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


# $NO_2$ and natural organic matter affect both soot aggregation behavior and sorption of S-metolachlor

## Supporting Information

Gabriel Sigmund,[1,2] Stephanie Castan,[2] Christopher Wabnitz,[1] Rani Bakkour,[1] Thorsten Hüffer,[2] Thilo Hofmann,[2] Martin Elsner[1,3]

[1] *Chair of Analytical Chemistry and Water Chemistry, Technical University of Munich, Marchioninistrasse 17, 81377 Munich, Germany*

[2] *Department of Environmental Geosciences, Centre for Microbiology and Environmental Systems Science, University of Vienna, Althanstraße, 1090 Wien, Austria*

[3] *Institute of Groundwater Ecology, Helmholtz Zentrum München, Ingolstädter Landstrasse 1, 85764 Neuherberg, Germany*

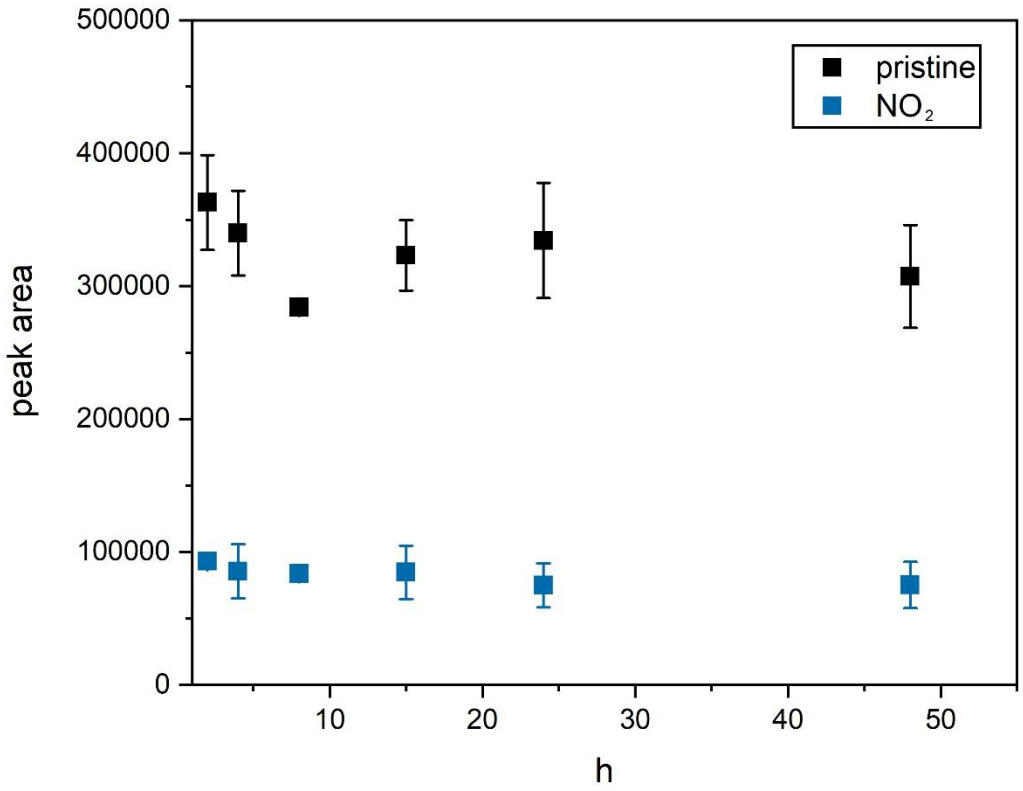


**Figure S1:** Kinetics of sorption of S-metolachlor to pristine soot (black symbols) and $NO_2$ transformed soot (blue symbols) showed that sorption equilibrium was reached after 16 h.

