Comments Concerning “A Possible Simplification of the Goss-Modified Abraham Solvation Equation”

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Key Words: Linear free energy relationship; partition coefficient, solute descriptors

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In a paper appearing in this Journal, van Noort (2013a) suggested a possible simplification of the Goss-modified Abraham equation by eliminating the $v \cdot V$ term from the derived mathematical correlation for describing experimental air-solvent, water-solvent and organic solvent-organic solvent partition coefficients. The simplification was proposed after comparing the statistics of correlations based on the Goss-modified Abraham equation:

$$\log P = c + s \cdot S + a \cdot A + b \cdot B + l \cdot L + v \cdot V \quad (1)$$

to those of the simplified correlation:

$$\log P = c + s \cdot S + a \cdot A + b \cdot B + l \cdot L \quad (2)$$

obtained by removal of the $v \cdot V$ term. For the specific systems studied the author found that the $v \cdot V$ term could be omitted from the air-solvent partition coefficient correlations with no loss of statistical quality. For air-solvent and water-organic solvent, as well as solute partitioning in organic biphasic systems, elimination of the $v \cdot V$ term led to a fairly small deterioration of statistical quality. We concur that these conclusions hold for the most part for the specific systems considered by van Noort. Moreover, Mintz et al. (2008, 2009) and van Noort (2013a) have noted that the Abraham model L and V solute descriptors are highly inter-correlated. It is poor statistical practice to include these two highly inter-correlated descriptors in a single correlation equation.

Our purpose is not criticize the excellent work of van Noort (2013a), but rather we wish to clarify what may be an unintended consequence of the suggested simplification. The Goss-modified Abraham equation was obtained by substitution of the $v \cdot V$ term (or $l \cdot L$ term) into the Abraham solvation parameter for the $e \cdot E$ term. The Abraham model is based on two linear

free energy relationships (LFERs), eqns. (3) and (4) (Abraham, 1993; Abraham et al., 2004, 2010):

$$SP = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V}, \quad (3)$$

$$SP = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L}, \quad (4)$$

where SP denotes some property of a series of solutes in a given solvent, a given partitioning system, or a given biological or pharmaceutical process. In the present application SP refers to the logarithm of the solute's partition coefficient between two condensed phases, SP is $\log P$ in eqn. (3), or the logarithm of the solute's partition coefficient into a condensed phase from the gas phase, SP is $\log K$ in eqn. (4). We prefer to distinguish between the two types of partitioning processes by the different symbols P and K , while van Noort used the same symbol for both. Removal of the $e \cdot \mathbf{E}$ term from eqn. (4) gives the simplified version of the Goss-Modified Abraham model that van Noort suggested as the simplified version of Goss-Modified Abraham model for correlating both $\log P$ and $\log K$ values. Given the similarity between eqns. (2) - (4) the question arises is whether one should remove the $e \cdot \mathbf{E}$ term from the Abraham model? While van Noort did not suggest the removal of the $e \cdot \mathbf{E}$ term from the Abraham model, the possibility is perhaps an unintended, logical consequence resulting from the conclusions put forth by van Noort.

For informational purposes, the solute descriptors in the Abraham model (denoted as $\mathbf{E}$, $\mathbf{S}$, $\mathbf{A}$, $\mathbf{B}$, $\mathbf{V}$ and $\mathbf{L}$) when multiplied by their respective solvent/process equation coefficients (c_p , e_p , s_p , a_p , b_p , v_p , c_k , e_k , s_k , a_k , b_k and l_k) describe a specific type of molecular interaction. For example, the $a \cdot \mathbf{A}$ term describes a hydrogen-bond interaction between an H-bond donor solute and an H-bond acceptor solvent molecule. The solute descriptor $\mathbf{A}$ is a measure of the solute's overall hydrogen acidity. Similarly, the $b \cdot \mathbf{B}$ term measures the interaction between an H-bond

acceptor solute and an H-bond donor solvent molecule, and the $e \cdot E$ term describes interactions involving the solute's π - and n-electron pairs. The remaining solute descriptors and equation coefficients are described in greater detail by van Noort (2012, 2013a,b), by Panayiotou (2013), and by Abraham et al. (Abraham, 1993, Abraham et al., 2004).

