Journal of Hazardous Materials, 13 (1986) 147–159
Elsevier Science Publishers B.V., Amsterdam — Printed in The Netherlands

EVALUATION OF BIODEGRADATION RANKS OF PRIORITY ORGANIC COMPOUNDS

KOHEI URANO and ZENJI KATO

Department of Safety and Environmental Engineering, Yokohama National University, Hodogaya-ku, Yokohama (Japan)

(Received June 20, 1985; accepted in revised form September 3, 1985)

Summary

Biodegradations of 78 priority organic compounds were tested with an electrolytic respirometer under the standard conditions determined in the preceding paper. The biodegradabilities of these numerous compounds were classified into ten ranks by the method proposed in the preceding paper. The results are discussed from the structures of the organic compounds and conventional knowledge on the biodegradation mechanisms, and propriety of the classification method for evaluating the biodegradabilities are substantiated.

Introduction

Synthetic organic compounds cause various environmental problems. Biodegradability is a most important characteristic of an organic compound for predicting its influence on the environment. A new method to evaluate the biodegradabilities of organic compounds was outlined in our previous paper [1]. In the proposed method, organic compounds could be classified into 10 biodegradability ranks by tests with an electrolytic respirometer. In this study, the biodegradabilities of 78 organic compounds are evaluated by the new method. The results are discussed from the structures of the organic compounds and conventional knowledge on the biodegradation mechanisms [2], and the suitability of the progressed method is substantiated.

Materials and methods

Aqueous solutions of 78 organic compounds whose names and properties are listed in Table 1 were used in this study. The sample number in Table 1 for each compound is used in the following figures and tables.

The electrolytic respirometer for the biodegradation tests and the testing procedures were the same as described in the preceding paper [1]. The test conditions which were determined in the preceding study are shown again in Table 2 because the test conditions exert a significant influence on the

0304-3894/86/$03.50

TABLE 1

Properties of organic compounds employed

Number	Compound name	Molecular formula	ThOD (g/g)	DOC (g/g)
1	D-(+)-Xylose	$C_5H_{10}O_5$	1.07	0.40
2	D-(+)-Glucose	$C_6H_{12}O_6$	1.07	0.40
3	L-α-Alanine	$C_2H_4(NH_2)COOH$	1.35	0.40
4	L-Glutamic acid	$C_2H_4(COOH)CH(NH_2)COOH$	1.37	0.41
5	Ethylalcohol	C_2H_5OH	2.08	0.52
6	n-Butylalcohol	C_4H_9OH	2.59	0.65
7	iso-Butylalcohol	$C_2H_4(CH_3)CH_2OH$	2.59	0.65
8	Ethylene glycol	$C_2H_4(OH)_2$	1.29	0.39
9	Glycerol	$CH(CH_2OH)_2OH$	1.22	0.39
10	Acetic acid	CH_3COOH	1.07	0.53
11	Propionic acid	C_2H_5COOH	1.51	0.49
12	n-Butyric acid	C_3H_7COOH	1.82	0.55
13	n-Valeric acid	C_4H_9COOH	2.04	0.59
14	iso-Valeric acid	$CH(CH_3)_2COOH$	2.04	0.59
15	Adipic acid	$C_4H_8(COOH)_2$	1.40	0.49
16	Sodium stearate	$C_{17}H_{35}COONa$	2.68	0.69
17	Sodium oleate	$C_9H_{18}C_8H_{16}COONa$	2.68	0.71
18	Propionaldehyde	C_2H_5CHO	2.48	0.62
19	n-Butylaldehyde	C_3H_7CHO	2.44	0.67
20	Acetone	CH_3COCH_3	2.20	0.62
21	Methylethylketone	$CH_3COC_2H_5$	2.44	0.67
22	Ethylacetate	$CH_3COOC_2H_5$	1.82	0.55
23	n-Butylacetate	$CH_3COOC_4H_9$	2.20	0.62
24	Ethylether	$C_2H_5OC_2H_5$	2.59	0.65
25	n-Propylether	$C_3H_7OC_3H_7$	2.82	0.71
26	Hexaoxyethylene-hexylether	$C_6H_{13}O(C_2H_4O)_6H$	1.32	0.74
27	n-Hexylamine	$C_6H_{13}NH_2$	3.40	0.71
28	Hexamethylene-diamine	$C_6H_{12}(NH_2)_2$	3.30	0.62
29	Monoethanolamine	$C_2H_4(NH_2)OH$	2.23	0.39
30	Acetonitrile	CH_3CN	3.92	0.59
31	Acetamide	CH_3CONH_2	2.03	0.41
32	Tetramethyl-ammoniumchloride	$(CH_3)_4NCl$	2.26	0.44
33	Sodium dodecyl-sulfate	$C_{12}H_{25}OSO_3Na$	2.02	0.50
34	Sodium pentaoxy-ethylenedodecyl-sulfate	$C_{12}H_{25}O(C_2H_4O)_5SO_3Na$	1.93	0.52
35	Sodium α-tetra-decenesulfonate	$C_{14}H_{27}SO_3Na$	2.27	0.56
36	Benzene	C_6H_6	3.07	0.92
37	Chlorobenzene	C_6H_5Cl	1.78	0.53
38	Fluorobenzene	C_6H_5F	2.41	0.75
39	Benzoic acid	C_6H_5COOH	1.97	0.69
40	Benzaldehyde	C_6H_5CHO	2.41	0.79

