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Predicting physico-chemical properties of polychlorinated diphenyl ethers (PCDEs): potential persistent organic pollutants (POPs)

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Abstract: Polychlorinated diphenyl ethers (PCDEs) have received more and more concerns as a category of potential persistent organic pollutants (POPs). Modeling its environmental fate and exposure assessment require a number of fundamental physico-chemical properties. However, the experimental data are currently limited due to the difficulty in analysis caused by the complexity of PCDE congeners. As an alternative, the quantitative structure property relationship (QSPR) approach could be used. In this paper, twelve kinds of molecular connectivity indices (MCIs) of all 209 possible molecular structure patterns of PCDEs were calculated. Based on 106 PCDEs with three observed physico-chemical properties—vapour pressure (P_L^0), aqueous solubility (S_w) and *n*-octanol/water (K_{ow}) and their MCIs data, a series of QSPR equations were established using multiple linear regression (MLR) method. As a result, three equations with best performance were selected mainly from the view of high regression coefficient (R) and low standard error (SE). All of them showed significant relationship and high accuracy. With these equations the properties of other 103 patterns of PCDEs without the reported observed values were predicted. Furthermore, three partition properties for PCDE congeners—Henry's Law constants (H), partition coefficients between gas/water (K_{gw}) and gas/*n*-octanol (K_{go}) were calculated according to the internal relationship among these six properties. These observed and predicted values, in contrast with the criteria listed in the Stockholm treaty about POPs which has been signed by more than ninety countries in May 2001, illustrated that most of PCDEs congeners are potential persistent organic pollutants. As all descriptors/predictors are derived just from the molecular structure itself and without the import of any empirical parameters, this method is impersonal and promising for the estimation of physico-chemical properties of PCDEs.

Keywords: PCDEs; POPs; QSPR; molecular connectivity indices

Introduction

Polychlorinated diphenyl ethers $C_{12}H_{10-x}OC_{lx(x=1-10)}$ (PCDEs, ClxDEs) represent a group of halogenated aromatic compounds, which are structurally located between polychlorinated biphenyls (PCBs) and polychlorinated dibenzo-*p*-furans (PCDFs). PCDEs have been found as by-products in widely used chlorinated phenols and chlorinated phenoxyacetic acids, where they have been identified at a level of 100—1000 mg/kg (Kurz, 1995a). Also PCDEs come from all processes of incomplete combustion e.g. municipal waste incinerators. As a result PCDEs have been detected in a wide range of environmental samples (Kurz, 1995b).

PCDEs have recently been reported to be immunotoxic and to induce microsomal enzymes. Also, the persistence and bioaccumulation in laboratory animals are quite similar to the PCBs. PCDEs are regarded as additional persistent indicator molecules for a global pollution of the environment by organochlorine compounds (Kurz , 1999). Persistent organic pollutants (POPs) are now of great concerns, especially after more than ninety countries all over the world signed the Stockholm Convention about POPs in May, 2001. As potential POPs, PCDEs' risk assessment and exposure evaluation have received more and more researchers' interest.

Physico-chemical properties, especially those partitioning properties, of micropollutants play a major role in their transport and mobility in the global environments. This is particularly true for those POPs chemicals like PCDEs. According to the numbers and position difference of constituted chlorine atoms, there are 209 possible structural patterns of PCDEs. This complexity had caused the difficulty both for the qualitative and for the quantitative analysis, and so does the determination of physico-chemical properties. Traditional experimental determination methods usually need special equipment and samples, cost large amounts of money, time and manpower. As a result, there is limited number of PCDEs to be determined currently (Kurz, 1999; Ruelle, 1997; 2000), which could not meet the needs of the risk assessment of PCDEs. Thus, the technology of quantitative structure-property relationship (QSPR), which correlate and predict property data of pollutants from their structural descriptors, may be used to study the physico-chemical properties and generate predicted data efficiently.

Molecular connectivity indices (MCIs) are well known topological indices, which have numerous successful applications in various areas of physics, chemistry, biology, drug design, as well as environmental sciences. Sabljic and his colleagues have focused on applying MCIs in estimation of various partitioning properties of POPs during recent 15 years. And they have successfully developed a series of reliable QSPR models (Sabljic, 2001).

