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Prediction of Environmental Properties in Water–Soil–Air Systems for Phthalates

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Abstract In this paper, environmentally key properties including aqueous solubilities (S_W), vapor pressures (V_P), sorption coefficients (K_{OC}), octanol–water (K_{OW}), octanol–air (K_{OA}) and air–water (K_{AW}) partition coefficients of 53 phthalates are studied by the quantitative structure-property relationship models by means of previously proposed *Lu* index. Reliable models are obtained to estimate Log S_W, solubility in air (Log S_A), Log K_{OC} and Log K_{OW} for phthalates with the correlation coefficients of estimations (R) being 0.9869, 0.9461, 0.8880 and 0.9836, and the standard errors being 0.44, 0.27, 0.52 and 0.40, respectively. The predictive ability of the constructed models is demonstrated by the correlation coefficients (R_{CV}) in the leave-one-out cross validation procedures being 0.9709, 0.9218, 0.8089 and 0.9784, and the corresponding standard errors (s_{CV}) being 0.47, 0.34, 0.67 and 0.47, respectively. The properties of K_{AO} and K_{AW} for the phthalates are calculated by the predicted S_W, S_A, and K_{OW} values.

Keywords Phthalates · Environmental properties · QSPR · *Lu* index

The evaluation of the environmental behavior of phthalates has become a principle goal in order to predict the environmental risk. The key physical–chemical properties including aqueous solubilities (S_W), vapor pressures (V_P), sorption coefficient (K_{OC}), octanol–water (K_{OW}), octanol–air (K_{OA}) and air–water (K_{AW}) partition are of great importance in evaluating their environmental transport and fate. Therefore the availability and reliability of these physical–chemical data seems especially important. In recent years, some scientists have developed various quantitative structure-property relationship (QSPR) models to estimate physical–chemical properties for phthalate esters. Thomsen et al. (1999) described solubility, octanol–water partitioning and soil sorption coefficient of a series of phthalates through various structure-activity/quantitative structure-activity relationship (SAR/QSAR) concepts including molecular connectivity indices (MCI), electro-topological atomic state indices (EASI) and group-contribution (UNIFAC). Cousins and Mackay (2000) developed a QSPR method for the correlation of physical–chemical properties and partition coefficients, namely the "three solubility" approach for 22 phthalates. Sacan et al. (2005) presented QSPR models for water solubility, *n*-octanol-water partition coefficient and Henry's law constant for polychlorinated dibenzo-*p*-dioxins (PCDDs) and dibenzo-*p*-furans (PCDFs) and phthalates based on the characteristic root index (CRI) and three semi-empirical molecular orbital (E_{HOMO} and E_{LUMO}), and dipole moment (μ). Definitely, those researchers have made significant contributions to provide the reliable physical–chemical properties for phthalates.

The objective of this study was to develop reliable and predictive QSPR models for a set of 53 phthalates. It is noteworthy that nearly 20 phthalates, e.g., Monomethyl phthalate, Di(6-methylheptyl) phthalate, Hexyl 8-methylnonyl phthalate, etc., which have not been studied in previous QSPR models, were included in this work. The *Lu* index, which was proposed by our previous research group and has been successfully used in various QSPR studies (Lu et al. 2006a, b, c), was employed to build QSPR models. The predictive ability of the final models was verified by Leave-One-Out (LOO) cross validation procedures.

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Table 1 Chemical names, abbreviations, Chemical Abstract Registry (CAS) and European Inventory of Existing Commercial Substance (EINECS) numbers, chemical formulations, and calculated *Lu* indices for 53 phthalates

