathrm{SST}} \qquad (5)$$

Where f_i is the predicted value, y_{av} is the mean of the experimental data y_i is the data w_i is the weight of each data point, usually w_i=1. SSE is defined in relation (4) and SST is the total sum of squares.

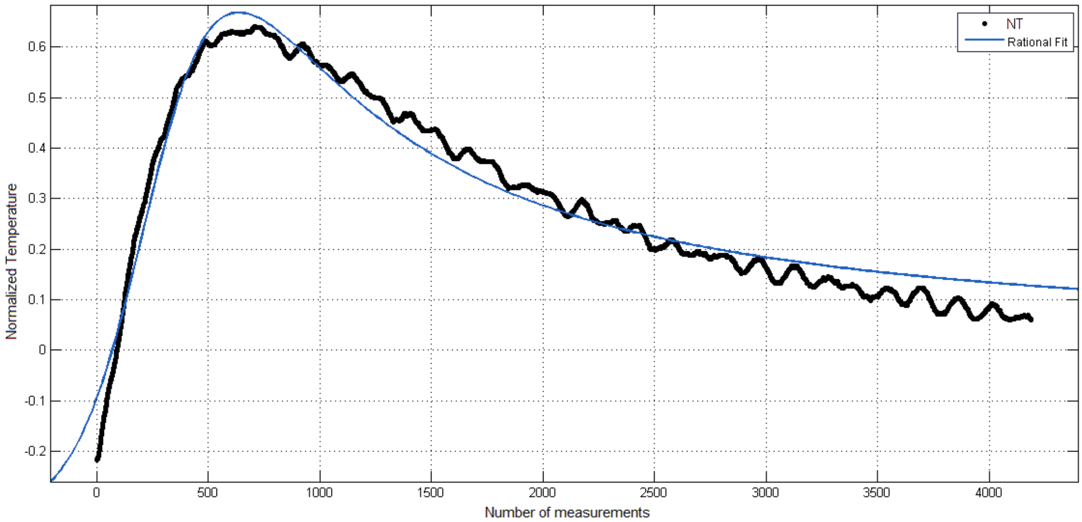

Fig. 3. Curve fitting for the rational function.

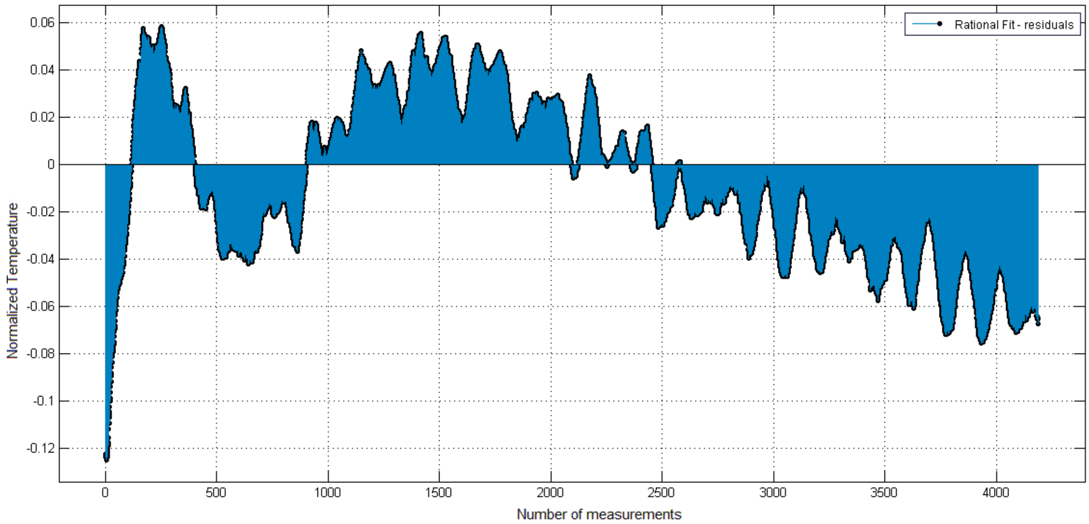

Fig. 4. Diagram of errors for the rational function.