In this study, we extended the work of Sabljic *et al*. and introduced MCIs into the QSPR study of physico-chemical properties of PCDEs. Multiple stepwise regression (MLR) technique was used, and the models with best performances respectively for three physico-chemical properties were selected: vapour pressure (P_L^0), aqueous

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solubility(S_w) and *n*-octanol/water(K_{ow}). And other three partition properties of PCDE congeners-Henry's law constants (H), partition coefficients between gas/water(K_{gw}) and gas/*n*-octanol (K_{go}) were calculated according to the internal relationship among these six properties.

1 Materials and method

1.1 Sample set

The data set from Kurz *et al*.(Kurz, 1999) were used in this study, which contains three physico-chemical properties of 106 PCDE congeners: vapour pressure(P_L^0), aqueous solubility(S_w) and *n*-octanol/water(K_{ow}).

1.2 Calculation of MCIs

The calculation method of MCIs has been well documented both in textbooks and literatures (Karelson, 2000; Sabljic, 2001). In this study, 12 MCIs were used, which can be classified into four categories: (1) The 0—2 order simple molecular connectivity indices(SMCI): ${}^0\chi$, ${}^1\chi$, ${}^2\chi$; (2) The average 0—2 order simple molecular connectivity indices(ASMCI): ${}^0\chi_A$, ${}^1\chi_A$, ${}^2\chi_A$; (3) The 0—2 order valence molecular connectivity indices(VMCI): ${}^0\chi^V$, ${}^1\chi^V$, ${}^2\chi^V$; (4) The average 0—2 order valence molecular connectivity indices(AVMCI): ${}^0\chi_A^V$, ${}^1\chi_A^V$, ${}^2\chi_A^V$.

The average MCIs are calculated from the ratio of the corresponding MCIs and the number of total atoms. 0, 1 and 2 order MCIs represent the contribution of atom, bond and inter-bond to the specific property respectively. Dragon software version 1.1(Todeschini, 2000) was used to generate all these 12 MCIs above for all 209 possible patterns.

1.3 Modeling and selection of models with best performance

Based on the sample set of 106 PCDE congeners and their corresponding MCIs calculated from Dragon software, a series QSPR models were established using origin software Version 6.0 (Microcal Software, Inc., http://www.microcal.com/, 1999) to performing multiple linear regression analysis.

Three equations with best performance were selected by seeking for maximum adjusted regression coefficient (R_{adj}) and minimum standard deviation(S_d).

1.4 Prediction on samples outside the sample set

With the selected three equations from 1.3, three physico-chemical properties of 103 samples outside the sample set were predicted. Furthermore, other three physico-chemical properties were also calculated according to the internal relationship among these six properties described by Kurz *et al*.(Kurz, 1999):

Henry's Law constants(H): $H = \frac{P_L^0}{S_w}$,

Partition coefficients of gas/water(K_{gw}): $K_{gw}(T) = \frac{H}{R \cdot T}$,

Gas/*n*-octanol(K_{go}): $K_{go} = \frac{K_{gw}}{K_{ow}}$.

2 Results and discussions

The QSPR models for three physico-chemical properties are shown below: (1) For vapour pressure(P_L^0)

$$-\log P_L^0 = 1.434\ {}^0\chi - 2.901\ {}^1\chi + 0.287\ {}^2\chi - 1.074, \quad (1)$$

($n = 106$, $R_{adj} = 0.975$, $S_d = 0.177$, $F = 1380.076$, $p < 0.0001$)

$$-\log P_L^0 = 21.947\ {}^0\chi_A - 159.992\ {}^1\chi_A - 44.953\ {}^2\chi_A + 71.509, \quad (2)$$

($n = 106$, $R_{adj} = 0.973$, $S_d = 0.184$, $F = 1282.381$, $p < 0.0001$)

$$-\log P_L^0 = 5.030\ {}^0\chi^V - 8.716\ {}^1\chi^V - 0.457\ {}^2\chi^V + 3.013, \quad (3)$$

($n = 106$, $R_{adj} = 0.975$, $S_d = 0.177$, $F = 1380.076$, $p < 0.0001$)

$$-\log P_L^0 = 68.839\ {}^0\chi_A^V - 85.521\ {}^1\chi_A^V - 23.978\ {}^2\chi_A^V - 5.243, \quad (4)$$

