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QSAR studies on biological oxygen demand of alcohols

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A model for predicting the biological oxygen demand, and hence biodegradibility of chemical substances, is proposed for some alcohols. A novel parameter, ThOD, has been used along with some other topological indices for construction of regression models. Statistical evaluation of the agreement between model predictions show that the compounds can be classified as highly degradable, moderately degradable and low-degradable alcohols.

Keywords: QSAR, theoretical oxygen demand, BOD, alcohol, topological indices, regression model

IPC: **Int.Cl.[7] C 07 C**

Organic matters upon oxidation degrade into gaseous compounds like carbon dioxide, sulphur dioxide, nitrogen dioxide and to water vapours. Oxidation may be carried out either by applying conventional chemical oxidants like potassium dichromate and potassium permanganate or by several micro-organisms, which apply enzymes for the purpose. When water containing organic matter is discharged into river, lake or sea natural decomposition of organic matter through oxidation by biological agents takes place. The biochemical oxidation is brought about by naturally occurring microorganisms, which use the organic matter as a source of carbon.

Dissolved oxygen in water sustains respiration of aquatic organisms. Naturally, this is a simplified picture of a complex set of reactions, the rates of which depend on the temperature, the type of organic matter present, the type of microorganisms, the aeration, and the amount of light available[1]. The biological oxygen demand (BOD) test of a sample containing organic matters is an empirical bioassay type procedure, which measures the dissolved oxygen consumed by microbial organisms while assimilating and oxidizing the organic matters present. The sample in an appropriate dilution is incubated for 5 days at 20°C. The reduction in amount of dissolved oxygen results in the evaluation of BOD. The five days test has been generally adopted with the knowledge that this does not necessarily represent the time required for total oxidation of the organic matter present. In some cases, a test period of longer than five days is specified. However, there is no acceptable procedure for determining the accuracy of the BOD test.

With so much of dependable factors, BOD has become a rare candidate for structure activity relationship (SAR) studies. Literature is almost silent in this area of research. Herein, an attempt has been made to model BOD using molecular parameters. Theoretical oxygen demand, ThOD (non-empirical, but based on chemical reaction), a novel molecular parameter has been proposed for the use in QSAR studies.

Database

The biological oxygen demand (BOD) values collected from literature[1] are results of five days incubation of the organic matters at 20°C and are given in **Table I**.

Evaluation of Theoretical Oxygen Demand (ThOD)

Microorganisms consume carbon from organic matter to convert it to carbon dioxide. Theoretical oxygen demand (ThOD) for the constituent carbon can be calculated by stoichiometric conversion of carbon to carbon dioxide and, hydrogen and oxygen to water. ThOD is a ratio of oxygen in grams required for complete oxidation of the organic molecule to corresponding oxides and the molecules in gram. For hydrocarbons the ThOD can be calculated by considering the following reaction.