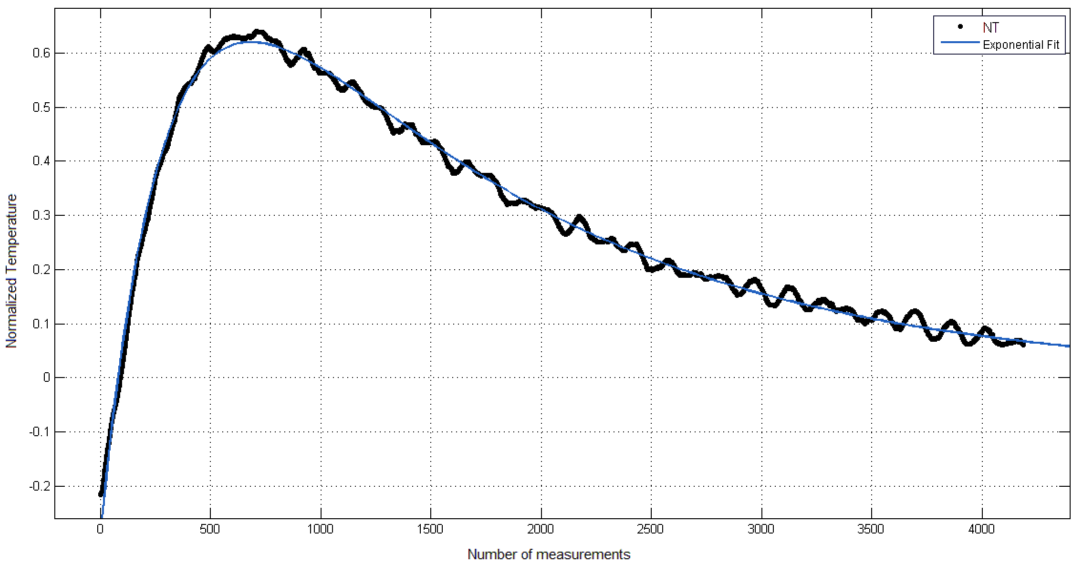

Fig. 5. Curve fitting for the exponential function.

