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

Electronic Supplement Material for

The molecular interactions of organic compounds with tire crumb materials differ substantially from those with other microplastics

Thorsten Hüffer[a,b]*, Maren Wehrhahn[a], Thilo Hofmann[a,b]*

[a]Department of Environmental Geosciences, Center for Microbiology and Environmental Systems Science

[b]Research Platform Plastics in the Environment and Society (PLENTY), University of Vienna, Althanstrasse 14, 1090 Vienna, Austria

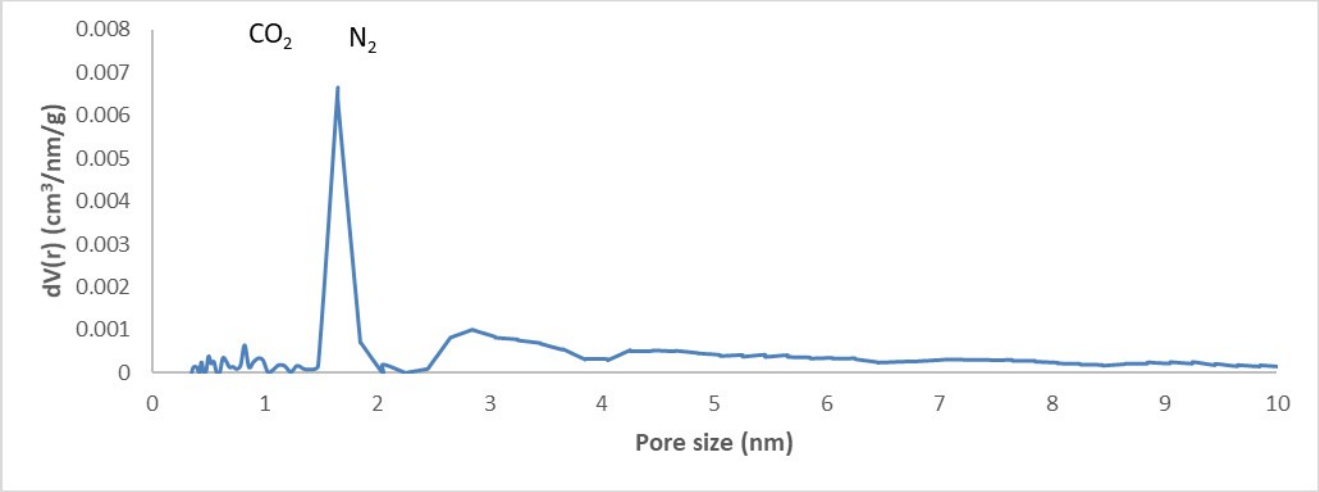

Figure S1: Pore size distribution of CB measured using N_2 and CO_2 physisorption BET.

