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Supplementary Information

Comparison of Atmospheric Travel Distances of Several PAHs Calculated by Two Fate and Transport Models (The Tool and ELPOS) with Experimental Values Derived from a Peat Bog Transect. *Atmosphere* 2014, *5*, 324–341.

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Supporting Material

Comparison of atmospheric travel distances of several PAHs calculated by two fate and transport models (The Tool and ELPOS) with experimental values derived from a peat bog transect.

Table S1. Coordinates of Greater Sudbury and sampling locations.

Site Name	Latitude	Longitude	Distance from Superstack (km)
Sudbury (Superstack)	N 46.48011	W 81.056506	-
Giant Bog *	N 46.42422	W 79.937056	81
Eagle Lake Bog	N 45.80572	W 79.444830	140
Spruce Bog	N 45.59050	W 78.373055	220
Green Lake Bog	N 45.68517	W 77.151194	310

Note: * While the names of the other sampling sites have previously been reported, the name Giant Bog was assigned to this site as no previous description and thus no established name was available.

Table S2. Original and adjusted settings in The Tool.

	Temperature (K)	Area of Water (%)	Depth of Water (m)	Wind Speed ($km \cdot h^{-1}$)	Height of Air (m)	Precipitation Rate ($mm \cdot a^{-1}$)
original	298.15	71	100	14.4	6000	850
adjusted	276.95	10	10	13.1	1000	1008

Table S3. Original and adjusted settings in ELPOS.

	Length of Study Region (m)	Wind Speed ($km \cdot h^{-1}$)	Precipitation Rate ($mm \cdot a^{-1}$)	Area of Water (%)	Depth of Water (m)	Area of Industry (%)
original	200,000	14.4	760	3	3	10
adjusted	450,000	13.1	1008	10	10	3

Table S4. Input values for The Tool at 4 °C. Partition coefficients were taken from Ma *et al*. (2009) [24] and temperature adjusted as described in the manuscript, half-life times were calculated with AOPWIN [40] and adjusted for OH-radical concentration and daytime length. Partition coefficients and degradation rates for particles are hypothetical values.

	Molar Mass	log K_{AW}			log K_{OW}			Half-Life Air	Half-Life Water	Half-Life Soil
	(g/mol)	0 °C	4 °C	13 °C	0 °C	4 °C	13 °C	(h)	(h)	(h)
Phen	178.23	−4.27	−4.14	−3.86	4.68	4.58	4.39	14.44	1440	2880
Flt	202.26	−4.95	−4.82	−4.53	5.31	5.19	4.95	6.42	1440	2880
B[a]A	228.30	−7.06	−6.89	−6.53	4.86	4.74	4.50	1.49	1440	2880
Chry	228.29	−5.38	−5.24	−4.91	6.61	6.46	6.17	3.76	1440	2880
B[b]F	252.31	−6.27	−6.11	−5.76	6.58	6.47	6.25	10.12	1440	2880
B[a]P	252.31	−6.27	−6.11	−5.76	7.03	6.87	6.55	3.76	1440	2880
Ind	276.33	−7.15	−6.99	−6.62	7.33	7.14	6.76	2.91	1440	2880
particles	63.55	−9.00	−9.00	−9.00	10.00	10.00	10.00	10×10^9	10×10^9	10×10^9

Table S5. Input values for ELPOS. Partition coefficients (25 °C) were taken from Ma *et al*. (2009) [24], half-life times were calculated with AOPWIN [40] and adjusted for OH-radical concentration and daytime length. The partition coefficients and degradation rates for particles are hypothetical values.

