Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Table S1: Surfactant sorption data where direct analysis of both the sediment and water phase have been applied.

Substance	Type of sediment (fraction)	Ionic strength	Conc range of surfactant	Type of sorption isotherm	$K_{p,0}^{total}$ (L/kg)	K_p^{hydr} (L/kg)	oc%	$K_{p,0}^{elec}$ (L/kg)	C_s^{max} (mg/kg)	Reference
C10-LAS	aquifer sediment (< 1 mm)	no	5-8000 mg/L (mixture)	Langmuir			0.17	26	1989	Istok 1999
C11-LAS	aquifer sediment (< 1 mm)	no	5-8000 mg/L (mixture)	Langmuir			0.17	93	3449	Istok 1999
C12-LAS	aquifer sediment (< 1 mm)	no	5-8000 mg/L (mixture)	Langmuir			0.17	211	2770	Istok 1999
C13-LAS	aquifer sediment (< 1 mm)	no	5-8000 mg/L (mixture)	Langmuir			0.17	2115	396	Istok 1999
^{14}C10-LAS	EPA-12	0.01 M NaN3	0 - 7 μmol/L	Virial	15.1		2.3		0.465 mmol/kg	Westall 1999
^{14}C12-LAS	EPA-12	0.01 M NaN3	0 - 4 μmol/L	Virial	77		2.3		0.465 mmol/kg	Westall 1999
^{14}C14-LAS	EPA-12	0.01 M NaN3	0 - 0.5 μmol/L	Virial	709		2.3		0.465 mmol/kg	Westall 1999
C10-comm LAS	2 river sediments (< 0.125 mm)	10 mM NaHCO3	1 - 12 mg/L	Henry's law region		15	TOC =22.2 %			Marchesi 1991
C11-comm LAS	2 river sediments (< 0.125 mm)	10 mM NaHCO3	1 - 12 mg/L	Henry's law region		54	TOC =22.2 %			Marchesi 1991
C12-comm LAS	2 river sediments (< 0.125 mm)	10 mM NaHCO3	1 - 12 mg/L	Henry's law region		317	TOC =22.2 %			Marchesi 1991
C13 comm LAS	2 river sediments (< 0.125 mm)	10 mM NaHCO3	1 - 12 mg/L	Henry's law region		23700	TOC =22.2 %			Marchesi 1991
^{14}C-LAS comm	river sediment 1	0.01 M KCl	0.25 - 7.5 mg/L	Langmuir	343		1.13		3125	Matthijs 1985
^{14}C-LAS comm	river sediment 2	0.01 M KCl	0.25 - 9 mg/L	Langmuir	211		1		1923	Matthijs 1985
^{14}C-LAS comm	river sediment 3	0.01 M KCl	0.25 - 7 mg/L	Langmuir	347		1		4348	Matthijs 1985
^{14}C-LAS comm	river sediment 4	0.01 M KCl	0.25 - 6.5 mg/L	Langmuir	440		3.41		4000	Matthijs 1985
^{14}C-LAS comm	river sediment 5	0.01 M KCl	0.25 - 10 mg/L	Langmuir	176		0.34		1471	Matthijs 1985
^{14}C-LAS comm	river sediment 6	0.01 M KCl	0.25 - 8.5 mg/L	Langmuir	256		0.67		2326	Matthijs 1985
^{14}C-LAS comm	river sediment 7	0.01 M KCl	0.25 - 8.5 mg/L	Langmuir	218		1.34		3125	Matthijs 1985
^{14}C-LAS comm	kaolin	0.01 M KCl	0.25 - 5 mg/L	Langmuir	18		0		131	Matthijs 1985
^{14}C-LAS comm	Aldrich humic acid	0.01 M KCl	0.25 - 2 mg/L	Langmuir	1200		n.s.		8568	Matthijs 1985
$C_{10}EO_8$	Marine (Frisian Front)	100 mg/L NaN3	0.005-111 mg/L	Independent		9.4	0.27	663	0.61 - 0.95	Droge 2007