Each term in the Abraham model is based on a type of molecular interaction believed to be present in solution. Each term does have physical significance. One can always eliminate terms from the Abraham model whenever the term's contribution is negligible; however, this should be done only after obtaining the correlation equation and only after assessing whether or not the term is indeed negligible. Small terms mean that the molecular interaction is weak for the given solute-solvent interaction. One should not presume ahead of time that the term will be negligible. Abraham, Acree and coworkers (Abraham and Acree, 2013; Abraham et al., 2010; Grubbs et al., 2010; Jiang et al., 2013; Stephens et al., 2012a,b) have assembled water-organic partition coefficient (as $\log P$) and air-condensed phase partition coefficients (as $\log K$) for water for more than 90 different organic solvents and for several ionic liquids. Poole and coworkers (Ariyasena and Poole, 2013; Poole et al., 2013) determined partition coefficients of a diverse series of organic solutes in numerous totally organic biphasic systems. Organic biphasic systems are used in the separation of compounds that decompose in an aqueous environment and in the determination of solute descriptors of compounds having insufficient aqueous solubility to permit accurate quantification. A partial listing of the published equation coefficients is given in Table 1. Examination of the numerical values shows that there are a large number of partitioning systems for which the e -coefficient is fairly large. Many of the water-alkane systems have e -coefficients in the $e \approx 0.56$ to $e \approx 0.82$ range, the water-wet/dry alcohol systems have e -

coefficients that range from $e \approx 0.17$ to $e \approx 0.62$, and the e -coefficients of the water-isopropyl myristate and water-carbon disulfide systems are $e \approx 0.92$ and $e \approx 0.69$, respectively.

To illustrate the effect that removal of the $e \cdot \mathbf{E}$ term can have on the descriptive ability of the derived Abraham model we will consider two representative examples using the equation coefficients provided in Table 1. For water-organic solvent partition coefficients we will also consider the $\mathbf{V}$ descriptor correlations for the reasons to be discussed shortly. In the case of the water-heptane partition system:

$$\begin{aligned} \log P = & 0.297(0.029) + 0.634(0.039) \mathbf{E} - 1.755(0.049) \mathbf{S} - 3.571(0.050) \mathbf{A} - 4.946(0.063) \mathbf{B} \\ & + 4.488(0.040) \mathbf{V} \end{aligned} \quad (5)$$

(N = 185, SD = 0.141, $R^2 = 0.996$, F = 7941)

$$\begin{aligned} \log P = & 0.153(0.043) - 1.116(0.047) \mathbf{S} - 3.531(0.078) \mathbf{A} - 5.454(0.085) \mathbf{B} + 4.759(0.056) \mathbf{V} \end{aligned} \quad (6)$$

(N = 185, SD = 0.221, $R^2 = 0.989$, F = 4019)

$$\begin{aligned} \log P = & 1.766(0.041) - 0.395(0.086) \mathbf{E} - 2.925(0.097) \mathbf{S} - 4.159(0.096) \mathbf{A} - 4.694(0.121) \mathbf{B} \\ & + 1.102(0.019) \mathbf{L} \end{aligned} \quad (7)$$

(N = 185, SD = 0.274, $R^2 = 0.983$, F = 2066)

$$\begin{aligned} \log P = & 1.756(0.042) - 3.188(0.083) \mathbf{S} - 4.167(0.101) \mathbf{A} - 4.417(0.110) \mathbf{B} + 1.049(0.016) \mathbf{L} \end{aligned} \quad (8)$$

(N = 185, SD = 0.290, $R^2 = 0.981$, F = 2318)

the best descriptive correlation is obtained with the $\mathbf{V}$ solute descriptor. Our past experience in using the Abraham model has shown that the $\mathbf{V}$ solute descriptor gives the better correlations for water-organic solvent partition coefficients, while the $\mathbf{L}$ descriptor gives the better correlations

for gas-organic solvent partition coefficients. This should not be too surprising as the numerical values of the solute descriptors were computed within this framework. The statistical information associated with the derived correlation equations include the number of experimental data points in the regression analysis (N), the standard deviation (SD), the squared correlation coefficient (R^2), and the Fisher-F statistic (F). Standard errors in the calculated coefficients are given in parenthesis immediately after the respective equation coefficient. The experimental partition coefficient data and solute descriptors used in the regression analyses were taken from a study by Stephens et al. (2012b).

