Prediction of Adsorption Isotherms of Organic Compounds from Water on Activated Carbons

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(Received January 22, 1981)

Synopsis. An adsorption equation is postulated for predicting the adsorption isotherms of organic compounds from water on activated carbons.

It is known that the prediction of adsorption isotherms for a given adsorbent from the physical properties of the adsorbate is important for adsorbent-adsorbate interaction. For gas-phase adsorption, Dubinin[1] showed that the physical constants such as molar volume and parachor are useful for predicting the isotherms. Reucroft *et al.*[2] studied the relationship between the adsorbability and physical constants and concluded that the molecular refraction gives a good correlation. In liquid-phase adsorption, Abe *et al.*[3] have calculated partition coefficient of 93 organic compounds between the solution and the adsorbed phases at an infinite dilution and examined the correlation with various physical constants. We present the following adsorption equation for predicting the adsorption isotherms of organic compounds from water on activated carbons in terms of a physical constant.

$$\log X = \alpha\Phi + \beta + \gamma \log C, \quad (1)$$

where X is the weight of solute adsorbed (mg/g), C the equilibrium concentration of the solute (mg/l), and α, β, γ are constants. The constant Φ represents the adsorbability of the adsorbate and is independent of the nature of adsorbent. We have tried to replace the Φ value with a physical constant such as molecular refraction or parachor.

Equation 1 was applied to the adsorption isotherms of 22 aliphatic monofunctional compounds from water on an activated carbon at 25 °C,[4] the data of 122 plots being given to a HITAC 10—II computer to determine the α, β, γ values by means of multiple regression analysis. The constants and statistic analysis for several physical constants are given in Table 1. High correlation coefficients have been obtained for molecular refraction and parachor. The result resembles that in gas-phase adsorption. Standard deviations, the t values in the Student test and the overall goodness of fit expressed by means of the F values indicate that Eq. 1 in which the Φ value is replaced with molecular refraction or parachor provides a satisfactory approximation. Figure 1 shows a plot of log X observed *vs.* log X calculated by means of

$$\log X_{\text{calcd}} = 0.08111R - 1.230 + 0.4895 \log C. \quad (2)$$

We see from Fig. 1 that the molecular refraction gives a good prediction of the isotherms as shown by

$$\log X_{\text{obsd}} = 0.99998 \log X_{\text{calcd}} - 0.000066. \quad (3)$$

(r=0.9685, s=0.09400, F=1018, t=42.63)

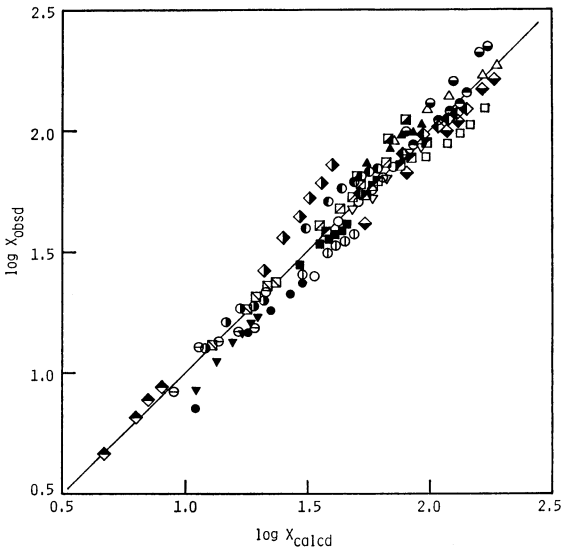

Fig. 1. Prediction of adsorption isotherms of 22 aliphatic monofunctional compounds from water on an activated carbon.
●: 1-Propanol, ○: 1-butanol, ◓: 1-pentanol, ◒: 1-hexanol, ◑: propionic acid, ◐: butyric acid, ▲: valeric acid, △: hexanoic acid, ▼: acetone, ■: 2-butanone, ▽: 2-pentanone □: 2-Hexanone, ⓓ: diethyl ether, ◆: dipropyl ether, ▧: methyl acetate, ◰: ethyl acetate, ◩: propyl acetate, ◈: butyl acetate, ◆: acetaldehyde, ⊖: propionaldehyde, ◈: butyraldehyde, ◪: valeraldehyde.

