ISSN 1001-0742
CN 11-2629/X

JES

JOURNAL OF ENVIRONMENTAL SCIENCES

April 1, 2015 Volume 30
www.jesc.ac.cn

MBR in Wastewater Reclamation

ELSEVIER
Science Press

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Research Center for Eco-Environmental Sciences
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Journal of Environmental Sciences Volume 30 2015

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Quantitative structure–biodegradability relationships for biokinetic parameter of polycyclic aromatic hydrocarbons

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ARTICLE INFO

Article history:
Received 14 June 2014
Revised 29 July 2014
Accepted 31 July 2014
Available online 31 January 2015

Keywords:
Leave-one-out cross-validation
Stepwise multiple linear regression
Polycyclic aromatic hydrocarbons
QSBR

ABSTRACT

Prediction of the biodegradability of organic pollutants is an ecologically desirable and economically feasible tool for estimating the environmental fate of chemicals. In this paper, stepwise multiple linear regression analysis method was applied to establish quantitative structure biodegradability relationship (QSBR) between the chemical structure and a novel biodegradation activity index (q_{max}) of 20 polycyclic aromatic hydrocarbons (PAHs). The frequency B3LYP/6-311+G(2df,p) calculations showed no imaginary values, implying that all the structures are minima on the potential energy surface. After eliminating the parameters which had low related coefficient with q_{max}, the major descriptors influencing the biodegradation activity were screened to be Freq, D, MR, E_{HOMO} and ToIE. The evaluation of the developed QSBR mode, using a leave-one-out cross-validation procedure, showed that the relationships are significant and the model had good robustness and predictive ability. The results would be helpful for understanding the mechanisms governing biodegradation at the molecular level.

Introduction

Polycyclic aromatic hydrocarbons (PAHs) are produced by chemical industry for a variety of applications, including pharmaceuticals, cosmetics, pesticides, disinfectants, agro-chemicals, dyestuffs, antifreeze, corrosion inhibitor, coal–tar wastes and creosote wood preservation (Wang et al., 2007; Haritash and Kaushik, 2009). Several PAHs have been reported to display toxic, mutagenic and carcinogenic properties even when present in low concentrations. These compounds pose a serious threat to humans and marine animals and have received increasing awareness in the aquatic environment (Mearns et al., 2009). Their fate in environment includes volatilization, photo-oxidation, chemical oxidation, adsorption on soil particles, leaching, and microbial degradation which are the major degradation processes for PAHs (Zheng et al., 2007; Augulyte et al., 2009; Kalmykova et al., 2014).

The quantitative structure–biodegradability relationship (QSBR) developed from the quantitative structure activity relationships (QSAR) is a tool used to describe and predict the biodegradability of organic compounds (Okey and Stensel, 1996). The objectives of QSBR studies are to understand mechanisms of biodegradation, to classify chemicals according to relative biodegradability, and to predict the biodegradability of new organic compounds. It is also valuable for estimating the environmental fate of pollutants and the risk assessment of PAHs (Raymond et al., 2001; Baboshin and Golovleva, 2012). Toward these objectives, much research has been performed to develop reliable QSBR models. Ferreira (2001) performed a structure based study of the

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http://dx.doi.org/10.1016/j.jes.2014.07.030
1001-0742/

biodegradation rates of 22 benzene derivatives in aqueous systems. They revealed that the computed averaged dipole polarizabilities and the summation of the Raman activities over vibrational degrees of freedom of benzene derivatives are in excellent linear correlation with the observed first-order biomass-normalized rate coefficient of benzene derivatives. A negative correlation (correlation coefficient 0.99) between denitrification rate and molecular connectivity index $^1X^v$ reflected that the degradation of aromatic heterocyclic compounds in activated sludge was substantially influenced by molecular size and the electronic properties (Wammer and Peters, 2005). Meanwhile, during O_3/UV degradation process, a QSAR model was established which revealed that the degradation rate depended on the highest occupied molecular orbital and delocalization energy (Chen et al., 2001).