				mode					mmol/kg	
$C_{12}EO_8$	Marine (Frisian Front)	100 mg/L NaN3	0.03 - 40.1 mg/L	Independent mode		103	0.27	3540	0.40 - 0.93 mmol/kg	Droge 2007
$C_{14}EO_8$	Marine (Frisian Front)	100 mg/L NaN3	0.0004-2.77 mg/L	Independent mode		1402	0.27	39170	0.18 - 0.66 mmol/kg	Droge 2007
$NPEO_3$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	1460	230	0 and 20			John 2000
$NPEO_4$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	930	270	0 and 20			John 2000
$NPEO_5$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	750	320	0 and 20			John 2000
$NPEO_6$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	700	360	0 and 20			John 2000
$NPEO_7$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	590	330	0 and 20			John 2000
$NPEO_8$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	550	400	0 and 20			John 2000
$NPEO_9$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	540	460	0 and 20			John 2000
$NPEO_{10}$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	450	480	0 and 20			John 2000
$NPEO_{11}$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	550	530	0 and 20			John 2000
$NPEO_{12}$	native sed (normal+org free) (<0.125 mm)	10 mM NaHCO3	0.1 - 5 μM	Henry’s law	750	590	0 and 20			John 2000

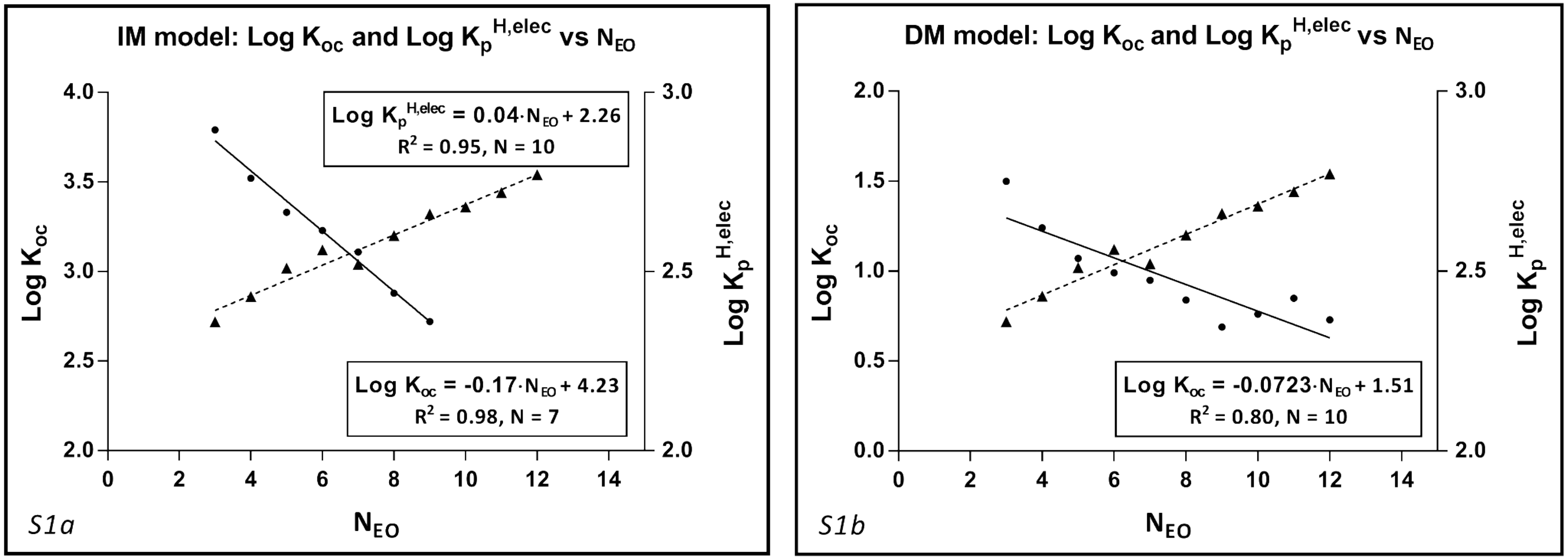

Fig S1. log K_{oc} and log $K_p^{H,elec}$ with the EO number (N_{EO}) for $NPEO_x$ based on partition coefficients derived according to the IM model (S1a) and DM model (S1b). Data taken from Table 4a and 4b adapted from John[1].

