INDICATION OF BIOCATALYTIC MECHANISMS IN ENVIRONMENTAL REMEDIATION BY STATISTICAL METHODS

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INTRODUCTION

The remediation of the soil and ground water caused by chlorinated hydrocarbon derivatives is one of our most important tasks. Bioremediation researches intensively go in for the utilization of enzyme products to the degradation of hydrocarbon pollutants in groundwater [1]. Based on Michaelis-Menten kinetic data series of degradation of some chlorinated hydrocarbons, our paper focuses on the statistical methods that are able to reveal the presence of latent inhibition or activation from the modeled biodegradations. Inhibition or activation mechanisms during enzymatic demolition can influence the correlation of kinetic curves as well as their regression. Application of principal component analysis (PCA) to kinetic data series of individual substrates also results in extra information that is shown in loading plot diagrams.

MATERIALS AND METHODS

Detection of possible enzymatic mechanisms is represented through degradations of dichloromethane (DCM) and dichloroethane (EDC) [2,3,4].

In the case of meeting the limitations above, the decrement of concentration of chlorinated hydrocarbon (*S*) is proportional to concentration increment of the intermediate (*P*) accruing from it. Decreasing the amount of chlorinated compound in time can be expressed by equation

$$\frac{dS}{dt} = \left(-\frac{dP}{dt}\right) = -v_{max}\frac{S}{K_M + S} \quad (1)$$

,where *S* symbolizes the chlorinated substrate, K_M is the Michaelis constant of dehalogenation, v_{max} is maximal reaction rate of dehalogenation step. The solutions of the model were equally reproduced to the conditions with and without inhibition and activation. The kinetic data series of the substrates ($S=S(t)$) were supplied by ODE solver inserted in SCILAB 5.3.3 software. The amplitudes of the superposed noise to original differential solutions are about 2.5 % of the average concentrations of the substrates.

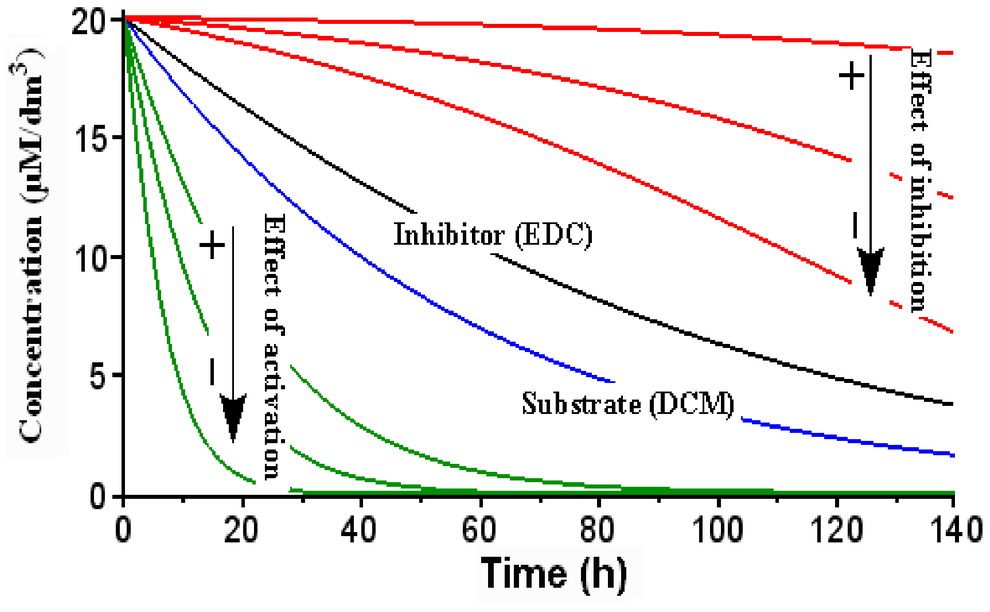

Fig. 1. *Effect of inhibition and activation on the degradation of substrate (DCM)*

CONCLUSION

Modelled the enzymatic demolition of concrete pollutants, applications of some statistical methods have been developed to the recognition of the potential mechanisms modifying the velocities of enzymatic degradations. Appearance of inhibition effects can be made to be detected by assessing the correlations of kinetic data series belonging to different substrates. Presence of the inhibition become visible in the increment of the slope and in the decrement of the intercept.