Examination of eqns. (5) - (8) further reveals that removal of the $e \cdot E$ term increases the standard deviation from $SD = 0.141$ log units (eqn. 5) to $SD = 0.221$ log units (eqn. 6). Expressed in terms of the partition coefficient, P , the average error goes from 38 relative percent to 66 relative percent. Much smaller differences were noted in the case of the two L descriptor equations, $SD = 0.274$ log units (eqn. (7)) versus $SD = 0.290$ log units (eqn. (8)), but these are not the preferred equations for water-organic solvent partitions anyway. If the goal is to have a mathematical equation for predicting log P values of additional compounds for which measured experimental data are not available, then removal of the $e \cdot E$ term from eqn. (5) in this case defeats the purpose for deriving the Abraham model correlation. Since the numerical values of the E solute descriptor is easily calculable from the refractive index or group fragment values there is really no computational advantage for removing the $e \cdot E$ term from the model, except in those instances where the term is truly negligible.

The standard deviation for each derived correlation expression does not always provide the complete picture regarding the equation's descriptive ability. One needs to compare the measured log P values of individual solutes to calculated values based on each correlation

equation. We provide in Table 2 such comparisons for eqns. (5) - (8). Examination of the numerical entries in the second and sixth columns of the table reveals that replacement of the **V** descriptor by the **L** descriptor, combined with removal of the $e \cdot \mathbf{E}$ term from the Abraham model, leads to deviations of 0.55 log units or more for common solutes like helium, neon, sulfur dioxide, iodine, cyclohexane, ethylamine, propylamine, 2-nitropropane, pyrene and benzil. Even though the standard deviation increased by only 0.15 log units in going from eqn. (5) to eqn. (8), the deviations for several of the individual compounds increased much more.

The second dataset that we consider pertains to solute transfer from water into isopropyl myristate (Abraham and Acree, 2005). The dataset contains experimental log *P* values for 141 different solutes, many of which are derivatives of known pharmaceutical compounds. The log *P* values were determined either directly through practical partition coefficient measurements, or indirectly through solubilities of the solutes in both water and isopropyl myristate. Regression analysis of the 141 experimental log *P* values yielded the following two Abraham model correlations:

$$\begin{aligned} \log P = & -0.605(0.080) + 0.930(0.059) \mathbf{E} - 1.153(0.062) \mathbf{S} - 1.682(0.090) \mathbf{A} - 4.093(0.080) \mathbf{B} \\ & + 4.249(0.060) \mathbf{V} \end{aligned} \quad (9)$$

(N = 141, SD = 0.265, R² = 0.990, F = 1393)

$$\begin{aligned} \log P = & -0.282(0.130) - 0.843(0.099) \mathbf{S} - 1.604(0.151) \mathbf{A} - 4.113(0.135) \mathbf{B} + 4.414(0.099) \mathbf{V} \end{aligned} \quad (10)$$

(N = 185, SD = 0.439, R² = 0.946, F = 593)

The **L** solute descriptors were not available for most of the compounds of the compounds in the isopropyl myristate dataset, hence, our discussion is limited to the removal of the $e \cdot \mathbf{E}$ term from the Abraham model **V**-descriptor correlation. Examination of eqns. (9) and (10) reveals that the

equation containing the $e \cdot \mathbf{E}$ term provides the better mathematical correlation for the partition coefficients in the water-isopropyl myristate system.

