Retention Volumes of Organic Substances on Ester Phases

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ABSTRACT: Reliable methods of agreement does not exist between the chromatographic retention volumes of substances and their physicochemical properties. That is why it is impossible to predict these characteristics for unstudied substances. Well-known works in this field have either qualitative character or give the results suitable only for homologous series. That is why it was very interesting to consider the available arrays of experimental data of gas-liquid chromatography by means of Koppel-Palm multi-parameter equations. The individual characteristics of this equation are determined experimentally. The final multi-parameter equation proposed by us was adequate for generalizing the retention-time data for the polyester phase of substances with different structures and also for calculating this value for other (unstudied) substances on the basis their physicochemical characteristics. The generalizing equations permit us to draw conclusions about the nature of the processes taking place during the adsorption-desorption of the substances in the stationary phase. © 2007 Wiley Periodicals, Inc. J Appl Polym Sci 106: 1595–1600, 2007

Key words: retardation time; solution properties

There are no reliable methods for correlating the chromatographic retention volume (V_R) values of various substances and their physicochemical properties at this time. That is why it is impossible to predict these characteristics for unstudied substances. Well-known works in this field[1,2] either present qualitative characteristics or provide results suitable only for ranges of similar substances (predominantly for homologous series); the latter is caused by the complicated character of the interactions taking place in the stationary chromatographic phase-absorbed substance system, which is impossible to describe adequately by the influence of one parameter.

Abraham and coworkers[3–5] proposed considering the data for the retention of substances on stationary phases via the processes of gas–liquid chromatography (GLCh) according to the principle of linearity of free energy. However, the characteristics of the substances used in their works to a great extent were obtained by means of different additive schemes.

For this reason, it is very interesting to consider the available arrays of experimental data from GLCH with the Koppel–Palm enlarged multiple-parameter equation; the separate characteristics of this equation are determined experimentally:[6]

$$\lg Q = a_0 + a_1 \frac{n^2 - 1}{n^2 + 2} + a_2 \frac{\varepsilon - 1}{2\varepsilon + 1} + a_3 B + a_4 E_T \quad (1)$$

In this equation, Q is a determinate value, such as the constant rate or equilibrium constant. a_1 is the numerical coefficient at separate terms, the numerical values of which are calculated by the generalization of quantitative experimental data. They reflect the significance of these terms on the magnitude of $\lg Q$. n and ε are the refractive index and permittivity, respectively, of the investigated substances, and they determine the polarizability and polarity; that is, they are the factors responsible for nonspecific solvation. B and E_T are the basicity according to Palm[7] and the electrophilicity accordingly to Reichardt,[8] respectively, and they determine the capacity of a substance for acid–base interactions, that is, for specific solvation.

We have shown in previous works[7–9] that this approach is also effective for the generalization of data concerning the solubility of gases as well as polymer and coal swelling in different solvents if we take into account the factors of the cohesion energy, which is proportional to the square of Hildebrand's solubility parameter (δ_H^2) and the molar volume (V_M)

