Benchmarking the SPARC software program for estimating solubilities of naphthalene and anthracene in organic solvents

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The solubility of polyaromatic hydrocarbons (PAHs) and their derivatives in organic solvents is of substantial interest for the upstream and downstream petroleum sectors [1-4]. Knowledge of this physico-chemical property helps guide the development and optimization of existing and proposed extraction and processing operations. In addition to extensive experimental work determining the solubilities of various PAHs (see, e.g., ref. [5-21]), a number of studies have developed quantitative structure-property relationships (QSPRs) and employed associated software programs (see, e.g., ref. [22-28]) for predicting the solubility of these compounds in a wide range of solvent systems.

To date, despite its broad applications towards predicting the partitioning behavior and reactivity of various organic compounds, the SPARC software program [29-36] has not been previously benchmarked for its capacity to estimate the solubility of representative PAHs in organic solvents. Consequently, in the current work we investigate the ability of SPARC to predict the solubilities of naphthalene (**1**) and anthracene (**2**) (Figure 1) in a range of organic solvents at various temperatures.
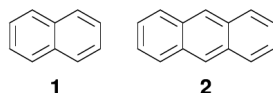

Fig. 1. Structures of naphthalene (**1**) and anthracene (**2**).

Mole fraction solubilities (log_{10} X_A^{sat}) of **1** and **2** were estimated using SPARC (August 2011 release w4.6.1646-s4.6.1646; http://ibmlc2.chem.uga.edu/sparc/) with the default settings and solvent profiles. We have previously examined the ability of this program to estimate the pK$_a$ values, hydrolysis rate constants, and partitioning behavior of several classes of organic compounds [37-46].

We began our studies using the X_A^{sat} of naphthalene obtained in chloroform, t-butanol, cyclohexanol, 2-propanol, 1-propanol, and ethanol at 40°C under atmospheric pressure (Table 1). Poor agreement between the experimental and SPARC predicted X_A^{sat} was found for t-butanol, cyclohexanol, and 2-propanol (errors of +0.78, +0.41, and +0.45 log_{10} units, respectively), with reasonable X_A^{sat} agreement for chloroform, 1-propanol, and ethanol (errors of +0.11, -0.15, and -0.02 log_{10} units, respectively).

Table 1. Comparison between experimental and SPARC estimated mole fraction solubilities (log_{10} X_A^{sat}) of naphthalene in selected organic solvents at 40°C under atmospheric pressure.

	expt.	SPARC
chloroform	-0.33 [47]	-0.22
t-butanol	-1.00 [47]	-0.22
cyclohexanol	-0.63 [47]	-0.22
2-propanol	-1.12 [47]	-0.67
1-propanol	-1.03 [47]	-1.28
ethanol	-1.14 [47]	-1.16

However, a recurring problem with SPARC appears to be its inconsistency in reproducing results between different sessions of the online program. For example, during one session, X_A^{sat} of -0.16,

-0.16, -0.16, -0.16, -0.94, and -0.84 were obtained for chloroform, t-butanol, cyclohexanol, 2-propanol, 1-propanol, and ethanol at 40°C, respectively. Later the same day, different corresponding X_A^{sat} values of -0.22, -0.22, -0.22, -0.67, -1.28, and -1.16 were obtained. We have previously reported on the temporal instability of the SPARC program for predicting partitioning properties [40]. Several concerns arise from this software behavior. The first issue is that solvents with such widely differing physico-chemical properties as chloroform, t-butanol, and cyclohexanol should not have equivalent predicted X_A^{sat} to two significant figures for PAHs. Additionally, temporal inconsistencies in the prediction performance of any software program renders it of little utility, and suggests substantial code errors as the source of the anomalous and unpredictable responses.

We then considered the solubility behavior of naphthalene in a suite of additional organic solvents of varying polarity and for which broad temperature range specific X_A^{sat} values were available (Table 2). With the single exception of methanol, SPARC overestimates the solubility of naphthalene in all solvents (i.e., log_{10} $X_{A,SPARC}^{sat}$>log_{10} $X_{A,expt}^{sat}$). Similarly, with the exception of methanol, the SPARC prediction performance improves with increasing temperature, as the solute becomes more soluble in the solvent. While the errors in predicted versus experimental log_{10} X_A^{sat} are typically on the order of several tenths of a log_{10} unit at low temperatures, at higher temperatures the error is reduced (with the exception of methanol) to <0.1 log_{10} units.

