



Supplement of

Modelling the impact of climate change on the atmospheric transport and the fate of persistent organic pollutants in the Arctic

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Tables

Table S1. Total mass of the studied compounds emitted to the atmosphere over the 10 year simulated periods applied in the 'ES' and 'E' simulations¹. Total mass of the studied compounds in air, snow, vegetation, water and soil in the entire model domain applied in the 'ES' and 'S' simulations.

Compound	Total 10 year atmospheric emissions applied in the 'ES' and 'E' simulations [t]	Initial mass in air applied in the 'ES' and 'S' simulations [t]	Initial mass in snow applied in the 'ES' and 'S' simulations [t]	Initial mass in vegetation applied in the 'ES' and 'S' simulations [t]	Initial mass in water applied in the 'ES' and 'S' simulations [t]	Initial mass in soil applied in the 'ES' and 'S' simulations [t]
α -HCH	1,149.5	27.33	18.79	6.25	7519.10	228.56
β -HCH	191.6	0.86	0.05	2.49	3611.60	3.08
γ -HCH	14,256.3	28.46	14.86	23.63	3324.00	234.43
PCB008	796.7	2.97	0.86	1.49	7.51	8.29
PCB028	285.7	1.05	0.60	0.83	2.32	11.43
PCB031	231.9	0.73	0.57	0.67	1.63	9.66
PCB052	145.3	0.46	0.49	0.51	1.40	18.42
PCB101	74.7	0.21	0.33	0.35	1.95	83.80
PCB118	105.1	0.25	0.50	0.53	4.29	133.60
PCB138	68.9	0.16	0.27	0.45	2.09	163.78
PCB153	76.0	0.16	0.26	0.50	3.30	189.34
PCB180	23.7	0.04	0.06	0.17	1.94	78.03
PCB194	5.3	0.01	0.01	0.03	0.91	23.43

¹The temporal resolution of emissions of the α -HCH, β -HCH and γ -HCH emissions is monthly and the temporal resolution of the emissions of the PCB congeners is annual.

Table S2. Physical-chemical properties applied in the model studies.

	Log K_{OA}	Log K_{AW}	Log K_{OW}	OH reaction rates in air on the form: $K_{OH}=A \exp(-E_a * 1000/(R*T))$		Reaction half-life in soil [h]	Reaction half-life in water [h]
				A	E_a		
α -HCH	7.48	-3.59	3.88	1.4E-11	11.2	459	2117
β -HCH	8.74	-4.83	3.91	1.4E-11 ^a	11.2 ^a	459	2117
γ -HCH	7.72	-3.96	3.76	6.0E-10	14.2	409	2425
PCB8	7.35	-2.06	5.11	4.48E-10	13.72 ^b	5500	4200
PCB28	7.86	-1.93	5.66	2.7E-10	13.72	10000	5500
PCB31	7.94	-1.87	5.78	1.4E-11	6.07	10000	5500
PCB52	8.22	-1.96	5.95	4.97E-11	10.46	17000	10000
PCB101	8.83	-2.08	6.38	6.15E-11	12.92	100000	31000
PCB118	9.44	-2.36	6.65	6.15E-11	12.92	100000	31000
PCB138	9.67	-1.97	7.19	8.12E-11	15.38	550000	55000
PCB153	9.45	-2.13	6.86	8.12E-11	15.38	550000	55000
PCB180	10.17	-2.51	7.15	1.4E-10	17.84	1000000	55000
PCB194	11.13	-2.77	7.78	8.44E-11	17.84 ^c	1700000	55000

^a assumed to the same as α -HCH.^b same value of E_a as for PCB28, A adjusted according to estimates from (Wöhrnschimmel. Personal communication).^c same value of E_a as for PCB180, A adjusted according to estimates from Wöhrnschimmel et al., 2013 (ref. 16).

Table S3. t-values according to the Student's t-test and significance level (p). Bold phase show significance levels lower than 0.01.