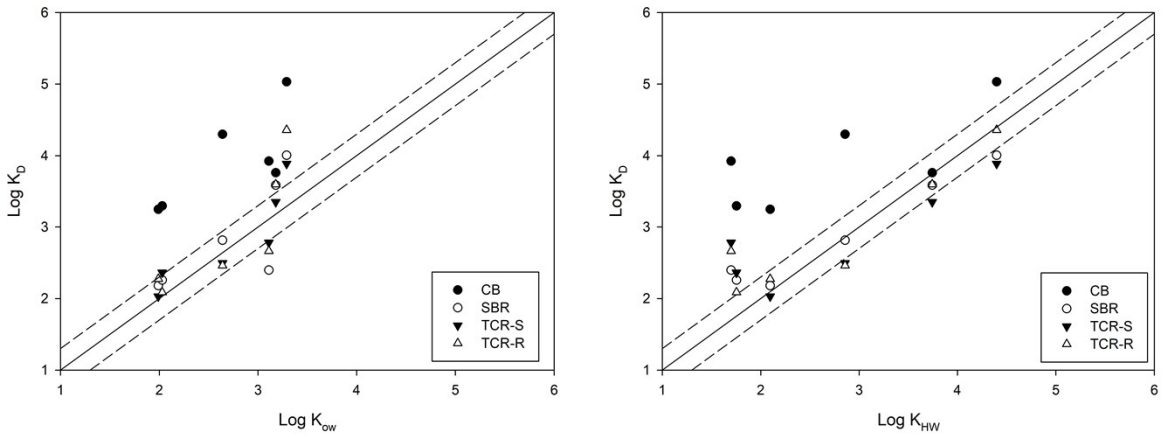

Figure S2: log K_{OW}-log K_D (left) and log K_{HW}-log K_D (right) correlations for sorption by carbon black (CB), styrene butdiene rubber (SBR), and the two tire crumb materials (TCR-S and TCR-R). Solid line indicates 1:1 correlation, and dashed lines indicate 0.3 log unit deviations.

Table S1: Fitting parameters ± standard errors, root mean square error, and Akaike's Information Criterion (AIC) for non-linear sorption model fits to the experimental isotherm data of n-hexane.

Freundlich Model (FM)

Sorbent	K_F	n	R^2	RMSE	AIC	N
CB	1.40E+05 ± 1.51E+04	0.518 ± 0.032	0.951	0.3142	-29.48	14
SBR	1.03E+04 ± 1.49E+03	0.963 ± 0.038	0.969	0.2255	-41.82	15
TCR-S	7.80E+03 ± 8.36E+02	0.977 ± 0.030	0.962	0.2336	-46.71	17
TCR-R	2.48E+04 ± 4.83E+03	0.844 ± 0.404	0.918	0.3708	-22.77	13

Langmuir Model (LM)

Sorbent	Q_{max}	K_L	R^2	RMSE	AIC	N
CB	1.43E+06 ± 1.43E+05	9.70E-02 ± 1.70E-02	0.967	0.2080	-41.04	14
SBR	2.17E+08 ± 3.92E+07	4.19E-05 ± 7.58E-04	0.966	0.2328	-40.88	15
TCR-S	1.38E+07 ± 1.53E+07	5.51E-04 ± 6.35E-04	0.963	0.2307	-47.14	17
TCR-R	1.18E+07 ± 2.50E+06	2.00E-03 ± 4.48E-04	0.973	0.2171	-36.68	13

Dual-Mode-Langmuir Model (DML)

Sorbent	log Q_{max}	K_L	K_P	R^2	RMSE	AIC	N
CB	1.00E+06 ± 1.45E+05	1.48E-01 ± 3.00E-02	4.42E+03 ± 1.33E+03	0.974	0.3303	-25.99	14
SBR	5.38E+03 ± 1.41E+04	5.33E+00 ± 1.23E+02	8.58E+03 ± 7.02E+02	0.974	0.2149	-41.29	15
TCR-S	1.38E+07 ± 3.14E+08	5.52E-04 ± 7.00E-03	7.00E-03 ± 8.12E+04	0.963	0.2388	-44.15	17
TCR-R	1.18E+07 ± 3.19E+06	2.00E-03 ± 5.05E-04	3.89E-05 ± 7.27E+02	0.973	0.2277	-33.21	13

Polanyi-Manes Model (PMM)

Sorbent	log Q_{max}	a	d	R^2	RMSE	AIC	N
CB	6.34 ± 0.11	-2.16E-07 ± 6.95E-07	2.964 ± 0.599	0.976	0.1839	-42.40	14
SBR	9.86 ± 1.87	-2.38E-01 ± 3.91E-01	0.609 ± 0.253	0.979	0.1929	-44.53	15
TCR-S	7.65 ± 0.58	-8.00E-03 ± 1.40E-02	1.167 ± 0.290	0.963	0.2388	-44.14	17
TCR-R	7.14 ± 0.12	-1.18E-04 ±1.37E-04	1.933 ± 0.218	0.978	0.2061	-35.81	13

Table S2: Fitting parameters ± standard errors, root mean square error, and Akaike's Information Criterion (AIC) for non-linear sorption model fits to the experimental isotherm data of cyclo-hexane.

