Indication of biocatalytic mechanisms in environmental remediation by statistical methods

Zoltán HERKE[1] , Tibor CSERNY[2] , Balázs MAGYAR[3] , Zsolt István NÉMETH[1]

[1]Institute for Chemistry, Faculty of Forestry, University of West Hungary, H-9400, 4 Bajcsy-Zs, Sopron, Hungary
[2]Earth Sciences Section, Hungarian Academy of Sciences, H-1050, 9 Széchenyi, Budapest, Hungary
[3]Elgoscar-2000 Ltd, H-1134, 1-3 Klapka, Budapest, Hungary

Abstract

Pollution of the soil and the underground medium by synthetic hydrocarbons and their derivatives is one of civilization problems. The soil pollutions can damage the local ecosystem. The pollutants may threaten both the supply of drinking water and natural water resources with a relevant risk. There is promising feasibility for environmental remediation of the soil that is called bioremediation. Its operation underlies the capability of biological systems that some enzymes are also able to demolish a number of *xenobiotic* compounds since they have such conformations which are very similar to those of natural substrates of the enzymes. Although many times with smaller reaction rates, thus, a few enzymes can catalyze the degradation of the pollutants from, for example, the processes chemical industry. Efficiency of applying the bioremediation mostly depends on the chemical features of the pollution including the heterogeneity of material quantity, physical and chemical properties of the medium, etc. Taking the interactions of the pollutants and the enzymatic system into account, to work out efficiently applications of bioremediation is necessary to clear the sensitivity of kinetic parameters in the catabolism and to recognize the modifications of enzyme activities induced by the pollutions. Based on the dependences of biochemical reactions on the substrate and enzyme concentrations as well as on the Michaelis constants, the speed of degradation can be optimized and the bioremediation efficiency can in turn be maximized.

Modelled by Michaelis kinetic is also obvious that the effects of inhibition on enzymatic reactions influence the monitoring the kinetic curves of the degradations of the pollutants. Inhibition mechanisms appearing in the enzymatic bioremediation can be detected in the parameter alterations of the regressions of the various kinetic curves. The correlations and the regression relationships of kinetic curves of the *xenobiotic* pollutants taking part in the simultaneous biochemical degradations are potential information sources. Any kind of inhibitions can change the slope and the intercept of the regression straight lines. The correlations of the same substrates including both some type of inhibitions of reaction kinetics with respect to inhibition free biochemical catabolism show significantly different slopes and intercepts. After data pre-processing, there is a possibility to carry out principal component analysis (PCA) on the data set (object matrix) being created from kinetic data series. With its application, an alternative method is introduced for the detections of inhibition and/or activation mechanisms. This novel approximation is based on the fact that the monotony of the kinetic curves affects the loadings of PCA method. The loading plots allow us to see significant alterations of inhibitions or activations in the enzymatic degradations in visual ways. The steps of revealing the extra information hidden in primary kinetic results of any complex enzymatic systems are depicted in some figures.