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¹⁴C-LABELED CHEMICAL PURITY CHECK.

Methods. Purity checks for ¹⁴C-labeled solutes were conducted using a HPLC with UV-detection (Waters Corp., detector model # 418, pump model # 515, and autosampler model # 717 plus) and a μ Bondpak C18 3.9 x 300 mm column (Waters Corp., Milford, MA). Elution was under a constant condition of 70% acetonitrile and 30% water at 1.0 mL/minute. 20 μ L of a stock solution (~12000 DPM) was spiked and the eluent was collected every minute for 12 min and analyzed by scintillation counting.

Results. UV and radiochemical (scintillation counting) responses both showed only one major peak for each solute tested, occurring at the same retention times as the corresponding peak of standard solutions. A mass balance calculation showed that more than 97% of radioactivity was accounted in the eluted peak in all cases. More specifically, two tests of phenanthrene showed recoveries of 97.18% and 97.44%, and a single measurement with 1,2,4-trichlorobenzene (TCB) showed 102.37% recovery.

CHARACTERIZATION OF BLACK CARBON MATERIALS.

Methods. Quantification of organic carbon in all soot samples was conducted by high temperature combustion under oxygen at 950°C (Model CM5120, UIC Corp., Joliet, IL) followed by coulometric quantification of the CO₂ produced (Model CM5012, UIC corp., Joliet, IL). Percentages of carbon in samples following thermal treatment in air for 24 hours at 375°C (gC/100g sample) were determined through an implementation of the approaches published by Gustafsson *et al.* (1). Details of the thermal pretreatment and the elemental analysis for soot samples are reported in Nguyen *et al.* (2).

X-ray photoelectron spectra were obtained with a Physical Electronics (Eden Prairie, MN) 10-360 Precision Energy Analyzer using the Mg K α line (1253.6 eV) of a Φ 04–500 Dual Anode X-ray Source at 15 kV and 300 W. Specific surface area was measured using conventional BET analysis techniques (Coulter 3100 BET instrument, Miami, FL), and the reported surface areas are based on standard BET analysis of multipoint nitrogen adsorption data obtained at 77°K (3). Prior to analysis, the samples were outgassed at 300°C for 5 hours, in accordance with American Society for Testing and Materials (ASTM) Standard D4820-97 (4) for powdered black carbon samples. Electrophoretic mobilities of the soot suspensions in synthetic groundwater containing 5 mM CaCl₂ and 0.02% NaN₃ (pH=6.7) were measured with a Zeta Potential Analyzer (Brookhaven Instruments, Holtsville, NY). The temperature of suspensions in electrophoretic mobility experiments was constant at 22°C.

Samples of diesel particulate material (SRM 2975) were analyzed for PAHs by Dr. Poster (NIST) using methods described by Poster et al. (5-7). Briefly, pressurized fluid extraction with dichloromethane and gas chromatography with mass spectrometry were used to determine the concentrations of 40 individual PAHs with molecular weights (MW) ranging from 128 amu (naphthalene) to 300 amu (coronene). The following PAHs were examined: (1) naphthalene, (2) 2-methylnaphthalene, (3) 1-methylnaphthalene, (4) biphenyl, (5) acenaphthene, (6) 2,6-dimethylnaphthalene, (7) acenaphthylene, (8) 2,3,5-trimethylnaphthalene, (9) fluorene, (10) phenanthrene, (11) anthracene, (12) 3-methylphenanthrene, (13) 2-methylphenanthrene, (14) 9-methylphenanthrene, (15) 1- + 4-methylphenanthrene, (16) fluoranthene, (17) pyrene, (18) cyclopenta[*def*]phenanthrene, (19) retene, (20) benzo[*ghi*]fluoranthene, (21) cyclopenta[*cd*]pyrene, (22) benzo[*c*]phenanthrene, (23) benz[*a*]anthracene, (24) triphenylene, (25) chrysene, (26) benzo[*b*]fluoranthene, (27) benzo[*j*]fluoranthene, (28) benzo[*k*]fluoranthene,

(29) benzo[*a*]fluoranthene, (30) benzo[*e*]pyrene, (31) benzo[*a*]pyrene, (32) perylene, (33) indeno[1,2,3-*cd*]pyrene, (34) benzo[*ghi*]perylene, (35) benzo[*c*]chrysene + dibenz[*a,j*]anthracene, (36) dibenz[*a,c*]anthracene, (37) dibenz[*a,h*]anthracene, (38) benzo[*b*]chrysene, (39) picene, and (40) coronene. Note that 1- + 4-methylphenanthrene and benzo[*c*]chrysene + dibenz[*a,j*]anthracene were analyzed in combination.