Freundlich Model (FM)

Sorbent	K_F	n	R^2	RMSE	AIC	N
CB	9.33E+03 ± 1.92E+03	0.671 ± 0.038	0.914	0.3663	-31.42	17
SBR	4.84E+03 ± 9.75E+02	0.847 ± 0.037	0.956	0.2688	-31.13	13
TCR-S	2.44E+03 ± 4.56E+02	0.941 ± 0.035	0.959	0.2603	-40.28	16
TCR-R	5.18E+03 ± 7.33E+02	0.815 ± 0.028	0.956	0.2567	-40.73	16

Langmuir Model (LM)

Sorbent	Q_{max}	K_L	R^2	RMSE	AIC	N
CB	1.44E+06 ± 1.31E+05	3.00E-03 ± 3.86E-04	0.983	0.1647	-58.59	17
SBR	3.47E+06 ± 9.13E+05	8.97E-04 ± 2.92E-04	0.971	0.2203	-36.30	13
TCR-S	5.62E+06 ± 2.34E+06	3.81E-04 ± 1.78E-04	0.968	0.2288	-44.42	16
TCR-R	3.77E+06 ± 4.11E+05	8.13E-04 ± 1.06E-04	0.991	0.1194	-65.21	16

Dual-Mode-Langmuir Model (DML)

Sorbent	log Q_{max}	K_L	K_P	R^2	RMSE	AIC	N
CB	1.36E+06 ± 3.05E+05	3.00E-03 ± 7.62E-04	3.66E+01 ± 1.26E+02	0.983	0.1700	-55.69	17
SBR	1.43E+06 ± 1.19E+06	2.00E-03 ± 1.00E-03	6.65E+02 ± 5.16E+02	0.973	0.2199	-34.13	13
TCR-S	1.70E+06 ± 4.33E+06	8.37E-04 ± 2.00E-03	7.52E+02 ± 1.20E+03	0.969	0.2353	-41.62	16
TCR-R	2.40E+06 ± 8.27E+05	1.00E-03 ± 3.57E-04	3.09E+02 ± 2.01E+02	0.992	0.1152	-64.48	16

Polanyi-Manes Model (PMM)

Sorbent	log Q_{max}	a	d	R^2	RMSE	AIC	N
CB	6.23 ± 0.06	-2.33E-06 ± 2.65E-06	2.548 ± 0.209	0.987	0.2831	-38.36	17
SBR	6.73 ± 0.02	-1.57E-04 ± 2.82E-04	1.181 ± 0.324	0.975	0.2113	-35.15	13
TCR-S	6.56 ± 0.13	-2.43E-05 ± 3.56E-05	2.174 ± 0.270	0.983	0.1728	-51.51	16
TCR-R	6.72 ± 0.06	-1.37E-04 ± 8.10E-05	1.841 ± 0.108	0.994	0.1021	-68.33	16

Table S3: Fitting parameters ± standard errors, root mean square error, and Akaike's Information Criterion (AIC) for non-linear sorption model fits to the experimental isotherm data of benzene.

Freundlich Model (FM)

Sorbent	K_F	n	R^2	RMSE	AIC	N
CB	4.30E+04 ± 8.35E+03	0.398 ± 0.026	0.964	0.2056	-41.35	14
SBR	1.95E+02 ± 3.51E+01	0.953 ± 0.025	0.962	0.2571	-57.24	22
TCR-S	1.42E+02 ± 4.35E+01	0.946 ± 0.044	0.921	0.3769	-30.45	17
TCR-R	2.33E+02 ± 2.75E+01	0.959 ± 0.016	0.989	0.1385	-72.48	19

Langmuir Model (LM)