TABLE I
Experimental Values of V_R for Various Substances and ΔH_{evap} Values

No.	Substance	ΔH_{evap} (kJ/mol) at 25°C	V_R at 120°C[b] DEG-A	DEG-S
1	*n*-Hexane	31.56	1.6	3.6
2	*n*-Octane	41.49	4.9	12.5
3	*n*-Decane	51.38	14.0	39.6
4	*n*-Dodecane	61.51	38.4	122.0
5	*n*-Tetradecane	71.30	107.0	373.0
6	*n*-Hexadecane	81.38	297.0	1110
7	Cyclohexane	33.01	4.6	8.8
8	Benzene	33.83	17.0	22.7
9	Toluene	38.01	28.8	42.6
10	*o*-Xylene	43.43	62.1	98.1
11	*m*-Xylene	42.65	48.6	79.6
12	*p*-Xylene	42.40	47.0	77.1
13	Ethyl benzene	42.24	44.0	71.5
14	Dichloromethane	28.82	10.8	13.1
15	Chloroform	31.28	17.6	22.9
16	Tetrachloroform	32.43	10.2	15.8
17	1,2-Dichloroethane	35.16	26.6	31.7
18	Methanol	37.43	9.5	8.1
19	Ethanol	42.32	11.7	11.2
20	Propanol-1	47.45	20.8	21.6
21	Propanol-2	45.39	12.4	12.7
22	Butanol-1	52.35	37.1	41.6
23	2-Methyl propanol-1	50.82	27.2	30.8
24	Butanol-2	49.72	20.7	23.7
25	2-Methyl propanol-2	46.69	11.4	12.9
26	Pentanol-1	57.02	63.9	77.6
27	3-Methyl butanol-1	55.61	49.7	61.4
28	Pentanol-2	54.21	33.9	42.4
29	Hexanol-1	61.61	107.0	141.0
30	4-Methyl pentanol-1	60.47	88.5	114.0
31	Heptanol-1	66.81	182.0	253.0
32	Octanol-1	70.98	321.0	477.0
33	2-Ethyl hexanol-1	69.80[a]	231.0	343.0
34	Cyclohexanol	62.01	164.0	194.0
35	Propene-2-ol	47.13[a]	29.4	27.5
36	2-Chloroethanol	49.20[a]	127.0	110.0
37	2-Methoxy ethanol	49.34[a]	53.1	47.7
38	Ethylene glycol	75.33[a]	481.0	—
39	Diethylene glycol	80.40[a]	—	—
40	Diethyl ether	27.10	2.4	3.7
41	Dipropyl ether	35.79[a]	5.2	—
42	Diisopropyl ether	32.26[a]	2.8	5.3
43	Dibutyl ether	44.97	14.6	31.2
44	Diamyl ether	45.00[a]	45.8	106.0
45	Diisoamyl ether	44.70[a]	27.2	63.8
46	Tetrahydropyran	34.67[a]	—	—
47	Tetrahydrofuran	31.99	12.6	16.0
48	Furan	27.45	6.3	7.5
49	1,4-Dioxane	38.60	37.9	41.7
50	Dimethoxyethane	36.39	15.6	19.3
51	Acetone	30.99	9.1	9.0
52	Butanone-2	34.79	14.2	16.0
53	Pentanone-3	38.52	20.9	26.6
54	Hexanone-2	43.14	36.5	49.3
55	Cyclopentanone	42.72	77.8	84.8
56	Cyclohexanone	45.06	133.0	160.0
57	Ethyl formate	31.96	8.0	8.6
58	Methyl acetate	32.29	—	9.2
59	Ethyl acetate	35.60	11.2	13.9
60	*n*-Propyl acetate	39.72	18.6	24.5
61	*n*-Butyl acetate	43.86	30.9	42.8

TABLE I *Continued*

| No. | Substance | ΔH_{evap} (kJ/mol) at 25°C | V_R at 120°C[b] | |
			DEG-A	DEG-S
62	*n*-Amyl acetate	48.00[a]	50.8	79.1
63	*iso*-Amyl acetate	46.70[a]	39.6	61.7
64	Ethyl propionate	39.21	16.3	22.3
65	Vinyl acetate	34.38[a]	11.3	13.2
66	Methyl acrylate	29.20[a]	15.2	17.7
67	Water	43.98	19.4	14.0

[a] Calculated value.
[b] Under GLCh conditions on the fixed phases.

of the solvents, reflecting the influence of the structural factors in accordance with eq. (2):

$$\lg Q = a_0 + a_1 f(n^2) + a_2 f(\varepsilon) + a_3 B \\ + a_4 E_T + a_5 \delta_H^2 + a_6 V_M \quad (2)$$

In this equation, Q is the solubility of the gases in the liquids (in molar parts) or the number of moles of the absorbed solvent. This equation is also effective for the generalization of data concerning the diffusion coefficients of organic liquids into polymers.[10]

Equation (2) can be expected to also be suitable for the generalization of data concerning the V_R values of substances in the stationary phases via their separation by the GLCh method because the gas sorption–desorption quasi-equilibrium processes, proceeding under dynamic conditions in the stationary phases, are the basis of GLCH. We have used the respective data from ref. 11 for 60 substances, knowing all the characteristics used in eq. (2) (see Table I), to check this assumption. Taking into account the different characteristics of the investigated substances (from nonpolar hydrocarbons to alcohols able to form hydrogen bonds), we can consider this set sufficiently representative of the ability of the substances to introduce both physical interactions and processes for the formation of hydrogen bonds or complexes with charge transfer. With the aim of generalization, we have used the values of V_R at 120°C in polar polymeric phases: diethylene glycol esters with adipinic acid [diethylene glycol adipinate (DEG-A)] and sebacic acid [diethylene glycol sebacinate (DEG-S)]. The characteristics of the retention of the liquid substances have been taken from reviews,[12,13] and the calculation have been performed in accordance with the recommendations of the International Union of Pure and Applied Chemistry for group correlation analysis in chemistry.[14]