Results. Scanning electron microscopy (SEM) of SRM 2975 has shown the soot to be comprised of roughly 1 μm sized aggregations of primary spherical particles that are roughly 30 nm in size (2). Although the aggregated particle size in aqueous solution is not well known, we observed that a substantial fraction of this material exists as visible particles when suspended in 5 mM CaCl_2 solution, and that another fraction of visible soot particles remains at the air/water surface.

The percentages of carbon remaining after thermal treatment in air for 24 hours at 375°C (f_{sc}), was higher for the fresh hexane soot (84.0 ± 8.1 ; N=6) than for diesel soot SRM 2975 (81.7 ± 4.8 ; N=6) and the oxidized hexane soot (80.9 ± 4.4 ; N=6). As reported in our previous work (2), the thermal pretreatment method for f_{sc} quantification is best viewed as a semi-quantitative tool for detecting primarily the presence of soot.

Both bulk and surface O/C ratios showed that diesel soot (0.08 and 0.20) and oxidized hexane soot (0.08 and 0.21) have similar O/C ratios, and that these values are twice as high as those in the fresh hexane soot (0.04 and 0.10). Electrophoretic mobility tests showed that the microscopically visible particle aggregates for all three materials had negative surface charges under the water chemistry condition of the synthetic groundwater, with electrophoretic mobility increasing on the order of: hexane soot ($-1.13 \pm 0.06 \times 10^{-8}$ m/sec/V/m; N=3), diesel soot (-1.38

± 0.08 ($\times 10^{-8}$ m/sec/V/m); N=3), and oxidized hexane soot (-1.50 ± 0.02 ($\times 10^{-8}$ m/sec/V/m); N=3). The summed concentration of 40 identified PAHs for SRM 2975 was 120×10^{-6} g PAHs /g soot. BET surface area for diesel soot SRM 2975, hexane soot, oxidized hexane soot, and char NC2 was 127 ± 16 (N=3), 91 ± 19 (N=5), 82 ± 5 (N=5), and 118 ± 20 (N=3) m²/g, respectively.

CONTROL STUDIES FOR THE FLOCCULATION-BASED BATCH SORPTION METHODOLOGY.

Methods.

(i) **A control study to test completeness of solid-liquid separation** was conducted. In order to confirm that the collected supernatant was effectively soot-free, we compared solute activity in the supernatant with that of a soot-free control using a modification of the air-bridge technique applied by Bucheli and Gustafsson (8). For this test, approximately 1.2 mg of soot SRM 2975 was mixed with 125 mL of synthetic groundwater for 59 days. After this mixing, the soot/water suspension was subjected to the flocculation and centrifugation procedure described above, and 1 mL of the clarified supernatant was withdrawn and injected into a 2-mL vial. This open 2-mL vial was then placed into a sealed 22-mL vial together with two other open 2-mL vials containing soot-free synthetic ground water. ¹⁴C-labeled tetrachloroethylene (PCE) was then spiked into one of the two soot-free vials. The entire system was then sealed with a Teflon-lined cap and the PCE allowed to equilibrate by means of gas-phase (headspace) mass transfer among the three vials. After two weeks, 1 mL of water from each vial was taken for scintillation counting.

(ii) **A control study to test for flocculant effects on solute loss in sorbent-free systems** was conducted using two sets of solid-free experiments with TCB and phenanthrene. A volume of 5 μ L of ¹⁴C-labeled solution of the test solute in methanol was spiked into 50 mL centrifuge tubes filled with synthetic groundwater. For each solute, a total of twelve tubes were rotated end-over-end at a speed of 12 RPM overnight (roughly 14 hours), followed by the addition of 2 μ L of

PACl solutions at varying PACl concentration (Table 2S) and then by continuous shaking and centrifugation as for the flocculation step of sorption experiments. A set of blank samples without PACl addition was simultaneously evaluated for comparison.

(iii) **A comparative study with and without flocculant in a char system** was conducted to check for possible effects of the flocculant and flocculation on sorption, as might result, for example, from modification of sorbent surface chemistry or from the particle aggregation. To test for such effects, we conducted a comparative sorption study using a natural char material of comparable surface characteristics as the SRM 2975 soot, but for which effective solid-liquid separation could also be achieved without PACl addition. For this comparative study, we used the char NC2, which has similar BET surface area (118 ± 20 vs. 127 ± 16 m²/g) and the same surface O/C (0.20) as soot SRM 2975.