	Molar Mass (g/mol)	melting Point (°C)	log K_{AW}	log K_{OW}	log K_{OC}	Half-Life (h) Air	Half-Life (h) Water	Half-Life (h) Soil	Half-Life (h) Sediment
Phen	178.23	372	−2.76	4.47	3.65	14.44	1440	2880	1,3000
Flt	202.26	382.00	−3.27	4.97	4.52	6.42	1440	2880	1,3000
B[a]A	228.30	431.80	−3.59	5.83	4.61	1.49	1440	2880	1,3000
Chry	228.29	530.00	−3.82	5.67	5.06	3.76	1440	2880	1,3000
B[b]F	252.31	441.20	−4.58	5.86	5.73	10.12	1440	2880	1,3000
B[a]P	252.31	452.00	−4.51	6.05	5.73	3.76	1440	2880	1,3000
Ind	276.33	436.00	−4.70	6.57	6.40	2.91	1440	2880	1,3000
particles	63.55	1084.62	−9.00	10.00	−0.5	10×10^9	10×10^9	10×10^9	10×10^9

Table S6. Input values for ELPOS calculated by the implemented temperature adjustment; log K_{OW} and K_{OC} are not presented as they were not changed.

	log K_{AW}			Half-Life (h) Air			Half-Life (h) Water			Half-Life (h) Sediment			Half-Life (h) Soil		
	0 °C	4 °C	13 °C	0 °C	4 °C	13 °C	0 °C	4 °C	13 °C	0 °C	4 °C	13 °C	0 °C	4 °C	13 °C
Phen	−3.72	−3.56	−3.20	1.82	1.50	1.00	4359.06	3602.44	2392.04	3,9352.67	3,2522.02	2,1594.76	8718.13	7204.88	4784.07
Flt	−4.23	−4.07	−3.71	0.81	0.67	0.44	4359.06	3602.44	2392.04	3,9352.67	3,2522.02	2,1594.76	8718.13	7204.88	4784.07
B[a]A	−4.55	−4.39	−4.03	0.19	1.06	0.10	4359.06	3602.44	2392.04	3,9352.67	3,2522.02	2,1594.76	8718.13	7204.88	4784.07
Chry	−4.78	−4.62	−4.26	0.47	0.39	0.26	4359.06	3602.44	2392.04	3,9352.67	3,2522.02	2,1594.76	8718.13	7204.88	4784.07
B[b]F	−5.54	−5.38	−5.02	1.28	1.06	0.70	4359.06	3602.44	2392.04	3,9352.67	3,2522.02	2,1594.76	8718.13	7204.88	4784.07
B[a]P	−5.47	−5.31	−4.95	0.47	0.39	0.26	4359.06	3602.44	2392.04	3,9352.67	3,2522.02	2,1594.76	8718.13	7204.88	4784.07
Ind	−5.66	−5.50	−5.14	0.37	0.30	0.20	4359.06	3602.44	2392.04	3,9352.67	3,2522.02	2,1594.76	8718.13	7204.88	4784.07
particles	−9.96	−9.80	−9.44	3×10^{10}	2.5×10^{10}	1.6×10^{10}	3×10^{10}	2.5×10^{10}	1.6×10^{10}	3×10^{10}	2.5×10^{10}	1.6×10^{10}	3×10^{10}	2.5×10^{10}	1.6×10^{10}

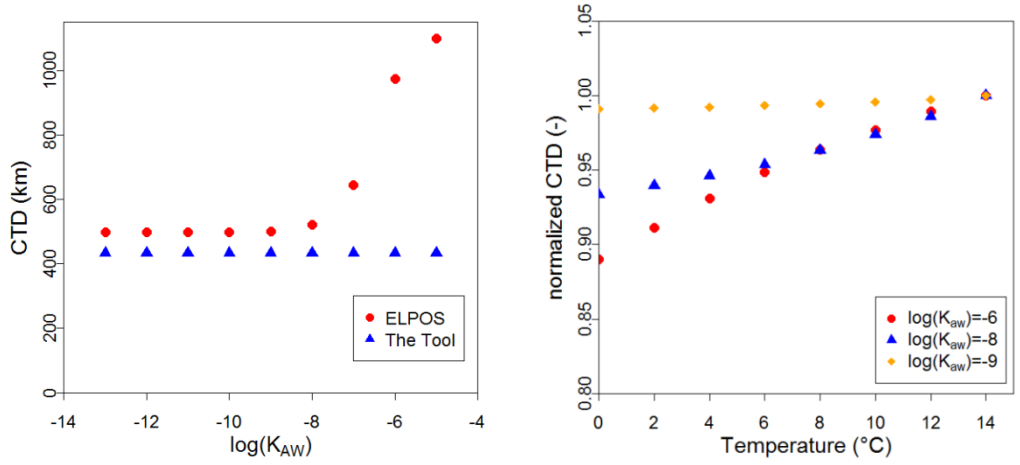
Table S7. Maximum deposition rates of PAHs ($\mu g \cdot m^{-2} \cdot a^{-1}$) and metals ($mg \cdot m^{-2} \cdot a^{-1}$) in each of the sampled peat cores and calculated ETD (km).