Sorbent	Q_{max}	K_L	R^2	RMSE	AIC	N
CB	1.37E+06 ± 1.15E+05	2.00E-03 ± 4.57E-04	0.966	0.1998	-42.16	14
SBR	7.38E+06 ± 4.92E+06	2.06E-05 ± 1.47E-05	0.959	0.2641	-56.05	22
TCR-S	1.47E+06 ± 9.04E+05	8.16E-05 ± 5.79E-05	0.922	0.3753	-30.59	17
TCR-R	2.74E+07 ± 1.90E+07	6.59E-06 ± 4.74E-06	0.986	0.1515	-69.08	19

Dual-Mode-Langmuir Model (DML)

Sorbent	log Q_{max}	K_L	K_P	R^2	RMSE	AIC	N
CB	1.02E+06 ± 1.08E+05	4.00E-03 ± 7.52E-04	4.83E+01 ± 1.36E+01	0.983	0.1487	-48.35	14
SBR	8.53E+05 ± 1.89E+05	6.35E-04 ± 1.00E-03	1.33E+02 ± 2.28E+01	0.965	0.2508	-56.76	22
TCR-S	1.01E+05 ± 4.15E+05	5.45E-04 ± 2.00E-03	7.01E+01 ± 5.08E+01	0.930	0.3693	-29.32	17
TCR-R	5.24E+03 ± 3.92E+03	2.60E-02 ± 3.70E-02	1.62E+02 ± 6.84E+00	0.991	0.1261	-74.36	19

Polanyi-Manes Model (PMM)

Sorbent	log Q_{max}	a	d	R^2	RMSE	AIC	N
CB	6.34 ± 0.07	-8.45E-08 ± 2.14E-07	2.881 ± 0.437	0.989	0.1211	-54.10	14
SBR	7.51 ± 0.46	-2.00E-03 ± 3.00E-03	1.332 ± 0.259	0.964	0.2540	-56.18	22
TCR-S	6.23 ± 0.33	-3.08E-06 ± 1.06E-06	2.390 ± 0.585	0.939	0.3452	-31.62	17
TCR-R	8.98 ± 0.49	-4.30E-02 ± 3.30E-02	0.834 ± 0.117	0.990	0.1347	-71.84	19

Table S4: Fitting parameters ± standard errors, root mean square error, and Akaike's Information Criterion (AIC) for non-linear sorption model fits to the experimental isotherm data of chlorobenzene.

Freundlich Model (FM)

Sorbent	K_F	n	R^2	RMSE	AIC	N
CB	2.64E+05 ± 1.80E+04	0.299 ± 0.010	0.985	0.1178	-82.94	20
SBR	7.54E+02 ± 5.62E+01	0.961 ± 0.011	0.991	0.1185	-87.03	21
TCR-S	2.95E+02 ± 2.98E+01	1.016 ± 0.015	0.982	0.1708	-82.33	24
TCR-R	2.27E+02 ± 4.00E+01	1.066 ± 0.026	0.956	0.2781	-56.35	23

Langmuir Model (LM)

Sorbent	Q_{max}	K_L	R^2	RMSE	AIC	N
CB	2.50E+06 ± 2.92E+05	1.30E-02 ± 4.00E-03	0.872	0.3339	-41.28	20
SBR	2.44E+07 ± 5.77E+06	2.62E-05 ± 6.56E-06	0.994	0.1014	-93.56	21
TCR-S	2.54E+08 ± 1.72E+09	1.28E-06 ± 8.68E-06	0.981	0.1755	-81.04	24
TCR-R	2.87E+08 ± 3.71E+09	1.17E-06 ± 1.52E-06	0.939	0.3240	-49.34	23

Dual-Mode-Langmuir Model (DML)

Sorbent	log Q_{max}	K_L	K_P	R^2	RMSE	AIC	N
CB	1.76E+06 ± 1.79E+05	3.20E-02 ± 9.00E-03	1.78E+02 ± 3.65E+01	0.943	0.2325	-54.10	20
SBR	1.14E+06 ± 1.55E+06	2.40E-04 ± 2.16E-04	4.19E+02 ± 8.51E+01	0.995	0.0969	-93.87	21
TCR-S	2.74E+08 ± 7.83E+09	2.34E+01 ± 1.45E+01	3.24E+02 ± 6.57E+01	0.976	0.1795	-78.45	24
TCR-R	7.22E+08 ± 6.20E+09	2.56E+02 ± 3.92E+02	3.34E+02 ± 4.95E+2	0.964	0.3304	-46.89	23