For this control study, twenty 63 mL sorption bottles containing 6.0-6.3 mg of char NC2 were spiked with TCB. After 28 days of equilibration, these sorption bottles were divided equally into four sets of five samples each. Solid-liquid separation by only centrifugation was used for the first set. For the other three sets, solid-liquid separation was achieved by means of flocculation and centrifugation using three different PACl doses (0.10, 0.25, and 0.35 mg/L as Al).

(iv) In order to make **a comparative study of the flocculation-based with the air-bridge technique**, we applied the experimental set-up described by Bucheli and Gustaffson (8), using an initial aqueous concentration (C_o) on the order of 0.02 µg/mL. For this experiment, four air-bridge systems were created, each consisting of an open 60 mL glass serum bottle (Wheaton #223746) inside of a cap-sealed 250 mL amber glass jar (Wheaton #217892). From 1.0 to 1.2 mg of soot was added to each serum bottle. Approximately 50 mL of sorption water was then added to each serum bottle and to the space outside the bottle within each glass jar. For each system 5

μL of ¹⁴C-labeled phenanthrene solution was spiked into each serum bottle and the glass jar was immediately sealed with an aluminum foil-lined plastic screw cap. The exchange of phenanthrene between the serum bottle and the external water was then allowed to occur via the headspace. Using the results of Bucheli and Gustafsson (8) as a guide, we allowed an equilibration time of 123 days.

Results

(i) For the **control study to test completeness of solid-liquid separation**, the ratios of PCE concentration in the soot-free control relative to that in the soot-sample supernatant were 0.99 ± 0.02 (N=4). In this control study, if the supernatant were to contain soot particles, then the concentration of PCE in the supernatant solution would be higher than that in water because of sorption of PCE to colloidal soot, which would be sampled and subsequently extracted into the scintillation cocktail. If we assume a K_{oc} of 9000 mL/g for PCE at the given aqueous concentration of 10^{-4} of solubility (as based on prior results with soils --- see Figure 10a, in Ref. (9)), then sorption to colloidal soot should be sufficiently strong to reveal soot at 6.8 μg/mL or 0.56% of the original amount added. Thus, the lack of detectable concentration difference between soot-sample supernatant and soot-free water indicates that soot concentrations were less than this amount. Using a relation published elsewhere for evaluating the potential for colloid effects (10), one can show that such low concentration of suspended soot would not affect the measured K_d of phenanthrene or TCB. Clearly, the method achieved a sufficient degree of soot-water separation.

(ii) For the **control studies to test for flocculant effects on solute loss in sorbent-free systems**, the fractions of recovery from tubes spiked with different amounts of PACl solution were similar to those from tubes without PACl (Table 2S). The similarity indicates that the addition of PACl

alone did not cause sorbate loss from solution. Similar observations have been reported by Laor and Rebhun (11) and by Hong et al. (12), even at higher flocculation doses that were specifically designed to cause aluminum hydroxide precipitation.

(iii) For the **comparative study with and without flocculant in a char system**, average K_d values for the three sets spiked with 0.10, 0.25, and 0.35 mg/L of PACl were 12000 ± 1000 ; 12000 ± 1000 ; and 11000 ± 600 mL/g, respectively. The average K_d value for samples without the addition of PACl was 11000 ± 1000 mL/g. This statistical equivalency of these results proved that flocculation did not affect the sorption results.

(iv) Our implementation of the **air-bridge method** for measuring sorption of phenanthrene to SRM 2975 gave an average K_d of 727000 ± 221000 mL/g after 123 days of equilibration (based on 4 replicates) at $C_e/S_w=0.001$. At the same equilibrium concentration, the flocculation-based method gave an average K_d of 683000 ± 148000 mL/g (5 replicates). These results are also shown in Table 1, where they can be compared with results obtained by other investigators. Overall, the results confirmed the equivalency of the two methods within the errors of the estimates.

METHODS USED FOR ANALYZING BATCH SORPTION DATA.