Currently, in the model development process of the QSBR, the half-lives, theoretical oxygen demand (ThOD) and biological oxygen demand (BOD) were commonly used as the biodegradability indexes (Okey and Stensel, 1996). Although some models are available for the %BOD predictions, their applicability is limited to specific classes (Philipp et al., 2007). No attention has been paid to the theoretical considerations of the relationship between biokinetic parameters of compound and the descriptors. The objective of the present study was to develop valid QSBR for appropriate parameter expressing the kinetics of bacterial biotransformation of PAHs. The relationship between specific biodegradation rate (q_{max}) and molecular structure descriptors was gradually established using multiple linear regression analysis.

1. Materials and methods

1.1. Biodegradation data

Experiments were designed to measure biodegradation rates of 20 PAHs in aqueous systems. These experiments were performed individually for each PAH at a concentration significantly below its aqueous solubility to ensure that no separate PAH phase was present. Experimental measurement of the biokinetic parameters was based on the Andrews model, an extension of the Monod model that accounts for substrate inhibition (Wammer and Peters, 2005):

$$q = \frac{q_{max} \times C}{K_S + C + C^2/K_I} \quad (1)$$

where, q (mg/(L·hr)) is the specific biotransformation rate, C (mg/L) is the substrate concentration, q_{max} (mg/(L·hr)) is the maximal specific biotransformation rate, K_S (mg/L) is the biotransformation affinity coefficient, and K_I (mg/L) is the substrate inhibition coefficient. The fitting parameters in the above equation are presented in Table 1. The biokinetic of q_{max} was used as the biodegradability index. The values of

Table 1 – Structure and biodegradation activity value of 20 PAHs.

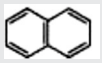
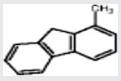
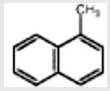
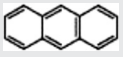
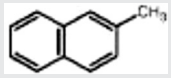
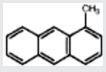
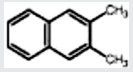
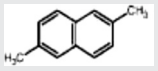
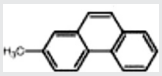
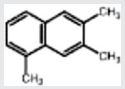
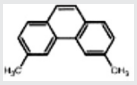
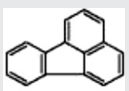
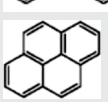
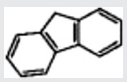
Compound	Structure	q_{max} (mg/(L·hr))	Compound	Structure	q_{max} (mg/(L·hr))
Naphthalene		61.36	1-Methylfluorene		161.54
1-Methylnaphthalene		210.52	Anthracene		178.19
2-Methylnaphthalene		240.97	1-Methylanthracene		76.33
1,5-Dimethylnaphthalene		152.63	Phenanthrene		108.94
2,3-Dimethylnaphthalene		101.49	1-Methylphenanthrene		72.85
2,6-Dimethylnaphthalene		172.23	2-Methylphenanthrene		138.39
2,3,5-Trimethylnaphthalene		92.28	3,6-Dimethylphenanthrene		159.64
Acenaphthene		89.59	Fluoranthene		95.48
Acenaphthylene		189.41	Pyrene		61.41
Fluorene		81.47	1-Methylpyrene		32.75

Table 2 – Descriptors of PAHs used in QSBR study.