Table 2. Comparison between experimental and SPARC estimated mole fraction solubilities (log_{10} X_A^{sat}) of naphthalene in selected organic solvents at various temperatures under atmospheric pressure.

benzene			chlorobenzene		
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
6.1	-0.76 [48]	-0.31	4.2	-0.73 [48]	-0.32
15.0	-0.65 [48]	-0.27	8.8	-0.68 [48]	-0.30
21.7	-0.57 [48]	-0.24	22.1	-0.53 [48]	-0.24
29.1	-0.49 [48]	-0.20	29.4	-0.46 [48]	-0.20
39.6	-0.38 [48]	-0.16	40.0	-0.35 [47]	-0.16
40.0	-0.37 [47]	-0.16	42.8	-0.33 [48]	-0.14
48.8	-0.28 [48]	-0.12	49.0	-0.27 [48]	-0.12
61.2	-0.16 [48]	-0.071	62.6	-0.15 [48]	-0.066
methanol			acetone		
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
0.8	-1.97 [48]	-2.33	6.3	-0.90 [48]	-0.69
13.5	-1.79 [48]	-2.08	14.3	-0.78 [48]	-0.28
26.3	-1.59 [48]	-1.85	24.2	-0.64 [48]	-0.23
33.6	-1.48 [48]	-1.72	32.6	-0.52 [48]	-0.19
40.0	-1.36 [47]	-1.61	39.3	-0.44 [48]	-0.16
43.9	-1.29 [48]	-1.55	40.0	-0.42 [47]	-0.16
56.7	-0.99 [48]	-1.34	47.2	-0.33 [48]	-0.13
68.4	-0.41 [48]	-1.14	58.5	-0.21 [48]	-0.081
74.3	-0.086 [48]	-1.03	69.5	-0.094 [48]	-0.039
n-butanol			nitrobenzene		
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
11.7	-1.31 [48]	-1.23	2.9	-0.79 [48]	-0.59
22.0	-1.24 [48]	-1.04	13.8	-0.66 [48]	-0.28
31.6	-1.09 [48]	-0.80	24.0	-0.54 [48]	-0.23
40.0	-0.94 [47]	-0.16	40.0	-0.36 [47]	-0.16
46.5	-0.80 [48]	-0.13	45.3	-0.31 [48]	-0.14
56.9	-0.56 [48]	-0.088	60.2	-0.17 [48]	-0.075
68.1	-0.22 [48]	-0.045	65.3	-0.12 [48]	-0.055
76.0	-0.04 [48]	-0.015	71.8	-0.070 [48]	-0.031

Table 2 cont'd.

	aniline			n-hexane	
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
0.6	-1.16 [48]	-0.34	8.7	-1.21 [48]	-0.45
10.6	-0.99 [48]	-0.29	14.8	-1.10 [48]	-0.41
22.0	-0.81 [48]	-0.24	19.5	-1.02 [48]	-0.38
29.9	-0.68 [48]	-0.20	27.7	-0.88 [48]	-0.33
37.4	-0.56 [48]	-0.17	36.1	-0.73 [48]	-0.28
40.0	-0.51 [47]	-0.16	40.0	-0.65 [47]	-0.25
50.8	-0.35 [48]	-0.11	45.8	-0.54 [48]	-0.13
60.8	-0.20 [48]	-0.072	57.9	-0.30 [48]	-0.084
65.4	-0.15 [48]	-0.055	64.6	-0.18 [48]	-0.058
74.4	-0.055 [48]	-0.021	72.5	-0.072 [48]	-0.028
	carbon tetrachloride			toluene	
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
0.4	-0.92 [48]	-0.36	8.2	-0.74 [48]	-0.31
6.0	-0.84 [48]	-0.32	17.3	-0.63 [48]	-0.26
13.0	-0.75 [48]	-0.28	34.8	-0.43 [48]	-0.18
19.5	-0.66 [48]	-0.25	40.0	-0.37 [47]	-0.16
28.2	-0.55 [48]	-0.21	43.9	-0.33 [48]	-0.14
39.5	-0.41 [48]	-0.16	52.1	-0.25 [48]	-0.11
40.0	-0.40 [47]	-0.16	67.4	-0.13 [48]	-0.047
46.9	-0.32 [48]	-0.13			
58.3	-0.20 [48]	-0.082			
64.8	-0.14 [48]	-0.057			
72.4	-0.067 [48]	-0.028			

