Additions and Corrections

Christopher P. Higgins and Richard G. Luthy*: Modeling Sorption of Anionic Surfactants onto Sediment Materials: An a priori Approach for Perfluoroalkyl Surfactants and Linear Alkylbenzene Sulfonates

There are errors in the estimated aqueous solubilities (C_w^{sat} (L)) for the perfluoroalkanes and the associated free energies of phase transfer per CF_2 unit reported in Table 1 due to an incorrect application of the superheated liquid solubility equation for the perfluoroalkanes of interest. This alters the magnitude of the corresponding hydrophobic components to the Gibbs free energy of sorption reported in Table 2. This change is consistent with previously reported values of the free energy of phase transfer per CF_2 unit reported by Goss and Bronner (*J. Phys. Chem. A* **2006**, *110*, 9518−9522), as corrected in a subsequent erratum to their original paper (*J. Phys. Chem. A* **2006**, *110*, 14054). A corrected version of Table 2 is included below. For Table 1, the correct value for the $\Delta\Delta G_{sol}$ per CF_2 unit from air to water is 2.7 kJ/mol, while the $\Delta\Delta G_{sol}$ per CF_2 unit from liquid to water is 5.3 kJ/mol. The reference to this 5.3 kJ/mol free energy change in the text (p 3256) should refer to change from the pure liquid phase to the aqueous phase, rather than from the gaseous phase to the aqueous phase.

This correction also modifies the magnitude of two coefficients used in the model. First, the correct n multiplier for the perfluoroalkanes listed in footnote b of Table 2 is 0.62. As a result, the correct F_{access} fitting parameter, while still 0.34 for LAS, is 0.01 for the PFC surfactants. This in turn results in a slightly modified Figure 4, shown below.
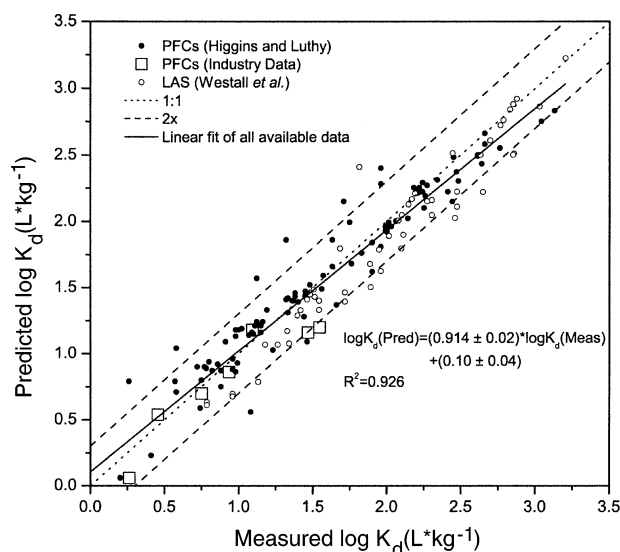

FIGURE 4. Predicted versus measured distribution coefficients for PFCs and LAS using F_{access} values of 0.01 and 0.34, respectively.

While the discussion of the F_{access} parameter on pp 3258 and 3259 is still valid, the magnitude of this parameter and the difference in this parameter between PFCs and LAS suggest physicochemical differences in the interactions of these chemicals with sediment organic matter. These corrected values do not change the conclusions of the paper.

TABLE 2. Chemical-Specific Model Inputs

surfactant	formula	tail log C_{sat}^w(L) (M)	tail log P (kPa)	uncharged head group formula −[X]− O^-	uncharged head group $\Delta\bar{V}$ (cm³/mol)[a]	$-\Delta G_{hyd}$ (kJ/mol)[b]
PFOA	C_7F_{15}−X	-7.49^d	1.02^f	−[CO]−	9.74	34.1
[PFHpS)^c				−[SO$_2$]−	22.17	35.8
PFNA	C_8F_{17}−X	-8.41^d	0.57^g	−[CO]−	9.74	37.3
PFOS				−[SO$_2$]	22.71	39.1
PFDA	C_9F_{19}−X	-9.33^e	0.11^g	−[CO]−	9.74	40.6
[PFNS)^c				−[SO$_2$]−	22.17	42.3
PFUnA	$C_{10}F_{21}$−X	-10.26^e	-0.34^f	−[CO]−	9.74	43.8
PFDS				−[SO$_2$]−	22.17	45.6
PFDoA	$C_{11}F_{23}$−X	-11.17^e	-0.79^f	−[CO]−	9.74	47.1
[PFUnS)^c				−[SO$_2$]−	22.17	48.8
C10LAS	$C_{16}H_{25}$−X	-7.07^h	N/A	−[SO$_2$]−	25.94	34.8
C12LAS	$C_{18}H_{29}$−X	-8.30^h	N/A	−[SO$_2$]−	25.94	39.2
C14LAS	$C_{20}H_{33}$−X	-9.52^h	N/A	−[SO$_2$]−	25.94	43.5

[a] Estimated using approach of Abraham and McGowan (*17*) with recommended modification (*18*). [b] Calculated via $-\Delta G_{hyd} = RT \cdot n \cdot \ln \gamma_{sat}^w(L)$, with $n = 0.62$ for perfluoroalkanes and for hydrocarbons, and $\log \gamma_{sat}^w(L) = \log 55.6 - \log C_{sat}^w(L) + 0.04 \Delta\bar{V}$. [c] For predictive purposes only. No sorption data available for this surfactant. [d] Obtained from Horvath and Getzen (*20*). [e] Estimated from shorter chain analog data provided in Horvath and Getzen (*20*). [f] Estimated from analog data provided in Dias et al. (*22*) and Dias et al. (*23*). [g] Obtained from Dias et al. (*22*) or Dias et al. (*23*). [h] As estimated from Sherblom et al. (*24*).