Compound	LogK_{OW}	D (Å)	$^0X^v$	$^1X^v$	MR (m^3/mol)	NRB	E_{HOMO} (eV)	E_{LUMO} (eV)	ToIE (eV)	Freq (cm^{-1})	DE (kJ/mol)
Naphthalene	1.37	2	9.342	3.114	4.0418	4	−8.7429	−2.8212	−1473.2851	867.125	89.384
1-Methylnaphthalene	0.19	2	8.903	2.945	5.5604	3	−6.9381	−1.9214	−987.0517	743.439	95.527
2-Methylnaphthalene	1.24	2	9.013	3.048	6.1983	3	−6.5742	−1.5890	−926.1428	698.381	82.018
1,5-Dimethylnaphthalene	2.19	3	6.438	1.917	4.3195	4	−8.4719	−2.3461	−1293.4271	723.014	103.284
2,3-Dimethylnaphthalene	0.73	3	5.189	1.482	3.0873	4	−7.7943	−1.8472	−1738.0924	807.725	64.893
2,6-Dimethylnaphthalene	1.68	4	6.724	2.049	4.2981	5	−10.3725	−2.9425	−1095.3758	715.293	71.582
2,3,5-Trimethylnaphthalene	1.35	3	4.024	1.273	2.9946	5	−6.9318	−1.8219	−1437.4978	791.785	87.017
Acenaphthene	1.87	2	2.571	0.842	3.4571	6	−9.5321	−2.0481	−1631.8567	780.269	60.491
Acenaphthylene	0.94	3	5.617	1.891	5.0278	6	−7.8736	−1.7832	−1037.2154	738.153	79.279
Fluorene	0.57	3	3.506	1.139	2.9012	5	−12.6981	−4.2704	−1537.2803	803.942	93.493
1-Methylfluorene	0.81	2	1.783	0.582	4.1254	6	−8.8364	−2.4378	−1358.0874	758.236	81.572
Anthracene	1.48	4	2.946	0.947	2.5031	6	−7.1734	−2.0941	−2088.6796	705.293	76.249
1-Methylanthracene	1.09	4	6.178	2.014	2.7988	6	−11.8942	−3.8926	−1948.1732	805.179	99.027
Phenanthrene	3.04	5	8.934	3.173	3.1806	7	−9.9576	−3.4123	−1703.9718	772.895	82.687
1-Methylphenanthrene	2.95	5	3.016	0.927	4.3189	7	−12.5638	−4.9831	−1439.0267	791.073	94.284
2-Methylphenanthrene	0.79	4	5.284	1.893	3.7923	7	−9.4932	−3.0874	−1580.2693	772.038	103.912
3,6-Dimethylphenanthrene	0.18	6	5.013	1.378	2.6847	6	−8.4271	−2.4892	−1274.3281	718.386	127.103
Fluoranthene	2.84	4	4.820	1.694	3.0956	8	−10.4831	−3.0461	−1892.5286	829.591	86.268
Pyrene	2.41	5	1.849	0.593	3.2153	8	−15.2911	−4.9783	−2105.3924	815.675	93.891
1-Methylpyrene	1.58	6	7.135	2.439	2.8539	8	−13.9804	−4.2935	−2379.5871	873.248	110.392

the kinetic parameters for Andrews equation were obtained using nonlinear regression analysis in MINITAB 14.0

1.2. Geometry optimization and molecular descriptors

The equilibrium geometries of all PAHs were fully optimized using the density functional theory (DFT) method. The DFT calculations were run using a moderate basis set size (6-311+G(2df,p)) In all optimizations, the initial structures were pre-minimized using a force-field in Gaussian 09 program. Since the structures are relatively rigid, the precise starting geometries were not considered to be particularly important. We performed the optimizations in the framework of the C1 and C2 point groups. The frequency B3LYP/6-311+G(2df,p) calculations showed no imaginary values, implying that all the structures are minima on the potential energy surface.

There are 11 molecular descriptors used in this article. Six descriptors such as octanol/water partition coefficient (K_{OW}), zero molecular connective index ($^0X^v$), first molecular connective index ($^1X^v$), molecular diameter (D), molar refractivity (MR) and number of rotatable bonds (NRB) were calculated by Algorithms Builder 1.0. The quantum chemical descriptors of the highest occupied molecular orbital (E_{HOMO}), the energy of lowest unoccupied molecular orbital (E_{LUMO}), total energy of electronics (ToIE), the wagging vibration frequency of the whole molecule (Freq) and delocalization energy (DE) were calculated by using the software of Chemofiice 6.0. on energy-minimized structures at a semi-empirical level (AM1). The related chemical descriptors of 20 PAHs are listed in Table 2.

1.3. Development of QSBR equation

The stepwise regression analysis was carried out by MINITAB 14.0, including dependent variable q_{max} and independent variables mentioned above obtained from calculating results. Procedures for stepwise regression analysis were described by Xu et al. (2012). The goodness of the established model was accessed by the following statistical parameters: R (correlation coefficient), R^2 (coefficient of determination), S.E. (standard error of regression estimation), F (Fisher check value) and RMSE (the root mean squared error).