Our comments should not be construed as a criticism of van Noort's paper. We are in full agreement with van Noort in that there is no need to use the two highly correlated solute descriptors $\mathbf{V}$ and $\mathbf{L}$ in the same mathematical correlation. The comparisons presented in this communication are intended to show the importance of retaining the $e \cdot \mathbf{E}$ term in the Abraham solvation parameter equations. We do recognize that there will be instances when the $e \cdot \mathbf{E}$ term can be removed from the derived correlations because of a small numerical value for the e -coefficient, in which case its contribution to the calculation of $\log P$ (or $\log K$) will be small. This will be true for other terms in the Abraham model as well. We prefer to use the $\mathbf{V}$ descriptor in the $\log P$ correlation and the $\mathbf{L}$ descriptor in the $\log K$ correlation, rather than using the $\mathbf{L}$ descriptor in both correlations as suggested by van Noort. As stated above our past experience with the Abraham model has been that the $\mathbf{V}$ descriptor provides the better of the two correlations for $\log P$ values and that the $\mathbf{L}$ -descriptor provides the better of the two correlations for $\log K$ values. The only exception is the gas-water system where the $\mathbf{V}$ -descriptor and the $\mathbf{L}$ -descriptor equations yield very nearly the same statistical fits. One of the objectives in deriving mathematical correlations is to predict unmeasured values for additional compounds. If this is the case then it makes sense to use the better of the derived correlations in making predictions for additional compounds. Moreover we (Abraham and Acree, 2010a,b,c; Abraham and Zhao, 2004) have extended the $\log P$ correlation:

$$\text{Log } P = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} + j^+ \cdot \mathbf{J}^+ + j^- \cdot \mathbf{J}^- \quad (11)$$

to include the partition of simple ions (such as Na^+ , Cl^-) and ionic species (such as substituted benzoates, tetraalkylammonium cations, pyridinium ions). The term $j^+ \cdot \mathbf{J}^+$ applies to cations and

the term $j^- \cdot \mathbf{J}^-$ term applies to anions. The two new descriptors do not appear in the equation at the same. Equation (11) applies also to neutral molecules for which the solute parameters $\mathbf{J}^+ = \mathbf{J}^- = 0$, and that the coefficients c_p , e_p , s_p , a_p , b_p , and v_p in eqn. (11) are the same as those in eqn (3). It is not possible to use correlations that contain the $\mathbf{L}$ descriptor for predictions involving simple ions and ionic species because there are no values of the $\mathbf{L}$ descriptor for these chemical entities.

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Table 1. Abraham model correlations for select water-organic solvent, water-ionic liquid, organic biphasic and air-organic solvent partition systems

Solvent	c	e	s	a	b	l	v
Water-organic solvent							
Butanol (wet)	0.376	0.434	-0.718	-0.097	-2.350	0.000	2.682
Pentanol (wet)	0.185	0.367	-0.732	0.105	-3.100	0.000	3.395
Hexanol (wet)	-0.006	0.460	-0.940	0.142	-3.284	0.000	3.792
Heptanol (wet)	0.041	0.497	-0.976	0.030	-3.438	0.000	3.859
Octanol (wet)	0.088	0.562	-1.054	0.034	-3.460	0.000	3.814
Nonanol (wet)	-0.041	0.562	-1.103	0.090	-3.540	0.000	3.922
Decanol (wet)	-0.136	0.542	-0.989	0.046	-3.722	0.000	3.996
Isobutanol (wet)	0.249	0.480	-0.639	-0.050	-2.284	0.000	2.758
Methanol (dry)	0.276	0.334	-0.714	0.243	-3.320	0.000	3.549
Ethanol (dry)	0.222	0.471	-1.035	0.326	-3.596	0.000	3.857
Propan-1-ol (dry)	0.139	0.405	-1.029	0.247	-3.767	0.000	3.986
Butan-1-ol (dry)	0.165	0.401	-1.011	0.056	-3.958	0.000	4.044
Pentan-1-ol (dry)	0.150	0.536	-1.229	0.141	-3.864	0.000	4.077
Hexan-1-ol (dry)	0.115	0.492	-1.164	0.054	-3.978	0.000	4.131
Heptan-1-ol (dry)	0.035	0.398	-1.063	0.002	-4.342	0.000	4.317
Octan-1-ol (dry)	-0.034	0.489	-1.044	-0.024	-4.235	0.000	4.218
Decan-1-ol (dry)	-0.058	0.616	-1.319	0.026	-4.153	0.000	4.279
Propan-2-ol (dry)	0.099	0.344	-1.049	0.406	-3.827	0.000	4.033
iso-Butanol (dry)	0.188	0.354	-1.127	0.016	-3.568	0.000	3.986
2-Butanol (dry)	0.127	0.253	-0.976	0.158	-3.882	0.000	4.114
tert-Butanol (dry)	0.211	0.171	-0.947	0.331	-4.085	0.000	4.109
3-Methylbutan-1-ol (dry)	0.073	0.360	-1.273	0.090	-3.770	0.000	4.273
2-Pentanol (dry)	0.115	0.455	-1.331	0.206	-3.745	0.000	4.201
Pentane	0.369	0.386	-1.568	-3.535	-5.215	0.000	4.514
Hexane	0.333	0.560	-1.710	-3.578	-4.939	0.000	4.463
Heptane	0.297	0.634	-1.755	-3.571	-4.946	0.000	4.488
Octane	0.231	0.738	-1.840	-3.585	-4.907	0.000	4.502
Nonane	0.240	0.619	-1.713	-3.532	-4.921	0.000	4.482
Decane	0.186	0.722	-1.741	-3.449	-4.970	0.000	4.476
Undecane	0.058	0.603	-1.661	-3.421	-5.120	0.000	4.619
Dodecane	0.114	0.668	-1.644	-3.545	-5.006	0.000	4.459
Hexadecane	0.087	0.667	-1.617	-3.587	-4.869	0.000	4.433
Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	0.000	4.577

