Equations for Correlating Vapor Pressures with Temperature

Sir,

Equation 1 deals with an important property (vapor pressure, P) and an important relationship (P vs. temperature, t, °C or T, K). Equation 1, which is much simpler than previously proposed P vs. T equations (1–3), was used here to correlate P with t, °C, for more than 100 chemicals:

$$P^e = b + mt, \text{°C} \quad [1]$$

where e is an exponent, b is the intercept, and m is the slope of the line.

During the past 120 yr numerous equations have been proposed (1–3) for correlating P with t, °C, or T, K. The limitations of the frequently preferred Antoine Equation 2 (published in 1888) have been described by Riddick *et al.* (3). The more common of the equations published since 1888 are Equations 2–8 (3).

$$\log P = A - B/[(t, \text{in °C}) + C] \quad [2]$$

$$\log P = A - B/T + CT \quad [3]$$

$$\log P = A - B/T + C/T^2 + D/T^3 \quad [4]$$

$$\log \mathrm{P} = A - B/T - CT + DT^2 \quad [5]$$

$$\log P = A - B/T - C \log T \quad [6]$$

$$\log P = A - B/T + C \ln T \quad [7]$$

$$\log P = A - B/T + 1.75 \log T + CT \quad [8]$$

where A, B, C, and D are constants

In addition to being simple and user-friendly, Equation 1 has these advantages: P^e is linear with temperature and hence should be linear also with other temperature-linear properties; vapor pressures at additional temperatures can be calculated

TABLE I.
Ethers, Ketones, and Aldehydes: Equations[a] Correlating Vapor Pressures (*P*) with Temperature (*t*, °C)[b,c]

	Temp., °C	Exponent, *e*	Intercept, *b*	Slope, *m*	Corr. coeff., *r*
Diethyl ether	–25/50	0.20	1.904	0.01784	5, 77
Diisopentyl ether	–75/150	0.15	0.5719	0.00826	6, 10
Tetrahydrofuran	–25/100	0.21	1.459	0.01787	5, 62
Tetrahydropyran	0/88	0.17	1.178	0.01154	5, 56
Glycol dibutyl ether	100/203	0.20	0.0296	0.01225	5, 58
1,4-Dioxane	25/125	0.17	1.025	0.01151	5, 36
Anisole	25/150	0.17	0.6239	0.01021	5, 29
Diphenyl ether	200/258	0.20	–0.3204	0.01100	1.00
Acetone	0/100	0.20	1.562	0.01706	5, 33
Methyl propyl ketone	0/150	0.17	1.037	0.01126	4, 78
Methyl hexyl ketone	50/150	0.14	0.5061	0.00816	5, 74
Diethyl ketone	50/150	0.20	0.9707	0.01520	5, 69
Acetylacetone	25/125	0.21	0.6383	0.01455	4, 89
Cyclopentanone	50/151	0.20	0.7407	0.01363	5, 63
Cyclohexanone	100/155	0.18	0.6044	0.01088	5, 63
Acetaldehyde	–25/25	0.20	2.135	0.01880	6, 60
Propanal	0/48	0.17	1.557	0.01325	5, 62
Butanal	25/75	0.176	1.307	0.01267	1.00
Isobutanal	0/65	0.21	1.488	0.01784	4, 89
Acrolein	0/75	0.20	1.636	0.01660	5, 87
Furfural	75/162	0.20	0.3369	0.01353	4, 45
Benzaldehyde	50/150	0.17	0.4737	0.00963	4, 85
Salicylaldehyde	100/197	0.17	0.3530	0.00934	5, 74

[a] $P^e = b + m\,t$, °C, where P is vapor pressure (kPa), e is an exponent, b is the intercept, and m is the slope.
[b] Data from Reference 5.
[c] The correlation coefficient r, of for example, 0.9999977 given as 5, 77.