2. Results and discussion

2.1. Unitary linear regression

Prior to stepwise multiple linear regression analysis, the monadic linear correlation between 11 chemical descriptors and q_{max} was studied respectively. The related coefficients are shown in Table 3. As can be seen in Table 3, there is the highest linear correlation coefficient ($R = -0.844$) between q_{max} and Freq. Meanwhile there is the lowest linear correlation coefficient ($R = 0.368$) between q_{max} and DE. The scatter diagram of Freq and DE with q_{max} was shown as Fig. 1. After eliminating the parameters which had low related coefficient ($|R| < 0.5$) with q_{max}, we found that the major descriptors influencing the biodegradation activity were Freq, D, MR, E_{HOMO} and ToIE.

Table 3 – Correlation coefficients of descriptors used in this study.

	LogK_{OW}	D	$^0X^v$	$^0X^v$	MR	NRB	E_{HOMO}	E_{LUMO}	ToIE	Freq	DE
q_{max}	0.493	0.601	−0.402	−0.398	0.573	−0.389	0.837	−0.413	0.701	−0.844	0.368

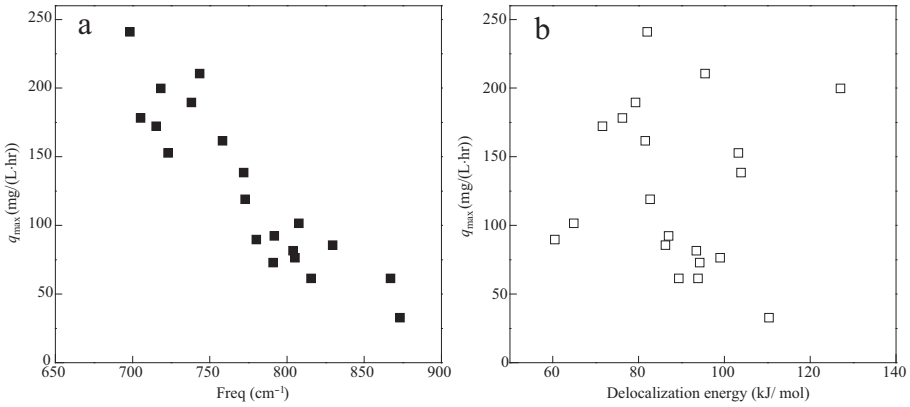


Fig. 1 – Scatter diagram of (a) vibration frequency and (b) delocalization energy with q_{max}.

2.2. Quantitative structure–biodegradability relationship

In order to get the best QSBR model, Freq and *D* were initially taken as independent variables to carry out linear regression analysis, and we got Eq. (2):

$$q_{max} = 147.2–0.11\ \text{Freq} + 31.6\ \text{D} \quad (2)$$

n = 20, R = 0.871, R^2 = 0.703, S.E. = 10.18, F = 27.69, RMSE = 7.89.

To investigate the influence of adding variables to QSBR, we added MR as an independent variable and got Eq. (3) based on Eq. (2). Moreover, by adding E_{HOMO} as an independent variable we got Eq. (4) based on Eq. (3), and by adding ToIE as an independent variable we got Eq. (5) based on Eq. (4).

$$q_{max} = 109.3–0.15\ \text{Freq} + 27.5\ \text{D} + 4.52\ \text{MR} \quad (3)$$

n = 20, R = 0.921, R^2 = 0.852, S.E. = 5.084, F = 23.51, RMSE = 3.782

$$q_{max} = 172.9–0.31\ \text{Freq} + 19.6\ \text{D} + 8.97\ \text{MR} + 3.82\ E_{HOMO} \quad (4)$$

n = 20, R = 0.951, R^2 = 0.901, S.E. = 4.72, F = 25.38, RMSE = 2.23

$$q_{max} = 382.1 –0.57\ \text{Freq} + 13.4\ D + 6.08\ MR + 13.24\ E_{HOMO} + 0.017\ \text{ToIE} \quad (5)$$

n = 20, R = 0.969, R^2 = 0.946, S.E. = 2.73, F = 34.38, RMSE = 1.032.

