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Prediction of biodegradability for selected organic chemicals

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SUMMARY

The 5-day BODs of 45 organic chemicals were determined using acclimated mixed microbial cultures. These chemicals included alcohols, acids, esters, ketones, aromatics and miscellaneous compounds. The BOD data were correlated with (1) water solubilities, (2) log of 1-octanol/water partition coefficients, (3) molar refractivities and volumes, (4) melting (m.p.) and boiling points, (5) number of carbon (C No.), hydrogen and oxygen atoms, (6) molecular weights, and (7) theoretical (Th) BODs of chemicals. Linear and second-order polynomial regression analyses were used; the latter was also attempted with two or more independent variables. All prediction equations were compared for statistical merits. The equations, one from each regression type, with the highest prediction power were: log 5-day mmol BOD/mmol chemical = (1) $-0.183+0.813$ (log ThBOD), (2) $-0.391+1.560$ (log ThBOD) -0.532 (log ThBOD)^2, and (3) $-0.4060+0.2470$ (C No.) -0.0133 (C No.)^2 -0.0005 (m.p.). The measured BOD data for 43 additional chemicals were compared with the predicted values calculated through the above equations. The three equations predicted the BODs for 84–88% of the test chemicals within 80% of the experimental values. The mean percent relative standard deviations between predicted and experimental BOD values were statistically compared for these equations, and no significant difference ($P \leq 0.01$) in their predictive utility was found. The acclimation potential of an autochthonous microbial community cannot yet be predicted, but this study demonstrates that the process of active biodegradation for structurally dissimilar chemicals appears to correlate quantitatively with certain physicochemical parameters.

INTRODUCTION

The universe of synthetic chemicals is large and expanding, in terms of both production volumes and the variety of chemicals commercially available. Effective assessment of ecological impacts requires rapid screening of chemicals for their treatability, environmental persistence, and toxicity so that testing resources can be focused on the potentially hazardous chemicals. One screening technique is to predict biological activities of chemicals from their physicochemical properties. Chemical

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structure-activity models have been developed for a variety of biological endpoints including rat oral LD_{50}, mutagenicity, carcinogenicity, teratogenicity [4], fish toxicity [15] and biodegradability [2,4, 10,12,13,17].

Inspection of the literature reveals both quantitative and qualitative structure-biodegradation correlations. The former, however, included only similar chemicals [2,12,17], while in contrast, the latter considered diverse classes of chemicals [4,10]. Quantitative structure-biodegradation relationships applicable to various structural configurations are desired for the fate assessment of chemicals. Thus, this investigation was conducted (1) to determine the possibility of developing quantitative relationships between the physicochemical properties and biodegradation of model organic chemicals, and (2) to test comparatively the usefulness of these relationships in predicting biodegradation of various test chemicals.

MATERIALS AND METHODS

Preparation of microbial seeds

Mixed microbial cultures capable of using 45 model organic chemicals (analytical grade) as sole carbon and energy sources were separately isolated by an enrichment culture technique [14]. Similarly, additional cultures were obtained that were capable of degrading 43 test chemicals. Microbial seeds for the BOD tests were prepared from the culture growth (10^5–10^6 cells/ml) in mineral salts medium [11] containing 100 mg/l (solid) or 100 μl/l (liquid) chemical substrate. The culture was diluted (1:1) with physiological saline and incubated on a shaker (150 rpm) for 24 h prior to its use.

Measuring biodegradation of model chemicals

Biodegradation of 45 model chemicals by acclimated microbes was measured separately by the BOD technique [1]. A test chemical and 1 ml of the seed were added to 20 ml of dilution water contained in a 300-ml BOD bottle. Bottles were filled to capacity with the same water, and sealed and incubated for 20 days at 21 ± 3°C. Each test was run in duplicate. A seed control and two or more chemical concentrations ranging from 0.4 to 3.2 mg or μl/l were employed in each test. Glucose-glutamic acid controls for assessing the dilution water quality were included. Initial and 5, 10 or 11, 14 or 15, and 20-day dissolved oxygen (DO) concentrations were determined using a YSI 54 oxygen meter equipped with a self-stirring probe. The DO concentrations in randomly selected bottles were measured by the azide modification of the iodometric method [1]. The test BOD values showing DO depletions of at least 2 mg/l and residual DO of at least 1 mg/l were acceptable. These values were adjusted for the seed control and used for calculating the 5-day mmol BOD/mmol chemical at various chemical concentrations. For some chemicals, insufficient DO depletions occurred within 5 days and thus their 5-day BODs were estimated from the most linear regions of the relationships between BOD values and incubation times. The mean 5-day mmol BOD/ mmol chemical values were used for developing biodegradation prediction models.