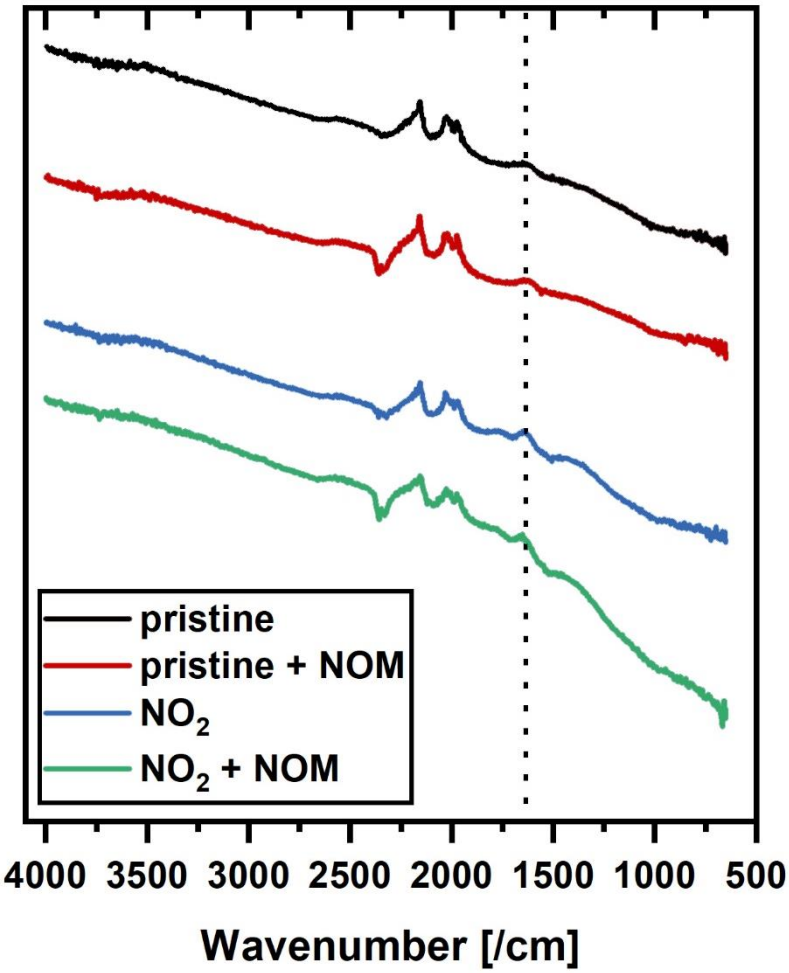


**Figure S2:** Fourier transform infrared spectra of dried samples indicate the formation of C=O and/or COOH groups following $NO_2$ transformation, as indicated by the increase of the peak at the wavelengths of 1620 to 1670, which can be attributed to a conjugated C=O group and/or a COOH group.[1,2]

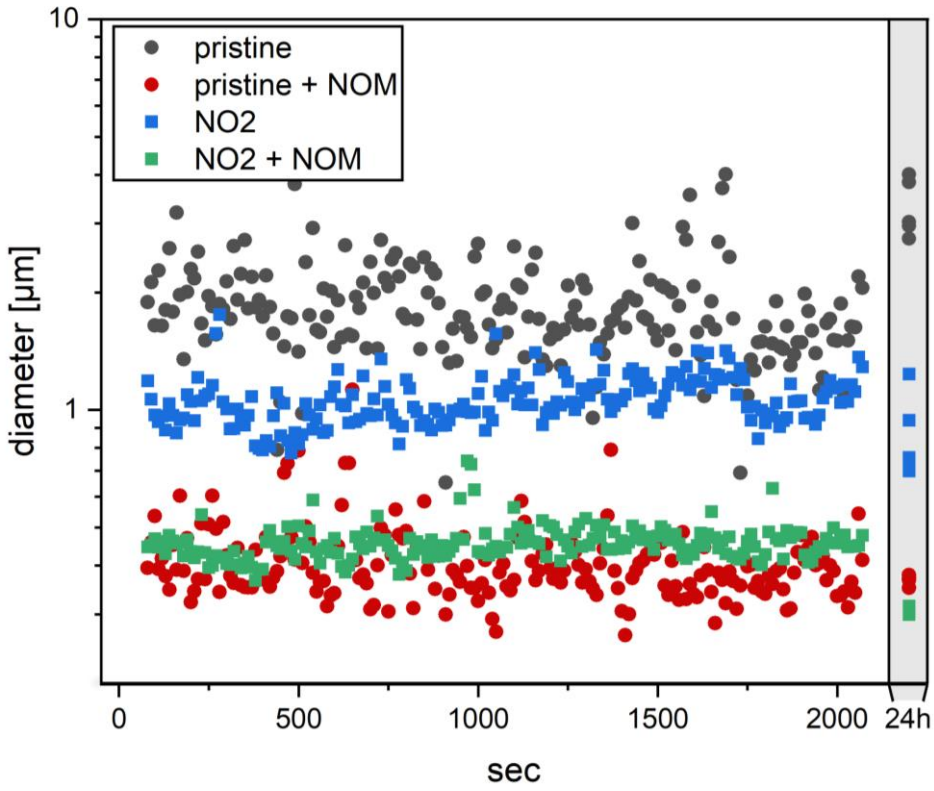


**Figure S3:** Aggregation kinetics of pristine and transformed soot for 30 min after introduction into water and after 24h of shaking (grey area). The similarity from 80 sec. to 2000 sec. indicates that most aggregation occurred during the first 80 sec. of the measurement which could not be measured due to the sample preparation protocol.

**Table S1:** ppLFER calculation according to Lu et al. (2016) for aqueous S-metolachlor concentration of 10 mg/L.

$$\mathbf{Log\ K_{Csoot} = (3.74 \pm 0.11)V + ((-0.35 \pm 0.02)log\ ai)E + (-0.62 \pm 0.10)A + (-3.35 \pm 0.11)B + (-1.45 \pm 0.09)}$$

$$\mathbf{log\ K_D = (10^{log\ KCsoot} * f_{sootC})}$$

Reference:


1 J. M. O'Reilly and R. A. Mosher, "Functional groups in carbon black by FTIR spectroscopy," Carbon, vol. 21, no. 1, pp. 47–51, 1983.

2 C. Moreno-Castilla, M.. López-Ramón and F. Carrasco-Marín, "Changes in surface chemistry of activated carbons by wet oxidation," Carbon, vol. 38, no. 14, pp. 1995–2001, 2000.

3 Z. Lu, J. K. MacFarlane, and P. M. Gschwend, 2016, "Adsorption of Organic Compounds to Diesel Soot: Frontal Analysis and Polyparameter Linear Free-Energy Relationship," Environ. Sci. Technol., vol. 50, no. 1, pp. 285–293, 2016.