Table 1 (continued)

Number	Compound name	Molecular formula	ThOD (g/g)	DOC (g/g)
41	Benzylalcohol	$C_6H_5CH_2OH$	2.52	0.78
42	Toluene	$C_6H_5CH_3$	3.13	0.91
43	Benzonitrile	C_6H_5CN	2.87	0.82
44	Acetophenone	$C_6H_5COCH_3$	2.53	0.80
45	Phenol	C_6H_5OH	2.38	0.77
46	Aniline	$C_6H_5NH_2$	3.01	0.77
47	Benzenesulfonic acid	$C_6H_5SO_3H$	2.33	0.46
48	Nitrobenzene	$C_6H_5NO_2$	1.88	0.59
49	Ethylphenylether	$C_6H_5OC_2H_5$	2.62	0.79
50	Benzenesulfoamide	$C_6H_5SO_2NH_2$	1.78	0.46
51	Phenylacetate	$C_6H_5OCOCH_3$	2.11	0.71
52	Acetanilide	$C_6H_5NHCOCH_3$	2.54	0.71
53	Benzyltrimethylammoniumchloride	$C_6H_5(CH_3)_3NCl$	2.61	0.63
54	*o*-Hydroxybenzoic acid	$o\text{-}C_6H_4(OH)COOH$	1.62	0.62
55	*m*-Hydroxybenzoic acid	$m\text{-}C_6H_4(OH)COOH$	1.62	0.62
56	*p*-Hydroxybenzoic acid	$p\text{-}C_6H_4(OH)COOH$	1.62	0.62
57	*o*-Aminobenzoic acid	$o\text{-}C_6H_4(NH_2)COOH$	2.04	0.61
58	*m*-Aminobenzoic acid	$m\text{-}C_6H_4(NH_2)COOH$	2.04	0.61
59	*p*-Aminobenzoic acid	$p\text{-}C_6H_4(NH_2)COOH$	2.04	0.61
60	*o*-Nitrobenzoic acid	$o\text{-}C_6H_4(NO_2)COOH$	1.38	0.50
61	*m*-Nitrobenzoic acid	$m\text{-}C_6H_4(NO_2)COOH$	1.38	0.50
62	*p*-Nitrobenzoic acid	$p\text{-}C_6H_4(NO_2)COOH$	1.38	0.50
63	*o*-Aminophenol	$o\text{-}C_6H_4(NH_2)OH$	2.42	0.66
64	*m*-Aminophenol	$m\text{-}C_6H_4(NH_2)OH$	2.42	0.66
65	*p*-Aminophenol	$p\text{-}C_6H_4(NH_2)OH$	2.42	0.66
66	*o*-Nitrophenol	$o\text{-}C_6H_4(NO_2)OH$	1.55	0.52
67	*m*-Nitrophenol	$m\text{-}C_6H_4(NO_2)OH$	1.55	0.52
68	*p*-Nitrophenol	$p\text{-}C_6H_4(NO_2)OH$	1.55	0.52
69	*o*-Nitroaniline	$o\text{-}C_6H_4(NO_2)NH_2$	1.97	0.52
70	*m*-Nitroaniline	$m\text{-}C_6H_4(NO_2)NH_2$	1.97	0.52
71	*p*-Nitroaniline	$p\text{-}C_6H_4(NO_2)NH_2$	1.97	0.52
72	*p*-Pentaoxyethylene nonylphenylether	$p\text{-}C_6H_4(C_9H_{19})(C_2H_4O)_5H$	2.40	0.72
73	*m*-Aminobenzene-sulfonic acid	$m\text{-}C_6H_4(NH_2)SO_3H$	1.53	0.42
74	*p*-Phenolsulfonic acid	$p\text{-}C_6H_4(OH)SO_3H$	1.19	0.41

Table 1 (continued)

Number	Compound name	Molecular formula	ThOD (g/g)	DOC (g/g)
75	*p*-Toluenesulfonic acid	$p\text{-}C_6H_4(CH_3)SO_3H$	1.43	0.44
76	*p*-Dodecylbenzene-sulfonic acid	$p\text{-}C_6H_4(C_{12}H_{25})SO_3H$	2.53	0.66
77	β-Naphthol	$\beta\text{-}C_{10}H_7OH$	2.77	0.83
78	β-Naphthalene-sulfonic acid	$\beta\text{-}C_{10}H_7SO_3H$	1.77	0.58

TABLE 2

Standard conditions for biodegradation tests

Concentration of compound	100 mg/l
pH of solution	7 ± 1
Concentration of activated sludge[a]	30 mg/l
Culture mediums	JIS inorganic mediums, 1 ml/300 ml
Temperature	20 ± 1°C
Period	within 14 days

[a] Not acclimatized sludge.

evaluation of the biodegradabilities. The measurements of the biochemical oxygen demand (BOD) curves and the concentrations of dissolved organic carbon (DOC) were repeated two or three times for the same compound, and the reproducibilities were confirmed.