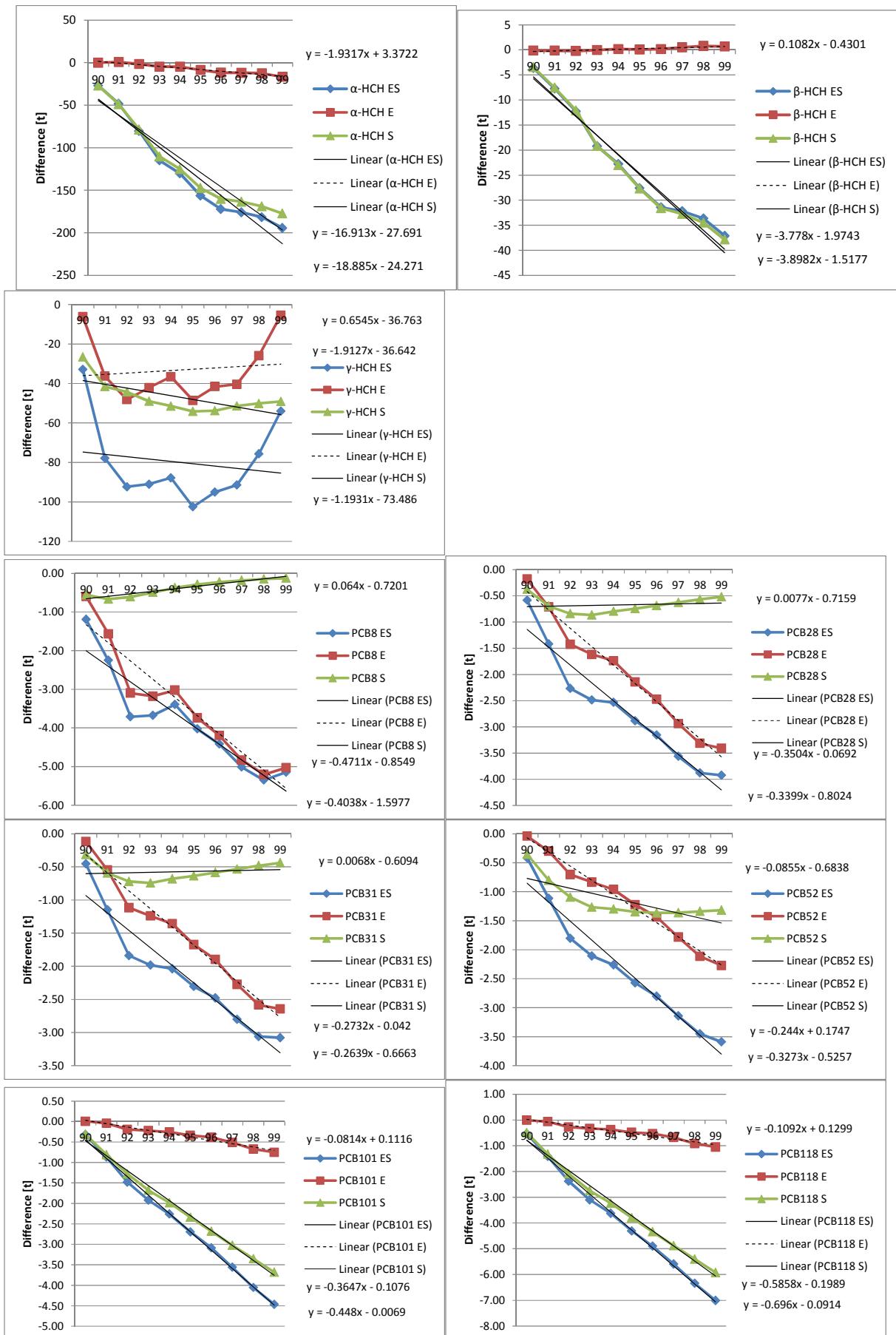
	'ES' simulations				'E' simulations			
	Whole domain t	Whole domain p	Arctic t	Arctic P	Whole domain t	Whole domain p	Arctic t	Arctic P
α -HCH total	-11.06	3.99E-06	-21.24	2.54E-08	-14.49	5.03E-07	21.57	2.24E-08
α -HCH air	-6.56	1.77E-04	-3.66	0.006	2.46	0.039	0.99	0.354
α -HCH sea	-9.93	8.97E-06	-7.82	5.13E-05	-9.89	9.24E-06	40.30	1.58E-10
α -HCH soil	-13.58	8.30E-07	-19.79	4.42E-08	-3.48	0.008	-3.27	0.011
β -HCH total	-14.11	6.20E-07	11.89	2.29E-06	7.16	9.65E-05	14.90	4.06E-07
β -HCH air	-0.08	0.938	-0.89	0.402	0.44	0.671	-1.34	0.218
β -HCH sea	-14.27	5.68E-07	17.25	1.30E-07	19.48	5.00E-08	19.79	4.42E-08
β -HCH soil	-1.63	0.142	-6.49	1.91E-04	-3.25	0.012	-0.00	0.997
γ -HCH total	-0.49	0.640	28.61	2.41E-09	0.36	0.73	27.06	3.75E-09
γ -HCH air	0.68	0.517	0.48	0.645	1.30	0.231	0.70	0.504
γ -HCH sea	6.66	1.60E-04	32.20	9.44E-10	16.87	1.55E-07	33.92	6.23E-10
γ -HCH soil	-3.61	0.007	-4.51	0.002	-4.20	0.003	-1.85	0.102
PCB8 total	-7.27	8.67E-05	-2.07	0.072	-8.90	2.00E-05	-2.61	0.031
PCB8 air	-0.55	0.601	0.43	0.678	-0.47	0.650	0.51	0.626
PCB8 sea	-3.55	0.007	-2.00	0.080	-3.78	0.005	-2.59	0.032
PCB8 soil	-10.38	6.42E-06	-14.86	4.15E-07	-17.12	1.37E-07	-7.09	1.03E-04
PCB28 total	-10.41	6.30E-06	-3.27	0.011	-19.05	5.98E-08	-3.19	0.013
PCB28 air	0.07	0.946	0.20	0.848	0.09	0.934	0.25	0.810
PCB28 sea	-2.22	0.058	-2.10	0.069	-2.95	0.018	-3.14	0.014
PCB28 soil	-12.53	1.55E-06	-14.74	4.42E-07	-46.69	4.89E-11	-1.56	0.158
PCB31 total	-9.56	1.19E-05	-2.39	0.044	-18.20	8.53E-08	-2.20	0.059