($n = 106$, $R_{adj} = 0.976$, $S_d = 0.175$, $F = 1414.902$, $p < 0.0001$)

(2) For aqueous solubility(S_w)

$$-\log S_w = 3.337\ {}^0\chi - 4.149\ {}^1\chi - 0.620\ {}^2\chi + 3.44966, \quad (5)$$

($n = 106$, $R_{adj} = 0.94728$, $S_d = 0.36633$, $F = 629.86962$, $p < 0.0001$)

$$-\log S_w = 17.779\ {}^0\chi_A - 265.511\ {}^1\chi_A - 66.861\ {}^2\chi_A + 132.921, \quad (6)$$

($n = 106$, $R_{adj} = 0.929$, $S_d = 0.424$, $F = 461.430$, $p < 0.0001$)

$$-\log S_w = 2.408\ {}^0\chi^V - 2.833\ {}^1\chi^V - 0.288\ {}^2\chi^V - 0.463, \quad (7)$$

($n = 106$, $R_{adj} = 0.947$, $S_d = 0.366$, $F = 629.004$, $p < 0.0001$)

$$-\log S_w = 91.030\ {}^0\chi_A^V - 106.197\ {}^1\chi_A^V - 33.229\ {}^2\chi_A^V - 4.954, \quad (8)$$

($n = 106$, $R_{adj} = 0.933$, $S_d = 0.414$, $F = 485.653$, $p < 0.0001$)

(3) For *n*-octanol/water(K_{ow})

$$\log K_{ow} = 2.656\ {}^0\chi - 4.595\ {}^1\chi + 0.036\ {}^2\chi + 9.820, \quad (9)$$

($n = 106$, $R_{adj} = 0.94522$, $S_d = 0.1834$, $F = 629.870$, $p < 0.0001$)

$$\log K_{ow} = -55.698\ {}^0\chi_A - 357.509\ {}^1\chi_A - 55.406\ {}^2\chi_A + 223.556, \quad (10)$$

($n = 106$, $R_{adj} = 0.94534$, $S_d = 0.1832$, $F = 606.300$, $p < 0.0001$)

$$\log K_{ow} = 3.908\ {}^0\chi^V - 7.888\ {}^1\chi^V + 0.129\ {}^2\chi^V + 8.694, \quad (11)$$

($n = 106$, $R_{adj} = 0.939$, $S_d = 0.194$, $F = 537.968$, $p < 0.0001$)

$$\log K_{ow} = 43.781\ {}^0\chi_A^V - 61.724\ {}^1\chi_A^V - 5.309\ {}^2\chi_A^V - 0.169. \quad (12)$$

($n = 106$, $R_{adj} = 0.930$, $S_d = 0.208$, $F = 463.097$, $p < 0.0001$)

Eq.(4), (5) and (10) were selected as optimal equations with best performance from the view of maximum adjusted regression coefficient(R_{adj}) and minimum standard deviation(S_d). Judged by the performance parameters such like high R_{adj}, which seems quite low S_d, large F and small p, Eq.(4),(5) and(10) are all of significant related at the confidence level $\alpha = 0.05$ and quite satisfying accuracy. The relationships between predicted values from these three equations and observed values of 106 PCDE congeners in sample set are shown in Fig. 1, which seems quite close.

Table 1 Predicted P_L^0, S_w, K_{ow} values of other 103 PCDEs outside the sample set