Results and discussion

Sugars and aliphatic compounds

Examples of the BOD/ThOD curves of sugars and aliphatic compounds are shown in Figs. 1—4. The characteristic indexes of the lag time (t_l), the rate constant (k) for the geometrical biodegradation, the biodegradation time (t_d) before the endogenous respiration period, the degradation ratio at t_d (BOD_d/ThOD), and the DOC ratio at t_d (DOC_d/DOC_0) are listed in Table 3. The biodegradation ranks of those compounds were determined by the new method proposed in the preceding paper and are also shown in Table 3.

Biodegradation ranks of sugars and amino acids

The biodegradation ranks of the sugars were A-a. It is generally known that sugars are easily biodegraded through the Embdem—Meyerhof path-

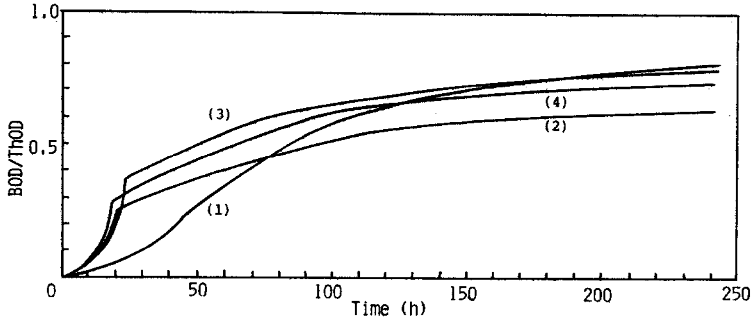

Fig. 1. Change of BOD/ThOD with time for xylose (1), glucose (2), alanine (3) and glutamic acid (4). (Numbers in Figs. 1—8 show compound numbers which are the same as in Table 1.)

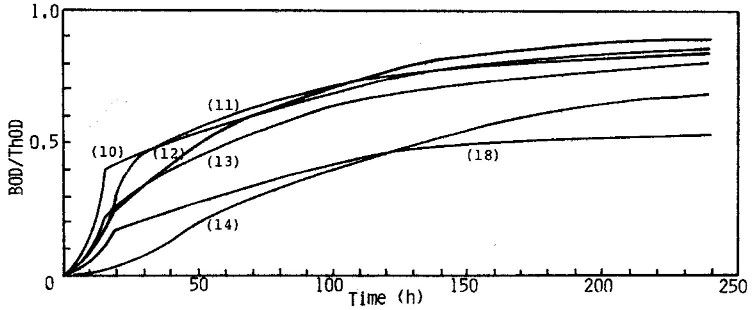

Fig. 2. Change of BOD/ThOD with time for acetic acid (10), propionic acid (11), n-butyric acid (12), n-valeric acid (13), iso-valeric acid (14), and propionaldehyde (18).

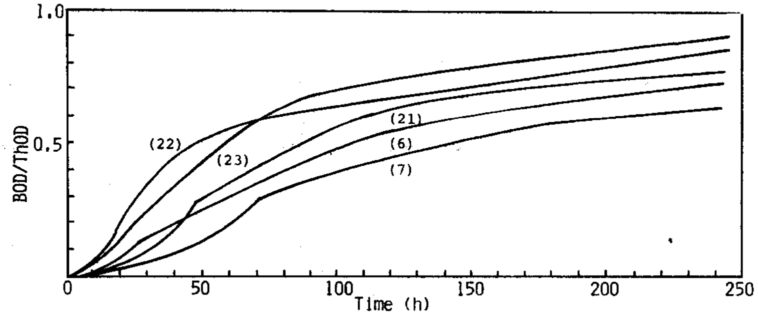

Fig. 3. Change of BOD/ThOD with time for n-butylalcohol (6), iso-butylalcohol (7), methylethylketone (21), ethylacetate (22), and n-butylacetate (23).

way, the pentose—phosphate pathway or the Entner—Doudoroff pathway, and the TCA cycle.

The biodegradation ranks of the amino acids were also A-a. It is known that amino acids are easily biodegraded through deamination, the glycolytic pathway, and the TCA cycle.

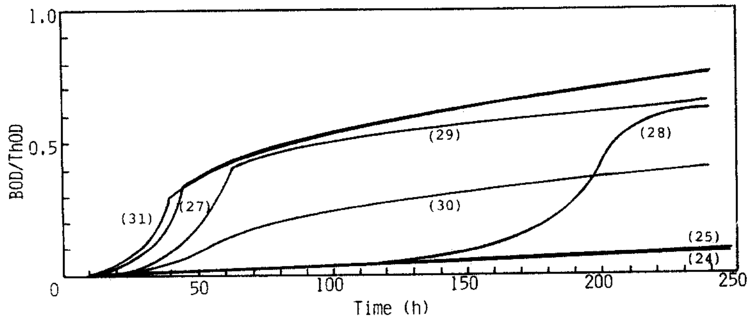

Fig. 4. Change of BOD/ThOD with time for ethylether (24), n-propylether (25), n-hexylamine (27), hexamethylenediamine (28), monoethanolamine (29), acetonitrile (30), and acetamide (31).