Table I — BOD, ThOD, PC_1, PC_2 and PC_3 values of 29 different alcohols

Sl.No.	Compd	Mol. formula	BOD	ThOD	PC_1	PC_2	PC_3
1	Methanol	CH_4O	1.12	1.50	6.650	1.349	-1.663
2	Ethanol	C_2H_6O	1.67	2.10	4.293	-0.054	-0.372
3	2-Chloro ethanol	C_2H_5OCl	0.5	1.093	3.205	1.020	-1.432
4	Ethylene glycol	$C_2H_6O_2$	0.81	1.26	3.095	0.755	-1.183
5	Ethanol amine	C_2H_7ON	1.1	2.49	3.356	2.117	2.229
6	Allyl alcohol	C_3H_6O	0.2	2.20	3.254	1.003	0.727
7	Isopropanol	C_3H_8O	2.0	2.40	2.882	-1.473	-0.321
8	Ethylene glycol monomethyl ether	$C_3H_8O_2$	0.50	1.684	1.539	0.269	-0.317
9	Glycerol	$C_3H_8O_3$	0.87	1.217	0.715	1.184	-0.589
10	*n*-Butanol	$C_4H_{10}O$	2.04	2.594	1.111	-1.716	0.297
11	*sec*-Butanol	$C_4H_{10}O$	1.87	2.594	1.303	-1.748	0.261
12	*iso*-Butanol	$C_4H_{10}O$	1.66	2.60	1.346	-1.729	0.253
13	Ethylene glycol mono ethyl ether	$C_4H_{10}O_2$	1.58	1.955	-0.051	-0.807	-0.372
14	Diethylene glycol	$C_4H_{10}O_3$	0.15	1.51	-1.301	-0.052	-0.849
15	Diethanol amine	$C_4H_{11}O_2N$	0.1	2.13	-1.184	0.902	1.181
16	Furfuril alcohol	$C_5H_6O_2$	0.534	1.796	-0.534	3.320	1.729
17	1-Pentanol	$C_5H_{12}O$	1.61	2.727	-0.478	-2.472	0.245
18	*iso*-Amyl alcohol	$C_5H_{12}O$	0.162	2.740	-0.020	-1.911	0.630
19	2-Isopropoxy ethanol	$C_5H_{12}O_2$	0.12	2.154	-0.985	-0.936	0.176
20	Phenol	C_6H_6O	1.68	2.26	-1.865	0.110	-0.267
21	Resorcinol	$C_6H_6O_2$	1.5	1.89	-1.563	1.505	0.062
22	Quinol	$C_6H_6O_2$	1.00	1.89	-1.415	1.435	0.373
23	Phloroglucinol	$C_6H_6O_3$	0.468	1.523	-2.343	2.158	-0.020
24	Cyclohexanol	$C_6H_{12}O$	0.379	2.828	-1.487	-3.227	-0.162
25	Diacetone alcohol	$C_6H_{12}O_2$	0.68	2.538	-1.980	-0.687	0.994
26	*d*-Gluconic acid	$C_6H_{12}O_7$	0.350	0.900	-7.238	3.295	-1.837
27	Butyl cellosolve	$C_6H_{14}O_2$	1.68	2.305	-3.233	-1.349	-0.049
28	Hexylene glycol	$C_6H_{14}O_2$	0.02	2.305	-2.231	-0.992	-0.430
29	Diethylene glycol mono ethyl ether	$C_6H_{14}O_3$	0.58	2.173	-4.840	-1.268	-0.797

$C_c H_h + (c+h/4) O_2 \rightarrow cCO_2 + h/2 H_2O$

ThOD of $C_cH_h = 32 (c + h/4)/(12c + h)$ ... (1)

When the molecule contains oxygen, the oxygen demand from the atmosphere decreases and it is reflected in the denominator of the equation. For a compound $C_cH_hO_o$ the ThOD value can be evaluated from Eqn (2).

$$ThOD (C_cH_hO_o) = 32 (c+ h/4 – o/2) /(12c + h + 16o) \quad \ldots (2)$$

Similarly, when the organic molecule contains sulphur and nitrogen the ThOD can be determined by considering the conversion of sulphur to sulphur dioxide and nitrogen to nitrate (NO_3^-) (Eqn 3).

$$ThOD (C_cH_hO_oN_nS_s)= 32 (c + h/4 – o/2 + 3n/2 + s) / (12c + h + 16o + 14n + 32s) \quad \ldots (3)$$

In the standard BOD_5 day test, nitrification does not occur within the time frame. Hence the compound containing nitrogen has a very low BOD_5 value when compared to theoretical oxygen demand (ThOD).

Evaluation of molecular descriptors

Molecular descriptors derived from structural graph have been applied successfully on QSAR studies[2-6]. Fungicidal and mutagenic activities have been well correlated with molecular parameters[8-10].