	Chry	B[b+k]F	B[a]P	Ind	Cu	Zn
GB 1	15	30	15	33	6	55
GB 2	24	15	14	32	5	35
GB 3	24	22	6	17	4	71
ELB 1	31	13	7	15	2	42
ELB 2	10	14	5	30	2	40
ELB 3	10	15	6	28	2	31
SB 1	7	9	10	19	2	23
SB 2	14	10	7	11	2	37
SB 3	7	9	5	14	1	31
GLB 1	7	6	2	8	2	34
GLB 2	12	12	7	21	1	16
GLB 3	11	11	6	15	1	10
ETD (km)	292	281	321	310	173	222

Table S8. Empirically determined travel distances of several metals derived from other studies with standard error (SE), significance level (p), and coefficient of determination (R^2).

Study	Metal	ETD (km)	SE (km)	p (-)	R^2 (-)
Freedman *et al*. [43]	Ni	23.53	1.25	0.000	0.92
	Cu	22.36	1.12	0.000	0.91
Nieboer *et al*. [44]	Cu	30.74	5.75	0.001	0.78
	Ni	21.31	4.74	0.002	0.72
	Zn	67.15	24.64	0.026	0.48
Kettles and Bonham-Carter [45]	Cu	32.56	4.14	0.000	0.64
	Pb	21.32	2.69	0.000	0.64
	Zn	66.47	12.71	0.000	0.44

Figure S1. (**A**) Particle-CTD calculated by both models as a function of the air-water partition coefficient (K_{AW}); and (**B**) Particle-CTD (normalized to the CTD at 14 °C) calculated with ELPOS as a function of temperature for three air-water partition coefficients. The CTD of a completely particle bound substance should not depend on the air-water partition coefficient and also not on the temperature (as in both models, wet and dry deposition are not implemented as temperature-dependent processes). For The Tool, no dependence of CTD on K_{AW} was observed, whereas the CTD calculated by ELPOS was increasing with temperature for $\log(K_{AW}) > -9$. Therefore, we chose a K_{AW} of −9 to simulate the particle behavior in both models. Moreover, the temperature dependence of CTD in ELPOS was negligible for this $\log(K_{AW})$, whereas a clear dependence on temperature (caused by apparent partitioning into the gas phase) was observed for $\log(K_{AW}) > -9$.



(**A**) (**B**)

Table S9. Characteristic travel distances of PAHs and particles, 95% confidence intervals (CI) and fraction bound to particles calculated by The Tool for different temperature scenarios and with regionalized settings.

	0 °C			4 °C			13 °C		
	CTD (km)	95% CI	Particle Fraction (%)	CTD (km)	95% CI	Particle Fraction (%)	CTD (km)	95% CI	Particle Fraction (%)
Phen	1633	483–5514	0.7	325	51–2066	0.4	258	50−1329	0.2
Flt	596	212–1673	13.4	149	33–675	8.0	116	29−458	2.5
B[a]A	66	13–329	87.4	44	6–298	78.4	28	4−205	47.4
Chry	378	295–483	89.2	225	75−672	80.9	113	31−409	50.0
B[b]F	355	305–405	98.4	336	231−489	97.0	293	153−559	89.6
B[a]P	375	346–405	99.4	355	220−571	98.8	285	142−572	94.5
Ind	380	364–398	100	375	343−410	99.9	352	257−487	99.5
particles	388	388–388	100	388	388−388	100	388	388−388	100

Figure S2. Time trends of reconstructed deposition rates of Ind in the sampled bogs (Giant Bog (GB). Eagle Lake Bog (ELB). Spruce Bog (SB) and Green Lake Bog (GLB)). The three data series per bog represent the three replicate cores per site.