Biodegradation ranks of carboxylic acids, aldehydes, and alcohols

The biodegradation ranks of most of the carboxylic acids were A-a, but the rank of iso-valeric acid was B-a, and the ranks of sodium stearate and sodium oleate were also B-a. It is known that linear carboxylic acids are easily biodegraded through β-oxidation and the TCA cycle. Branched carboxylic acids, however, are known to be biodegraded through α-oxidation, β-oxidation, and the TCA cycle [3]. Because of these many steps, the biodegradation times of the branched compounds may be longer than those of the linear compounds. Sodium stearate and sodium oleate formed insoluble salts with the inorganic culture mediums, but those fatty acid salts were easily biodegraded by adding sodium tripolyphosphate for the masking of the hardness ions in the inorganic mediums [4]. Therefore, the reason for the large t_d of these fatty acid salts is the formation of insoluble salts with inorganic mediums, and those compounds are substantially biodegradable. In specific cases like this, the conditions of the biodegradation test should be appropriately altered.

The biodegradation ranks of the linear aldehydes were A-a. It is generally known that aldehydes are oxidized into carboxylic acids and are then biodegraded further. Therefore, the lower biodegradation ranks of branched aldehydes may be the same as of branched carboxylic acid. Further, several aldehydes may not be biodegraded because of their toxicity to microorganisms.

The biodegradation ranks of the linear alcohols were A-a, but the rank of a branched alcohol, iso-butylalcohol, was B-a. It is generally known that alcohols are also oxidized into carboxylic acids through aldehydes, and are then biodegraded further. The cause of the lower biodegradation rank of iso-butylalcohol is the same as the case of the branched carboxylic acids.

Biodegradation ranks of ketones, esters, and ethers

The biodegradation ranks of acetone and methylethylketone were B-b and A-a, respectively. It is generally known that ketones are changed into

TABLE 3

Characteristic indexes and biodegradation ranks of sugars and aliphatic compounds

Compound number	t_l (h)	k (h^{-1})	t_d (h)	$\frac{BOD_d}{ThOD}$	$\frac{DOC_d}{DOC_0}$	Biodegradation rank
1	5 ~ 10	0.032 ~ 0.047	100 ~ 110	0.46 ~ 0.56	0.11 ~ 0.21	A-a
2	~5	0.050 ~ 0.076	120 ~ 130	0.44 ~ 0.54	0.06 ~ 0.19	A-a
3	~5	0.051 ~ 0.078	80 ~ 90	0.40 ~ 0.53	0.11 ~ 0.26	A-a
4	5 ~ 10	0.095 ~ 0.11	100 ~ 130	0.58 ~ 0.60	0.20 ~ 0.24	A-a
5	5 ~ 10	0.043 ~ 0.055	90 ~ 120	0.42 ~ 0.51	0.13 ~ 0.14	A-a
6	5 ~ 10	0.036 ~ 0.046	70 ~ 100	0.42 ~ 0.57	0.17 ~ 0.28	A-a
7	5 ~ 10	0.015 ~ 0.020	140 ~ 185	0.54 ~ 0.55	0.07 ~ 0.14	B-a
8	10 ~ 15	0.026 ~ 0.035	70 ~ 90	0.69 ~ 0.81	0.06 ~ 0.11	A-a
9	~5	0.050 ~ 0.078	60 ~ 70	0.52 ~ 0.62	0.06 ~ 0.07	A-a
10	~5	0.066 ~ 0.074	135 ~ 140	0.73 ~ 0.81	0.27 ~ 0.31	A-a
11	~5	0.051 ~ 0.069	100 ~ 135	0.68 ~ 0.83	0.06 ~ 0.14	A-a
12	~5	0.047 ~ 0.067	135 ~ 145	0.58 ~ 0.82	0.10 ~ 0.24	A-a
13	~5	0.070 ~ 0.072	120 ~ 160	0.55 ~ 0.79	0.11 ~ 0.17	A-a
14	5 ~ 10	0.016 ~ 0.022	185 ~ 200	0.58 ~ 0.66	0.19 ~ 0.39	B-a
15	10 ~ 15	0.044 ~ 0.060	90 ~ 100	0.50 ~ 0.75	0.12 ~ 0.21	A-a
16[a]	10 ~ 20	not obtained	90 ~ 120	0.20 ~ 0.35	—	B-b
17[a]	5 ~ 10	not obtained	80 ~ 130	0.25 ~ 0.45	—	B-b
18	~5	0.046 ~ 0.063	135 ~ 140	0.35 ~ 0.53	0.22 ~ 0.31	A-a
19	~5	0.044 ~ 0.069	90 ~ 135	0.46 ~ 0.57	0.21 ~ 0.30	A-a
20	20 ~ 25	0.016 ~ 0.020	155 ~ 210	0.42 ~ 0.74	0.19 ~ 0.22	B-a
21	~5	0.025 ~ 0.031	140 ~ 165	0.60 ~ 0.64	0.05 ~ 0.10	A-a
22	~5	0.042 ~ 0.051	50 ~ 70	0.43 ~ 0.53	0.08 ~ 0.15	A-a
23	~5	0.048 ~ 0.051	90 ~ 120	0.58 ~ 0.65	0.07 ~ 0.23	A-a
24	>240	—	—	—	—	D
25	>240	—	—	—	—	D
26	5 ~ 20	0.059 ~ 0.10	50 ~ 80	0.37 ~ 0.45	0.10 ~ 0.19	A-b
27	5 ~ 10	0.047 ~ 0.057	70 ~ 110	0.52 ~ 0.61	0.06 ~ 0.07	A-a
28	120 ~ 140	0.011 ~ 0.013	220 ~ 265	0.41 ~ 0.56	0.04 ~ 0.21	C-a
29	15 ~ 20	0.034 ~ 0.036	75 ~ 90	0.40 ~ 0.45	0.07 ~ 0.14	A-a
30	20 ~ 25	0.023 ~ 0.024	80 ~ 90	0.17 ~ 0.21	0.28 ~ 0.38	B-b
31	5 ~ 15	0.047 ~ 0.050	70 ~ 80	0.44 ~ 0.49	0.19 ~ 0.20	A-a
32	>240	—	—	—	—	D
33	5 ~ 15	0.078 ~ 0.098	60 ~ 80	0.46 ~ 0.55	0.10 ~ 0.15	A-a
34	30 ~ 50	0.050 ~ 0.060	100 ~ 150	0.20 ~ 0.25	0.50 ~ 0.65	B-c
35	10 ~ 25	0.015 ~ 0.025	100 ~ 120	0.28 ~ 0.35	0.28 ~ 0.35	B-b