The generalization of all the data presented in Table I for lg V_R for 64 substances in accordance with eq. (2) and GLCh for DEG-A leads to an expression with a relatively low value of the multiple correlation coefficient: $R = 0.915$. Consecutive exclusion from consideration of most divergent data in accordance with the technique[14] leads correspondingly to expressions with higher R values: for dioxane, $R = 0.931$; for ethylene glycol, $R = 0.940$; for vinyl acetate, $R = 0.948$; and for dimethoxyethane, $R = 0.956$. Hence, exclusion from consideration of four substances (only 7% of the general primary quantity) permits us to obtain a six-parameter equation with adequate accuracy for determining the relation between the logarithms of the V_R values of the substances and their physicochemical characteristics (according to ref. 14, the equation is considered adequate if $R \geq 0.95$):

$$\lg V_R = -6.48 + (18.12 \pm 1.08)f(n^2) + (3.75 \pm 0.54)f(\varepsilon) \\ - (0.203 \pm 0.300) \times 10^{-3} B + (0.20 \pm 0.007)E_T \\ + (0.349 \pm 0.116) \times 10^{-3}\delta_H^2 \\ + (9.01 \pm 0.54) \times 10^{-3}V_M \quad (3)$$

where N is 60, R is 0.956, and S is ± 0.149 (i.e., the root-mean-square deviation).

Positive signs for all the terms of the equation, with the exception of B, show that the retention times increase with the extension of the numerical values of these characteristics. Because the coupled correlation coefficient (r) between lg V_R and any term from eq. (3) is extremely low [a maximum of $r = 0.490$ was obtained with $f(n^2)$], it does not permit us to estimate the separate terms of the equation contribution to the value of lg V_R. That is why, in accordance with the meaning in ref. 14, the terms of the equation have been determined by means of their exclusion in turn from the calculations of the R values for the obtained equations with a lower number of terms. Thus, basicity parameter B is nonsignificant (with its exclusion, R of the obtained five-parameter equation is equal to 0.956; i.e., it remains practically invariable). The low significance of this parameter agrees with the large standard deviation for the value of the regression coefficient at the corresponding term exceeding its absolute value. The nonsignificant influence of the term δ_H^2 is also

relative (with its exclusion, R decreases to 0.949). Also, the exclusion of E_T has practically the same influence; R decreases to 0.948.

The obtained four-parameter equation [eq. (4)] is adequate; this is confirmed by the determination of Fisher's criterion according to recommendations[14] for the corresponding number of points at the confidence probability of 0.95:

$$\lg V_R = -6.39 + (17.37 \pm 1.09)f(n^2) \\ + (2.87 \pm 0.44)f(\varepsilon) + (0.035 \pm 0.005)E_T \\ + (8.52 \pm 0.54) \times 10^{-3}V_M \quad (4)$$

where N is 60, R is 0.949, and S is ± 0.160.

However, the exclusion of any remaining parameters practically destroys the correlation (R decreases below 0.9).

An analysis of eqs. (3) and (4) permits us to conclude that the factors determining the retention time are the physical interaction of the absorbed substances with the stationary phase and first of all the dipole–dipole interaction of more polar substrates with polar polyester. At the same time, the formation of hydrogen bonds practically does not take place, presumably as a result of the relatively high temperature (120°C) in the chromatographic column. Also, a greater volume of the molecules (V_M) increases their retention time; probably with the increasing size of the molecules absorbed to the structure of the stationary phase, their diffusion to the surface and desorption in the gas-carrier flow are complicated. This can involve the surprise that the V_R values of the substances are increased with increasing self-association, which is characterized by δ_H^2. However, this fact becomes understandable if we take into account $\delta_H^2 = (\Delta H_{\mathrm{evap}} - RT)/V_m$; that is, this factor depends on the evaporation enthalpy (ΔH_{evap}). Correspondingly, the energy needed for substance evaporation will increase; the desorption of the substances by gas-carrier flow from the film of the liquid phase will be complicated.

That is why we carried out the recalculation of the data from Table I with the change in eq. (2), using δ_H^2 of the substances with the corresponding values of ΔH_{evap} at 298 K. The values of ΔH_{evap} (298 K) used in the calculation are presented in Table I. After such a change, the following calculation can be performed:

$$\lg V_R = a_0 + a_1f(n^2) + a_2f(\varepsilon) + a_3B + a_4E_T \\ + a_5\Delta H_{\mathrm{evap}} + a_6V_M \quad (5)$$

The results are better than those of eq. (2). Thus, the data for the retention of all 64 substances on DEG-A are generalized by the six-parameter equation [eq. (5)] with $R = 0.933$, and consecutive exclusion from the calculation of the most deviating data permits us to increase its value to the recommended value

of $R > 0.95$ under the exclusion in the next order: dioxane, 0.942; *tert*-butanol, 0.946; vinyl acetate, 0.949; and water, 0.954. In this way, for the remaining 60 substances, eq. (6) is adequate:

$$\lg V_R = -4.20 + (13.86 \pm 1.45)f(n^2) + (2.91 \pm 0.54)f(\varepsilon) \\ + (0.224 \pm 0.317) \times 10^{-3}B - (6.557 \pm 10.523) \\ \times 10^{-3}E_T + (24.70 \pm 5.21) \times 10^{-3}\Delta H_{\mathrm{evap}} \\ + (1.888 \pm 1.478) \times 10^{-3}V_M \quad (6)$$

where N is 60, R is 0.954, and S is ± 0.159.

