Journal of Bioremediation & Biodegradation

Review Article Open Access

Utilising Chemical Compounds of Biodegradation Modeling Process

Hurn Carfes J*

Depatment of Biochemistry of Fiji University, Fiji

Abstract

The biodegradation kinetics of BTEX (benzene, toluene, ethylbenzene and xylene isomers) compounds were studied individually and as mixtures by using models with different levels of sophistication. In order to evaluate the performances of the unstructured models we used experimental data from literature. The system description was based on the material balances of key components for batch uncompetitive inhibitions were applied along with the sum kinetics with interaction parameters models. The kinetic parameters were estimated via a global search method known as Particle Swarm Optimization (PSO). Successfully described by applying a SKIP model, with the main advantage being the consideration of the substrate interactions.

Keywords: Biodegradation kinetics; SKIP model; Inhibitions

Introduction

The values of kinetic parameters of biodegradation process have been obtained by using the nonlinear least squares regression analysis available in several software packages. The aromatic hydrocarbons known collectively as BTEX are extremely toxic, and can contaminate the environment as a consequence of industrial discharges and leakage from underground fuel tanks. Compared to the physical–chemical processes of remediation of the impacted areas, the biodegradation of these compounds is a very cost-effective technique and the authors experimentally observed the phenomena of non-interaction, stimulation, inhibition and substrate co-metabolism [1]. The main reasons for these synergetic and/or antagonistic interactions during the biodegradation of BTEX compounds can be attributed to the competitive inhibition, toxicity and formation of toxic intermediates. The microbial growth on substrate mixture is a key subject of studies in the field of bioremediation, effluents treatment and fermentation processes. Bielefeld and Stensel were the first to give the quantitative evaluation of the biodegradation of a mixture of five BTEoXpX substrates. Deeb and Alvarez-Cohen focused their studies on characterization of the effect and interaction of the ethylbenzene on a biodegradation of the benzene, toluene and xylene isomers. Throughout complex experimental studies, the authors have observed negative and positive interactions between substrates [2], and have suggested the presence of non-interactive, competitive inhibition, non-competitive inhibition, stimulation and co-metabolism.

Their work highlighted the possible mechanisms involved, and thus opened more space to model this sophisticated system and to study in details the complex substrate interactions. An accurate determination of biodegradation kinetics is very important in order to design cost effective and reliable bioreactors for treatment of contaminated groundwater and industrial effluents [3]. A crucial step and a difficult task in this procedure are to obtain reliable estimated values of the model parameters. Nonlinear parameter fitting methods have been shown to yield mathematically superior kinetic estimates of the coefficients comparatively to the linear transformation methods such as the.. The Levenberg–Marquardt local optimization algorithm is used. The synthetic wastewater biodegradation experimental data were used as a basis of the fitting process done with MATLAB optimization toolbox. A hybrid genetic algorithm has been use in a nonlinear parameters estimation procedure for modeling of the simultaneous saccharification and fermentation of starch to ethanol. Recently, a methodology for statistical identification of the substrate interactions during a removal of BTEX mixture was presented, where the Minitab software was used [4].

The objective of this work was to evaluate diverse microbial growth kinetics models describing the BTEX biodegradation processes. The sets of experimental data used in the study were kindly provided by Deeb and Alvarez-Cohen. In addition, a modern global search method called Particle Swarm Optimization. The performance of the unstructured kinetic models was evaluated assuming that the mixture of BTEX as homologous substrates can be represented by competitive inhibition and SKIP models and by applying the models of non-competitive and uncompetitive inhibition considered by Sigel. These models were proposed to describe dual substrate interaction, and have been extended to various substrates presented in the system. Recently, and Abuhamed have modelled aerobic biodegradation kinetics of Pseudomonas putida on benzene, toluene and phenol mixture. SKIP model was applied by Ballesteros for modeling the growth of P. putida on mixtures of formic acid, vanillin, phenol and oxalic acid. The model of competitive inhibition describes processes where the inhibitor and the substrate, which generally possess similar chemical structure, compete for the same enzyme active site responsible for the compounds metabolization [5]. The acceleration constants $\mathbf{c}_1$ and $\mathbf{c}_2$ represent the weighting of the stochastic acceleration terms that pull each particle toward individual and group best positions. The parameters' values of PSO method are empirical, but they have direct influence on the search space and their careful adjustment for any particular kinetic model allows a quick and good convergence. Several constant values were tested, and a good convergence was obtained using the optimized values for the initialization of the population, the following parameters values are predefined: particle number, number of iterations, number of parameters, inertia factors, acceleration constants and the search limit. During the search of objective function minimum, when the specified number of iterations was reached, the best search solution was used as

***Corresponding author:** Hurn Carfes J, Depatment of Biochemistry of Fiji University, Fiji, E-mail: carfes.j.@gmail.com