[a] Formed insoluble salts with the inorganic culture mediums.

carboxylic acids by the following reactions, and are biodegraded further.

$$R{-}COCH_3 + O \rightarrow R{-}COCH_2OH + 3\ O \rightarrow R{-}COOH + CO_2 + H_2O \qquad (1)$$

Since several ketones, however, have weak toxicity to microorganisms, the biodegradation times of these compounds may be long.

The biodegradation ranks of the esters were A-a. It is known that esters are easily decomposed into alcohols and carboxylic acids by hydrolysis and are biodegraded further.

The biodegradation ranks of the two alkylethers were D. These ethers have not toxicity, but it is known that alkylethers are stable like alkylhydrocarbons, and are difficult to be biodegraded. The rank of dioxyethylenehexylether, a nonionic surfactant, was A-b. The reason for this slightly low degradation ratio may be that the polyoxyethylene group is difficult to be biodegraded [5].

Biodegradation ranks of nitrogen compounds

The biodegradation ranks of mono-amine and mono-amide were A-a, but the rank of diamine, hexamethylenediamine, was C-a. It is known that acetoamide is easily changed into acetic acid by deamination, and monoethanol amine is easily changed into acetoaldehyde by deamination, and then into acetic acid by oxidation. Hexylamine may be easily biodegraded by deamination and ω-oxidation. The reason for the long biodegradation time of hexamethylenediamine may be that the deamination-rate of diamine is low.

The biodegradation rank of a nitril was B-a. Since the biodegradation of a nitril may pass through amine, the biodegradation time may be longer than that of the amine.

Biodegradation ranks of sulfur compounds

The biodegradation ranks of the sulfonates and the sulfates were various. The rank of α-olefinesulfonate was B-b. It is known that aliphatic sulfonates are biodegraded into aldehyde and sulfite by the following reaction and are then biodegraded further [6].

$$\begin{aligned} \mathrm{R{-}CH_2CH_2SO_3Na + O} &\rightarrow \mathrm{R{-}CH_2CH(OH)SO_3Na} \\ &\rightarrow \mathrm{RCH_2CHO + NaHSO_3} \end{aligned} \tag{2}$$

Because of these many degradation steps, the biodegradation time of alifatic sulfonates may be slightly longer. The rank of the pentaoxyethylenedodecylsulfonate was B-c. The reason for its low biodegradation ratio may be that the polyoxyethylene group is difficult to be biodegraded. The rank of the dodecylsulfate was A-a. It is known that alkylsulfates are easily biodegraded into alcohol and inorganic sulfate, and are then biodegraded further.

Aromatic compounds

Examples of the BOD/ThOD curves for the aromatic compounds are shown in Figs. 5—8. The characteristic indexes of t_l, k, t_d, $\mathrm{BOD_d/ThOD}$ and $\mathrm{DOC_d/DOC_0}$ and the biodegradation ranks are listed in Table 4.