No.	-Phthalate	Abbreviations	EINECS no.	CAS no.	*Lu*
1	Monomethyl	SMP	224-476-6	4376-18-5	10.8174
2	Dimethyl	DMP	205-011-6	131-11-3	11.6642
3	Diethyl	DEP	201-550-6	84-66-2	13.4351
4	Monobutyl	SBP	205-036-2	131-70-4	13.6682
5	Diallyl	DAP	205-016-3	131-17-9	15.1772
6	Di-*n*-propyl	DPP	205-015-8	131-16-8	15.2049
7	Diisopropyl	DIPP	210-086-3	605-45-8	15.0030
8	Methyl 2-ethoxy-2-oxoethyl	MeoOeP	201-625-3	85-71-2	16.0282
9	Di-*n*-Butyl	DBP	201-557-4	84-74-2	16.9499
10	Diisobutyl	DIBP	201-553-2	84-69-5	16.6995
11	Butyl-2-methylpropyl	BMPP	241-802-2	17851-53-5	16.7896
12	Ethyl 2-ethoxy-2-oxoethyl	EeoOeP	201-555-3	84-72-0	16.8090
13	Di(2-methoxyethyl)	DMEP	204-212-6	117-82-8	16.9132
14	Butylcyclohexyl	BCP	201-548-5	84-64-0	18.2949
15	Di-*n*-pentyl	DPeP	205-017-9	131-18-0	18.6607
16	Di(3-methylbutyl)	DMBP	210-088-4	605-50-5	18.5144
17	Di(2-ethoxyethyl)	DEEP	210-090-5	605-54-9	18.6115
18	Butylbenzyl	BBzP	201-662-7	85-68-7	18.8412
19	Diphenyl	DPhP	201-546-4	84-62-8	19.5532
20	Butylbutoxyethyl	BboEP	251-483-1	33374-28-6	19.5154
21	Dicyclohexyl	DCHP	201-545-9	84-61-7	19.6276
22	Butyl 2-ethylhexyl	BEHP	201-623-2	85-69-8	19.9919
23	Butyloctyl	BOP	201-562-1	84-78-6	20.4128
24	Di-*n*-hexyl	DHP	201-559-5	84-75-3	20.3148
25	Diisohexyl	DIHP	276-090-2	146-50-9	20.1878
26	Di(2-ethylbutyl)	DEBP	230-741-7	7299-89-0	19.8625
27	Butyl 2-butoxy-2-exoethyl	BboOeP	201-624-8	85-70-1	20.1141
28	Dibenzyl	DBzP	208-344-5	523-31-9	19.8289
29	Dimethyl cyclohexyl	DMCHP	248-765-1	27987-25-3	20.8417
30	Di-*n*-heptyl	DHpP	222-885-4	3648-21-3	21.9713
31	Diisoheptyl	DIHpP	276-15-8	71888-89-6	21.8616
32	Butyldecylphthalate	BDcP	201-885-8	89-19-0	22.1093
33	Di(2-butoxyethyl)	DBEP	204-213-1	117-83-9	21.9111
34	Di-*n*-octyl phthalate	DOP	204-214-7	117-84-0	23.5930
35	Diisooctyl phthalate	DIOP	248-523-5	27554-26-3	23.4971
36	Di(2-ethylhexyl)	DEHP	204-210-0	117-81-7	22.9124
37	Decylhexyl	DeHP	247-21-01	25724-58-7	23.6364
38	Di(6-methylheptyl)	DMHpP	205-014-2	131-15-7	23.1354
39	Hexyldecylphthalate	HDcP	247-210-0	25724-58-7	23.6233
40	Hexyl 8-methylnonyl	HMNP	262-926-3	61702-81-6	23.5745
41	Di-*n*-nonyl	DNP	201-560-0	84-76-4	25.1411
42	Diisononyl	DINP	249-079-5	28553-12-0	25.0556
43	Octyldecyl	ODP	204-295-9	119-07-3	25.1695
44	6-Methylhepthyl-8-methylnonyl	MHpMNP	204-293-8	119-05-1	25.0663
45	Octyl 8-methylnonyl	OMNP	215-554-0	1330-96-7	25.1084
46	2-Ethylhexyl 8-methylnonyl	EHMNP	201-883-7	89-13-4	24.9332
47	Di-*n*-decyl	DDP	201-561-6	84-77-5	26.6779
48	Diisodecyl	DIDP	247-977-1	26761-40-0	26.6015
49	Di-*n*-undecyl	DUP	222-884-9	3648-20-2	28.1854
50	Diisoundecyl	DIUP	306-165-8	96507-86-7	28.1166
51	Didodecyl	DDdP	219-415-5	2432-90-8	29.6654

Table 1 continued

No.	-Phthalate	Abbreviations	EINECS no.	CAS no.	*Lu*
52	Di-*n*-tridecyl	DTDP	204-294-3	119-06-2	30.9747
53	Diisotridecyl	DITDP	248-368-3	68515-47-9	30.9167