Batch equilibration bottles without solid were used to estimate the losses from solution and in the presence of PACl, as might occur by sorption to glassware and diffusion of sorbate into and through the Teflon-lined septa. For this analysis, the mass losses from solution are assumed to be proportional to the aqueous concentration at the time of sampling and are represented by the variable X defined below (13).

$$X = \frac{M_t - M_r}{C_e} \quad (1S)$$

Here, X is the mass lost from solution per unit of concentration ($\mu\text{g}/(\mu\text{g}/\text{mL})$), M_t is the total mass spiked to the bottle (μg), M_r is the mass recovered at the time of sampling (μg), and C_e is the aqueous concentration at the time of sampling ($\mu\text{g}/\text{mL}$).

The ratio of solute mass lost over solute mass in aqueous solution is given by X/V_w , where V_w is the volume of water in the bottle. For our samples, this ratio ranged from $2.3\% \pm 0.2\%$ for 3 days equilibration time to $6.8\% \pm 1.9\%$ for 88 days equilibration time.

Solid uptake was calculated to account for the loss factor as follows:

$$q_e = \frac{M_t - C_e(V_w + X)}{M_s} \quad (2S)$$

Here M_s is the mass of solid in the vessel, M_t is the total mass of solutes injected, and other variables are as defined above.

COMPARISON WITH PRIOR RESULTS: K_{oc} AT LOW C_e FOR PHENANTHRENE WITH SOOT.

Table 1 (main text) shows the values of $\log K_{oc}$ measured for SRM 2975, together with prior results for soot formed from different fuels. For diesel soot SRM 2975, values of K_d and $\log K_{oc}$ measured using both an air-bridge method and our new flocculation-based method give very similar values at similar aqueous concentration ($C_e/S_w=10^{-3}$). For phenanthrene, our results with SRM 2975 also compare reasonably well with those obtained previously on SRM 1650 by Bucheli and Gustafsson using an air-bridge method (8), and by Jonker and Koelmans using a method based on three phase equilibration and solid phase extraction (14), when comparison is made at similar aqueous concentrations (see Table 1). For phenanthrene, the $\log K_{oc}$ measured previously for SRM 1650 by the other techniques is in the range of 5.25 to 5.30 at $C_e/S_w = 10^{-2}$,

and thus slightly higher than that obtained in our work for SRM 2975 at similar C_e/S_w (5.11). The value for $\log K_{oc}$ previously obtained on SRM 1650 by the cosolvent HPLC column method is 6.19, which is especially high relative to all other measures. Although the reason for these differences are not known, it is likely that the pretreatment with 100% methanol in the co-solvent HPLC study removed some natively-bound organic chemicals and thus uncovered some strong sorption sites that were otherwise unavailable for phenanthrene sorption, at least within the time frames of the air-bridge and three-phase studies. Other types of soot materials have also been studied for phenanthrene sorption. Among soot materials, coal soot, oil soot and wood soot had the lowest $\log K_{oc}$ values of 3.85, 4.57, and 4.61.. The traffic soot had the highest $\log K_{oc}$ value of 5.73 (14).

201 **TABLE 1S. Physiochemical Properties of Studied Solutes^a**

Chemical	log K_{ow}	Aqueous Solubility S_w (mg/L)	Density (g/mL)	Molar Volume V_s (mL/mol) ^b	Molar Volume V_b (mL/mol) ^c	Molecular Volume (\AA^3) ^d
1,2,4-trichloro-benzene (TCB)	4.0	34.6 ^e	1.45 ^g	125	158.7	160
phenanthrene	4.57	1.29 ^e (6.18) ^f	1.17 ^g	152	199	213

202 ^a All properties are at 25°C and from Schwarzenbach et al.(10), except where otherwise noted.
 203 ^b Molar volume as calculated by dividing the molecular weight by density of the pure chemical.
 204 ^c Molar volume at the boiling point, as estimated using LeBas increments.
 205 ^d Molecular volume calculated using the AM1 semiempirical method with PC Spartan Pro
 206 (Wavefunction, Inc. Irvine, CA).
 207 ^e Data taken from Karickhoff (15).
 208 ^f Solubility of subcooled liquid.
 209 ^g Data from Mackay et al., (16)

210 **TABLE 2S. Sorbate Recovery in Blank (Solid-free) Samples with and without PACl.**

Solutes	Al (mg/L)	Recovery (%) [*]
1,2,4-TCB	0	94.2 ± 1.4
1,2,4-TCB	0.07	94.2 ± 0.9
1,2,4-TCB	0.14	94.6 ± 1.0
1,2,4-TCB	0.21	94.4 ± 1.3
Phenanthrene	0	95.6 ± 2.0
Phenanthrene	0.05	97.0 ± 0.5
Phenanthrene	0.11	96.0 ± 0.7
Phenanthrene	0.16	95.1 ± 1.4

211 ^{*} Shown are average values ± standard deviation based on 3 replicates.