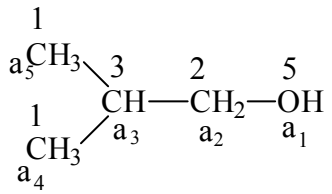
In the present study different types of molecular parameters have been evaluated for a set of alcohols with available BOD_5 values.

The molecular descriptors IC, SIC, CIC, W, $\overline{W}$, I_D^W, $I_D^{\overline{W}}$, $^1\chi$ and $^1\chi^v$ have been evaluated by using methods reported earlier[11]. For evaluation of V_c and V_{bc} the constitutional graph of a molecule is

considered where weightage to each constituting atom other than hydrogen is assigned as (Z_i-H) where Z_i is the valence of atom Z and, H is the number of hydrogen atom attached to it[11].

An illustration for evaluation of V_c and V_{bc} of *iso*-butanol is given below. In the constitutional graph the weights are given to each atom (vertex).

Illustration



Constitutional molecular graph of *iso*-butanol where the vertex weight is given by using the equation ($\delta_i^v = Z_i - H_i$).

$$V_c = \sum_{i=1}^{n} a_i \quad \text{... (4)}$$

$$a_i = \sum_{i=1}^{n} \prod_{i=1}^{n} \delta_i^{-1/2}$$

where n is the number of atoms other than hydrogen; and

$$V_{bc} = \sum_{i=1}^{k} \left(a_i a_j\right)^{-1/2} \quad \text{... (5)}$$

where k is the number of bonds and i and j are the adjacent atoms.

The ThOD and molecular parameters, calculated by the above methods are given in **Tables II** and **III**.

Multiple regression analysis was used to construct the regression models and the models were tested from student 't' test, F-statistics and correlation coefficient 'r'. In the regression model N stands for number of data points and RMS for root mean square.

Results and Discussion

Interrelationship of molecular parameters

The correlation matrix of BOD, ThOD and all molecular parameters is presented in **Table IV**. Among all parameters V_{bc} is found to correlate well with the BOD values (r = -0.3176) as well as with ThOD (r = -0.3813).

In each class of parameters the constituent parameters have correlation coefficients in the range of 0.5922-0.9925 except among IC and ThOD. Information content parameters derived from total molecular graph, do not correlate well with any of the molecular parameters. However, SIC and CIC have a good interrelationship with r = 0.9296. Similarly, ThOD derived from complete molecular formula, does not have good correlation with any other parameters (r = -0.0089 to - 0.4038). As the value depends on the constitution of the molecule, one can assume a good quantitative relationship of ThOD with the TIs. A multiple regression analysis of all the parameters evaluated here, with ThOD, however, resulted in a correlation coefficient of 0.8608 and F of 3.812. A large number of variables have 't' values less than 1. By excluding these variables a relatively good regression model is obtained (Eqn 6) with r = 0.8331 and F = 13.61 with 't' values greater than 1.8. The TIs, which contribute the most, are based on valence terms, which differentiate hetero-atoms from carbon.

$$\text{ThOD} = -0.038 + (2.682\pm1.251)\,\text{SIC} + (0.291\pm0.158)\,I_D^W + (0.796\pm0.246)\,{}^1\chi^v - (0.707\pm0.124)\,V_{bc} \quad \text{... (6)}$$

N= 29, r = 0.8331, F = 13.61, RMS = 0.101

To ordinate the parameters, the parameters have been subjected to principal component analysis (PCA). PCA helps in generating new parameters, which contain the characteristics of all the parameters to some extent and thus reduces the number of parameters. The results of PCA (**Table V**) reveal that the first principal component (PC_1) can explain 64.3% variance of the total data set whereas 97.5% variance can be explained by considering first five principal components (PC_1 to PC_5). The principal components are further correlated with the molecular parameters to find out the contribution of each parameter in corresponding PC (**Table VI**). This analysis also enables to classify the parameters into subgroups. The results reveal that IC constitutes a single class whereas ThOD, CIC and SIC can be clubbed to one class and all the other parameters constitute another class.