Application of PCA method provides an alternative way to indicate the enzyme mechanisms. This evaluation is based on revealing extra information out of loading plot diagrams where the substrate concentrations free from or under inhibition can be separated from each other. The effects modifying the enzyme activities can change the positions of substrate concentrations in the loading plot in significant manner.

RESULTS

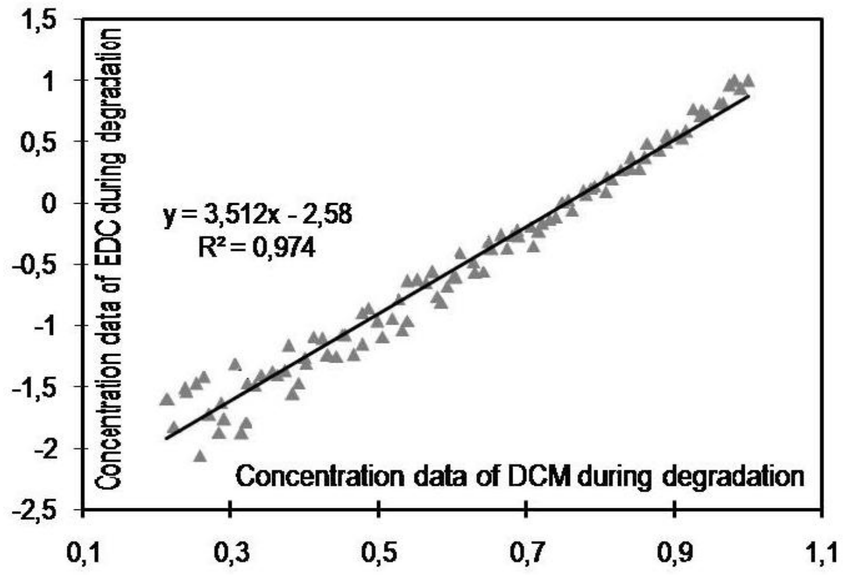

Fig. 2. (a) *Correlation between DCM and EDC data without inhibition*

Both the correlation of the substrates and their regression straight line are potential indicators of inhibition Significant alterations of the slope and the intercept can reflect the appearance of inhibition mechanism in an exact way. The monotony of kinetic data under inhibition deviates from that of inhibition free. In the case regression of DCM and EDC kinetic curves, inhibition effects on the slope and the intercept are depicted in *Figures 2.a.* and *2.b.*