212

212 **TABLE 3S. Fitted Parameters of Observed Sorption Data by Freundlich Isotherms***

Solutes	N	K_f^* (μg/g)	n	MWSE
1,2,4-TCB	41	35000 ± 1280	0.66 ± 0.01	0.02
Phenanthrene	36	21300 ± 490	0.43 ± 0.02	0.07

213 *Shown are average values ± standard deviation. N = number of observations. MWSE =mean
214 weighted square error = $1/v \sum [(q_{\text{measured}} - q_{\text{model}})^2] / q_{\text{measured}}^2$ where v is the number of degree of
215 freedom; here v=N-2. All fitted parameters were generated using Sigma Plot 2000 (SPSS Inc.,
216 Chicago, IL).

217

217 **TABLE 4S. Fitted Parameters of Observed Sorption Data by Dual Domain Model with a**
218 **Polanyi-Based Adsorption Isotherm^a**

Solutes	Assumed f_{oc}^b	$K_{op}f_{op}$ or $K_{oc}f_{oc}$	$q_{ad,max}$ (µg/g)	c	d	MWSE
1,2,4-TCB (N=41)	0	0	35000±7680	-0.0336±0.04	1.00±0.27	0.020
1,2,4-TCB ^c	0.027 ^c	670 ^c	21000±2500	-0.0322±0.02	1.00±0.10	0.028
1,2,4-TCB ^d	0.00012 ^d	3.0 ^d	35000±7600	-0.0335±0.03	1.00±0.276	0.020
1,2,4-TCB	0.2	502	27000±2800	-0.0347±0.015	1.00±0.09	0.043
1,2,4-TCB	0.6	1505	1300±380	-3.1×10 ⁻⁵ ±0.0002	2.15±0.96	0.040
1,2,4-TCB	0.65	1630	0.1×10 ⁻³ ±3900	-0.5943±2.6 ×10 ⁶	5.17±1.7 ×10 ⁷	0.263
1,2,4-TCB	0.817	2049	1.2×10 ⁻³ ±3.0 ×10 ⁴	-1.0×10 ⁶ ±1.1 ×10 ⁷	2.86±5.5 ×10 ⁷	0.282
Phenanthrene (N=36)	0	0	19000±900	-0.0115±0.005	1.18±0.1	0.031
Phenanthrene ^c	0.027 ^c	3700 ^c	15000±720	-0.004±0.002	1.42±0.1	0.030
Phenanthrene ^d	0.00012 ^d	16.0 ^d	19000±900	-0.0117±0.005	1.19±0.1	0.031
Phenanthrene	0.2	6777	12000±600	-0.0016±0.001	1.59±0.12	0.034
Phenanthrene	0.4	13554	7800±480	-2.3×10 ⁻⁴ ±2.3×10 ⁻⁴	2.08±0.25	0.044
Phenanthrene	0.7	23719	3800±580	0.0±0.0	2.93±1.37	0.063
Phenanthrene	0.817	27684	2700±700	0.0±0.0	3.01±2.77	0.069

219 ^a Shown are average values ± standard deviation. Maximum sorbed volume ($q'_{ad,max}$) can be obtained by
220 dividing maximum sorbed mass ($q_{ad,max}$) by the sorbate density given in Table 1S. MWSE =mean
221 weighted square error = $1/v \sum [(q_{measured} - q_{model})^2] / q_{measured}^2$ where v is the number of degree of freedom;
222 here v=N-3. All fitted parameters were generated using Sigma Plot 2000 (SPSS Inc., Chicago, IL). Other
223 parameters are defined in text.

224 ^b Except where otherwise noted (see footnote (^c) and (^d), $K_{oc}f_{oc}$ was calculated using the assumed f_{oc} and
225 using maximum reported log K_{oc} for sediment organic matter 3.40 for TCB and 4.53 for phenanthrene.

226 ^c Fitting parameters for Case 1 with $f_{op} = 0.027$ and $K_{op} = 137000$ for phenanthrene and 25000 for TCB.