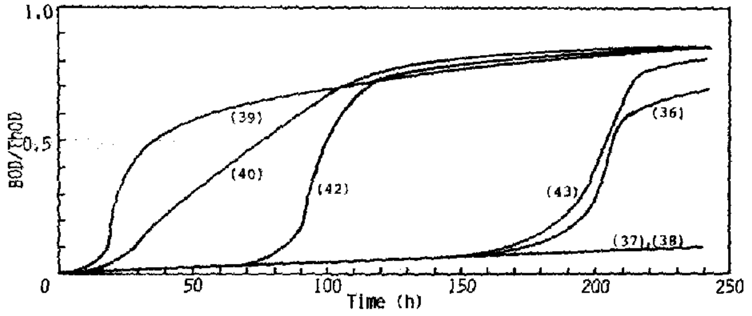

Fig. 5. Change of BOD/ThOD with time for benzene (36), chlorobenzene (37), fluorobenzene (38), benzoic acid (39), benzylalcohol (40), toluene (42), and benzonitrile (43).

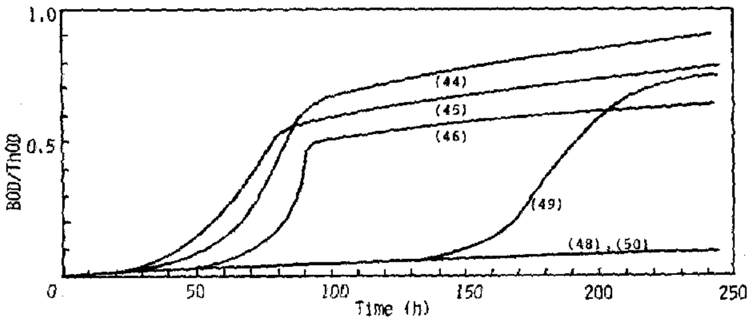

Fig. 6. Change of BOD/ThOD with time for acetophenone (44), phenol (45), aniline (46), nitrobenzene (48), ethylphenylether (49), and benzenesulfoamide (50).

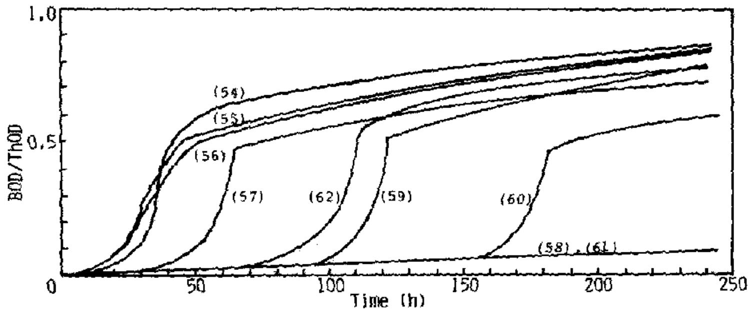

Fig. 7. Change of BOD/ThOD with time for *o*-hydroxybenzoic acid (54), *m*-hydroxybenzoic acid (55), *p*-hydroxybenzoic acid (56), *o*-aminobenzoic acid (57), *m*-aminobenzoic acid (58), *p*-aminobenzoic acid (59), *o*-nitrobenzoic acid (60), *m*-nitrobenzoic acid (61), and *p*-nitrobenzoic acid (62).

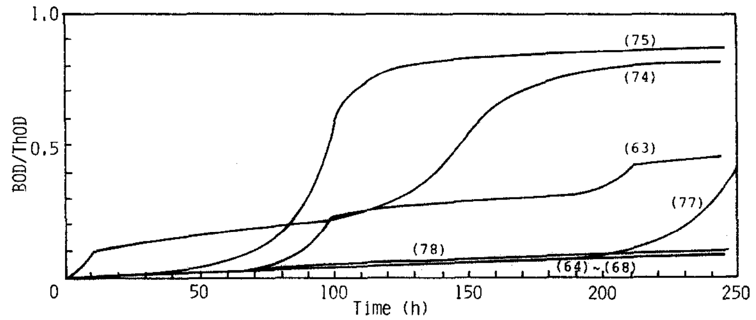

Fig. 8. Change of BOD/ThOD with time for *o*-aminophenol (63), *m*-aminophenol (64), *p*-aminophenol (65), *o*-nitrophenol (66), *m*-nitrophenol (67), *p*-nitrophenol (68), *p*-phenolsulfonic acid (74), *p*-toluenesulfonic acid (75), *β*-naphthol (77), and *β*-naphthalenesulfonic acid (78).

Biodegradation ranks of benzene and monosubstituted benzenes

The biodegradation ranks of benzoic acid, benzaldehyde, benzylalcohol, acetophenone, and phenol were A-a. The ranks of toluene, aniline, and acetoamide were B-a, and the ranks of benzene, benzonitrile, and phenylethylether were C-a. The ranks of phenylacetate and benzenesulfonate were A-c and C-c, respectively. The ranks of the other compounds, chlorobenzene, fluorobenzene, nitrobenzene, and benzenesulfoamide were D. It is known that most of the benzene substitutes are biodegraded by the two pathways through protocatechuic acid or catechol to the TCA cycle [7]. An intermediate, catechol, is known to be also biodegraded by another pathway through formic acid, pyruvic acid, and acetoaldehyde [8]. It is also known that several benzene substitutes are biodegraded by the pathway through phenol [9]. The monosubstituted benzenes whose carbon of the substituted groups combine with the benzene ring may be biodegraded through benzoic acid by oxidation. The biodegradation order of these monosubstituted benzenes were as follows, and this order seemed to agree with the order of easy oxidizing.