By comparing the various parameters in Eqs. (3) to (5), it can be found that Eq. (5) is an ideal QSBR model. This is because with the increase of the variable, correlation coefficient R, determination coefficient R^2 and Fisher check value F become bigger; while standard deviation S.E. and root mean squared error RMSE become smaller. In order to validate the predictive ability of different models, predicted values calculated by different models and experimental values were listed in Table 4. The relationship between experimental results and predicted values calculated by Eq. (5) was shown as Fig. 2. The results show good agreement between predictions and experimental data. Validation is a crucial aspect of any QSBR modeling. It is the process by which the reliability and

Table 4 – Experimental and predicted biodegradabilities.

Compound	q_{max} (exp.)	q_{max} (calcd.)					
		By Eq. (3)	Residual	By Eq. (4)	Residual	By Eq. (5)	Residual
Naphthalene	61.36	49.32	12.04	82.69	−21.33	53.24	8.12
1-Methylnaphthalene	210.52	199.84	10.68	227.59	−17.07	202.98	7.54
2-Methylnaphthalene	240.97	262.04	−21.07	253.61	−12.64	231.42	9.55
1,5-Dimethylnaphthalene	152.63	172.42	−19.79	133.4	19.23	141.02	11.61
2,3-Dimethylnaphthalene	101.49	111.44	−9.95	114.64	−13.15	88.48	13.01
2,6-Dimethylnaphthalene	172.23	158.17	14.06	152.38	19.85	180.48	−8.25
2,3,5-Trimethylnaphthalene	92.28	114.05	−21.77	77.36	14.92	102.11	−9.83
Acenaphthene	89.59	94.28	−4.69	84.15	5.44	80.53	9.06
Acenaphthylene	189.41	218.24	−28.83	191.71	−2.3	178.42	10.99
Fluorene	81.47	102.18	−20.71	70.78	10.69	70.84	10.63
1-Methylfluorene	161.54	206.85	−45.31	150.74	10.8	174.32	−12.78
Anthracene	178.19	202.98	−24.79	163.2	14.99	191.05	−12.86
1-Methylanthracene	76.33	88.45	−12.12	86.62	−10.29	90.84	−14.51
Phenanthrene	108.94	139.83	−30.89	94.67	14.27	124.23	−15.29
1-Methylphenanthrene	72.85	82.94	−10.09	59.37	13.48	60.53	12.32
2-Methylphenanthrene	138.39	108.24	30.15	119.43	18.96	129.74	8.65
3,6-Dimethylphenanthrene	159.64	176.54	−16.9	138.66	20.98	147.43	12.21
Fluoranthene	95.48	104.28	−8.8	86.09	9.39	90.34	5.14
Pyrene	61.41	83.93	−22.52	39.6	21.81	72.04	−10.63
1-Methylpyrene	32.75	46.03	−13.28	43.46	−10.71	40.95	−8.2

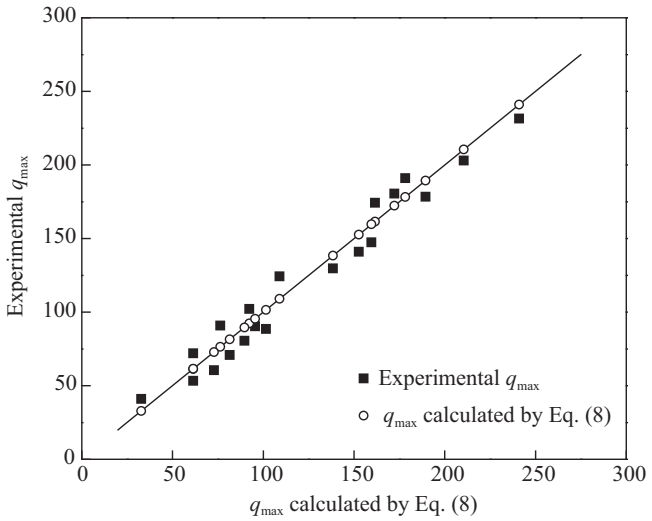


Fig. 2 – Plots of experimental q_{max} *versus* those predicated by Eq. (8).