Interrelationship of BOD with ThOD

From the scatter plot of BOD and ThOD (**Figure 1**) the alcohols are further classified into four sets.

When subjected to multiple regression analysis the BOD data of set I (**Table VII**) are found to correlate well with ThOD value (r = 0.98) with a slope of 0.9389 and intercept –0.3790 (Eqn 7). The slope ensures the complete decomposition of organic materials of this set by the concerned micro-organisms within the stipulated time period. This set

Table II — IC, SIC, CIC, W, $\overline{W}$ and I_D^W values of 29 different alcohols

Sl.No	Compd	IC	SIC	CIC	$\overline{W}$	W	I_D^W
1	Methanol	1.7925	0.6934	0.7925	1.00	0.0000	0.0000
2	Ethanol	1.8800	0.5931	1.2900	4.00	1.3333	6.0000
3	2-Chloroethanol	1.8800	0.5931	1.2900	10.00	1.6666	24.4644
4	Ethylene glycol	1.9219	0.5785	1.4000	10.00	1.6666	24.4644
5	Ethanol amine	2.5503	0.7372	0.9091	10.00	1.6666	24.4644
6	Allyl alcohol	2.1610	0.6505	1.1610	10.00	1.6666	24.4644
7	*iso*-Propanol	1.7807	0.4967	1.8043	9.00	1.5000	22.5293
8	Ethylene glycol monomethyl ether	2.0349	0.5499	1.6655	20.00	2.0000	62.9288
9	Glycerol	2.1560	0.5663	1.6514	31.00	2.0667	116.5605
10	*n*-Butanol	1.8716	0.4790	2.0353	20.00	2.0000	62.9288
11	*sec*-Butanol	1.8716	0.4790	2.0353	18.00	1.8000	57.5489
12	*iso*-Butanol	1.8716	0.4790	2.0353	18.00	1.800	57.5489
13	Ethylene glycol mono ethyl ether	1.9197	0.4799	2.0803	35.00	2.3333	129.6505
14	Diethylene glycol	1.9698	0.4819	2.1176	56.00	2.6667	233.4633
15	Diethanol amine	2.3921	0.5737	1.7777	56.00	2.6667	233.4633
16	Furfuril alcohol	2.6535	0.7171	1.0469	51.00	2.4286	222.2741
17	1-Pentanol	1.7917	0.4297	2.3783	35.00	2.3333	129.6505
18	*iso*-Amyl alcohol	1.9447	0.4664	2.2252	32.00	2.1333	119.7353
19	2-Isopropoxy ethanol	2.0346	0.4789	2.2133	52.00	2.4762	218.184
20	Phenol	1.9143	0.5173	1.7861	88.00	2.4444	443.3713
21	Resorcinol	2.3513	0.6175	2.0000	61.00	2.1786	284.4908
22	Quinol	2.2359	0.5872	1.5714	62.00	2.2143	288.2663
23	Phloroglucinol	2.3219	0.5943	1.5850	84.00	2.3333	422.1607
24	Cyclohexanol	1.6341	0.3847	2.6139	42.00	2.0000	178.7029
25	Diacetone alcohol	2.1815	0.5047	2.1404	66.00	2.3571	307.1556
26	*d*-Gluconic acid	2.4627	0.5303	2.1812	200.0	2.5641	1191.087
27	Butyl cellosolve	1.9658	0.4408	2.4937	84.00	3.0000	383.6803
28	Hexylene glycol	2.1060	0.4723	2.3534	66.00	2.3570	307.1556
29	Diethylene glycol mono ethyl ether	1.8403	0.4068	2.6833	120.0	3.3333	590.0267

Table III — $\bar{I}_D{}^w$, $^1I_D{}^w$, $^1\chi$, $^1\chi^v$, V_c and V_{bc} values of 29 different alcohols