Benzoic acid > benzaldehyde > benzylalcohol
> acetophenone > toluene > benzonitrile

The other monosubstituted benzenes may be biodegraded through catechol by hydroxylation. Since the hydroxylation is an electron-attractive reaction, the compounds which have electron-repellent groups may be biodegraded easily. Hansch et al. [10] reported that the electron-repellent strength of the substituted group might be related with the values of F constant which are shown in Table 5 for each of the substituted groups. From this table, it was found that the monosubstituted benzenes, whose values of F constant were smaller than 0.3, were more biodegradable than benzene, but the compounds of larger F constants were less biodegradable than benzene.

TABLE 4

Characteristic indexes and biodegradation ranks of aromatic compounds

Compound number	t_l (h)	k (h^{-1})	t_d (h)	$\frac{BOD_d}{ThOD}$	$\frac{DOC_d}{DOC_0}$	Biodegradation rank
36	100 ~ 140	0.051 ~ 0.057	200 ~ 220	0.41 ~ 0.59	0.03 ~ 0.09	C-a
37	>240	—	—	—	—	D
38	>240	—	—	—	—	D
39	5 ~ 20	0.11 ~ 0.12	65 ~ 80	0.61 ~ 0.69	0.03 ~ 0.07	A-a
40	5 ~ 10	0.065 ~ 0.074	100 ~ 130	0.77 ~ 0.85	0.03 ~ 0.09	A-a
41	5 ~ 15	0.042 ~ 0.062	130 ~ 200	0.79 ~ 0.87	0.05 ~ 0.18	A-a
42	45 ~ 60	0.057 ~ 0.074	130 ~ 135	0.67 ~ 0.74	0.03 ~ 0.07	B-a
43	130 ~ 145	0.036 ~ 0.037	220 ~ 240	0.70 ~ 0.71	0.09 ~ 0.10	C-a
44	15 ~ 20	0.029 ~ 0.042	85 ~ 115	0.65 ~ 0.73	0.05 ~ 0.08	A-a
45	15 ~ 25	0.025 ~ 0.028	85 ~ 105	0.52 ~ 0.62	0.05 ~ 0.09	A-a
46	50 ~ 55	0.042 ~ 0.046	110 ~ 130	0.47 ~ 0.49	0.10 ~ 0.18	B-a
47	100 ~ 110	0.013 ~ 0.034	170 ~ 180	0.12 ~ 0.27	0.49 ~ 0.73	C-c
48	>240	—	—	—	—	D
49	130 ~ 150	0.024 ~ 0.036	225 ~ 270	0.52 ~ 0.69	0.03 ~ 0.15	C-a
50	>240	—	—	—	—	D
51	~ 5	0.060 ~ 0.064	30 ~ 50	0.13 ~ 0.16	0.39 ~ 0.44	A-c
52	20 ~ 30	0.022 ~ 0.025	130 ~ 140	0.66 ~ 0.69	0.05 ~ 0.18	B-a
53	>240	—	—	—	—	D
54	10 ~ 20	0.073 ~ 0.093	60 ~ 70	0.62 ~ 0.69	0.15 ~ 0.25	A-a
55	5 ~ 20	0.054 ~ 0.080	50 ~ 70	0.44 ~ 0.48	0.28 ~ 0.32	A-a
56	5 ~ 15	0.056 ~ 0.095	45 ~ 60	0.49 ~ 0.54	0.23 ~ 0.32	A-a
57	30 ~ 35	0.058 ~ 0.070	70 ~ 80	0.47 ~ 0.50	0.15 ~ 0.16	B-a
58	>240	—	—	—	—	D
59	80 ~ 90	0.053 ~ 0.064	130 ~ 140	0.50 ~ 0.52	0.12 ~ 0.17	C-a
60	120 ~ 150	0.040 ~ 0.053	190 ~ 210	0.41 ~ 0.45	0.16 ~ 0.31	C-a
61	>240	—	—	—	—	D
62	60 ~ 65	0.042 ~ 0.060	140 ~ 170	0.64 ~ 0.74	0.14 ~ 0.22	B-a
63[a]	150 ~ 170	0.037 ~ 0.039	200 ~ 230	0.39 ~ 0.46	0.18 ~ 0.27	C-a
64	>240	—	—	—	—	D
65	>240	—	—	—	—	D
66	>240	—	—	—	—	D
67	>240	—	—	—	—	D
68	>240	—	—	—	—	D
69	>240	—	—	—	—	D
70	>240	—	—	—	—	D
71	>240	—	—	—	—	D
72	50 ~ 70	0.038 ~ 0.048	105 ~ 120	0.14 ~ 0.18	—	B-c
73	>240	—	—	—	—	D
74[a]	76 ~ 95	not obtained	190 ~ 195	0.76 ~ 0.78	0.13 ~ 0.15	C-a
75	50 ~ 60	0.041 ~ 0.045	125 ~ 135	0.79 ~ 0.80	0.07 ~ 0.08	B-a
76	>240	—	—	—	—	D
77	155 ~ 180	0.020 ~ 0.028	260 ~ 295	0.58 ~ 0.65	0.23 ~ 0.25	C-a
78	>240	—	—	—	—	D

[a] Degraded by two steps.

