Supporting Information

Importance of Adsorption (Hole-Filling) Mechanism for Hydrophobic Organic Contaminants on an Aquifer Kerogen Isolate

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Figure caption for the Supporting Information:

Supplementary Figure S1. DCB recovery ratios for the initial sorbate concentrations ranging from 0.2 to 70 μg/ml in the sorption solutions. The sorption solutions were treated as controls and put in the flame-sealed ampules for 1d (circle) and 2 weeks (square), respectively.

Supplementary Figure S2. Sorption, residual sorption and desorption isotherms of Phen and DCB on the isolated kerogen and the model fitting. The lines respectively represent the best fitting of the Freundlich equation to the sorption, residual sorption and desorption data, and the best fitting of the linear partitioning equation to desorption data. (a) DCB, (b) Phen.

Supplementary Figure S3. K_{oc}-K_{ow} correlations for the various K_d values estimated from the dual-mode model fitting (circle), and desorption data (square), and cited from literature (*40*) for Phen and Naph, and (*39*) for DCB and TCB (diamond).

Supplementary Table S1. Selective Physicochemical Properties of the Sorbates.

Compound	MW[a] (g/mol)	S_w[a] (mg/L)	T_m[a] (°C)	H[a] (Pa m^3/mol)	S_{scl}[b] (mg/L)	log K_{ow}[a]	V_s[a] (cm^3/mol)	ρ (g/cm^3)	K_{oc} (L/g-oc)		
									c	***d***	***e***
Phenanthrene	178.2	1.12	101	3.98	5.18	4.57	152	1.170	22.9	17.4	6.03
Naphthalene	128.2	31.7	80	43.0	107.1	3.3	111	1.160	1.23	1.75	0.73
TCB	181.5	5.36	99.5	192	26.1	4.02	131	1.386	6.46	5.93	2.42
DCB	147.2	92.8	-17	245		3.38	113	1.305	1.48	0.84	0.84

[a] Cited from Mackay et al. (1992). [b] cited from Ran et al. (*12*). [c] log K_{OC} = log K_{OW} − 0.21from Karickhoff et al., [d] log K_{OC} = −0.686 log S_w+ 4.273 from Means et al. (*41*) , [e] log K_{OC} = 0.72 log K_{OW} + 0.49 from Schwarzenbach and Westall.

[a] From Mackay, D.; Shiu, W. Y.; Ma, K. C. *Illustrated Handbook of Physical–Chemical Properties and Environmental Fate for Organic Chemicals*; Lewis Publishers: Chelsea, MI, Vols.1 and 2., 1992.

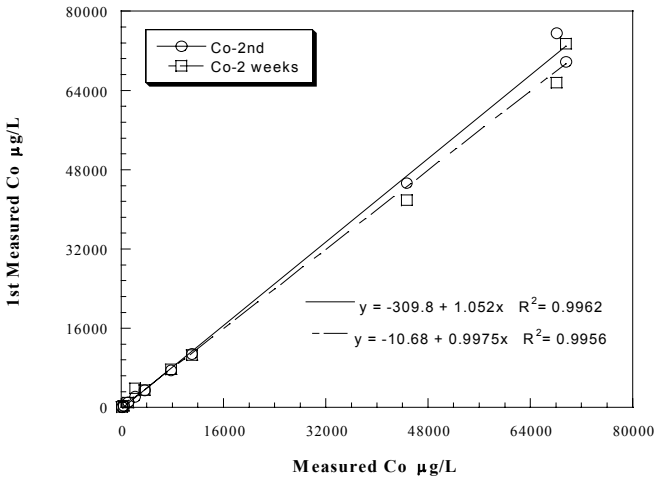
[c] Schwarzenbach, R. P.; Westall, J. C. *Environ. Sci. Technol.* **1981**, *15*, 1360-1367.

[e] Karickhoff, S. W.; Brown, D. S.; Scott, T. A. *Water Res.* **1979**, *13*, 241-248.

Supplementary Table S2. Dual-Mode Model Parameters for the Sorption Isotherms on the Isolated Kerogen.