PCB31 air	0.31	0.766	0.27	0.793	0.27	0.792	0.30	0.775
PCB31 sea	-1.62	0.144	-1.62	0.143	-2.54	0.035	-2.82	0.023
PCB31 soil	-11.10	3.88E-06	-9.40	1.34E-05	-42.57	1.02E-10	0.95	0.371
PCB52 total	-12.98	1.18E-06	-4.37	0.002	-27.28	3.51E-09	-0.97	0.360
PCB52 air	0.23	0.821	0.06	0.952	0.20	0.845	0.14	0.895
PCB52 sea	-1.51	0.169	-2.17	0.061	-3.41	0.009	-5.07	9.68E-04
PCB52 soil	-14.48	5.06E-07	-10.16	7.56E-06	-38.00	2.53E-10	9.00	1.85E-05
PCB101 total	-48.24	3.77E-11	-1.86	0.099	-15.14	3.58E-07	6.36	2.19E-04
PCB101 air	-0.24	0.820	-0.67	0.520	0.04	0.970	0.01	0.992
PCB101 sea	-2.10	0.069	-2.80	0.023	-6.60	1.70E-04	-9.37	1.37E-05
PCB101 soil	-122.98	2.14E-14	18.89	6.39E-08	-10.59	5.54E-06	70.98	1.73E-12
PCB118 total	-42.70	9.97E-11	-2.81	0.023	-14.23	1.13E-06	5.37	6.73E-04
PCB118 air	-0.90	0.392	-1.16	0.281	-0.69	0.510	-0.45	0.662
PCB118 sea	-2.98	0.018	-3.01	0.017	-7.42	7.48E-05	-5.39	6.53E-04
PCB118 soil	-157.72	2.92E-15	9.33	1.42E-05	-6.55	1.79E-04	41.35	1.29E-10
PCB138 total	-36.68	3.35E-10	1.48	0.178	-4.63	5.79E-07	7.38	7.78E-05
PCB138 air	-1.27	0.241	-1.63	0.141	-0.74	0.482	-0.32	0.754
PCB138 sea	-2.18	0.061	-1.58	0.152	-8.49	2.84E-05	-12.01	2.13E-06
PCB138 soil	-26.39	4.57E-09	27.78	3.04E-09	7.64	6.08E-05	42.78	9.82E-11
PCB153 total	-41.40	1.28E-10	1.98	0.083	-10.49	0.002	14.21	5.86E-07
PCB153 air	-1.18	0.273	-1.70	0.127	-0.46	0.660	0.09	0.933
PCB153 sea	-3.53	0.008	-3.16	0.013	-7.73	5.57E-05	-5.46	6.00E-04
PCB153 soil	-21.52	2.29E-08	41.67	1.21E-10	2.18	0.060	37.13	3.04E-10