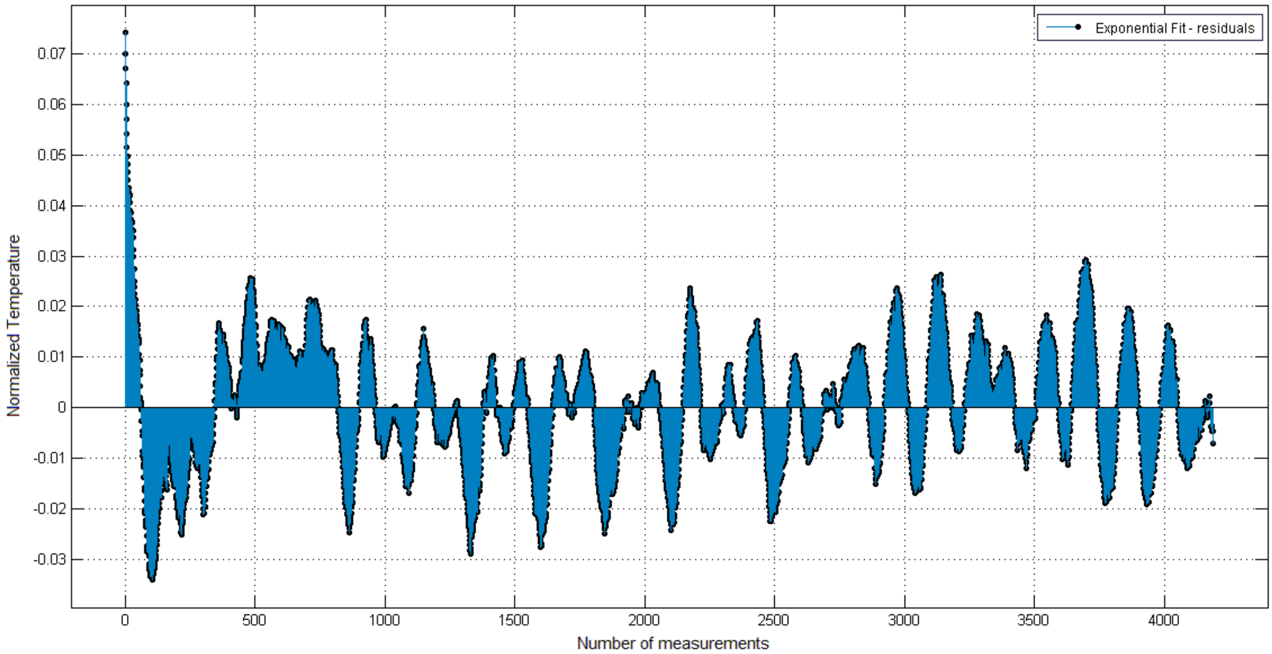

Fig. 6. Diagram of errors for the exponential function

C. Root Mean Squared Error

The Root Mean Squared Error is an estimate of the standard deviation, and is defined as

$$\mathbf{RMSE} = \mathbf{s} = (\mathbf{MSE})^{\frac{1}{2}} \quad (6)$$

MSE is the mean square error.

$$\mathbf{MSE} = \frac{\mathbf{SSE}}{\mathbf{v}} \quad (7)$$

Comparison of fitness parameters for the two candidate functions are given in table 1.

TABLE I.
COMPARISON BETWEEN FIT FUNCTIONS

Fit Function	SSE	R-square	RMSE
Rational	5.5780	0.9642	0.03652
Exponential	0.6873	0.9956	0.01282

IV. CONCLUSIONS

In our paper we searched a good fit for temperature measurement data collected in the field, looking to approximate the pattern of temperature curve after an injection event occurred. We found two candidate functions that seemed to fulfill the precision requirements for curve fitting. Using the CFTOOL Matlab functions we obtained the fit quality parameters for a rational and an exponential function. By result analysis we can conclude that the best fit function is the exponential function given by relation (3) with the corresponding coefficients. This function produces very good quality indicators for the fit and can be used to predict subsequent injection event scheduling. This scheduling allows an improvement of the bioremediation process by using smaller amounts of nutrients and also decrease the time necessary for the fulfillment of bioremediation process.

ACKNOWLEDGMENT

This research was supported by the European Union in the framework the Hungary-Romania Cross-Border Co-operation Programme 2007-2013 and co-financed by the States of Hungary and Romania, project number 0802/155_AF, acronym “Micromodel”.

REFERENCES

[1] I. Moga, I.Kiss, T. Vesselenyi, B. Fehér, “Data acquisition system for bioremediation laboratory”, in *Annals of The Oradea University Fascicle of Management and Technological Engineering* no.3, 2013, http://www.imtuoradea.ro/auo.fmte/
[2] T. Vesselenyi , I. Kiss , P. Mudura , I. Moga, “Subsurface flow modeling of a bioremediation laboratory test tank” *Annals of The Oradea University Fascicle Of Management And Technological Engineering* no.3, 2013, http://www.imtuoradea.ro/auo.fmte/
[3] National Semiconductor - *LM35A, Precision Centigrade Temperature Sensor*, 2000.
[4] M. H. Zwietering, I. Jongenburger, F. M. Rombouts, K. Van Triet, “Modelling of the bacterial growth curve” *Applied and environmental Microbiology* , 1990.
[5] J.U. Kreft, Ginger Booth, Julian W. T. Wimpenny “BacSim, a simulator for individual-based modelling of bacterial colony growth”, *Microbiology*, 1998.
[6] R.P. Benedict - *Fundamentals of temperature, pressure, and flow measurements*, 3rd ed. Wiley, New York, 1984
[7] MATLAB, *Programming Manual*, Mathworks, 2012.
[8] MATLAB CFTOOL *User manual*, Mathworks, 2012.