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

Biochar particle aggregation in soil pore water: influence of ionic strength and interactions with pyrene

Supporting Information

Stephanie Castan[a], *Gabriel Sigmund*[a,b,c], *Thorsten Hüffer*[a], *Thilo Hofmann*[a*]

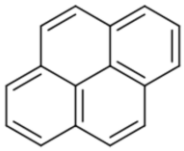
[a] *Department of Environmental Geosciences, Centre for Microbiology and Environmental Systems Science, University of Vienna, Althanstraße 14, 1090 Wien; *thilo.hofmann@univie.ac.at; Tel: +43-1-4277-53320*

[b] *Agroscope, Environmental Analytics, Reckenholzstrasse 191, CH-8046 Zurich, Switzerland*

[c] *Ithaka Institute for Carbon Strategies, Ancienne Eglise 9, Arbaz 1974, Switzerland*

Table S1: Selected pyrene properties.[1,2]

	Pyrene
CAS – No.	129-00-0
Molar mass [Da]	202.26
Log K_{OW}	4.88
Solubility [µg/L]	135
Molar volume [cm^3/mol]	159.3



Sorption isotherms were fitted with the Polanyi-Manes model (Equation 1), which is applicable for isotherm fits over large concentration ranges.[2,3]

Equation 1

$$log\ C_s = log\ Q^{max} + a * (\frac{RTln(\frac{S_W}{C_{aq}})}{V_S})^d$$

C_s……	mass of sorbate adsorbed per unit mass of sorbent
C_{aq}……..	sorbate concentration in aqueous phase
Q^{max}……	sorption capacity
a, d…….	fitting parameters
R…….	universal gas constant
T…….	absolute temperature
V_S……..	molar volume of solute
S_W……..	water solubility

For comparison among different isotherms, individual sorption coefficients (K_d, L/kg) were calculated at aqueous concentrations of 0.1, 1 and 10 µg/L. Standard deviations were calculated from duplicate measurements and unpaired t-tests were performed to test whether compared values are statistically different on a $p < 0.05$ level.

Figure S1: Sorption isotherms after 28 days in MQ (●) and 0.01 M $CaCl_2$ (■).

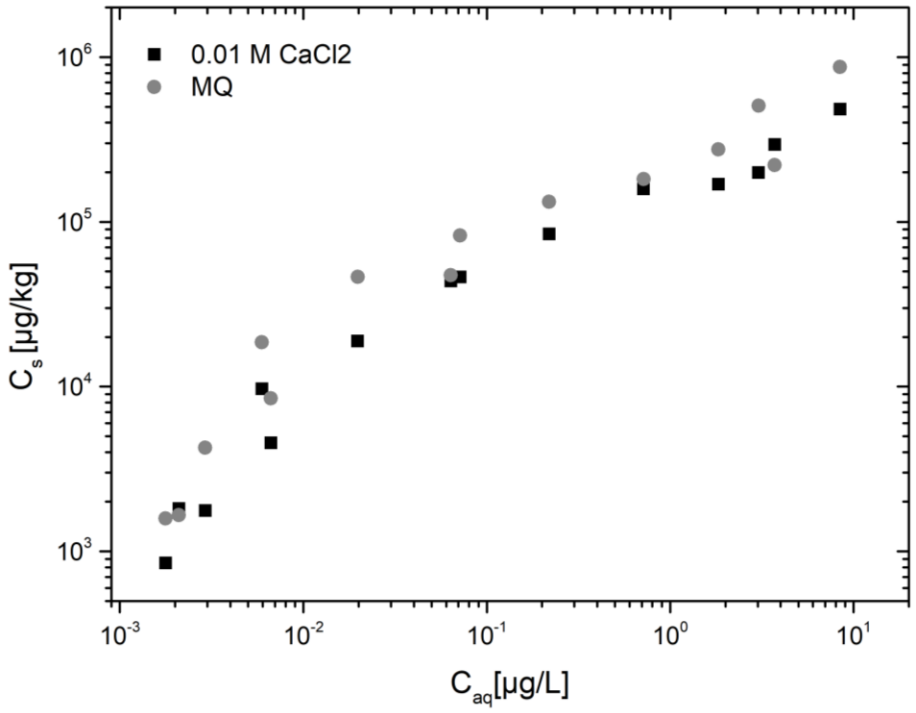
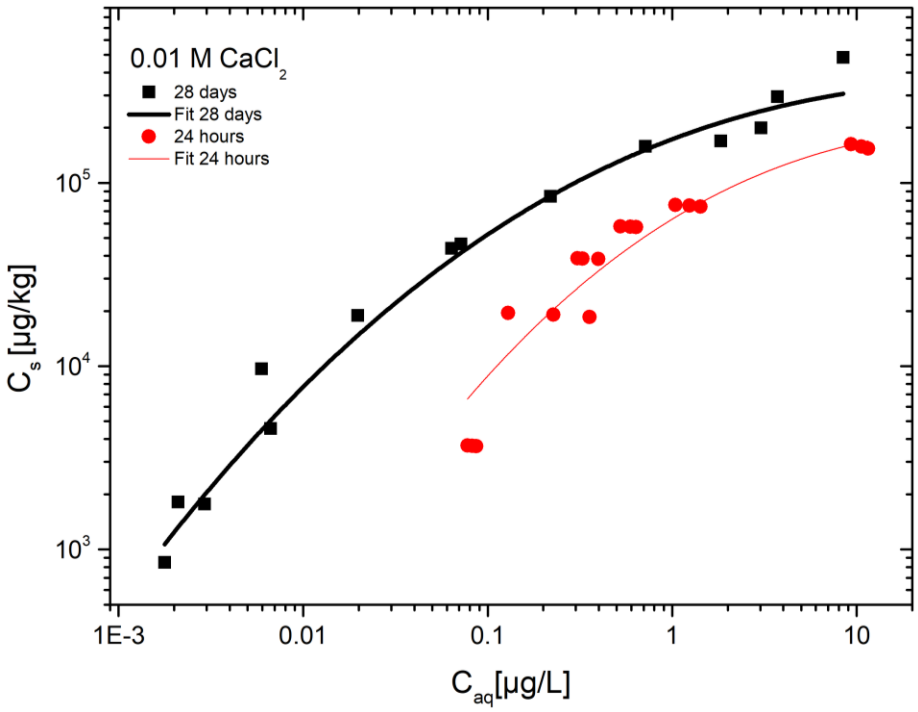


Figure S2: Sorption isotherms in 0.01 M $CaCl_2$ after 24 hours (●) and 28 days (■).



1. Chemspider database, Pyrene, *Royal Society of Chemistry* Available at: www.chemspider.com. (Accessed: 27th March 2019)

2. Yang, K., Zhu, L. & Xing, B., Adsorption of Polycyclic Aromatic Hydrocarbons by Carbon Nanomaterials, *Environ. Sci. Technol.*, 2006, **40**, 1855–1861

3. Kah, M., Zhang, X., Jonker, M. T. O. & Hofmann, T., Measuring and modeling adsorption of PAHs to carbon nanotubes over a six order of magnitude wide concentration range, *Environ. Sci. Technol.*, 2011, **45**, 6011–6017