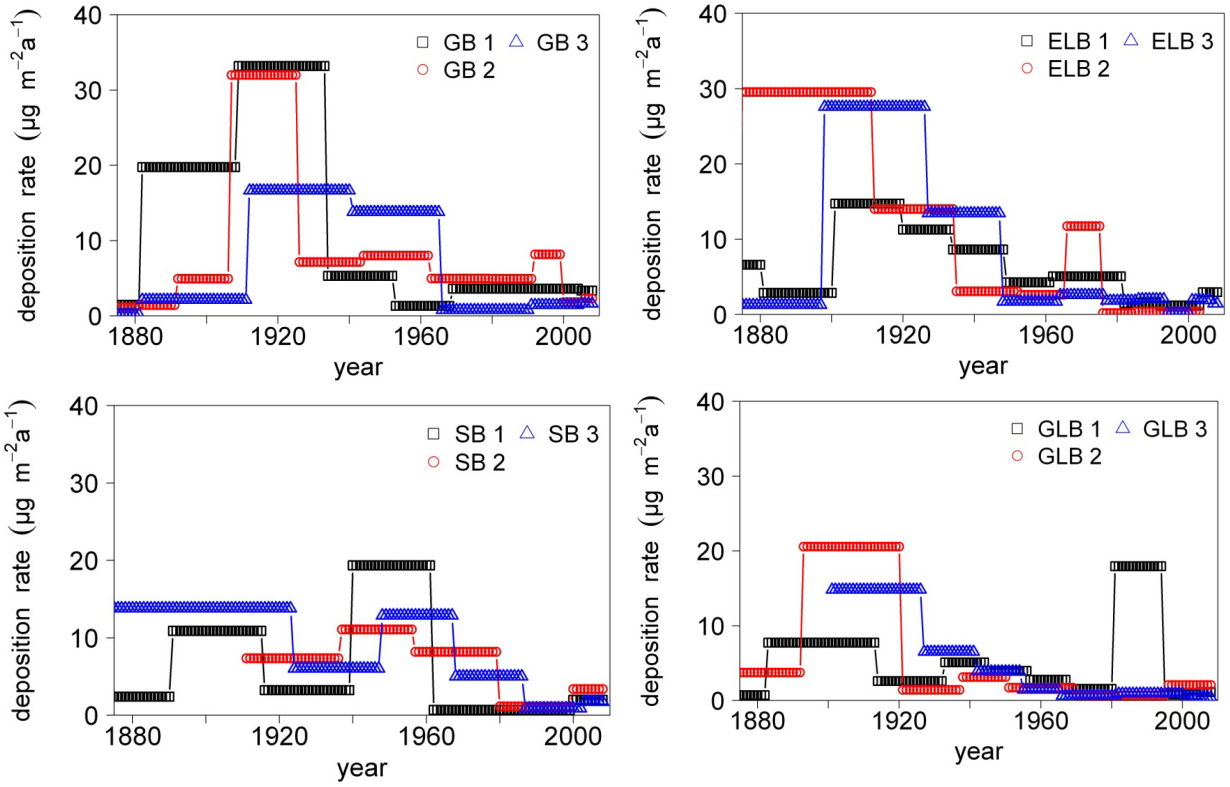


Figure S3. Average maximum PAH deposition rates along the transect; error bars indicate standard deviation of the three peat profiles per bog.