Substitute pattern	Predicted values						Substitute pattern	Predicted values					
	$-\log P_L^0$	$-\log S_w$	$\log K_{ow}$	H	$\log K_{gw}$	$\log K_{go}$		$-\log P_L^0$	$-\log S_w$	$\log K_{ow}$	H	$\log K_{gw}$	$\log K_{go}$
2,2'-	1.01	5.00	5.02	9.72	2.41	7.43	2,3,4,5,2',3'-	3.67	8.53	6.71	57.49	1.63	8.21
2,3'-	0.98	5.00	5.05	10.48	2.37	7.42	2,3,4,5,2',5'-	3.64	8.52	6.85	72.74	1.53	8.24
3,3'-	0.86	5.00	5.13	13.77	2.26	7.38	2,3,4,5,3',4'-	3.69	8.54	6.90	71.28	1.54	8.44
2,3,2'-	1.81	5.89	5.46	11.84	2.32	7.78	2,3,4,5,3',5'-	3.54	8.52	6.93	94.26	1.42	8.35
2,3,3'-	1.69	5.88	5.54	15.55	2.20	7.74	2,3,4,5,6,2'-	3.77	8.53	6.57	63.33	1.59	8.16
3,5,2'-	1.61	5.87	5.56	24.24	2.01	7.93	2,3,4,5,6,3'-	3.67	8.52	6.71	70.79	1.54	8.26
3,5,3'-	1.49	5.87	5.65	18.11	2.14	7.70	2,3,4,6,2',3'-	3.65	8.52	6.71	74.59	1.52	8.23
2,5,2'-	1.64	5.88	5.48	17.08	2.16	7.65	2,3,4,6,2',5'-	3.59	8.51	6.79	83.48	1.47	8.26
2,5,3'-	1.61	5.87	5.56	24.24	2.01	7.93	2,3,4,6,2',6'-	3.60	8.51	6.66	80.73	1.49	8.14
2,6,2'-	1.76	5.87	5.40	12.81	2.29	7.69	2,3,4,6,3',4'-	3.64	8.52	6.85	77.14	1.51	8.35
2,6,3'-	1.64	5.87	5.48	16.83	2.17	7.65	2,3,4,6,3',5'-	3.49	8.50	6.93	502.08	0.69	8.33
2,3,2',3'-	2.54	6.77	5.84	17.13	2.16	8.00	2,3,5,2',3',5'-	3.49	8.51	6.93	389.91	0.80	8.31
2,3,2',5'-	2.37	6.76	5.92	24.66	2.00	7.92	2,3,5,2',3',6'-	3.59	8.51	6.79	95.62	1.41	8.40
2,3,2',6'-	2.49	6.76	5.84	18.54	2.13	7.97	2,3,5,2',4',6'-	3.45	8.49	6.87	82.12	1.48	8.14
2,3,3',5'-	2.28	6.75	6.00	29.85	1.92	7.92	2,3,5,3',4',5'-	3.54	8.52	6.98	18.54	2.13	7.97
2,3,5,2'-	2.37	6.76	5.92	45.59	1.74	8.15	2,3,5,6,2',3'-	3.65	8.52	6.71	74.59	1.52	8.23
2,3,5,3'-	2.37	6.76	5.92	155.71	1.20	8.21	2,3,5,6,2',5'-	3.59	8.51	6.79	83.48	1.47	8.26
2,3,6,2'-	2.49	6.76	5.84	18.42	2.13	7.69	2,3,5,6,2',6'-	3.60	8.51	6.66	83.48	1.47	8.26
2,3,6,3'-	2.37	6.76	5.92	18.54	2.13	7.97	2,3,5,6,3',5'-	3.49	8.50	6.93	1025.46	0.38	8.02
2,4,2',6'-	2.32	6.75	5.86	26.69	1.97	7.83	2,3,6,2',3',6'-	3.60	8.51	6.66	80.73	1.49	8.14
2,4,6,2'-	2.32	6.74	5.86	26.24	1.98	7.84	2,3,6,2',4',6'-	3.54	8.50	6.74	188.21	1.12	8.32
2,4,6,3'-	2.20	6.74	5.94	34.14	1.86	7.81	2,3,6,3',4',5'-	3.64	8.52	6.85	212.34	1.07	8.35
2,5,2',5'-	2.23	6.75	6.00	33.34	1.87	7.87	2,4,6,2',4',6'-	3.40	8.48	6.87	490.27	0.70	8.34
2,5,2',6'-	2.32	6.75	5.86	26.69	1.97	7.83	2,4,6,3',4',5'-	3.49	8.51	6.93	88.36	1.45	8.49
2,5,3',5'-	2.19	6.74	6.08	35.36	1.85	7.93	3,4,5,3',4',5'-	3.59	8.54	7.04	502.08	0.69	8.33
2,6,2',6'-	2.42	6.75	5.78	21.20	2.07	7.85	2,3,4,5,2',3',5'-	4.13	9.41	7.34	212.34	1.07	8.35