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TABLE 2
Esters, Alcohols, and Acids: Equations[a] Correlating Vapor Pressures (*P*) with Temperature (*t*, °C)[b,c]

	Temp., °C	Exponent, *e*	Intercept, *b*	Slope, *m*	Corr. coeff., *r*
Propyl formate	0/100	0.19	1.210	0.01474	$\underline{4}$, 84
Methyl acetate	0/100	0.20	1.528	0.01740	$\underline{4}$, 85
Ethyl acetate	0/100	0.18	1.237	0.01370	$\underline{5}$, 05
Propyl acetate	25/125	0.19	0.9780	0.01403	$\underline{5}$, 48
Toluyl acetate	100/213	0.15	0.3029	0.00796	$\underline{5}$, 51
Isobutyl isobutanoate	25/150	0.15	0.6922	0.00887	$\underline{5}$, 19
Diethyl carbonate	50/125	0.17	0.8121	0.01100	$\underline{6}$, 10
Dimethyl phthalate	125/284	0.15	0.0581	0.00684	$\underline{6}$, 60
Ethyl acrylate	25/100	0.17	1.029	0.01171	$\underline{5}$, 41
Ethyl benzoate	100/212	0.15	0.3865	0.00760	$\underline{5}$, 43
Glycol diacetate	50/150	0.13	0.4935	0.00706	$\underline{5}$, 17
Butyl stearate	100/343	0.10	0.0516	0.00448	$\underline{5}$, 37
1-Hexanol	50/150	0.17	0.3245	0.01188	$\underline{5}$, 52
Glycol monoethyl ether	25/135	0.15	0.7121	0.00952	$\underline{5}$, 28
Cyclohexanol	100/161	0.22	−0.1142	0.01789	$\underline{5}$, 82
THF-OH[d]	100/178	0.19	0.2674	0.1201	$\underline{6}$, 30
Furfuryl alcohol	25/150	0.10	0.6549	0.00551	$\underline{4}$, 87
Glycerol	200/290	0.25	−2.022	0.01791	$\underline{5}$, 74
Acetic acid	25/125	0.17	0.8459	0.01141	$\underline{5}$, 71
Nonanoic acid	100/255	0.15	−0.0849	0.00817	$\underline{5}$, 66
Lauric acid[e]	182/299	0.20	−0.9440	0.01158	$\underline{4}$, 84
Stearic acid	224/355	0.19	−1.083	0.00934	$\underline{4}$, 74
Oleic acid	200/350	0.12	−0.0897	0.00508	$\underline{5}$, 65

[a] $P^e = b + m\,t$, °C, where *P* is vapor pressure (kPa), *e* is an exponent, *b* is the intercept, and *m* is the slope.
[b] Lauric and stearic acid data (6); other data (5).
[c] Correlation coefficient *r*, of 0.999984 given as $\underline{4}$, 84.
[d] Tetrahydrofurfuryl alcohol.
[e] Vapor pressure for 215°C omitted in equation formation.

by interpolation or prudent extrapolation; it has been used successfully with many types of compounds and hence is generally useful; calculated vapor pressures agree well with experimental and literature values; and it can be converted easily into Equation 9 for calculating *t*, °C from *P*:

$$t,\ ^\circ\mathrm{C} = (P^e - b)/m \qquad [9]$$

The vapor pressure vs. temperature equations of the present work are given as follows: ethers, ketones, and aldehydes, Table 1; esters, alcohols, and acids, Table 2; nitrogen compounds,

TABLE 3
Nitrogen Compounds: Equations[a] Correlating Vapor Pressures (*P*) with Temperature (*t*, °C)[b,c]