The determining factor of the retention time of the substances is ΔH_{evap}; the value of r between $\lg V_R$ and ΔH_{evap} is equal to 0.824 for all substances and is 0.832 if we take into account eq. (6). The influence of the rest of the equation terms has little significance; this is confirmed by the values of r between $\lg V_R$ and those ranging from 0.13 for B to 0.49 for $f(n^2)$.

After the exclusion of parameters of little significance, the dependence of the substance retention based on DEG-A at 120°C on their properties can be described with satisfactory accuracy by a four-parameter equation:

$$\lg V_R = -4.47 + (14.09 \pm 1.29)f(n^2) + (2.95 \pm 0.42)f(\varepsilon) \\ + (21.71 \pm 2.77) \times 10^{-3}\Delta H_{\mathrm{evap}} + (2.77 \pm 0.88) \\ \times 10^{-3}V_M \quad (7)$$

where N is 60, R is 0.953, and S is ± 0.161.

The experimental $\lg V_R$ values ($\lg V_{R,\mathrm{exp}}$), the corresponding values calculated in accordance with eq. (7) ($\lg V_{R,\mathrm{calcd}}$), and their divergence ($\Delta \lg V_R = \lg V_{R,\mathrm{calcd}} - \lg V_{R,\mathrm{exp}}$) are presented in Table II.

The influence of V_M has relatively little significance here because at its exclusion from the equation, R decreases to only 0.945. At the same time, although the retention time of the substances is determined mainly by the energy needed for evaporation (desorption) of the substances, the factors describing their ability for nonspecific interactions have an essential correcting influence on the value of $\lg V_R$, and the exclusion of the term $f(n^2)$ from eq. (7) reduces R to 0.851 and $f(\varepsilon)$ to 0.911.

With the aim of confirming these conclusions, we have considered in the same way the data for V_R of the same substances for DEG-S at 120°C (Table I). The results practically coincide with those for DEG-A. The following are presented: the quantities of the first generalized substances for N and R for all arrays of data and also of the substances for which the data disagree with the calculations and for which R increases with their exclusion, final generalizing expressions for six parameters and four parameters

TABLE II
Experimental and Calculated [Eq. (7)] Values of lg V_R for DEG-A at 120°C