PCB180 total	-77.55	8.52E-13	2.30	0.051	-55.31	5.94E-06	11.63	2.73E-06
PCB180 air	-3.95	0.004	-3.08	0.015	-3.04	0.016	-1.41	0.197
PCB180 sea	-10.18	7.42E-06	-5.31	7.16E-04	-20.45	3.42E-08	-2.80	0.023
PCB180 soil	-9.47	1.27E-05	30.08	1.62E-09	-5.06	9.80E-04	25.10	6.78E-09
PCB194 total	-24.62	7.90E-09	5.92	3.53E-04	-29.68	1.27E-11	-0.00	0.996
PCB194 air	-7.49	7.02E-05	-3.70	0.006	-7.49	6.97E-05	-3.52	0.008
PCB194 sea	-83.94	4.53E-13	-4.87	0.001	-50.49	2.62E-11	-4.07	0.004
PCB194 soil	-7.68	5.87E-05	35.44	4.40E-10	-15.52	2.96E-07	13.28	9.89E-07

	'S' simulations			
	Whole domain T	Whole domain p	Arctic t	Arctic P
α -HCH total	-9.96	8.73E-06	-22.67	1.52E-08
α -HCH air	-7.14	9.77E-05	-3.81	0.005
α -HCH sea	-8.41	3.03E-05	-9.59	1.16E-05
α -HCH soil	-14.58	4.79E-07	-20.02	4.04E-08
β -HCH total	-15.22	3.44E-07	4.49	2.03E-03
β -HCH air	-0.14	0.891	0.68	0.518
β -HCH sea	-14.99	3.86E-07	17.94	9.55E-08
β -HCH soil	0.02	0.987	-10.28	6.89E-06
γ -HCH total	-2.81	0.023	-2.04	0.076
γ -HCH air	-4.89	0.001	-2.14	0.065
γ -HCH sea	-4.00	0.004	11.85	2.35E-06
γ -HCH soil	5.32	7.15E-04	-3.81	0.005
PCB8 total	9.47	1.27E-05	4.97	0.001
PCB8 air	-1.49	0.176	-1.70	0.128
PCB8 sea	3.54	0.008	4.720	0.002
PCB8 soil	3.53	0.008	-0.75	0.475
PCB28 total	0.43	0.675	-2.11	0.067
PCB28 air	-1.52	0.168	-1.59	0.151
PCB28 sea	4.49	0.002	4.94	0.001
PCB28 soil	-0.11	0.912	-4.39	0.002
PCB31 total	0.44	0.672	-2.32	0.049
PCB31 air	-1.53	0.164	-1.64	0.139
PCB31 sea	4.62	0.002	4.96	0.001
PCB31 soil	-0.05	0.958	-4.43	0.002
PCB52 total	-3.55	0.008	-6.60	1.70E-04
PCB52 air	-1.74	0.120	-1.73	0.121
PCB52 sea	6.98	1.15E-04	5.76	4.27E-04
PCB52 soil	-3.75	0.006	-10.43	6.17E-06
PCB101 total	-39.09	2.02E-10	-4.92	0.001
PCB101 air	-3.40	0.009	-3.30	0.011
PCB101 sea	2.57	0.033	1.53	0.165
PCB101 soil	-56.91	1.01E-11	-58.89	7.68E-12
PCB118 total	-34.58	5.35E-10	-5.08	0.001
PCB118 air	-3.79	0.005	-4.00	0.004
PCB118 sea	1.09	0.306	0.004	0.997
PCB118 soil	-59.11	7.45E-12	-27.67	3.14E-09