Developing biodegradation prediction models

Relationships between biodegradation and selected physicochemical parameters of the model chemicals were established. The parameters included (1) estimated water solubilities [8] and log of 1-octanol/water partition coefficients (log P) [5,7], (2) calculated molar refractivities and volumes, number of carbon (C No.), hydrogen and oxygen atoms, molecular weights and theoretical (Th) BODs, and (3) measured melting (m.p.) and boiling points of chemicals. The above data, except ThBODs, were obtained through the QSAR interactive chemical information database system [6] at the Environmental Research Laboratory-Duluth, Duluth, MN. The ThBOD values were computed from the chemical empirical formulas.

The 5-day BOD values were correlated with all possible combinations of physicochemical characteristics of chemicals. This was done by linear and second-order polynomial regression analyses using Minitab® statistical software on a VAX 11/785 computer [9]. The latter regression was expanded with two or more independent variables. All prediction equations were evaluated by comparing (1) coefficients of determination (r^2), (2) t-ratios for independent variables, and (3) patterns in BOD residuals. A t-ratio is a square root of the F-statistic and is computed by dividing the coefficient for each variable by the standard deviation of that coefficient. The level of its significance is determined from t distribution tables and indicates the relative importance of that variable in the prediction equation [9]. Algebraic equations with the highest statistical merits, representing three types of regressions, were chosen and tested for their usefulness in predicting the 5-day BOD values of test chemicals.

Comparing predicted and measured biodegradation of test chemicals

A total of 43 test compounds from several chemical classes were selected and their physicochemical property data were compiled. These values were used in three equations to calculate 5-day BOD values for each chemical. Experimental 5-day BOD values of test chemicals were determined in the manner described for the model chemicals. Comparisons of three predicted BOD values with the corresponding experimental value for each chemical were made by computing percent relative standard deviation (%RSD) between predicted and measured values.

RESULTS AND DISCUSSION

Biodegradation of model chemicals

Biodegradation of 10 unsubstituted and 4 substituted alcohols, 3 carboxylic acids, 4 carboxylate esters, 4 ketones, 7 monosubstituted, 5 disubstituted and 3 trisubstituted benzenes, and 5 miscellaneous compounds was measured by the BOD technique. These chemicals were selected to include both structural diversity and broad ranges of physicochemical parameter values; that is, independent variables. Test concentrations for each chemical were less than the chemical water solubility limit for the chemical. The extent of biodegradation increased with increased chemical concentration, as was observed previously [3]. The mean 5-day mmol BOD/mmol chemical values were used for developing structure-biodegradation relationships. The coefficient of variation (CV) for the BOD values (Table 1) ranged from 0.0% for 1-chloro-3-hydroxypropane to 21.3% for methyl (2,4-dichlorophenoxy)acetate, with a mean of 7.9%.

Biodegradation prediction models

A total of 11 physicochemical parameters such as water solubility, log P and m.p. of model chemicals were correlated with the BOD values. Regression techniques were applied to derive prediction equations for linear and multidimensional second-order polynomial relationships. Data were fitted by exponential transformation where appropriate. All prediction equations within each regression type were compared for r^2, significance ($P \leq 0.1$) of t-ratios for independent variables, and pattern formations in BOD residuals. Combinations of more than two physicochemical parameters in the polynomial regression did not significantly improve r^2 or the t-ratios. The best-fit prediction equations, one from each regression type, were:

Linear regression ($n = 45$)

$$\log \text{5-day mmol BOD/mmol chemical} = -0.183 + 0.813 (\log \text{ThBOD});\ r^2 = 70.7\%;\ t\text{-ratio: } \log \text{ThBOD} = 10.19 \quad (1)$$

Polynomial regression with one independent variable ($n = 45$)

$$\log \text{5-day mmol BOD/mmol chemical} = -0.391 + 1.560 (\log \text{ThBOD}) - 0.532 (\log \text{ThBOD})^2;\ r^2 = 74.6\%;\ t\text{-ratios: } \log \text{ThBOD} = 5.16,\ (\log \text{ThBOD})^2 = -2.56 \quad (2)$$

Polynomial regression with two independent variables ($n = 41$)

$$\log \text{5-day mmol BOD/mmol chemical} = -0.4060 + 0.2470 (\text{C No.}) - 0.0133 (\text{C No.})^2 - 0.0005 (\text{m.p.});\ r^2 = 79.5\%;\ t\text{-ratios: C No.} = 9.13,\ (\text{C No.})^2 = -6.79,\ \text{m.p.} = -1.80 \quad (3)$$