Although the SPARC prediction errors for the solubilities of naphthalene at low temperatures in these organic solvents are larger than desired, they were sufficiently modest to warrant an examination into the solubilities of the next highest member of the [n]acene PAH series – anthracene – in various organic solvents (Tables 3 and 4). For this larger PAH, we find generally poor SPARC prediction performance at both low and moderately elevated temperatures, with $\log_{10} X_A^{sat}$ errors (always positive with the exceptions of ethylene glycol and 2,2,2-trifluoroethanol) typically on the order of one $\log_{10}$ unit or higher. In each of the solvents for which multiple temperature comparisons were made (toluene, 2-propanol, and n-heptane), the prediction errors all decline with increasing temperature, but not to the extent required to obtain reliable $\log_{10} X_A^{sat}$ estimates.

Table 3. Comparison between experimental and SPARC estimated mole fraction solubilities ($\log_{10} X_A^{sat}$) of anthracene in selected organic solvents at 25°C under atmospheric pressure.

solvent	expt.	SPARC
n-nonane	-2.68 [49]	-1.02
n-decane	-2.63 [49]	-1.02
chloroform	-1.96 [49]	-1.31
dichloromethane	-2.03 [49]	-1.17
chlorobenzene	-2.00 [49]	-0.80
methanol	-3.61 [49]	-3.21
ethanol	-3.34 [49]	-2.37
1-hexanol	-2.83 [49]	-1.70
cyclopentanol	-2.88 [49]	-2.07
ethylene glycol	-4.15 [49]	-4.86
2,2,2-trifluoroethanol	-4.06 [49]	-5.27
acetonitrile	-3.08 [49]	-2.26
benzonitrile	-2.07 [49]	-0.82
N,N-dimethylformamide	-2.11 [49]	-1.40
N,N-dimethylacetamide	-1.90 [49]	-1.16

Table 4. Comparison between experimental and SPARC estimated mole fraction solubilities ($\log_{10} X_A^{sat}$) of anthracene in selected organic solvents at various temperatures under atmospheric pressure.

solvent	Temperature (°C)	expt. $\log_{10} X_A^{sat}$	SPARC $\log_{10} X_A^{sat}$
toluene	20.0	-2.21 [50]	-1.07
	25.0	-2.14 [50]	-1.05
	30.0	-2.07 [50]	-1.00
	35.0	-1.98 [50]	-0.96
	40.0	-1.95 [50]	-0.93
	45.0	-1.85 [50]	-0.89
	50.0	-1.80 [50]	-0.85
2-propanol	20.0	-3.72 [50]	-1.90
	25.0	-3.43 [50], -3.39 [51], -3.47 [52]	-1.85
	30.0	-3.37 [50], -3.36 [52]	-1.75
	35.0	-3.24 [50], -3.21 [52]	-1.68
	40.0	-3.13 [50], -3.09 [52]	-1.61
	45.0	-3.13ᵃ [50]	-1.53
	50.0	-2.96 [50]	-1.47
n-heptane	20.0	-2.92 [50]	-1.09
	25.0	-2.87 [50], -2.80 [53]	-1.05
	30.0	-2.73 [50]	-1.00
	35.0	-2.75 [50]	-0.96
	40.0	-2.63 [50]	-0.92
	45.0	-2.49 [50]	-0.88
	50.0	-2.46 [50]	-0.84

ᵃ reported experimental X_A^{sat} value in ref. [50] is suspect as these authors report no change in X_A^{sat} between 40°C and 45°C, in contrast to expectations and the general trend between 20°C and 50°C.

Overall, the results suggest that the SPARC software program is currently not suitable for accurately predicting the solubilities of representative PAHs relevant for the petroleum sector in various organic solvents.

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