relevance of a procedure are established for a specific purpose. It is now being accepted that validation is an important process that includes assessment of issues such as data quality, applicability of the model and mechanistic interpretability in addition to statistical assessment (Nandy et al., 2013). A common method for internally validating a QSBR model is leave-one-out cross-validation. This has the advantage that each data point is used for both training and validation on each trail (Zhang et al., 2014). Leave-one-out cross-validation is normally restricted to applications where the amount of training data available is severely limited, such that even a small perturbation of the training data is likely to result in a substantial change in the fitted model. In the present study, it makes good sense to adopt a leave-one-out cross-validation strategy as it minimizes the perturbation to the data in each trial. The outcome from this procedure is a cross-validated correlation coefficient (Q^2_{LOO}), which is usually smaller than the overall R^2 for a QSBR mode (Kar and Roy, 2011). Frequently, Q^2_{LOO} is used as a criterion of both robustness and predictive ability of the model. Many authors consider high Q^2_{LOO} (for instance, $Q^2_{LOO} > 0.5$) as an indicator or even as the ultimate proof of the high predictive power of the QSBR mode. For Eq. (5), the Q^2_{LOO} of validation results is 0.927, which was significantly larger than 0.5. So the established QSBR model performed well with the aspects of goodness-of-fit, robustness and predictivity.

2.3. Mechanisms interpretation for the established QSBR mode

Freq is a parameter reflected the chemical bond strength. Biodegradation of PAHs included the fracture of the benzene ring. Therefore, chemical bond strength of the benzene ring must be closely correlated with biodegradation activity (Xu et al., 2012). E_{HOMO} is a parameter associated with the ability to donate electrons. All E_{HOMO} values are negative; therefore, smaller E_{HOMO} values indicate electrons that are more strongly bound to the system, which weakens the biodegradability of such compounds (Yang et al., 2004). TolE was the total energy of all electrons energy and repulsion energy between atomic nucleuses in a molecule. It was in direct proportion to the biodegradability of the compounds. When a PAH compound had lower TolE, the biodegradability would be poorer (Yang et al., 2006). Molecular diameter (*D*) indicated the spatial scale in where electrons in the molecule moved, and characterized the size of a molecule. Larger diameter molecules may interact with an enzyme more readily, thus increasing the biodegradability of this organic compound (Yang et al., 2006). Finally, MR was directly associated with its electronic property. If an aromatic compound had bigger MR, the electrons in this molecule was easier to be lost to form stronger electrostatic, so the biodegradability of this aromatic compound was better.

3. Conclusions

The theoretical relationship between biokinetic parameter (q_{max}) and molecular descriptors has been investigated based on stepwise multiple linear regression analysis. According to the experimental results, the major descriptors influencing the biodegradation activity were screened to be Freq, *D*, MR, E_{HOMO} and ToIE. Assessment based on leave-one-out cross-validation indicated that the established QSBR model had good robustness and predictive ability. Interpretation of the descriptors responsible for biodegradation activity can be useful tools for designing new biodegradable chemicals and/or predicting the biodegradability of new chemicals in the environmental hazard assessment.

Acknowledgments

This work was supported by the State Key Laboratory of Urban Water Resource and Environment, Harbin Institute of Technology (No. 2013DX10), the Sino-Dutch Research Program (No. zhmhgfs2011-001), and the Sino-American Coal Chemical Industry Program (No. ZMAGZ 2011001).

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Journal of Environmental Sciences (Established in 1989)
Volume 30 2015

Supervised by	Chinese Academy of Sciences	**Published by**	Science Press, Beijing, China
Sponsored by	Research Center for Eco-Environmental		Elsevier Limited, The Netherlands
	Sciences, Chinese Academy of Sciences	**Distributed by**	
Edited by	Editorial Office of Journal of	Domestic	Science Press, 16 Donghuangchenggen
	Environmental Sciences		North Street, Beijing 100717, China
	P. O. Box 2871, Beijing 100085, China		Local Post Offices through China
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Editor-in-chief	X. Chris Le	**Printed by**	Beijing Beilin Printing House, 100083, China

CN 11-2629/X **Domestic postcode: 2-580** **Domestic price per issue RMB ¥ 110.00**

ISSN 1001-0742