These equations depict correlations of BOD with parameters related to molecular size, ThBOD in Eqns. 1 and 2, and C No. in Eqn. 3. Inclusion of m.p. in Eqn. 3 explained 10% more variation in

Table 1

Model chemicals, their theoretical (Th) BODs, carbon contents (C No.), melting points (m.p.) and experimental BOD (mmol/mmol chemical) values

Chemical	ThBOD	C No.	m.p.	5-day BOD ± SD[a]
Unsubstituted alcohols				
1-butanol	6.00	4	−90	3.60±0.35
1-decanol	15.00	10	6	5.22±0.57
1-dodecanol	18.00	12	26	4.18±0.14
isopentyl alcohol	7.50	5	−117	4.46±0.21
isopropyl alcohol	4.50	3	−90	2.58±0.17
methanol	1.50	1	−94	0.92±0.08
1-nonanol	13.50	9	−6	6.28±0.66
1-octanol	12.00	8	−16	6.43±0.59
2-octanol	12.00	8	−39	6.13±0.23
1-undecanol	16.50	11	19	4.50±0.43
Substituted alcohols				
1-chloro-3-hydroxypropane	4.25	3	NF[b]	1.36±0.00[c]
N,*N*-diethylethanolamine	9.25	6	−70	5.50±0.24
2-(ethylamino)ethanol	6.25	4	−90	4.18±0.08
2-methyl-2,4-pentanediol	8.50	6	−50	4.79±0.32
Carboxylic acids				
capric acid	14.00	10	31	8.52±0.35
glycolic acid	1.50	2	80	0.89±0.08
trimethylacetic acid	6.50	5	34	1.59±0.21[c]
Carboxylate esters				
amyl acetate	9.50	7	−71	2.92±0.35
dibutyl fumarate	15.00	12	−19	5.75±0.46
2-hydroxyethyl acrylate	5.50	5	NF	3.35±0.13
isopropyl acetate	6.50	5	−73	3.40±0.25
Ketones				
acetone	4.00	3	−95	1.52±0.07
2-butanone	5.50	4	−86	3.23±0.13
2-decanone	14.50	10	15	6.97±1.01
2-octanone	11.50	8	−16	5.53±0.10
Monosubstituted benzenes				
acetophenone	9.50	8	21	5.61±0.17
benzyl alcohol	8.50	7	−15	5.93±0.17
biphenyl	14.50	12	69	4.11±0.60
N,*N*-dimethylaniline	10.75	8	2	4.63±0.45
ethyl benzene	10.50	8	−95	3.05±0.24
phenol	7.00	6	43	4.59±0.14
toluene	9.00	7	−95	3.40±0.42

Disubstituted benzenes				
4-*tert*-butyl benzoic acid	13.50	11	166	3.72±0.29
4-chlorophenol	6.75	6	44	3.85±0.58
4-cyanophenol	7.75	7	111	4.45±0.11
4-bromophenol	6.75	6	64	3.15±0.66
4-nitrophenol	5.75	6	113	4.65±0.43
Trisubstituted benzenes				
2,4-dichlorophenoxy acetic acid	8.00	8	140	4.64±0.51
3-ethoxy-4-hydroxy-benzaldehyde	10.00	9	77	5.29±0.20
Methyl(2,4-dichlorophenoxy) acetate	9.50	9	NF	1.74±0.37[c]
Miscellaneous compounds				
acetonitrile	2.00	2	− 45	1.15±0.17
benzene	7.50	6	6	2.73±0.19
formamide	1.25	1	3	0.42±0.04
1-methyl naphthalene	13.50	11	− 22	3.71±0.08
3-(3-pyridyl)-1-propanol	10.25	8	NF	2.71±0.11[c]

[a] $n \geq 4$.

[b] NF = not found.

[c] Estimated by linear regression technique from a 20-day test.

BODs than that accounted for by the polynomial regression with C No. alone. The m.p. and C No. were truly independent variables, with r^2 of 13.1% for their correlation. The influence of m.p. on chemical biodegradation cannot be rationalized, except that m.p. is possibly an indirect measure of a biologically relevant parameter not considered in this study.

Paris et al. [12,13] and Wolfe et al. [17] reported high r^2 values in correlating biodegradation rate constants and selected structural features of homologous series of chemicals. However, prediction models which incorporate a variety of distinct structures may have a useful screening level application in estimating environmental longevity of untested chemicals.