Table S2. Sorption of data of phenanthrene on sea sediment[2].

		$1/Q_0=1/C_s^{max}$	f_{oc} (%)	$C_{s,\ hydr}^{max}$ (mg/kg)	$C_{s,\ hydr}^{max}$ (mmol/kg)	$b = 1/K_LC_s^{max}$	$K_LC_s^{max}$	K_L (L/mmol)	$K^{L,hydr}_{p,0}$	K_{oc}
1		0.0127	0.58	78.7	0.44	0.0058	172.41379	3.90E+02	172	29727
2		0.012	0.42	83.3	0.47	0.0064	156.25	3.34E+02	156	37202
3	H20	0.0083	0.75	120	0.68	0.0049	204.08163	3.02E+02	204	27211
3	HCl	0.0098	0.81	102	0.57	0.0058	172.41379	3.01E+02	172	21286
3	H2O2	0.0496	0.08	20.2	0.11	0.0344	29.069767	2.57E+02	29	36337

The table above leads to an average K_L^{Hydr} = 316 L/mmol or an average K_{oc} of 30400 L/kg for phenanthrene in the applied experimental system.

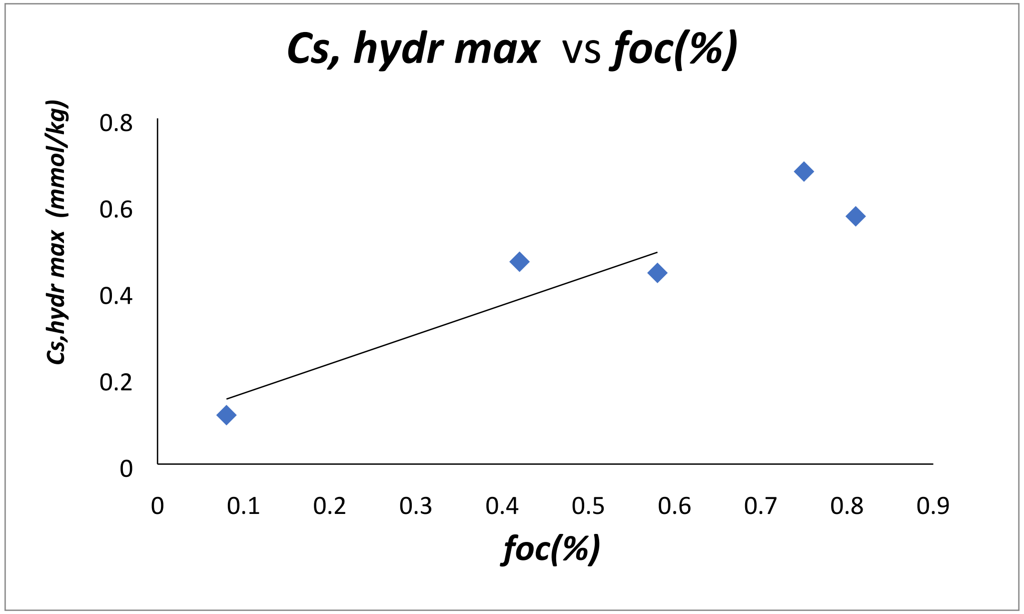

Fig S2: Correlation of $C_{s,hydr}^{max}$ vs f_{oc} *(%)* based on data from Table S2

References

1. W. W. John; G. Bao; W. P. Johnson; T. B. Stauffer *Environ. Sci. Technol.* 2000, **34**, 672-679.
2. G. Yang; X. Zheng *Environmental toxicology and chemistry* 2010, **29**, 2169-2176.