Methylcyclohexane	0.246	0.782	-1.982	-3.517	-4.293	0.000	4.528
Isooctane	0.320	0.511	-1.685	-3.867	-4.811	0.000	4.399
Benzene	0.142	0.464	-0.588	-3.099	-4.625	0.000	4.491
Toluene	0.125	0.431	-0.644	-3.002	-4.748	0.000	4.524
<i>o</i> -Xylene	0.083	0.518	-0.813	-2.884	-4.821	0.000	4.559
<i>m</i> -Xylene	0.122	0.377	-0.603	-2.981	-4.961	0.000	4.535
<i>p</i> -Xylene	0.166	0.477	-0.812	-2.939	-4.874	0.000	4.532
Ethylbenzene	0.093	0.467	-0.723	-3.001	-4.844	0.000	4.514
Nitrobenzene	-0.152	0.525	0.081	-2.332	-4.494	0.000	4.187
Isopropyl myristate	-0.605	0.930	-1.153	-1.682	-4.093	0.000	4.249
Water-Ionic Liquids							
([MBIm] ⁺ [BF ₄] ⁻) ^a (dry)	-0.082	0.454	0.541	-0.427	-4.583	0.000	2.961
([MBIm] ⁺ [(Tf) ₂ N] ⁻) ^b (dry)	-0.018	0.416	0.153	-1.312	-4.187	0.000	3.347
([MEIm] ⁺ [(Tf) ₂ N] ⁻) ^c (dry)	0.029	0.351	0.202	-1.684	-3.585	0.000	3.059
([MBPip] ⁺ [(Tf) ₂ N] ⁻) ^d (dry)	-0.129	0.494	0.235	-1.165	-4.385	0.000	3.422
([MBPyr] ⁺ [B(CN) ₄] ⁻) ^e (dry)	-0.071	0.354	0.562	-1.030	-4.415	0.000	3.346
([MeoeMPyr] ⁺ [FAP] ⁻) ^f (dry)	0.130	0.168	0.477	2.483	-4.245	0.000	3.215
Organic biphasic system							
Heptane - formamide	0.151	0.554	-2.169	-3.356	-1.671	0.000	2.257
Heptane - propylene carbonate	0.538	0.435	-2.087	-2.678	-0.441	0.000	0.796
Heptane - trifluoroethanol	-0.021	0.910	-1.581	-1.271	-2.852	0.000	1.307
Heptane - hexafluoroisopropanol	-0.372	0.914	-1.602	-0.633	-2.138	0.000	1.144
Isopentyl ether - formamide	0.135	0.570	-1.706	-1.314	-1.418	0.000	1.992
Triethylamine – formamide	-0.089	0.561	-1.100	-0.377	-1.601	0.000	1.733
Triethylamine - ethanolamine	0.067	-0.394	-0.640	-1.340	-1.282	0.000	1.406
Air-organic solvent							
Benzene	0.107	-0.313	1.053	0.457	0.169	1.020	0.000
Toluene	0.085	-0.400	1.063	0.501	0.154	1.011	0.000
<i>o</i> -Xylene	0.064	-0.296	0.934	0.647	0.000	1.010	0.000
<i>m</i> -Xylene	0.071	-0.423	1.068	0.552	0.000	1.014	0.000
<i>p</i> -Xylene	0.113	-0.302	0.826	0.651	0.000	1.011	0.000
Ethylbenzene	0.059	-0.295	0.924	0.573	0.098	1.010	0.000
Fluorobenzene	0.181	-0.621	1.432	0.647	0.000	0.986	0.000
Chlorobenzene	0.064	-0.399	1.151	0.313	0.171	1.032	0.000
Bromobenzene	-0.064	-0.326	1.261	0.323	0.292	1.002	0.000
Methyl <i>tert</i> -butyl ether (dry)	0.278	-0.489	0.801	2.495	0.000	0.993	0.000
Tetrahydrofuran (dry)	0.189	-0.347	1.238	3.289	0.000	0.982	0.000