	Dual Mode Model				
Chemicals	Q^o **(μg/g)**	b **(L/μg)**	K_d **(L/g)**	R^2	N^a
Phen	84.5±28.8 [b]	0.0207±0.0158 [c]	0.504±0.042[c]	0.997	24
Naph	135±83.0	0.00024±0.00019	0.0268±0.0034	0.999	24
TCB	116±135	0.002±0.002	0.100±0.038	0.992	20
DCB	134±56.1	0.00025±0.0002	0.030±0.001	1.000	20

[a] Number of observations. [b] 95% confidence interval of Q^o. [c] 95% confidence interval on b. [c] 95% confidence interval on K_d



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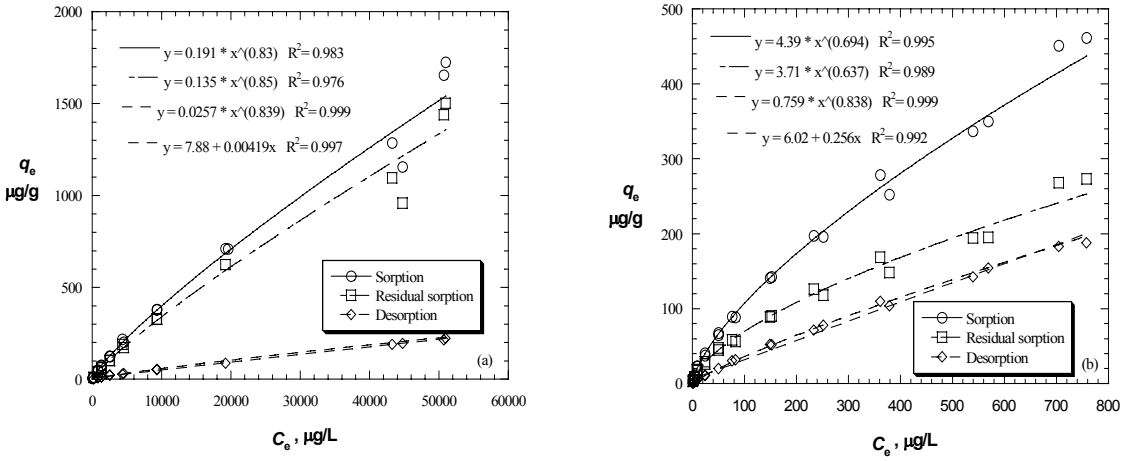

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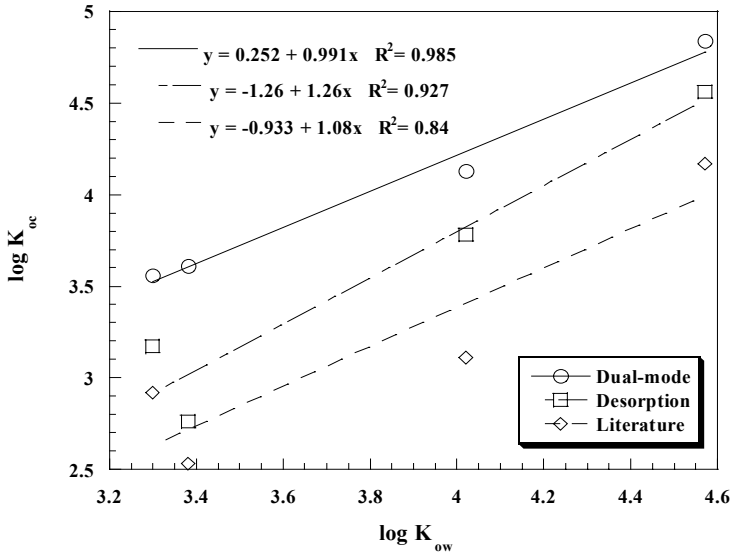

Supplementary Figure S3. K_{oc}-K_{ow} correlations for the various K_d values estimated from the dual-mode model fitting (circle), and desorption curves in Figure S2 (suqare), and cited from Karickhoff (*40*) for Phen and Naph, and Chiou et al. (*39*) for DCB and TCB (diamond).