Received: 10-Apr-2023, Manuscript No: jbrbd-23-100130, **Editor assigned:** 12-Apr-2023, PreQC No: jbrbd-23-100130 (PQ), **Reviewed:** 26-Apr-2023, QC No: jbrbd-23-100130, **Revised:** 01-May-2023, Manuscript No: jbrbd-23-100130 (R), **Published:** 08-May-2023, DOI: 10.4172/2155-6199.1000563

Citation: Hurn Carfes J (2023) Utilising Chemical Compounds of Biodegradation Modeling Process. J Bioremediat Biodegrad, 14: 563.

information in the process of restriction of the search space, where the most sensible parameters were considered. The parameters' sensitivity evaluation was possible in a graphical dialogue. In order to restrict the search space and hence to obtain fast convergence, the initial ranges of kinetic parameters were determined based on their real microbiological meaning. During the search of global optimum of the objective function, the ranges of kinetic parameters were systematically redefined and reduced, where the best evaluated values were preserved [6].

Method

On toxic substrate can be determined by taking the first derivative of the Andrews equation equal to zero. Thus, it can be demonstrated that the substrate concentration, i.e. the critical substrate concentration corresponding to the actual, can be calculated by Eq. In addition, the intensity of substrate inhibition can be measured by the **Ki** value and by the ratio between saturation and inhibition constants. The **Ks/ Ki** ratio was determined by using values presented in. The authors have reported that the cell yield on xylene was significantly lower than on the other BTEX biodegradable compounds at similar concentration. In the previous studies reported in the literature, the kinetics and stoichiometric parameters were obtained considering the and further these parameter values were used to fit experimental data of the mixture of substrates by applying complex models. In SKIP model identification, the information obtained during the identification procedure of Monod and Andrews models was preserved as initial parameter guess [7]. In the study of biodegradation kinetics of BTEX mixture, the main difficulty was to find the global minimum of objective function during the experimental data fitting procedure. This fact can be explained by the big number of estimated parameters. Analyzing the obtained OF residue for each model – SKIP, competitive inhibition, uncompetitive inhibition and noncompetitively inhibition– it was possible to determine the model that best describes the experimental data from the BTEX biodegradation process. SKIP model represented the experimental data better, resulting in a minimum value of objective function. The evaluation of 24 parameter values of the model needed sufficiently higher computational efforts. Moreover [8], the difficulty in identification procedure arose because the kinetic parameters are nonlinearly correlated. Hence, the usage of the information from microbial physiology studies helps to restrict the search on each parameter range where only biological meaningful values are considered. For more precise models' discrimination it is necessary to obtain sets of experimental data with repetitions.

Results

The experimental results from the literature were used with kind permission of the authors. The data on individual biodegradation compounds were based on the following initial conditions. The data on mixture substrate biodegradation process were based on the following initial conditions. In cases where the initial biomass concentration valu was not available, it was estimated by PSO method, together with the model parameters. It can be noticed, that evaluation of X0 during the identification procedure must be done with caution because the system response is very sensitive to the changes of initial conditions. The system of ordinary differential equations of each kinetic model was numerically solved.

The estimated parameter values of Monod and Andrews models are presented in Table 1. The search for best parameter values was restricted, and the initial ranges of kinetic parameters were determined based on their real microbiological meaning taken from the literature. Such approach helped tremendously the PSO search method to find the "global optimum" after few iterations. It can be seen that kinetic and stoichiometric parameters estimated in this work are similar to those found by other authors that have investigated the biodegradation of BTEX (Table 2) which proves the reliability of mentioned above procedure [9]. The value of previously determined in single substrates biodegradation process was used as an initial guess during the identification procedure when multiple substrates biodegradation kinetics was modelled. The low Ks value indicated that the culture had higher affinity to xylene than to the other compounds resulting in higher specific growth rate and yield coefficient. It was verified that Monod model predicts very well the biodegradation kinetics on single toxic substrate, mainly at low concentrations. The evaluated constant values of Monod model are very informative and can be used further as controls in all parameters' identification procedures. If the value of Ki is very high, the Andrews model is simplified to Monod form. By applying the Andrews model, it was verified that the maximum specific growth rate is higher on toluene (the experimental data indicates it has been consumed faster), whereas the xylene has been utilized slower and resulted in lower value. In addition, the estimated Ks value on toluene suggests higher culture affinity to toluene. The simulation results obtained with And rows model together with the experimental data represent the degradation of individual toxic substrates. The OF residues obtained by applying PSO global search method are shown as well. Both models have reached similar OF values for benzene, ethylbenzene and xylene compounds. The OF for toluene by applying Monod and Andrews models were equal to 0.010 and 0.0024, respectively. Initial substrate concentrations above 40 mg L−1 favor the adjustment obtained by Andrews's model; therefore the model supplies more information about the system. The initial substrate concentration above the critical one.