Predicted and measured biodegradation of test chemicals

Regression equations developed based on model chemicals were used for predicting the 5-day BOD values of test chemicals; 8 unsubstituted and 4 substituted alcohols, 6 ketones, 3 monosubstituted and 9 disubstituted benzenes, 7 ethers, and 6 miscellaneous compounds. Physicochemical property data for these chemicals were acquired and substituted in the prediction equations. Experimental 5-day BOD values of test chemicals were determined and compared with the predicted values (Table 2). Precision in these tests was comparable to that obtained with the model chemicals. The CV for the 5-day BODs ranged from 1.1% for 2,4-dihydroxybenzaldehyde to 28.6% for 2-hydroxyethyl ether, with a mean of 8.0%. The predictive power of each equation was assessed by examining the number of test chemicals distributed among various %RSD ranges (Table 3). The statistical equality ($P \leq 0.01$) of the mean %RSD values suggested that there was no distinctly superior correlation.

The power of a prediction model can be judged from the mean %RSD between predicted and measured biological endpoints for a given set of chemicals. For the data (Table 2) in this study, 80% RSD was chosen as a discriminator to separate predictable (≤80% RSD) and outlying (>80% RSD) chemicals. Eqns. 1, 2, and 3 predicted 86%, 88%, and 84%, respectively, of the test chemical BOD values within the acceptable range of 0–80% RSD (Table 3). There were several chemicals for which the above models could not adequately predict the BOD values. The mean ratios of predicted to experimental BODs for the outliers were 3.59 with

Table 2

Selected chemicals, their theoretical (Th) BODs, carbon contents (C No.), melting points (m.p.), and predicted and experimental BOD (mmol/mmol chemical) values

Chemical	ThBOD	C No.	m.p.	5-day BOD predicted by			Experimental 5-day BOD
				Eqn. 1	Eqn. 2	Eqn. 3	
Unsubstituted alcohols							
cyclohexanol	8.50	6	23	3.74	3.98	3.85	4.86
ethanol	3.00	2	−117	1.60	1.71	1.24	1.81
1-heptanol	10.50	7	− 36	4.44	4.44	4.89	5.91
1-hexanol	9.00	6	− 52	3.92	4.10	4.20	4.77
isobutyl alcohol	6.00	4	−108	2.82	3.17	2.65	3.92
1-pentanol	7.50	5	− 79	3.38	3.69	3.44	4.24
2-pentanol	7.50	5	NF[a]	3.38	3.69	NC[b]	4.12
1-propanol	4.50	3	−127	2.23	2.52	1.90	2.70
Substituted alcohols							
L-2-amino-1-butanol	6.25	4	− 2	2.91	3.26	2.35	2.88
2-ethyl-1-hexanol	12.00	8	− 76	4.95	4.71	5.71	4.98
3-furanmethanol	5.50	5	NF	2.62	2.97	NC	2.13
4-methyl-2-pentanol	9.00	6	− 90	3.92	4.10	4.39	5.07
Ketones							
cyclohexanone	8.00	6	− 45	3.56	3.84	4.17	3.98
2,6-dimethyl-4-heptanone	13.00	9	NF	5.28	4.86	NC	6.08
2-hexanone	8.50	6	− 57	3.74	3.98	4.22	5.22
4-hydroxy-4-methyl-2-pentanone	8.00	6	− 44	3.56	3.84	4.16	3.74
3-methyl-2-butanone	7.00	5	− 92	3.19	3.53	3.49	4.60
3-pentanone	7.00	5	− 39	3.19	3.53	3.28	4.65
Monosubstituted benzenes							
isopropylbenzene	12.00	9	− 96	4.95	4.71	6.13	4.91
N-methylaniline	9.25	7	− 57	4.00	4.16	5.01	3.54
n-propylbenzene	12.00	9	−100	4.95	4.71	6.16	3.06[c]
Disubstituted benzenes							
1,4-benzenedimethanol	9.50	8	114	4.09	4.22	4.59	6.05
2,2'-biphenol	13.50	12	109	5.44	4.93	3.88	10.25
4-*tert*-butylbenzyl alcohol	14.50	11	NF	5.77	5.05	NC	1.88[c]
4-chlorophenoxy-acetic acid	8.25	8	158	3.65	3.91	4.36	2.55
p-cresol	8.50	7	36	3.74	3.98	4.50	5.63
2,4-dihydroxy-benzaldehyde	7.50	7	202	3.38	3.69	3.72	4.67
4'-hydroxyacetophenone	9.00	8	109	3.92	4.10	4.62	5.51
4-methoxyphenol	8.00	7	57	3.56	3.84	4.39	4.59
xylenes (mixed isomers)	10.50	8	− 20	4.44	4.44	5.36	3.57