Polanyi-Manes Model (PMM)

Sorbent	log Q_{max}	a	d	R^2	RMSE	AIC	N
CB	6.85 ± 0.08	-3.54E-04 ± 3.88E-04	1.455 ± 0.188	0.989	0.1031	-86.65	20
SBR	7.73 ± 0.10	-3.00E-03 ± 1.00E-03	1.273 ± 0.065	0.996	0.0854	-99.17	21
TCR-S	7.45 ± 0.16	-2.00E-03 ± 1.00E-03	1.355 ± 0.103	0.989	0.1401	-90.35	24
TCR-R	7.37 ± 0.21	-8.01E-04 ± 7.96E-04	1.539 ± 0.173	0.971	0.3077	-50.17	23

Table S5: Fitting parameters ± standard errors, root mean square error, and Akaike's Information Criterion (AIC) for non-linear sorption model fits to the experimental isotherm data of di-n-propyl ether.

Freundlich Model (FM)

Sorbent	K_F	n	R^2	RMSE	AIC	N
CB	6.89E+04 ± 8.31E+03	0.338 ± 0.018	0.959	0.2958	-33.69	15
SBR	7.26E+02 ± 1.03E+02	0.741 ± 0.021	0.981	0.1495	-50.27	14
TCR-S	1.37E+03 ± 3.52E+02	0.667 ± 0.033	0.965	0.2483	-27.36	11
TCR-R	7.98E+01 ± 1.91E+01	1.079 ± 0.031	0.953	0.2702	-39.09	16

Langmuir Model (LM)

Sorbent	Q_{max}	K_L	R^2	RMSE	AIC	N
CB	1.02E+06 ± 1.42E+05	1.00E-02 ± 3.00E-03	0.882	0.3313	-30.29	15
SBR	8.62E+05 ± 2.38E+05	2.09E-04 ± 7.36E-05	0.926	0.2921	-31.52	14
TCR-S	7.82E+05 ± 1.91E+05	3.12E-04 ± 1.24E-04	0.931	0.3447	-20.14	11
TCR-R	2.82E+08 ± 4.53E+09	2.06E+06 ± 3.32E+07	0.930	0.3272	-32.96	16

Dual-Mode-Langmuir Model (DML)

Sorbent	log Q_{max}	K_L	K_P	R^2	RMSE	AIC	N
CB	6.78E+05 ± 1.02E+05	1.90E-02 ± 5.00E-03	7.28E+01 ± 1.71E+01	0.951	0.2263	-39.75	15
SBR	8.89E+04 ± 2.62E+04	2.00E-03 ± 8.64E-04	5.68E+01 ± 6.00E+00	0.984	0.1428	-49.47	14
TCR-S	2.17E+05 ± 1.08E+05	1.00E-03 ± 8.65E-04	3.99E+01 ± 1.20E+01	0.960	0.2816	-21.95	11
TCR-R	1.41E+06 ± 2.29E+13	6.51E+05 ± 5.30E+13	1.36E+02 ± 1.75E+06	0.931	0.3371	-30.12	16

Polanyi-Manes Model (PMM)

Sorbent	log Q_{max}	a	d	R^2	RMSE	AIC	N
CB	6.45 ± 0.19	-5.45E-05 ± 1.70E-04	1.859 ± 0.554	0.965	0.1908	-44.86	15
SBR	7.57 ± 0.66	-1.80E-02 ± 3.00E-02	0.990 ± 0.272	0.981	0.1561	-46.97	14
TCR-S	7.01 ± 0.70	-5.00E-03 ± 1.30E-02	1.195 ± 0.464	0.965	0.2608	-23.64	11
TCR-R	8.45 ± 0.17	-1.40E-02 ± 2.30E-02	1.100 ± 0.275	0.953	0.2790	-36.17	16

Table S6: Fitting parameters ± standard errors, root mean square error, and Akaike's Information Criterion (AIC) for non-linear sorption model fits to the experimental isotherm data of 2,6-dimethylheptan-2-ol.