Table 2 Experimental physical–chemical properties of phthalates

Phthalate	S_W (mg L^{-1})	V_P (Pa)	Log K_{OW}	Log K_{OC}
DMP	2,810	0.22	1.60	2.3
	4,000			
	4,248			
	4,290			
	4,320			
DEP	680	0.052	2.42	4.2
	869	0.0813		
	928	0.22		
	1,080			
DAP	182		3.23	
DPP	108		3.27	
DIPP			2.83	
DBP	9.15	2.27×10^{-3}	4.13	4.11
	10.1	2.53×10^{-3}		
	11.2	2.77×10^{-3}		
	13	4.67×10^{-3}		
		4.80×10^{-3}		
		5.47×10^{-3}		
		9.73×10^{-3}		
DIBP	6.2		4.11	3.14
	20			
	20.3			
DPeP			5.62	
BBzP	0.7	1.15×10^{-3}	4.73	3.997
	2.69	1.20×10^{-3}		
	2.82			
	2.9			
	40.2			
DCHP			4.90	
DHP	7.00×10^{-2}	1.87×10^{-3}	6.82	4.72
	4.60×10^{-2}	2.40×10^{-4}		4.718
DHpP	1.70×10^{-2}			
DOP	4.00×10^{-4}		8.10	
	5.10×10^{-4}		8.18	
DEHP			7.27	5.68
				5.72
DNP	1.3×10^{-4}			
DINP	1.1×10^{-4}			
	6.00×10^{-4}			
DIDP	1.7×10^{-4}			5.46
DDP	5.00×10^{-4}		8.91	
	2.20×10^{-4}			
DTDP				6.26

Materials and Methods

The definition of the *Lu* index is based on the shortest distance matrix, and expressed as:

$$Lu = n^{\frac{1}{2}} \log \left[\sum_{i}^{n} \sum_{i}^{n} D_{ij} + \sum_{i}^{n} \sum_{i}^{n} D_{ij}^{2} \right] \quad (1)$$

where n is the number of vertices in a molecular topological graph. D_{ij} is the shortest distance between vertices i and j, and is calculated by summing the relative bond length between two adjacent vertices in the shortest path. The single *Lu* index, which has an excellent discrimination power toward describing the molecular structures of isomers, mainly reflects the molecular sizes of chemicals. Since many physical–chemical properties, e.g., octanol–water partition and soil sorption coefficients, are much related to the molecular size, this index is definitely useful for QSPR studies.

The vapor pressure of a liquid substance, P_L^S (Pa), is equivalent to its solubility in air, S_A (mol m^{-3}), and can be obtained from the gas law

$$S_A = P_L^S / RT \quad (2)$$

where R is gas constant (8.314 Pa m^{-3} mol^{-1} K^{-1}) and T is the absolute temperature (298 K). The values of K_{OW}, K_{OA} and K_{AW} can be resulted from following equations:

$$K_{OW} = S_O / S_W \quad (3)$$

$$K_{OA} = S_O / S_A \quad (4)$$

$$K_{AW} = S_A / S_W \quad (5)$$

where S_O is solubility in octanol.

Results and Discussion

One of the most important concerns of QSPR study is to choose reliable experimental data for modeling. Cousins and Mackay (2000) have presented a thorough analysis for assessing physical–chemical measurements for phthalates and recommended the S_W and V_P values for QSPR modeling. The suggested data set was reasonable and included in our study. All data are taken from original papers (Defoe et al. 1990; Dobbs et al. 1984; Ellington and Floyd 1996; Ellington 1999; Frissell 1956; Grayson and Fosbraey 1982;