	Temp., °C	Exponent, *e*	Intercept, *b*	Slope, *m*	Corr. coeff., *r*
Butylamine	0/100	0.18	1.230	0.01367	$\underline{5}$, 32
Dibutyl amine	75/150	0.17	0.5365	0.01039	$\underline{5}$, 87
Triethyl amine	25/89	0.25	1.076	0.02358	$\underline{5}$, 32
Diethanolamine	200/269	0.17	−0.4948	0.01000	$\underline{5}$, 24
Triethanolamine	260/335	0.14	−0.3463	0.00672	$\underline{5}$, 55
Aniline	100/184	0.17	0.3705	0.00990	$\underline{5}$, 38
Piperidine	50/125	0.20	0.9407	0.01485	$\underline{6}$, 30
Pyridine[d]	25/150	0.19	0.8819	0.01319	$\underline{5}$, 47
Hexanenitrile	25/150	0.16	0.6210	0.00903	$\underline{5}$, 47
Octanenitrile	100/205	0.17	0.3033	0.00921	$\underline{5}$, 35
Acrylonitrile	0/100	0.20	1.314	0.01553	$\underline{4}$, 86
Benzonitrile	50/150	0.14	0.5463	0.00720	$\underline{5}$, 84
Nitroethane	25/100	0.18	0.8943	0.01236	$\underline{5}$, 58
2-Nitropropane	25/125	0.19	0.8450	0.01298	$\underline{5}$, 39
Nitrobenzene	25/211	0.16	0.3663	0.00820	$\underline{5}$, 62
N,*N*-Dimethyl formamide	50/153	0.18	0.5656	0.01131	$\underline{5}$, 88
N,N-Dimethyl acetamide	50/150	0.20	0.2169	0.01394	$\underline{4}$, 86

[a] $P^e = b + m\,t$, °C, where *P* is vapor pressure (kPa), *e* is an exponent, *b* is the intercept, and *m* is the slope.
[b] Data from Reference 5.
[c] Correlation *r*, of 0.9999932 given as $\underline{5}$, 32.
[d] Vapor pressure at 50°C omitted in equation formation.

TABLE 4
Hydrocarbons, Halogen, Sulfur, Phosphorus, Silicon, and Lead Compounds: Equations[a] Correlating Vapor Pressures (P) with Temperature (t, °C)[b,c]

	Temp., °C	Exponent, e	Intercept, b	Slope, m	Corr. coeff., r
n-Hexane	–25/125	0.20	1.441	0.01560	4, 66
Toluene	25/150	0.20	0.9473	0.01418	4, 87
Perfluoro-tributyl amine	50/150	0.15	0.4422	0.00883	5, 57
Dichloromethane	–25/20	0.18	1.701	0.01500	5, 25
1-Chlorobutane	0/100	0.20	1.305	0.01545	5, 28
1-Chloroctane	75/150	0.17	0.4263	0.00968	6, 80
1-Bromopentane	50/150	0.20	0.7457	0.01367	5, 31
1-Iodobutane[d]	25/150	0.19	0.8197	0.01213	5, 28
1-Butanethiol	0/100	0.18	1.076	0.01240	5, 34
Dimethyl disulfide	0/100	0.17	0.9806	0.01109	5, 35
Benzenethiol	60/150	0.17	0.5347	0.00984	5, 60
Thiophene	25/125	0.20	1.219	0.01542	5, 50
Tetrahydrothiophene	50/150	0.20	0.8272	0.01398	5, 73
Dimethyl sulfoxide	25/150	0.14	0.5198	0.00742	5, 00
Tributyl phosphate	225/289	0.14	0.09279	0.00628	6, 70
o-Tricresylphosphate	250/400	0.12	–0.1709	0.00457	5, 24
Tetraethylsilane	25/150	0.16	0.7271	0.00893	5, 09
Trichloromethylsilane	25/75	0.21	1.490	0.01731	7, 00
Tetraethyl lead[e]	75/187	0.15	0.3815	0.00884	5, 61

[a] $P^e = b + m\,t$, °C, where P is vapor pressure (kPa), e is an exponent, b is the intercept, and m is the slope.
[b] Tetraethyl lead data from Reference 2; other data from Reference 5.
[c] Correlation coefficient r, of 0.9999934 given as 5, 34.
[d] Vapor pressure at 50°C not used in equation formation.
[e] Vapor pressure at 112° and 162°C not used in equation formation.