Freundlich Model (FM)						
Sorbent	**K_F**	**n**	**R^2**	**RMSE**	**AIC**	**N**
CB	4.36E+04 ± 1.47E+04	0.593 ± 0.037	0.967	0.2081	-34.53	12
SBR	4.12E+02 ± 2.09E+02	0.876 ± 0.055	0.923	0.3937	-28.97	17
TCR-S	8.42E+02 ± 2.25E+02	0.918 ± 0.033	0.956	0.2467	-42.00	16
TCR-R	8.54E+02 ± 2.11E+02	0.848 ± 0.035	0.957	0.2712	-28.17	12

Langmuir Model (LM)						
Sorbent	**Q_{max}**	**K_L**	**R^2**	**RMSE**	**AIC**	**N**
CB	3.11E+07 ± 1.09E+07	6.00E-05 ± 3.45E-05	0.866	0.4071	-18.43	12
SBR	9.38E+07 ± 2.08E+08	1.43E-06 ± 3.29E-06	0.907	0.3729	-30.81	17
TCR-S	2.70E+08 ± 4.71E+08	1.62E-06 ± 2.90E-06	0.940	0.2895	-36.88	16
TCR-R	3.28E+06 ± 5.12E+05	1.39E-04 ± 2.69E-05	0.985	0.1608	-40.71	12

Dual-Mode-Langmuir Model (DML)							
Sorbent	**log Q_{max}**	**K_L**	**K_P**	**R^2**	**RMSE**	**AIC**	**N**
CB	2.75E+06 ± 5.32E+05	4.00E-03 ± 2.00E-03	5.73E+02 ± 4.37E+01	0.986	0.1433	-41.08	12
SBR	5.74E+04 ± 2.26E+04	6.70E-02 ± 2.12E-01	1.15E+02 ± 8.59E+00	0.969	0.2268	-45.90	17
TCR-S	5.62E+04 ± 4.94E+04	2.70E-02 ± 1.15E-01	3.77E+02 ± 3.10E+01	0.969	0.2174	-44.16	16
TCR-R	2.58E+06 ± 2.19E+06	1.65E-04 ± 1.09E-04	2.99E+01 ± 9.76E+01	0.985	0.1686	-37.18	12

Polanyi-Manes Model (PMM)							
Sorbent	**log Q_{max}**	**a**	**d**	**R^2**	**RMSE**	**AIC**	**N**
CB	10.63 ± 2.09	-1.08E+00 ± 1.36E+00	0.303 ± 0.172	0.987	0.1370	-42.16	12
SBR	9.14 ± 1.00	-4.19E-01 ± 4.20E-01	0.493 ± 0.165	0.951	0.2830	-38.37	17
TCR-S	9.04 ± 0.43	-1.58E-01 ± 1.02E-01	0.681 ± 0.115	0.972	0.2078	-45.61	16
TCR-R	6.63 ± 0.08	-4.04E-05 ± 3.74E-05	2.244 ± 0.184	0.993	0.1121	-46.98	12

Table S7: logK_D values calculated for the investigated sorbent-sorbate system at 10-3 of the sorbate solubility.

Sorbate	**Log K_D (carbon black)**	**Log K_D (styrene butadiene)**	**Log K_D (TCR-S)**	**Log K_D (TCR-R)**
nHex	5.03	4.01	3.89	4.36
cHex	3.76	3.59	3.35	3.60
Benz	3.25	2.18	2.03	2.27
cBenz	4.30	2.82	2.50	2.46
DNPE	3.30	2.26	2.36	2.09
DMH	3.92	2.40	2.78	2.66