Ethers							
2-(2-*n*-butoxyethoxy)ethanol	11.00	8	– 68	4.61	4.54	5.66	5.95
n-butyl ether	12.00	8	– 98	4.95	4.71	5.86	1.93
2,2-dimethoxypropane	7.00	5	NF	3.19	3.53	NC	4.34
2-(2-ethoxy-ethoxy)ethanol	8.00	6	NF	3.56	3.84	NC	5.50
ethoxytriglycol	10.50	8	– 80	4.44	4.44	5.74	1.15[c]
2-hydroxyethyl ether	5.00	4	– 10	2.43	2.75	2.37	0.35[c]
2-(2-methoxyethoxy)ethanol	6.50	5	– 70	3.01	3.35	3.40	0.95[c]
Miscellaneous compounds							
DL-aspartic acid	3.75	4	279	1.92	2.13	1.70	1.82
1-bromononane	13.75	9	– 29	5.52	4.96	5.68	6.12
indole	9.75	8	52	4.18	4.28	4.93	4.83
monoallylamine	4.75	3	– 88	2.33	2.64	1.82	1.68
sorbitol hexaacetate	18.50	18	102	7.03	5.39	0.48	3.65[c]
thymine	5.50	5	326	2.62	2.97	2.16	3.25

[a] NF = not found.

[b] NC = not calculated.

[c] Estimated by linear regression technique from a 20-day test.

Eqn. 1, 4.08 with Eqn. 2, and 3.42 with Eqn. 3 (Table 4).

Linear and second-order polynomial regressions using the same variables were also performed on the combined data for model and test chemicals. The outliers from both data sets were excluded. Coefficients and t-ratios for the independent variables changed somewhat, and the r^2 slightly decreased in these pooled correlations. For example, with model chemicals ($n=41$), in the polynomial regression with C No. and m.p. as predictors (Eqn. 3), r^2 was 79.5%, while in the pooled correlation ($n=69$) r^2 was 75.2%. The cumulative data set, however, expanded the ranges of independent variables and structural diversity in comparison to that with the model chemicals alone.

The BOD technique was found to be appropriate for measuring biodegradation if the initial substrate concentration was at or greater than approximately 1 mg/l. This precluded the testing of chemicals having very low water solubilities, that is, high (>5) log P values. However, the frequency distribution of log P values for industrial chemicals demonstrates that a large majority of compounds fall between log P of 0 and 5, and that 50% are between log P of 2 and less [16]. In view of the above, additional chemical structures can be selected for fitting their BOD data (1) at greater distances from

Table 3

Number of test chemicals distributed among five ranges of percent relative standard deviations (%RSD)

BOD prediction by	No. of chemicals with % RSD[a] between					Mean %RSD[c]
	0–20	21–40	41–60	61–80	>80[b]	
Eqn. 1	16	18	2	1	6	23
Eqn. 2	21	12	5	0	5	22
Eqn. 3	18	9	2	2	6	22

[a] %RSD = abs (BOD predicted by Eqn. 1, 2 or 3 – BOD experimental) × 100/BOD experimental.

[b] Chemicals with >80% RSD were considered outliers.

[c] Calculated for chemicals between 0 and 80% RSD; F-statistic for comparison of three means was insignificant at $P \leq 0.01$.

Table 4

Outlying chemicals and their predicted (P) to experimental (E) BOD ratios

Chemical[a]	P BOD/E BOD		
	Eqn. 1	Eqn. 2	Eqn. 3
4-*tert*-butylbenzyl alcohol	3.07	2.69	NC[b]
n-Butyl ether	2.56	2.44	3.04
Ethoxytriglycol	3.86	3.86	4.99
2-Hydroxyethyl ether	6.94	7.86	6.76
2-(2-Methoxyethoxy)-ethanol	3.16	3.53	3.58
n-Propylbenzene	(1.62)[c]	(1.54)	2.01
Sorbitol hexaacetate	1.93	(1.48)	0.13

[a] Chemical with relative standard deviation >80%.

[b] NC = not calculated, as m.p. was not found.

[c] Parenthetic ratio indicates that chemical was not an outlier when its BOD value was predicted using that particular equation.

the means of, and (2) giving equal weight to each discrete value for, the independent variables to determine the best regression order for biodegradation prediction. However, one must be cognizant that even the most powerful predictive models cannot supersede the need to test chemicals for biodegradation. These models at best can help prioritize substances for in-depth evaluation, especially when testing resources are limited.

From the modeling perspective, one may wish to resolve the occurrence of biodegradation into two steps, microbial acclimation to a given chemical, followed by biodegradation of that chemical. Thus, there is a need to develop structure-microbial acclimation relationships in addition to structure-biodegradation models. The first relationship can be of a qualitative nature, but the second must be quantitative.

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