Dioxane (dry)	-0.034	-0.354	1.674	3.021	0.000	0.919	0.000
Methyl acetate (dry)	0.134	-0.477	1.749	2.678	0.000	0.876	0.000
Ethyl acetate (dry)	0.182	-0.352	1.316	2.891	0.000	0.916	0.000
Propyl acetate (dry)	0.165	-0.383	1.264	2.757	0.000	0.935	0.000
Butyl acetate (dry)	0.147	-0.414	1.212	2.623	0.000	0.954	0.000
Dimethylformamide (dry)	-0.391	-0.869	2.107	3.774	0.000	1.011	0.000
Dimethylacetamide (dry)	-0.308	-0.736	1.802	4.361	0.000	1.028	0.000
Acetonitrile (dry)	-0.007	-0.595	2.461	2.085	0.418	0.738	0.000

^a 1-Methyl-3-butyylimidazolium tetrafluoroborate

^b 1-Methyl-3-butyylimidazolium *bis*(trifluoromethylsulfonyl)imide

^c 1-Methyl-3-ethyylimidazolium *bis*(trifluoromethylsulfonyl)imide

^d 1-Methyl-1-butylpiperidinium *bis*(trifluoromethylsulfonyl)imide

^e 1-Methyl-1-butylpyrrolidinium tetracyanoborate

^f 1-(2-methoxyethyl)-1-methylpyrrolidinium *tris*(pentafluoroethyl)trifluorophosphate

Table 2. Comparison of Experimental $\log P$ Data for the Water-Heptane Partition System to Predicted Values Based on Eqns. (5) - (8) for Select Solutes

Solute	Log P Values				
	Exp.	Eqn. (5)	Eqn. (6)	Eqn. (7)	Eqn. (8)
Helium	0.636	0.602	0.477	-0.153	-0.070
Neon	0.731	0.679	0.731	0.030	0.104
Nitrous oxide	0.710	0.493	0.554	0.427	0.371
Sulfur dioxide	-0.530	-0.566	-0.469	-1.087	-1.140
Iodine	1.555	1.813	1.391	2.146	2.315
Nonane	6.600	6.476	6.705	6.375	6.143
Cyclohexane	3.970	4.109	4.065	4.619	4.546
Carbon disulfide	2.590	2.449	2.034	3.130	3.281
Ethylamine	-1.770	-1.556	-1.797	-1.032	-0.962
Propylamine	-1.000	-0.930	-1.126	-0.516	-0.475
2-Nitropropane	0.520	0.354	0.684	0.251	0.040
Pyrene	5.022	4.803	4.259	4.075	4.334
Benzil	2.700	2.705	2.789	2.022	1.932