TABLE 5

Relation between biodegradabilities and the F constant for benzene monosubstitutes

Compound	Substituted group	Biodegradation ranks	F constant
Phenol	—OH	A-a	0.29
Aniline	$—NH_2$	B-a	0.02
Acetanilide	$—NHCOCH_3$	B-a	0.28
Ethylphenylether	$—OC_2H_5$	C-a	0.22
Benzene	(—H)	C-a	0.00
Fluorobenzene	—F	D	0.43
Chlorobenzene	—Cl	D	0.41
Benzene sulfoamide	$—SO_2NH_2$	D	0.41
Nitrobenzene	$—NO_2$	D	0.67

Biodegradation ranks of substituted benzoic acids

The biodegradation ranks of the three hydroxybenzoic acids were A-a. For aminobenzoic acid and nitrobenzoic acids, the ranks of *o*- and *p*-compounds were B-a or C-a, but the ranks of *m*-compounds were D. *o*-Hydroxybenzoic acid and *o*-aminobenzoic acid may be easily biodegradated through catechol, and *m*- and *p*-hydroxybenzoic acids may be easily biodegraded through protocatechuic acid. *o*-Nitrobenzoic acid may be gradually biodegraded through catechol the same as *o*-aminobenzoic acid and *p*-aminobenzoic acid. *p*-Nitrobenzoic acid may be gradually biodegraded through hydroxybenzoic acid.

From the other viewpoint, it was shown that the carboxylic group promoted biodegradation of phenol, aniline and nitrobenzene, but did not promote biodegradation of *m*-amino and *m*-nitro benzoic acids.

Biodegradation ranks of substituted phenols and nitroanilines

o-Aminophenol was biodegraded in two steps and its biodegradation rank was C-a. It is known that *o*-aminophenol is easily oxydized into *o*-benzoquinone and may be biodegraded through catechol. The rank of *p*-aminophenol, however, was D because it was oxidized into insoluble *p*-benzoquinone and might not be biodegraded further. *m*-Aminophenol was also not biodegraded like *m*-aminobenzoic acid and *m*-nitrobenzoic acid. None of the nitrophenols and nitroanilines were biodegraded at all within 240 h, and their ranks were D. Namely, it was shown that the nitro group restrained the biodegradation of phenol and aniline.

Biodegradation ranks of substituted benzenesulfonates

The biodegradation ranks of *p*-toluenesulfonic acid and *p*-dodecylbenzenesulfonate were B-a and D, respectively. It is known that *p*-toluenesulfonic acid is biodegraded by hydroxylation and desulfonation [11,12]. *p*-Dodecylbenzenesulfonate could be biodegraded at a lower concentration than 10 mg/l, but it was not biodegraded at 100 mg/l because of its inhibition to microorganisms [4].

Conclusion

Since the obtained biodegradation ranks by the proposed method were reasonable for the many organic compounds as described above, it is substantiated that the new method is useful in evaluating the biodegradabilities of organic compounds.

References

1 K. Urano and Z. Kato, A method to classify biodegradabilities of organic compounds, J. Hazardous Materials, 13 (1986) 135—145.
2 A. White, P. Handler and E.L. Smith, Principles of Biochemistry, 4th edn., McGraw-Hill, New York, 1968.
3 O. Stokke, The degradation of branched chain fatty acid by alteration between α- and β-oxidations, Biochim. Biophys. Acta, 176 (1969) 54—59.
4 K. Urano and M. Saito, Biodegradations of surfactants and inhibitions of surfactants to biodegradations of other pollutants, Chemosphere, 14 (1985) 1333—1342.
5 J.R. Nooi, M.C. Testa and S. Willemse, Biodegradation mechanism of fatty alcohol nonionics. Experiments with some C-labeled stearyl alcohol/ethylene oxide condensates, Tenside, 7 (1970) 61—65.
6 F.J.E. Thijesse and T.H. Wanders, Microbiological degradation of n-alkane-l-sulfonates, Fette, Seifen, Anstrichm., 74 (1972) 413—416.
7 R. Stanier, E. Aderberg and J. Ingraham, The Microbial World, 4th edn., Prentice-Hall, 1976.
8 R.D. Swisher, Surfactant Biodegradation, Marcel Dekker, 1970.
9 R.E. Mckinney, Metabolism of aromatic compounds by activated sludge, Sewage Ind. Waste, 28 (1956) 547—557.
10 C. Hansch, A. Leo, S.H. Unger, K.H. Kim, D. Nikaitani and E.J. Lien, Aromatic substituent constants for structure—activity correlations, J. Med. Chem., 16 (1973) 1207—1216.
11 R.B. Cain and D.R. Farr, Metabolism of arenesulfonates by microorganisms, Biochem. J., 106 (1968) 859—877.
12 D.D. Focht and F.D. Williams, Degradation of *p*-toluenesulfonate by a pseudomonas, Can. J. Microbiol., 16 (1970) 309—316.