2,6,3',5'-	2.20	6.74	5.94	34.14	1.86	7.81	2,3,4,5,2',4',6'-	4.10	9.40	7.28	196.21	1.10	8.38
3,4,5,2'-	2.42	6.77	5.98	22.40	2.04	8.02	2,3,4,5,6,2',3'-	4.26	9.41	7.07	483.32	0.71	8.35
3,4,5,3'-	2.32	6.76	6.06	27.58	1.95	8.01	2,3,4,5,6,2',5'-	4.14	9.41	7.15	77.14	1.51	8.35
3,5,3',5'-	2.07	6.73	6.16	45.66	1.73	7.90	2,3,4,5,6,2',6'-	4.21	9.40	7.01	90.34	1.44	8.17
2,3,4,5,2'-	3.09	7.65	6.27	36.67	1.83	8.10	2,3,4,5,6,3',5'-	4.13	9.40	7.28	191.60	1.11	8.45
2,3,4,5,3'-	2.99	7.65	6.41	77.14	1.51	8.35	2,3,4,6,2',3',4'-	4.14	9.41	7.20	502.08	0.69	8.33
2,3,4,6,2'-	3.04	7.64	6.22	39.69	1.80	8.02	2,3,4,6,2',3',5'-	4.10	9.40	7.28	143.68	1.24	8.30
2,3,4,6,3'-	2.94	7.63	6.36	49.33	1.70	8.06	2,3,4,6,2',3',6'-	4.10	9.40	7.28	196.21	1.10	8.38
2,3,5,2',3'-	2.94	7.64	6.36	50.04	1.69	8.05	2,3,4,6,2',4',5'-	4.10	9.40	7.34	196.21	1.10	8.38
2,3,5,2',5'-	2.88	7.63	6.44	56.09	1.65	8.08	2,3,4,6,2',4',6'-	4.05	9.38	7.28	199.03	1.10	8.43
2,3,5,2',6'-	2.89	7.63	6.30	54.16	1.66	7.96	2,3,4,6,3',4',5'-	4.13	9.41	7.34	191.60	1.11	8.45
2,3,5,3',5'-	2.76	7.62	6.57	72.43	1.53	8.11	2,3,5,6,2',3',5'-	4.10	9.40	7.28	186.20	1.12	8.41
2,3,5,6,2'-	3.04	7.64	6.22	39.69	1.80	8.02	2,3,5,6,2',3',6'-	4.09	9.40	7.15	196.21	1.10	8.38
2,3,5,6,3'-	2.94	7.63	6.36	49.33	1.70	8.06	2,3,5,6,2',4',6'-	4.05	9.38	7.28	203.68	1.09	8.23
2,3,6,2',3'-	3.04	7.64	6.22	40.37	1.79	8.01	2,3,5,6,3',4',5'-	4.13	9.41	7.34	103.48	1.38	8.31
2,3,6,2',5'-	2.89	7.63	6.36	55.09	1.65	8.01	2,3,4,5,2',3',4',6'-	4.60	10.29	7.64	191.60	1.11	8.45
2,3,6,2',6'-	2.99	7.63	6.22	43.69	1.75	7.97	2,3,4,5,6,2',3',5'-	4.60	10.28	7.64	523.06	0.68	8.26
2,3,6,3',5'-	2.88	7.63	6.44	55.29	1.65	8.09	2,3,4,5,6,2',3',6'-	4.69	10.29	7.50	111.99	1.35	8.22
2,4,6,2',3'-	2.89	7.63	6.30	54.16	1.66	7.96	2,3,4,5,6,2',4',6'-	4.55	10.27	7.58	446.61	0.74	8.44
2,4,6,2',5'-	2.84	7.62	6.44	60.70	1.61	8.05	2,3,4,5,6,3',4',5'-	4.65	10.30	7.69	1025.46	0.38	8.02
2,4,6,2',6'-	2.85	7.61	6.24	58.61	1.63	7.87	2,3,4,6,2',3',4',6'-	4.57	10.28	7.64	121.20	1.31	8.18
2,4,6,3',5'-	2.72	7.61	6.52	78.38	1.50	8.02	2,3,4,6,2',3',5',6'-	4.57	10.28	7.64	102.01	1.39	8.31
3,4,5,2',3'-	2.99	7.65	6.41	46.24	1.73	8.14	2,3,5,6,2',3',5',6'-	4.57	10.28	7.64	185.54	1.13	8.27
3,4,5,2',5'-	2.93	7.65	6.49	51.83	1.68	8.17	2,3,4,5,6,2',3',4',6'-	5.16	11.17	7.64	102.01	1.39	8.31
3,4,5,2',6'-	2.94	7.64	6.36	50.04	1.69	8.05	2,3,4,5,6,2',3',5',6'-	5.16	11.17	7.64	103.48	1.38	8.31
3,4,5,3',5'-	2.84	7.64	6.57	23.79	2.02	7.66							

