Solubility Parameters of Oil and Fat Chemicals

Sir:

Solubility parameters (solpars), important and useful (1,2), are scarce and frequently inaccurate for oil and fat chemicals. Solpars (δ), calculated by Equation 1, are useful in the coating industry to aid in the selection of solvents. They are used also to predict compatibility of polymers, chemical resistance, and permeation rates and even to characterize the surfaces of pigments, fibers, and fillers. Liquids with similar solpars are miscible, and polymers will dissolve in solvents having solpars similar to their own (1,2).

$$\delta, \text{MPa}^{1/2} = (\text{EvM}/V)^{1/2} \quad [1]$$

where EvM is vaporization energy, J/mol, and V is molar volume at 25°C.

Solpars for many oil and fat chemicals, calculated by Equation 2 (Table 1), are given in Table 2. Equation 2 was developed by dividing Equation 3 by Equation 4 (where C is total carbons and EvM/V is δ^2): EvM/$V = (b' + m'C)/(b + mC)$ multiplied by $(b + mC)$ gave $\delta^2 (b + mC) = b' + m'C$, which divided by m gave Equation 2.

$$\delta^2 (C + b/m) = b'/m + m'/mC \quad [2]$$

$$\text{EvM (J/mol)} = b' + m'C \quad [3]$$

$$V = b + mC \quad [4]$$

The relatively high solpars of the lower alcohols, acids, ketones, and nitriles decrease with increasing chain length; the reverse is true for the relatively low solpars of ethers and *t*-amines (Table 2). These trends suggest the ultimate or limiting solpar (δ_∞ for C_∞) is about 17 $\text{MPa}^{1/2}$.

Additional useful solpars, calculated by Equation 5 with Reference 4 data, are: acetic anhydride, 23.3; acetonitrile, 24.0; acetophenone, 20.8; adiponitrile, 23.4; allyl alcohol, 25.6; aniline, 24.1; benzene, 18.7; benzyl alcohol, 23.6; carbon disulfide, 20.3; carbon tetrachloride, 17.6; chloroform, 18.9; *m*-cresol, 23.8; cyclohexane, 16.8; dibutylphthalate, 17.0; diethanolamine, 25.5; diethylene glycol, 24.0; dimethyl sulfoxide, 26.6; 1,4-dioxane, 21.2; 2-ethoxyethanol, 21.7; ethylene glycol, 34.2; ethyl isobutyrate, 16.7; furfural, 24.1; glycerol, 33.7; hexane, 14.9; methyl benzoate, 20.6; *N*-methyl formamide, 30.2; methyl oleate, 17.5; methylene chloride, 21.1; nitrobenzene, 22.6; nitromethane, 25.8; pyridine, 21.6; styrene, 18.9; toluene, 18.2; triacetin, 21.0; and water, 47.9.

TABLE 1
Equations[a] Correlating Solubility Parameters (δ, $\text{MPa}^{1/2}$) with Total Number of Homolog Carbons (*C*)[b,c]

		k[a]	Intercept, *i*	Slope, *s*
Ethers:	MeOR	2.192	297.5	301.9
	EtOR	2.329	271.0	296.3
	BuOR	2.333	341.4	278.8
	ROR	2.389	286.0	288.7
Esters:	RCOOMe	1.941	562.9	301.1
	RCOOEt	2.052	785.8	272.9
	MeCOOR	2.027	730.4	292.9
Ketones:	MeCOR	1.412	698.5	285.6
Aldehydes:	RCHO	1.426	798.9	274.4
Alcohols:	ROH	1.611	1808	300.5
Acids:	RCOOH	1.572	2288	294.9
Amines:	RNH_2	2.021	844.5	288.4
	R_2NH	2.472	572.4	288.7
	R_3N	2.763	259.4	290.8
Nitriles:	RCN	1.339	1081	279.5

[a]$\delta^2 (C + k) = i + s\ C$, where δ is solubility parameter ($\text{MPa}^{1/2}$); C is total homolog carbons; and *k*, *i*, and *s* are *b*/*m*, *b*′/*m*, and *m*′/*m*, respectively, from Equation 2.
[b]*R* is *n*-alkyl with one or more carbons.
[c]Data from References 1–6.

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TABLE 2
Solubility Parameters (δ, $MPa^{1/2}$) Calculated by Table 1 Equations[a,b]

	Total homolog carbons, *C*								
	3	4	5	6	7	8	9	10	12
MeOR	15.2	15.6	15.9	16.1	16.2	16.3	16.4	16.5	16.6
EtOR	14.8	15.2	15.5	15.7	15.9	16.0	16.1	16.2	16.3
BuOR			15.4	15.6	15.7	15.8	15.9	15.9	16.0
ROR		15.0		15.5		15.8		16.0	16.1
RCOOMe	19.3	18.6	17.9	17.6	17.5	17.3	17.3	17.3	17.3
RCOOEt	19.1	18.3	17.8	17.4	17.3	17.2	17.1	17.1	17.0
MeCOOR	19.3	18.4	17.9	17.6	17.6	17.5	17.5	17.4	17.4
MeCOR	19.6	18.9	18.2	18.0	17.9	17.8	17.7	17.7	17.5
RCHO	19.3	18.7	18.4	18.2	18.0	17.8	17.7	17.6	17.5
ROH	24.2	23.2	22.4	21.8	21.3	20.9	20.6	20.4	19.9
RCOOH	26.3	25.0	23.9	23.2	22.5	22.0	21.6	21.3	20.7
RNH_2	18.5	18.2	18.1	17.9	17.8	17.7	17.7	17.6	17.5
R_2NH		16.5		16.5		16.6		16.7	16.7
R_3N	14.3			15.1			15.6		15.9
RCN	22.5	20.9	19.9	19.4	19.1	18.8	18.7	18.5	18.2

[a]*R* is *n*-alkyl with one or more carbons.
[b]Solubility parameters of some of the lower homologs were calculated by Equation 5 using Reference 4 data.

$$\delta = [(\text{HvM} - 2480)/V]^{1/2} \quad [5]$$

where HvM (J/mol) is vaporization heat, and 2480 is *RT* (gas constant 8.3144 and 298.15 K).

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