Sl.No.	Compd	$\bar{I}_D{}^w$	$^1I_D{}^w$	$^1\chi$	$^1\chi^v$	V_c	V_{bc}
1	Methanol	0.0000	0.0000	1.000	0.4472	2.3416	0.8789
2	Ethanol	1.5000	2.0000	1.4142	1.0233	4.8334	1.2660
3	2-Chloroethanol	2.4464	4.0774	1.9142	1.0835	5.4006	2.1253
4	Ethylene glycol	2.4464	4.0774	1.9142	1.1324	5.6679	2.0238
5	Ethanol amine	2.4464	4.0774	1.9142	1.2245	6.1705	1.8735
6	Allyl alcohol	2.4464	4.0774	1.9142	1.1327	5.9049	1.9858
7	*iso*-Propanol	2.5032	3.7549	1.4689	1.4129	8.0378	1.5539
8	Ethylene glycol monomethyl ether	3.1464	6.2929	2.4142	1.5131	9.4764	2.4098
9	Glycerol	3.7600	7.7707	2.8081	1.7071	9.6284	2.9263
10	*n*-Butanol	3.1464	6.2929	2.4142	2.0233	10.7928	1.8682

— Contd

Table III — $\bar{I}_D{}^W$, $^1I_D{}^W$, $^1\chi$, $^1\chi^v$, V_c and V_{bc} values of 29 different alcohols — *Contd*

Sl.No.	Compd	$\bar{I}_D{}^W$	$^1I_D{}^W$	$^1\chi$	$^1\chi^v$	V_c	V_{bc}
11	*sec*-Butanol	3.1972	5.7549	2.2700	1.9509	11.5879	1.7960
12	*iso*-butanol	3.1972	5.7549	2.2700	1.8792	11.3732	1.8120
13	Ethylene glycol mono ethyl ether	3.7043	8.64337	2.9142	2.1007	10.8987	2.7802
14	Diethylene glycol	4.1689	11.1173	3.4142	2.2098	11.6124	3.5320
15	Diethanol amine	4.1689	11.1173	3.4142	2.3396	12.4507	3.2974
16	Furfuril alcohol	4.3583	10.5843	3.4318	2.0649	11.3339	4.2480
17	1-Pentanol	3.7043	8.6433	2.9142	2.5233	13.7067	2.2125
18	*iso*-Amyl alcohol	3.7417	7.9823	2.7700	2.3792	14.4222	2.1335
19	2-Isopropoxy ethanol	4.1958	10.3897	2.1927	2.4953	14.8089	3.0625
20	Phenol	5.0383	12.3159	3.3938	2.1343	12.0231	4.0044
21	Resorcinol	4.6638	10.1604	3.7877	2.2686	13.4400	4.6058
22	Quinol	4.6494	10.2952	3.7877	2.2686	13.9204	4.5041
23	Phloroglucinol	5.0257	11.7267	4.1815	2.4029	14.5692	4.7568
24	Cyclohexanol	4.2548	8.5097	3.3938	3.0747	17.6806	2.7403
25	Diacetone alcohol	4.6539	10.9698	3.4165	2.6348	18.6833	2.8319
26	*d*-Gluconic acid	5.9550	15.2703	5.9128	3.4737	21.4759	6.7183
27	Butyl cellosolve	4.5676	13.7029	3.6503	3.1007	16.7272	3.4441
28	Hexylene glycol	4.6539	10.9698	3.4165	2.8209	18.6417	2.9801
29	Diethylene glycol mono ethyl ether	4.9169	16.3896	4.4142	3.1780	16.6401	4.3984