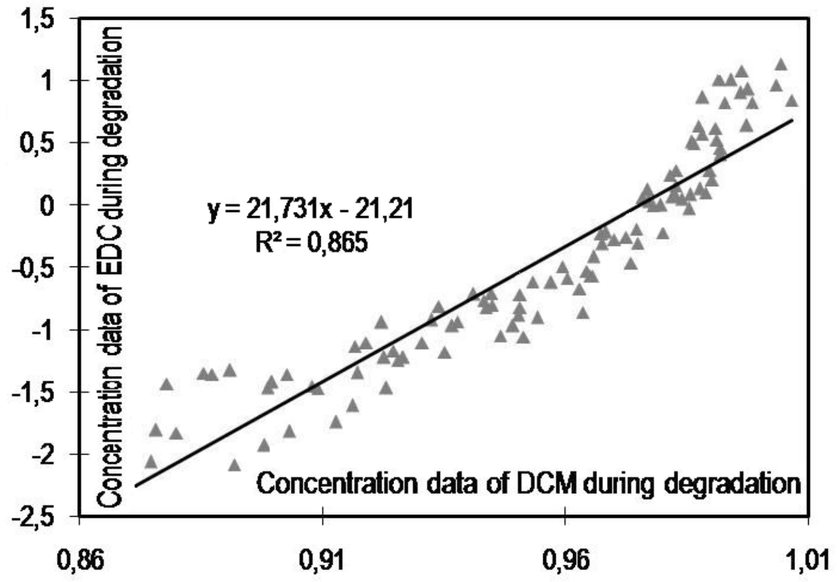

Fig. 2. (b) *Correlation between DCM and EDC data under inhibition*

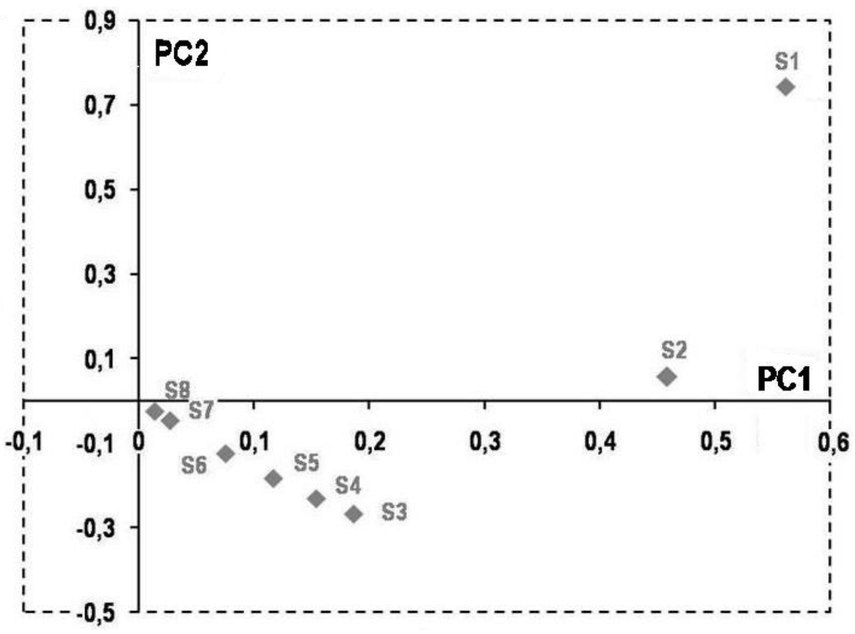

Fig. 3. (a) *Substrates under inhibiton effects (S_3 to S_8) in the loading plot of PC1 and PC2*

In the case of the inhibition, the points of substrate concentrations in the loading plot have smaller contributions to second principal component ($\mathbf{p}_2$) than the reference points (S_1, S_2) without inhibition (*Figure 3.a.*).
On the contrary, the activation enhances the contribution of the points to $\mathbf{p}_2$ component (*Figure 3.b.*).The points of reference substrate concentrations (S_1 and S_2) and the points of substrate concentration (S_3 to S_8) under various measures of competitive inhibition or activation effects are depicted in loading plots of *Figures 3.a.* and *3.b.*.

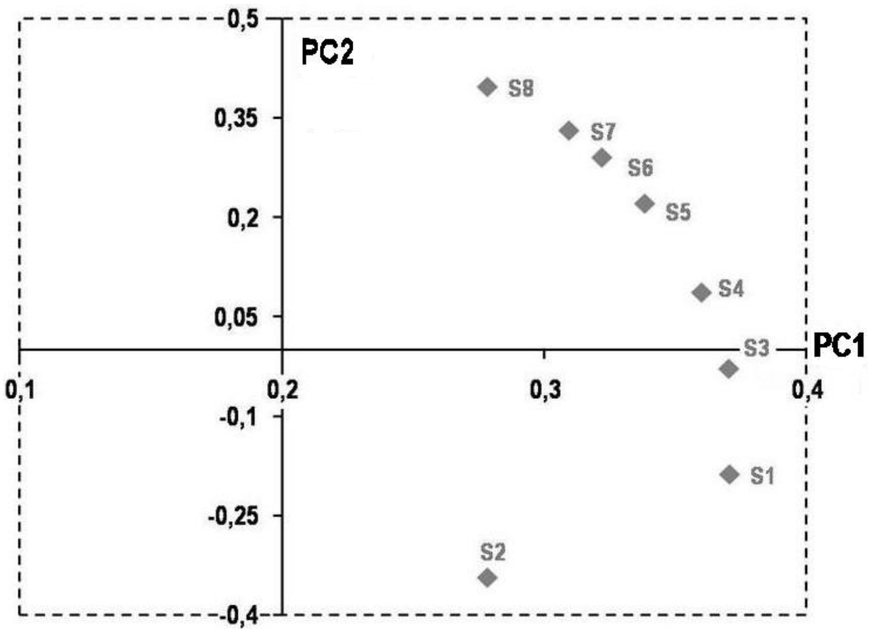

Fig. 3. (b) *Substrates under activation effects (S_3 to S_8) in the loading plot of PC1 and PC2*

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