Table 3 Predicted physical–chemical properties of phthalates

Phthalate	S_W (mg L^{-1})	V_P (Pa)	Log K_{OC}	Log K_{OW}	Log K_{OA}	Log K_{AW}
SMP	20,580	0.483	2.81	0.96	6.73	−5.77
DMP	7,273	0.258	2.97	1.41	6.97	−5.56
DEP	808	6.95×10^{-2}	3.31	2.35	7.46	−5.11
SBP	594	5.85×10^{-2}	3.35	2.47	7.52	−5.05
DAP	90	1.91×10^{-2}	3.63	3.27	7.95	−4.68
DPP	88	1.88×10^{-2}	3.64	3.29	7.96	−4.67
DIPP	115	2.18×10^{-2}	3.60	3.18	7.64	−4.46
MeoOeP	31	1.02×10^{-2}	3.79	3.73	7.96	−4.23
DBP	9.9	5.16×10^{-3}	3.97	4.22	8.45	−4.23
DIBP	13.8	6.20×10^{-3}	3.92	4.08	8.38	−4.30
BMPP	12.2	5.80×10^{-3}	3.94	4.13	8.40	−4.27
EeoOeP	11.4	5.70×10^{-3}	3.94	4.14	8.41	−4.27
DMEP	10.5	5.29×10^{-3}	3.96	4.20	8.44	−4.24
BCP	1.84	1.90×10^{-3}	4.22	4.93	8.83	−3.90
DPeP	1.15	1.45×10^{-3}	4.29	5.13	8.93	−3.80
DMBP	1.39	1.62×10^{-3}	4.26	5.05	8.89	−3.84
DEEP	1.24	1.51×10^{-3}	4.28	5.10	8.92	−3.82
BBzP	0.93	1.27×10^{-3}	4.32	5.22	8.98	−3.76
DPhP	0.37	7.50×10^{-4}	4.46	5.60	9.18	−3.58
BboEP	0.39	7.72×10^{-4}	4.45	5.58	9.17	−3.59
DCHP	0.35	7.10×10^{-4}	4.47	5.64	9.20	−3.56
BEHP	0.22	5.42×10^{-4}	4.54	5.83	9.30	−3.47
BOP	0.12	3.97×10^{-4}	4.62	6.06	9.43	−3.37
DHP	0.14	4.26×10^{-4}	4.60	6.00	9.39	−3.39
DIHP	0.17	4.69×10^{-4}	4.58	5.94	9.36	−3.42
DEBP	0.26	5.97×10^{-4}	4.51	5.76	9.26	−3.50
DBzP	0.18	4.95×10^{-4}	4.56	5.90	9.34	−3.44
BboOeP	0.28	6.12×10^{-4}	4.51	5.75	9.26	−3.51
DMCHP	7.59×10^{-2}	2.89×10^{-4}	4.70	6.28	9.54	−3.26
DHpP	1.73×10^{-2}	1.25×10^{-4}	4.91	6.89	9.87	−2.98
DIHpP	2.00×10^{-2}	1.36×10^{-4}	4.89	6.83	9.83	−3.00
BDcP	1.44×10^{-2}	1.13×10^{-4}	4.94	6.96	9.90	−2.94
DBEP	1.90×10^{-2}	1.31×10^{-4}	4.90	6.85	9.84	−2.99
DOP	2.24×10^{-3}	3.77×10^{-5}	5.22	7.75	10.32	−2.57
DIOP	2.51×10^{-3}	4.05×10^{-5}	5.20	7.70	10.29	−2.59
DEHP	5.41×10^{-3}	6.24×10^{-5}	5.09	7.39	10.13	−2.74
DeHP	2.09×10^{-3}	3.65×10^{-5}	5.22	7.77	10.33	−2.56
DMHpP	4.04×10^{-3}	5.29×10^{-5}	5.13	7.50	10.18	−2.68
HDcP	2.12×10^{-3}	3.69×10^{-5}	5.22	7.76	10.32	−2.56
HMNP	2.26×10^{-3}	3.82×10^{-5}	5.21	7.74	10.31	−2.57
DNP	3.08×10^{-4}	1.20×10^{-5}	5.51	8.57	10.75	−2.18
DINP	3.45×10^{-4}	1.28×10^{-5}	5.49	8.52	10.72	−2.20
ODP	2.97×10^{-4}	1.17×10^{-5}	5.51	8.59	10.77	−2.18
MHpMNP	3.40×10^{-4}	1.27×10^{-5}	5.49	8.53	10.73	−2.20
OMNP	3.22×10^{-4}	1.23×10^{-5}	5.50	8.55	10.74	−2.19
EHMNP	4.06×10^{-4}	1.40×10^{-5}	5.47	8.46	10.69	−2.23
DDP	4.35×10^{-5}	3.84×10^{-5}	5.80	9.39	11.19	−1.80
DIDP	4.82×10^{-5}	4.07×10^{-6}	5.78	9.35	11.17	−1.82