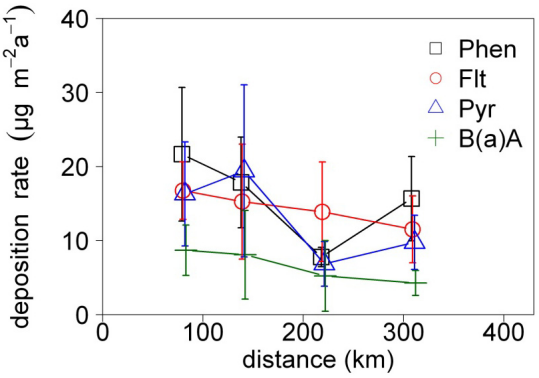


Table S10. Characteristic travel distances of PAHs and metals and fraction bound to particles calculated by ELPOS for different temperature scenarios and with regionalized settings.

	0 °C		4 °C		13 °C	
	CTD (km)	**Particle Fraction (%)**	**CTD (km)**	**Particle Fraction (%)**	**CTD (km)**	**Particle Fraction (%)**
Phen	2376	0.2	345	0.1	266	0.1
Flt	704	1.7	158	1.2	120	0.5
B[a]A	378	21.1	142	15.4	54	7.4
Chry	480	23.9	282	17.6	133	8.6
B[b]F	457	73.6	432	65.6	373	45.7
B[a]P	482	78.6	456	71.6	366	52.6
Ind	490	95.0	483	92.8	454	85.0
particles	517	100.0	517	100.0	517	100.0

Table S11. Sensitivity of the CTD to model input parameters estimated with The Tool.

	Windspeed	**Height of Air**	**Aerosol Deposition Velocity**	**Rain Rate**	**$t_{1/2}$ in Air**	**$t_{1/2}$ in Water**	**$t_{1/2}$ in Soil**	**K_{AW}**	**K_{OW}**
Phen	1.00	0.05	0.00	0.02	0.93	0.01	0.00	0.03	0.00
Flt	1.00	0.08	0.01	0.06	0.91	0.00	0.00	0.02	0.06
B[a]A	1.00	0.58	0.02	0.54	0.38	0.00	0.00	0.18	0.71
Chry	1.00	0.36	0.10	0.26	0.60	0.00	0.00	0.41	0.47
B[b]F	1.00	0.92	0.25	0.62	0.07	0.00	0.00	0.05	0.15
B[a]P	1.00	0.91	0.27	0.60	0.08	0.00	0.00	0.07	0.11
Ind	1.00	0.99	0.30	0.64	0.01	0.00	0.00	0.01	0.03
particles	1.00	1.00	0.31	0.64	0.00	0.00	0.00	0.00	0.00

Table S12. Sensitivity of the CTD to model input parameters estimated with ELPOS.

	Temperature	**Wind speed**	**Height of Air**	**Aerosol Deposition Velocity**	**Rain Rate**	**Vapor Pressure**	**$t_{1/2}$ in Air**	**$t_{1/2}$ in Water**	**$t_{1/2}$ in Soil**	**$t_{1/2}$ in Sed**	**K_{AW}**	**K_{OW}**	**K_{OC}**
Phen	0.18	1.00	0.02	0.00	0.02	0.00	0.97	0.00	0.00	0.00	0.02	0.00	0.00
Flt	0.07	1.00	0.02	0.00	0.02	0.00	0.96	0.00	0.00	0.00	0.01	0.00	0.00
B[a]A	0.09	1.01	0.04	0.00	0.02	0.00	0.98	0.00	0.00	0.00	0.11	0.14	0.00
Chry	0.08	1.00	0.08	0.01	0.08	0.00	0.90	0.00	0.00	0.00	0.08	0.13	0.00
B[b]F	0.03	1.00	0.64	0.05	0.57	0.00	0.32	0.00	0.00	0.00	0.00	0.22	0.00
B[a]P	0.08	1.00	0.43	0.04	0.39	0.00	0.52	0.00	0.00	0.00	0.25	0.37	0.00
Ind	0.05	1.00	0.71	0.08	0.61	0.00	0.25	0.00	0.00	0.00	0.19	0.25	0.00
particles	0.00	1.00	1.00	0.12	0.01	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00