TABLE 5
Equations ($y = b + mx$)[a] Correlating Vapor Pressure, (P, mm Hg or kPa) with Temperature (t, °C or T, K)[a,b,c]

	Pressure, P	y	x	Intercept, b	Slope, m	Corr. coeff., r
Ethyl hexaneoate	5–760 mm Hg	$P^{0.175}$	t,°C	0.68627	0.01494	4, 11
		log P	$1/(t + 190)$	6.9331	–1449.4	4, 38
Ethyl octaneoate	5–760 mm Hg	$P^{0.155}$	t,°C	0.45047	0.01126	4, 70
		log P	$1/(t + 210)$	7.4821	–1925.3	4, 84
Ethyl decaneoate	5–760 mm Hg	$P^{0.165}$	t,°C	0.05253	0.01200	4, 22
		log P	$1/(t + 175)$	7.2132	–1817.8	4, 13
Hexyl acetate	5–760 mm Hg	$P^{0.16}$	t,°C	0.70308	0.01284	4, 59
		log P	$1/(t + 210)$	7.2727	–1649.2	4, 76
Octyl acetate	5–760 mm Hg	$P^{0.15}$	t,°C	0.43106	0.01081	4, 64
		log P	$1/(t + 215)$	7.7000	–2049.4	4, 80
Decyl acetate	5–760 mm Hg	$P^{0.165}$	t,°C	0.01079	0.01218	4, 57
		log P	$1/(t + 170)$	7.2559	–1820.7	4, 74
Dodecyl acetate	5–760 mm Hg	$P^{0.155}$	t,°C	0.11789	0.01044	4, 87
		log P	$1/(t + 170)$	7.4570	–2054.5	4, 90
Hexadecanoic acid	4–256 mmHg	$P^{0.17}$	t,°C	0.99320	0.01174	4, 72
		log P	$1/(t + 75)$	6.7540	–1644.4	5, 03
1-Butanol	0.1–130 kPa	$P^{0.155}$	t,°C	0.69878	0.01138	4, 52
		log P	$1/(t + 180)$	6.5790	–1362.1	6, 50
Heptane	30–190 kPa	$P^{0.21}$	T,K	–3.3953	0.01624	6, 60
		log P	$1/(T - 52)$	6.0835	–1303.2	6, 71

[a] $P^e = b + m\,t$,°C (or T, K) or the Antoine equation $\log P = b + m/(t,°C + k)$.
[b] Ester data (6, p. 524); 1-butanol data, (5); hexadecanoic data (6, p. 514); and heptane data (7).
[c] Correlation coefficient, r, of 0.999911 given as 4, 11.

Table 3; and hydrocarbons, halogen, sulfur, phosphorus, silicon, and lead compounds in Table 4.

The frequently used Antoine Equation 2 [(with 700 organic chemicals (4)] was compared with Equation 1 for several esters, one carboxylic acid, one alcohol, and one hydrocarbon (Table 5). The Antoine Equation 2 was slightly more accurate than Equation 1 in some instances but vastly inferior with respect to simplicity and ease of use.

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REFERENCES

1. Reid, R.C., J.M. Prausnitz, and B.E. Poling, *Properties of Liquids and Gases*, 4th edn., McGraw-Hill, New York, 1987.
2. Partington, J.R., *An Advanced Treatise on Physical Chemistry of Liquids*, Longmans, Green Co., New York, 1955, Vol. 2.
3. Riddick, J.A., W.B. Bunger, and T.K. Sakano, *Organic Solvents*, 4th edn., John Wiley & Sons, New York, 1986.
4. Yaws, C.L., *Thermodynamic and Physical Property Data*, Gulf Publishing, Houston, 1992.
5. Lide, D.R., *Handbook of Organic Solvents*, CRC Press, Boca Raton, 1995.
6. Singleton, W.S., *Fatty Acids, Part 1*, edited by K.S. Markley, Interscience Publishers, New York, 1960.
7. Weber, L.A., Vapor Pressure of Heptane from the Triple Point to the Critical Point, *J. Chem. Eng. Data 45*:173–176 (2000).

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