Table IV — Cross-correlation matrix of TIs for a set of alcohols

	BOD	ThOD	IC	SIC	CIC	W	W	$I_D{}^W$	$\bar{I}_D{}^w$	$^1I_D{}^w$	$^1\chi$	$^1\chi^v$	V_c	V_{bc}
BOD	1													
ThOD	0.312	1												
IC	-0.235	0.039	1											
SIC	-0.090	-0.432	-0.125	1										
CIC	-0.015	0.404	0.143	-0.930	1									
W	-0.275	-0.249	0.025	-0.264	0.476	1								
W	-0.253	0.092	0.119	-0.490	0.666	0.673	1							
$I_D{}^W$	-0.259	-0.293	0.004	-0.214	0.416	0.992	0.592	1						
$\bar{I}_D{}^w$	-0.262	-0.008	0.082	-0.394	0.616	0.823	0.875	0.768	1					
^1I_D	-0.297	-0.032	0.098	-0.419	0.640	0.877	0.912	0.813	0.943	1				
$^1\chi$	-0.303	-0.180	-0.130	-.281	0.523	0.925	0.763	0.895	0.913	0.915	1			
$^1\chi^v$	-0.230	0.221	0.112	-0.940	0.835	0.793	0.825	0.738	0.885	0.900	0.854	1		
V_c	-0.265	0.216	0.097	-0.596	0.796	0.781	0.744	0.735	0.878	0.856	0.840	0.972	1	
V_{bc}	-0.318	-0.381	0.021	-0.050	0.302	0.903	0.681	0.885	0.866	0.855	0.932	0.695	0.678	1

of compounds contains the aliphatic alcohols, and hydroxy aromatic compounds like phenol and resorcinol.

$$BOD = -(0.3790 \pm 0.1113) + (0.9389 \pm 0.0574)\ ThOD \quad \ldots (7)$$

$r = 0.98$, $F = 267.1$, $RMS = 0.0139$

The second set of alcohols contains relatively complex alcohols and the BOD values are found to be significantly less than the ThOD values. In this set also a good correlation between BOD and ThOD is obtained with $r = 0.99$ (Eqn 8) (**Table VIII**). Plot of observed *vs*. predicted BOD values of two sets of alcohols is shown in **Figure 2**. Thus this set of

Table V — Eigen values, percent of variance and cumulative percent of variance of molecular parameters in principal component analysis

Molecular Parameters	Eigen values	Percent of variance	Cumulative percent of variance
PC_1	8.353	64.3	64.3
PC_2	2.341	18.0	88.3
PC_3	1.012	7.8	90.0
PC_4	0.5496	4.2	94.3
PC_5	0.4137	3.2	97.5
PC_6	0.1615	1.2	98.7
PC_7	0.0679	0.5	99.2
PC_8	0.0434	0.3	99.6
PC_9	0.0267	0.2	99.8
PC_{10}	0.0196	0.2	100.0
PC_{11}	0.0061	0.0	100.0
PC_{12}	0.0056	0.0	100.0
PC_{13}	0.0001	0.0	100.0

Table VI — Correlation coefficient of the TIs with PC_1, PC_2 and PC_3

Molecular parameters	PC_1	PC_2	PC_3
ThOD	0.0175	-0.7323	0.6002
IC	-0.2817	0.7938	0.5018
SIC	0.4817	0.8327	0.2365
CIC	-0.7028	-0.6799	-0.0886
W	-0.9150	0.2486	-0.1992
$\overline{W}$	-0.8649	-0.1059	0.1969
$I_D{}^W$	-0.8690	0.2947	-0.2475
$\bar{I}_D{}^W$	-0.9563	0.0576	0.1397
$I_D{}^W{}_1$	-0.9705	0.0404	0.0555
$^1\chi$	-0.9526	0.2510	-0.0326
$^1\chi^v$	-0.9494	-0.2518	0.0837
V_c	-0.9258	-0.2186	0.1051
V_{bc}	-0.8650	0.4543	-0.0703

alcohols can be considered under moderately biodegradable chemicals.

$$BOD = (0.1994\pm0.0163)\ ThOD + (0.1650\pm0.0322) \quad \ldots (8)$$

$r = 0.99$, $F = 150.2$, RMS = 0.0002

The alcohols having a wide difference of BOD and ThOD values constitute the third set of the series. This set contains the nitrogenous compounds and also compounds with higher complexity than sets I and II. The BOD values are low (0.02 to 0.379). The ThOD does not correlate well with the BOD values ($r = 0.45$). Similarly, the fourth set contains four alcohols with BOD values ranging from 1.00 to 1.61 and ThOD varies from 1.89 to 2.7. In this set also the correlation between BOD and ThOD is poor ($r = 0.201$).