Notes: The unit for P_L^0 is Pa, for S_w is mol/L, for H is Pa/(m^3·mol), all K_{gw} values are at 25℃

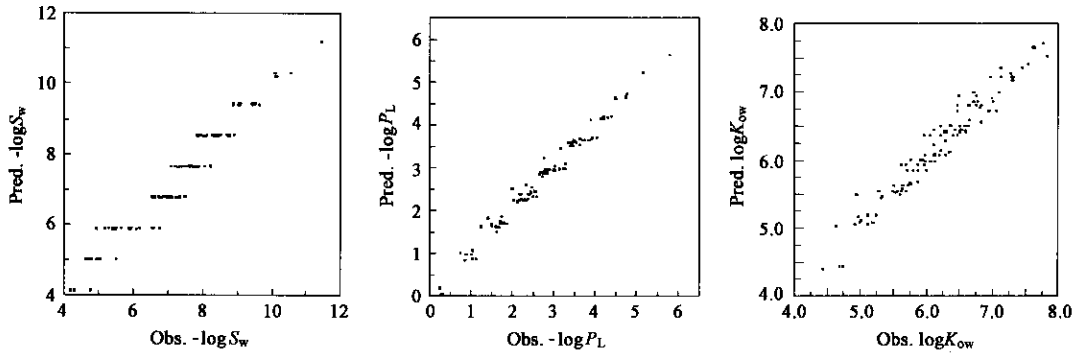

Fig. 1 Predicted value vs. observed values of P_L^0, S_w, K_{ow} for 106 PCDEs in the modeling sample set

To ensure the predicting capacity of selected equations, cross-validation test was done using MINITAB 13.1 software according to the methodology described by Carbo *et al.* (Carbo, 2000). The calculated R_{adj}^2 of Eq. (4), (5) and (10) were individually 0.9745, 0.9267, and 0.9400. Because R_{adj}^2 was expected to be close to the R_{adj}^2 and should be great than 0.5 (Carbo, 2000), these three equations were quite satisfactory in predicting capacity.

With the selected Eq. (4), (5) and (10), the P_L^0, S_w, K_{ow} of other 103 PCDE congeners outside the modeling sample set were predicted. And other three physico-chemical properties were further calculated according to the internal relationship among these six properties described by Kurz *et al.* (Kurz, 1999): Henry's Law constants (H), partition coefficients of gas/water (K_{gw}) and gas/n-octanol (K_{go}). All these results are shown in Table 1.

From the observed values in modeling sample set and predicted values in Table 1, low P_L^0 values of most PCDE congeners indicated they would not be at high levels in atmosphere. And low S_w and high K_{ow} values showed that they are hydrophobic/lipophilic, which means that PCDEs tend to accumulate in biota rather than in aqueous environment. K_{ow} values should be particularly of concerns because most of them have exceed the criteria (criteria = 5.0) in Stockholm Convention on Persistent Organic Pollutants (UNEP, 2001). High K_{go} values suggest that the tendency of accumulation from the atmosphere to lipids is also very high. As a result, the risk from PCDEs could not be omitted though they have not listed in Stockholm Convention yet.

3 Conclusions

The application of MCIs in the prediction of physico-chemical properties of persistent organic pollutants was extended in this study. A series of QSPR equations were established with high significance and accuracy, which shows this simple approach is effective and applicable in the estimation for properties needed for the risk assessment and exposure evaluation.

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