TABLE 1. MULTIPLE REGRESSION ANALYSIS FOR THE $\log X = \alpha\Phi + \beta + \gamma \log C$ EQUATION

Physical constant	Φ	α	β	γ	Multiple correlation coefficient r	Standard deviation s	Statistical test F	$t(\Phi)$	$t(\log C)$
Molecular refraction	R	0.08111	−1.230	0.4895	0.9685	0.09438	901.5	40.88	17.17
Parachor	P	0.009448	−1.445	0.5007	0.9671	0.09651	859.5	39.91	17.05
Molar-attraction constant	ΣF	0.002779	−1.683	0.4335	0.9337	0.1358	404.6	27.30	10.73
Molecular weight	M	0.02290	−1.146	0.4383	0.9198	0.1489	326.8	24.51	9.806
Molar volume	V	0.02067	−1.356	0.4704	0.9181	0.1397	300.5	23.61	10.69

$F(2, 60; 0.001)=7.76$, $t(60, 0.001)=3.460$.

Table 2. Multiple regression analysis for the $\log X=\alpha R+\beta+\gamma \log C$ equation

Activated carbon	α	β	γ	Number of data n	Multiple correlation coefficient r	Standard deviation s	Statistical test F	$t(R)$	$t(\log C)$
[A]	0.08407	−1.390	0.5461	12	0.9910	0.05971	247.3	22.22	7.506
[B]	0.06397	−0.4797	0.4312	13	0.9949	0.03543	487.6	31.21	11.14
[C]	0.06214	−0.4509	0.3823	13	0.9845	0.06103	157.7	17.76	5.590
[D]	0.07344	−1.328	0.5220	12	0.9650	0.09909	60.89	10.78	3.580
[E]	0.08439	−1.147	0.5137	13	0.9957	0.03989	578.4	33.53	11.64
[F]	0.07755	−1.117	0.5126	13	0.9948	0.04184	481.1	30.93	10.35
[G]	0.07095	−0.5225	0.4074	13	0.9943	0.04018	435.7	29.45	10.13
[H]	0.07318	−0.6517	0.4354	13	0.9921	0.04866	312.8	24.95	8.780
[I]	0.07232	−0.5587	0.4037	13	0.9893	0.05616	229.2	21.33	7.224
[J]	0.06798	−0.6728	0.4283	13	0.9905	0.05137	259.1	22.76	7.525
[K]	0.07390	−0.8544	0.4377	13	0.9932	0.04627	363.9	26.88	8.275
[L]	0.05782	−0.3705	0.4229	12	0.9858	0.05011	155.6	17.62	7.429
[M]	0.06805	−0.8374	0.4562	13	0.9887	0.05636	218.0	20.88	6.896
[N]	0.07847	−1.185	0.5622	13	0.9908	0.05577	267.6	23.07	8.514
[O]	0.08109	−0.9335	0.4906	13	0.9966	0.03400	724.5	37.58	13.70
[P]	0.07351	−0.9372	0.4527	13	0.9946	0.04128	459.9	30.28	9.383
[Q]	0.07543	−1.178	0.5277	13	0.9911	0.05439	275.9	23.48	8.019
[R]	0.07846	−1.050	0.5501	13	0.9933	0.04675	370.4	27.11	10.43
[S]	0.06239	−0.4707	0.4220	13	0.9977	0.05411	200.3	20.00	7.082
[T]	0.06926	−0.8454	0.5206	13	0.9836	0.06853	149.2	17.26	6.775

$F(2, 9; 0.001)=16.4$, $t(9, 0.001)=4.781$, $t(9, 0.01)=3.250$.

In order to examine whether Eq. 1 is applicable to the other activated carbons with different adsorption capacities, the adsorption experiments were carried out for 20 different activated carbons and 7 aliphatic monofunctional compounds (1-pentanol, butyric acid, hexanoic acid, 2-butanone, 2-pentanone, methyl acetate, butyl acetate). The results of multiple regression analysis for Eq. 1 with molecular refraction are given in Table 2. The high muliple correlation coefficients indicate that Eq. 1 is applicable to all the carbons.

If the α, β, and γ constants for a given activated carbon are determined from the adsorption data of several compounds, the adsorption isotherms of many other aliphatic monofunctional compounds can be predicted from only the molecular refraction constant.

References

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