Discussion

The advantage of SKIP model is that it makes possible the quantification of the interactions between BTEX substrates due to the presence of Iji parameters. In Table 1, the Ibe, Ite, Ixe interactive parameters' values show that benzene, toluene or xylene compounds present little or no effect of inhibition on ethylbenzene biodegradation. The degree of inhibition of toluene on benzene biodegradation was much higher than the degree of benzene inhibition on the toluene. Hence, the ethylbenzene can be considered as the strongest inhibitor between the BTEX biodegradable compounds based on the Ieb, Iet and Iex parameters' values. The xylene had almost insignificant inhibitory effect, as verified by Ixb, Ixt, and Ixe values.

The microbial association used in the experiments of Deeb and Alvarez-Cohen constituted of multiple species of microorganisms, hence the inhibition effect was an integral evaluation of the system behavior and could be modelled on the population level without taking into account particular metabolic controlling key steps. Bielefeld and Stensel have also reported inhibition interaction effects during BTEX biodegradation and the experimental data were fitted through competitive inhibition model proposed

The lack of specificity of SKIP model does not make it inadequate to describe the biodegradation of the BTEX mixture. Further metabolic engineering studies of the metabolic pathways of particular microorganisms will make possible to complete the understanding of interactions between substrates.

The excellent results obtained during the parameters estimation can be explained by determining the initial guess of kinetic parameters [10]. It was noted that the efficiency of PSO method was higher when the parameters' values were "far" from the global optimum ones, and when they were "close" to it the search procedure became "lost" between the local optimum values. Previously proposed a mathematical procedure

for parameters estimation through decomposition of the objective function. The basis of this methodology is a subdivision of a global search space where step-by-step local searches are performed. Thus, the dimensions of the search are reduced and the procedure becomes more robust to the initial parameter changes.

The global values evolution of the objective function through the iterative procedure of SKIP model parameters estimation when applying a global PSO method can be seen in All kinetic parameters were simultaneously estimated by using global search method by fitting experimental data of biodegradation process on single or mixed BTEX substrates. During the parameter identification procedure, the PSO performed with a higher efficiency compared with the local search methods. The PSO can be successfully applied for the optimization of upstream bioremediation process performance on a mixture of toxic compounds, as well as for the bioreactor design.

Conclusions

The developed in this work methodology can be considered as very efficient for prediction of the biodegradation kinetics of mixed toxic compounds, and therefore, it can be sufficiently useful in the modeling of complex microbial activities where multiple substrates are involved. On the other hand, the PSO method provided faster convergence for all cases of complex modeling of the BTEX biodegradation when 300 particles and 25 iterations were used during the search, the PSO method showed successful and fast search of a "global" minimum of the objective function, and as a result a good match between simulated and experimental profiles of BTEX biodegradation was achieved. These findings are in good agreement with other studies encountered in the literature.

Acknowledgement

None

References

1. Khan RMM, Chua ZJY, Tan JC, Yang Y, Liao Z (2019) From Pre-Diabetes to Diabetes: Diagnosis, Treatments and Translational Research. Medicina 55.
2. Gheith O, Farouk N, Nampoory N, Halim MA, Al Otaibi T (2016) Diabetic kidney disease: world wide difference of prevalence and risk factors. J Nephropharmacol 5: 49-56.
3. Williams R, Karuranga S, Malanda B, Saeedi P, Basit A, et al. (2020) Global and regional estimates and projections of diabetes-related health expenditure: Results from the International Diabetes Federation Diabetes Atlas, 9th edition. Diabetes Res Clin Pract 162: 108072.
4. Wang M, Yang Y, Liao Z (2020) Diabetes and cancer: Epidemiological and biological links. World J Diabetes 11: 227-238.
5. Wang M, Tan Y, Shi Y, Wang X, Liao Z, et al. (2020) Diabetes and Sarcopenic Obesity: Pathogenesis, Diagnosis, and Treatments. Front Endocrinol 11: 568.
6. Saeedi P, Petersohn I, Salpea P, Malanda B, Karuranga S, (2019) IDF Diabetes Atlas Committee. Global and regional diabetes prevalence estimates for 2019 and projections for 2030 and 2045: Results from the International Diabetes Federation Diabetes Atlas, 9th edition. Diabetes Res Clin Pract 157: 107843.
7. Williams R, Karuranga S (1992) Microalbuminuria Collaborative Study Group. Microalbuminuria in type I diabetic patients. Prevalence and clinical characteristics. Diabetes Care 15: 495-501.
8. Hovind P, Tarnow L, Rossing P, Jensen BR, Graae M, et al. (2004) Predictors for the development of microalbuminuria and macroalbuminuria in patients with type 1 diabetes: inception cohort study. BMJ 328: 1105.
9. Newman DJ, Mattock MB, Dawnay AB, Kerry S, McGuire A, et al. (2005) Systematic review on urine albumin testing for early detection of diabetic complications. HTA.
10. Astor BC, Matsushita K, Gansevoort RT, van der Velde M, Woodward M, et al. (2011) Lower estimated glomerular filtration rate and higher albuminuria are associated with mortality and end-stage renal disease. A collaborative meta-analysis of kidney disease population cohorts. Kidney Int 79: 1331-1340.