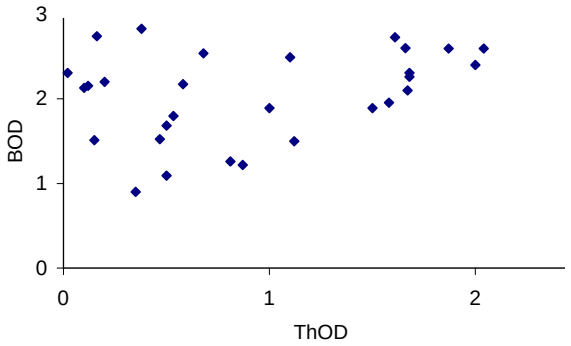


Figure 1 — Classification of alcohols from the plot of BOD *vs.* ThOD

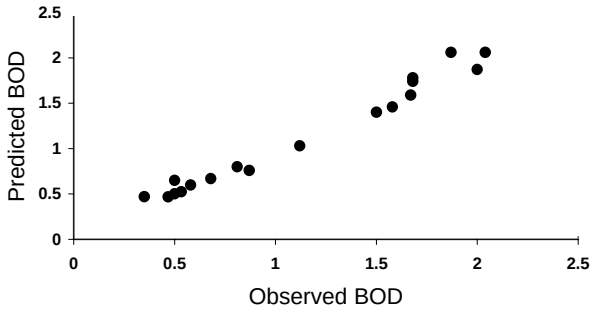


Figure 2 — Plot of observed *vs.* predicted BOD of two sets of alcohols

Table VII — Results of multiple regression analysis of data set I

Compd	Observed BOD	Predicted BOD
1	1.12	1.03
2	1.67	1.59
3	0.50	0.65
4	0.81	0.80
7	2.00	1.87
9	0.87	0.76
10	2.04	2.06
11	1.87	2.06
13	1.58	1.46
20	1.68	1.74
21	1.50	1.40
26	0.35	0.47
27	1.68	1.78

Table VIII — Results of multiple regression analysis of data set II

Compd	Observed BOD	Predicted BOD
8	0.500	0.501
16	0.534	0.523
23	0.468	0.469
25	0.680	0.671
29	0.580	0.598

Multiple regression analysis with molecular parameters

When all the BOD values were subjected to multiple regression analysis with the TIs a poor correlation coefficient (r = 0.6747) was obtained. Hence subsequently, the BOD values of individual set of compounds were analysed separately.

The BOD values of first set of compounds have a correlation coefficient of 0.999 with all the TIs but some TIs have 't' values less than 2.0 (selection of 2.0 is arbitrary). By excluding these variables an optimized equation is obtained with r = 0.999 and F = 138.1.

With a view to reducing the size of molecular parameters, principal components of the topological parameters have been derived and used in multiple regression analysis for each set of alcohols.

The first four principal components have been correlated with the BOD values to be assured that BOD values have some topological contributions. In the first set of data PC_1, PC_3 and PC_4 could explain the result significantly to an extent of 98%. All the PCs have significant 't' values ranging from 3.74 - 8.50. PC_2, which has a major contribution from ThOD and information contents exhibits a poor 't' value. Thus it can be suggested that molecular topology also contributes to the BOD values of this set of alcohols.

But in case of set II, the major contribution is due to PC_2 and PC_4 having 't' values –7.97 and 5.27, respectively. These principal components have major contributions from ThOD and information contents (SIC and CIC).

Thus the alcohols of set I can be classified as highly degradable, those of set II as moderately degradable and the rest as low-degradable alcohols.

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