227 ^d Fitting parameter for Case 2 with $f_{PAH} = 0.00012$ and $K_{PAH} = 137000$ for phenanthrene and 25000 for
228 TCB.

229

FIGURE 1S. Fitting of Observed 1,2,4-TCB Sorption Data by Dual-Domain Model with a Polanyi-Based Adsorption Isotherm and Six Alternative Assumptions for the Absorption Contribution: a) $f_{op}K_{op}=0$; (adsorption only). b) $f_{PAH}K_{PAH}=3.0$ (corresponding with case 2; c) $f_{op}K_{op}=607$ (corresponding with case 1); d) $f_{oc}K_{oc}=502$. e) $f_{oc}K_{oc}=1505$. f) $f_{oc}K_{oc}=2049$. Details of model fits are given in Table 4S.

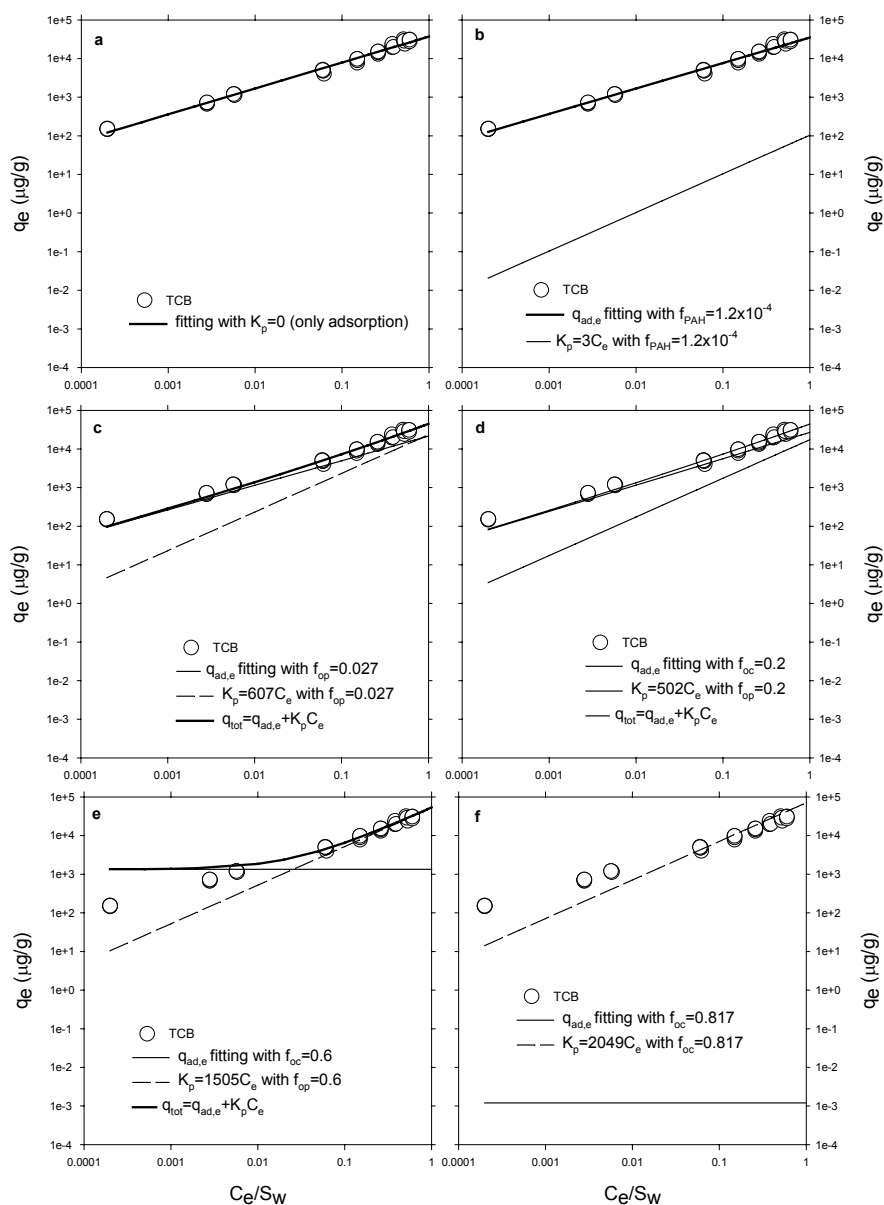
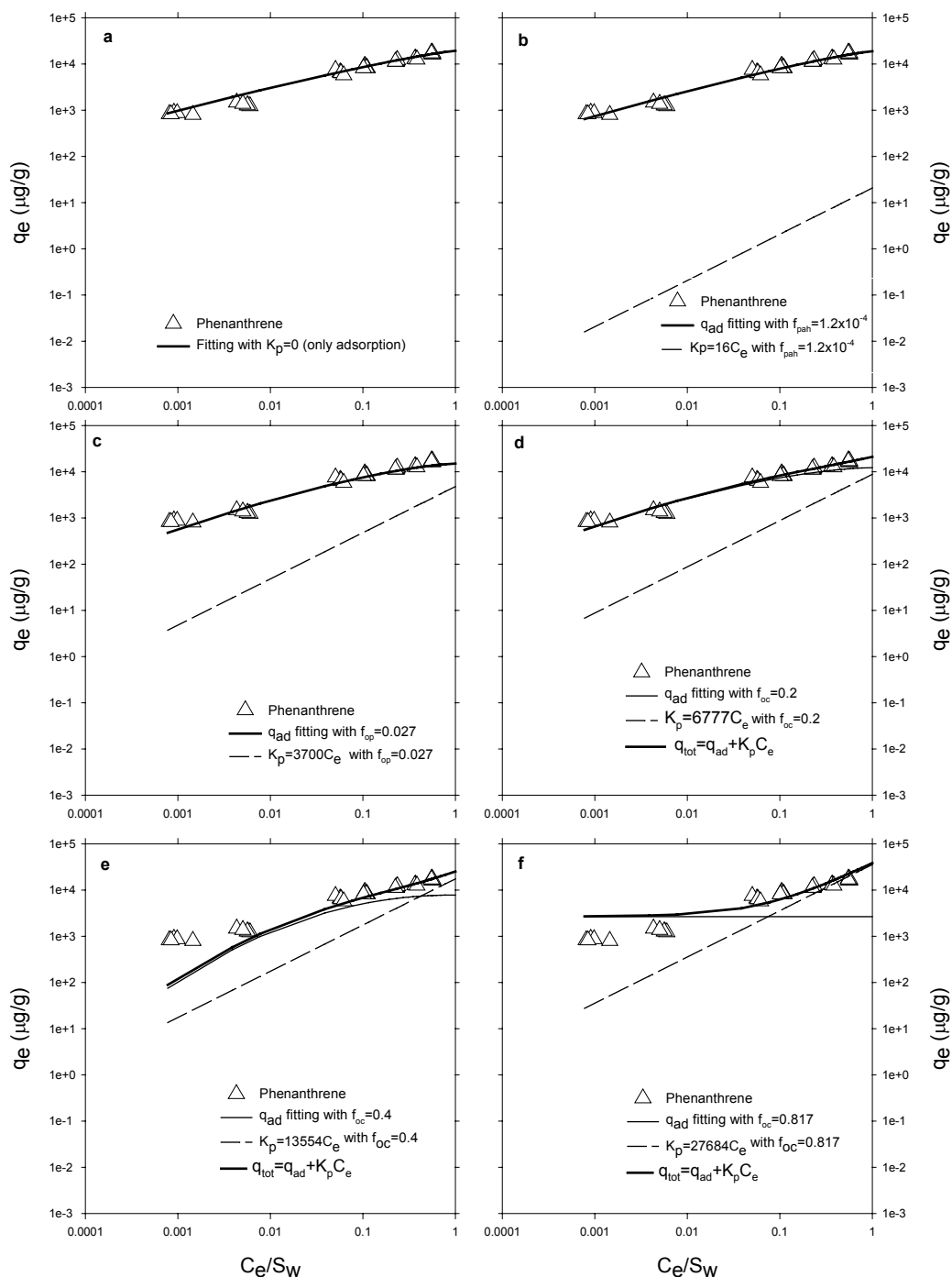


FIGURE 2S. Fitting of Observed Phenanthrene Sorption Data by Dual-Domain Model with a Polanyi-Based Adsorption Isotherm and Six Alternative Assumptions for the Absorption Contribution: a) $f_{op}K_{op}=0$; (adsorption only); b) $f_{PAH}K_{PAH}=16$ (corresponding with case 2; c) $f_{op}K_{op}=3700$ (corresponding with case 1); d) $f_{oc}K_{oc}=6777$. e) $f_{oc}K_{oc}=13554$. f) $f_{oc}K_{oc}=27684$. Details of model fits are given in Table 4S.



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