No.	Substance	Δlg V_R	lg V_R Experimental	lg V_R Calculated
1	*n*-Hexane	0.1463	0.2041	0.3504
2	*n*-Octane	0.1584	0.6902	0.8486
3	*n*-Decane	0.1320	1.1461	1.2781
4	*n*-Dodecane	0.0836	1.5843	1.6679
5	*n*-Tetradecane	0.0042	2.0294	2.0336
6	*n*-Hexadecane	−0.0806	2.4728	2.3922
7	Cyclohexane	0.0934	0.6628	0.7562
8	Benzene	0.0898	1.2304	1.3202
9	Toluene	0.0204	1.4594	1.4798
10	*o*-Xylene	−0.0486	1.7931	1.7445
11	*m*-Xylene	−0.0606	1.6866	1.6260
12	*p*-Xylene	−0.0893	1.6721	1.5828
13	Ethyl benzene	−0.0474	1.6435	1.5961
14	Dichloromethane	0.1446	1.0334	1.1780
15	Chloroform	−0.0186	1.2455	1.2269
16	Tetrachloroform	0.0629	1.0086	1.0715
17	1,2-Dichloroethane	0.1158	1.4249	1.5407
18	Methanol	−0.2652	0.9777	0.7125
19	Ethanol	0.0513	1.0682	1.1195
20	Propanol-1	0.1242	1.3181	1.4423
21	Propanol-2	0.2438	1.0934	1.3372
22	Butanol-1	0.1127	1.5694	1.6821
23	2-Methyl propanol-1	0.1784	1.4346	1.6130
24	Butanol-2	0.2580	1.3160	1.5740
25	2-Methyl propanol-2	0.3746	1.0569	1.4315
26	Pentanol-1	0.0743	1.8055	1.8798
27	3-Methyl butanol-1	0.1603	1.6964	1.8567
28	Pentanol-2	0.2529	1.5302	1.7831
29	Hexanol-1	0.0428	2.0294	2.0722
30	4-Methyl pentanol-1	0.3281	1.9469	2.2750
31	Heptanol-1	−0.0017	2.2601	2.2584
32	Octanol-1	−0.0951	2.5065	2.4114
33	2-Ethyl hexanol-1	−0.0397	2.3636	2.3229
34	Cyclohexanol	0.1621	2.2148	2.3769
35	Propene-2-ol	0.1603	1.4683	1.6286
36	2-Chloroethanol	−0.2009	2.1038	1.9029
37	2-Methoxy ethanol	−0.1311	1.7251	1.5940
38	Ethylene glycol	−0.2914	2.6821	2.3907
39	Diethylene glycol	—	—	2.7158
40	Diethyl ether	0.1182	0.3802	0.4984
41	Dipropyl ether	0.1707	0.7160	0.8867
42	Diisopropyl ether	0.3401	0.4472	0.7873
43	Dibutyl ether	0.0785	1.1644	1.2429
44	Diamyl ether	−0.2848	1.6609	1.3761
45	Diisoamyl ether	−0.0826	1.4346	1.3520
46	Tetrahydropyran	—	—	1.2429
47	Tetrahydrofuran	0.0232	1.1004	1.1236
48	Furan	−0.0639	0.7993	0.7354
49	1,4-Dioxane	−0.7078	1.5786	0.8708
50	Dimethoxyethane	−0.4013	1.1931	0.7918
51	Acetone	−0.0789	0.9590	0.8801
52	Butanone-2	−0.0082	1.1523	1.1441
53	Pentanone-3	0.0461	1.3201	1.3662
54	Hexanone-2	−0.0045	1.5623	1.5578
55	Cyclopentanone	−0.1790	1.8910	1.7120
56	Cyclohexanone	−0.1859	2.1239	1.9380
57	Ethyl formate	−0.1302	0.9031	0.7729
58	Methyl acetate	—	—	0.7469
59	Ethyl acetate	−0.1332	1.0492	0.9160
60	*n*-Propyl acetate	−0.1483	1.2695	1.1212

TABLE II *Continued*

| No. | Substance | $\Delta \lg V_R$ | lg V_R | |
			Experimental	Calculated
61	*n*-Butyl acetate	−0.1985	1.4900	1.2915
62	*n*-Amyl acetate	−0.2315	1.7059	1.4744
63	*iso*-Amyl acetate	−0.1699	1.5977	1.4278
64	Ethyl propionate	−0.1050	1.2122	1.1072
65	Vinyl acetate	−0.4526	1.0531	0.6005
66	Methyl acrylate	−0.1372	1.1818	1.0446
67	Water	−0.4073	1.2878	0.8805

(without B and E_T), and values of r between lg V_R and ΔH_{evap}.

For DGE-S at 120°C, N is 63 and R is 0.950; R at the exclusion for dioxane is 0.958:

$$\lg V_R = -4.55 + (13.86 \pm 1.41)f(n^2) + (1.85 \pm 0.47)f(\varepsilon)$$
$$+ (0.059 \pm 0.303) \times 10^{-3}B + (15.833 \pm 10.358)$$
$$\times 10^{-3}E_T + (11.79 \pm 6.19) \times 10^{-3}\Delta H_{\text{evap}}$$
$$+ (6.943 \pm 1.721) \times 10^{-3}V_M \quad (8)$$

N is 62, R is 0.958, r is 0.853, and S is ± 0.151:

$$\lg V_R = -3.76 + (12.51 \pm 1.13)f(n^2) + (2.08 \pm 0.38)f(\varepsilon)$$
$$+ (20.07 \pm 2.89) \times 10^{-3}\Delta H_{\text{evap}} + (4.727 \pm 0.847)$$
$$\times 10^{-3}V_M \quad (9)$$

N is 62, R is 0.956, and S is ± 0.154.

In this case, the exclusion of V_M reduces R to the undesirable low value of 0.933.

As we can see, the same parameters are significant in eqs. (3) and (4). For these parameters, both the signs and values of the coefficients are kept; factor ΔH_{evap} is determining in all cases. The calculations show that a multiple-parameter equation [eq. (5)] is adequate for generalizing the retention-time data for the polyester phase of substances with different structures and also for calculating this value for other (unstudied) substances on the basis of their physicochemical characteristics. Besides, the general-

izing equations permit us to draw conclusions about the nature of the processes taking place during the absorption–desorption of the substances in the stationary phase.

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