Table 3 continued

Phthalate	S_W (mg L^{-1})	V_P (Pa)	Log K_{OC}	Log K_{OW}	Log K_{OA}	Log K_{AW}
DUP	6.35×10^{-6}	1.26×10^{-6}	6.08	10.19	11.61	−1.42
DIUP	6.96×10^{-6}	1.32×10^{-6}	6.07	10.15	11.59	−1.44
DDdP	9.59×10^{-6}	4.21×10^{-7}	6.36	10.97	12.02	−1.05
DTDP	1.81×10^{-7}	1.60×10^{-7}	6.60	11.67	12.39	−0.72
DITDP	1.95×10^{-7}	1.67×10^{-7}	6.59	11.64	12.38	−0.74

Gledhill et al. 1980; Gückel et al. 1982; Hollifield 1979; Howard et al. 1985; Harnisch et al. 1983; Leyder and Boulanger 1983; Nielsen and Bundgaard 1989; Quackenbos 1954; Veith et al. 1980; Werner 1952). As for Log K_{OW}, we chose the most recent data, most of which are reported by Ellington and Floyd (1996). This operation was based on the assumption that the recently published data are believed to be more reliable because the measuring instrument and method used more recently may be better than older ones. The Log K_{OC} data used was taken from Williams et al. (1995) and Thomsen et al. (1999). The Log K_{OC} value of Di-ethyl phthalate given by Thomsen was omitted from the original data set because this value was clearly inconsistent with the measurements summarized by Williams and his collaborators (Williams et al. 1995).

Chemical names, abbreviations, Chemical Abstract Registry (CAS) and European Inventory of Existing Commercial Substance (EINECS) numbers, chemical formulations, and calculated *Lu* indces of studied phthalates are listed in Table 1. And the data set used in QSPR modeling, including 18 phthalates, is summarized in Table 2.

Models developed for Log S_W, Log S_A, Log K_{OC} and Log K_{OW} are shown below:

$$\begin{aligned} &\text{Log } S_W = 8.2431 - 0.5718\,Lu \\ &n = 34, R = 0.9869, s = 0.44, R_{CV} = 0.9709, \\ &s_{CV} = 0.47, F = 1,227 \end{aligned} \quad (6)$$

$$\begin{aligned} &\text{Log } S_A = -0.2324 - 0.3215\,Lu \\ &n = 15, R = 0.9461, s = 0.27, R_{CV} = 0.9218, \\ &s_{CV} = 0.34, F = 1,241 \end{aligned} \quad (7)$$

$$\begin{aligned} &\text{Log } K_{OC} = 0.7856 + 0.1880\,Lu \\ &n = 11, R = 0.8880, s = 0.52, R_{CV} = 0.8089, \\ &s_{CV} = 0.67, F = 43 \end{aligned} \quad (8)$$

$$\begin{aligned} &\text{Log } K_{OW} = -4.7875 + 0.5315\,Lu \\ &n = 15, R = 0.9836, s = 0.40, R_{CV} = 0.9784, \\ &s_{CV} = 0.47, F = 399 \end{aligned} \quad (9)$$

The correlation coefficients for constructed models are all larger than 0.88, and standard errors are all less than 0.52, which demonstrate the reliable correlation relationship between the *Lu* index and studied physical–chemical properties of phthalates. Meanwhile, the corresponding values of the leave-one-out cross validation procedure show the predictive ability of the developed models. On the other hand, the statistical results of the above presented models are comparable to previous results (Thomsen et al. 1999; Cousins and Mackay 2000). As mentioned above, other properties, such as Log K_{OA} and Log K_{AW} can be calculated from known Log S_W, Log S_A and Log K_{OW}. The predicted physical–chemical properties of 53 phthalates are listed in Table 3. It is worth noting that the physical–chemical properties of more than 20 compounds are not reported in previous studies.

In conclusion, the quantitative structure-property relationship models are developed for S_W, S_A, K_{OC} and K_{OW} of phthalates by using our previously proposed single *Lu* index, which has high resolution toward the structure of the chemicals. All presented models are highly related and have sound predictive ability. Other properties including K_{OA} and K_{AW} can be estimated by using the interrelationships between S_W, S_A and K_{OW}. The constructed models are used to predict physical–chemical properties of 53 phthalates, some of which have not been reported elsewhere.

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