PCB138 total	-35.34	4.50E-10	-0.32	0.756
PCB138 air	-4.13	0.003	-3.53	0.008
PCB138 sea	1.29	0.235	1.06	0.318
PCB138 soil	-43.94	7.94E-11	-4.97	0.001
PCB153 total	-65.50	3.28E-12	-2.11	0.068
PCB153 air	-4.57	0.002	-4.26	0.003
PCB153 sea	-0.63	0.548	-1.10	0.303
PCB153 soil	-34.03	6.08E-10	-0.63	0.546
PCB180 total	-75.14	1.10E-12	-2.03	0.077
PCB180 air	-5.30	7.25E-04	-4.31	0.003
PCB180 sea	-2.70	0.027	-3.36	0.010
PCB180 soil	-13.00	1.16E-06	7.39	7.71E-05
PCB194 total	-9.66	1.10E-05	9.26	1.50E-05
PCB194 air	-5.67	4.72E-04	-2.55	0.034
PCB194 sea	-25.32	6.34E-09	-3.18	0.013
PCB194 soil	2.92	0.019	19.83	4.35E-08

Figures



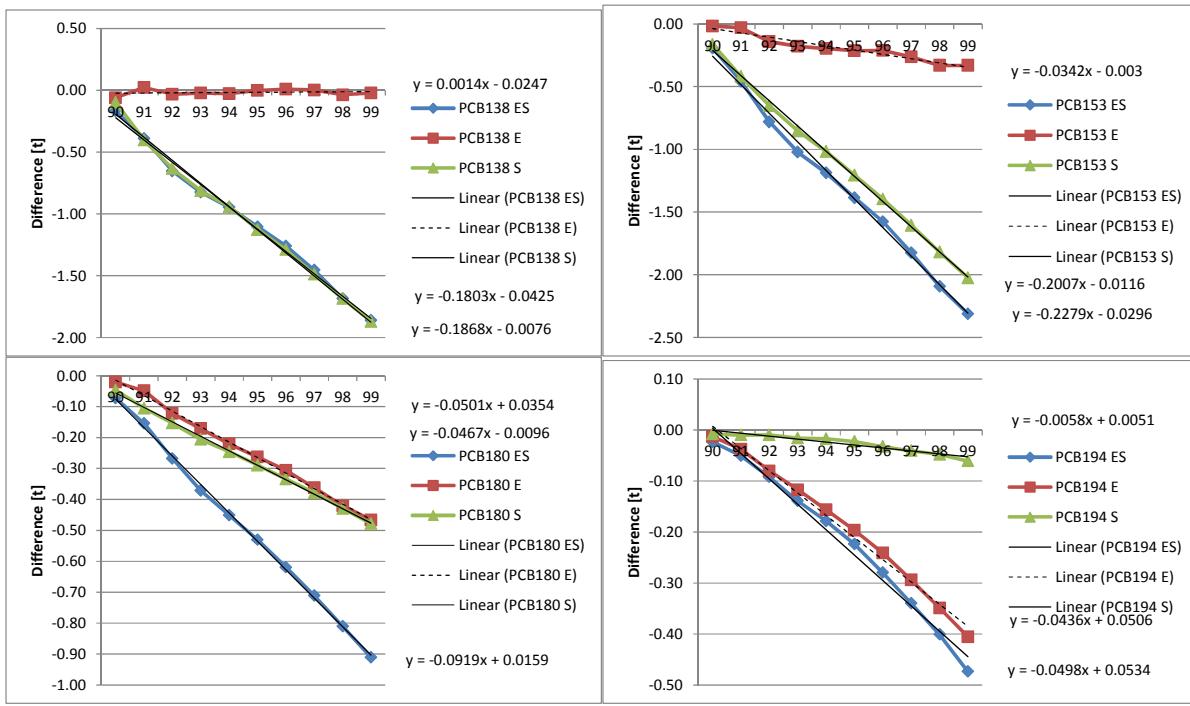
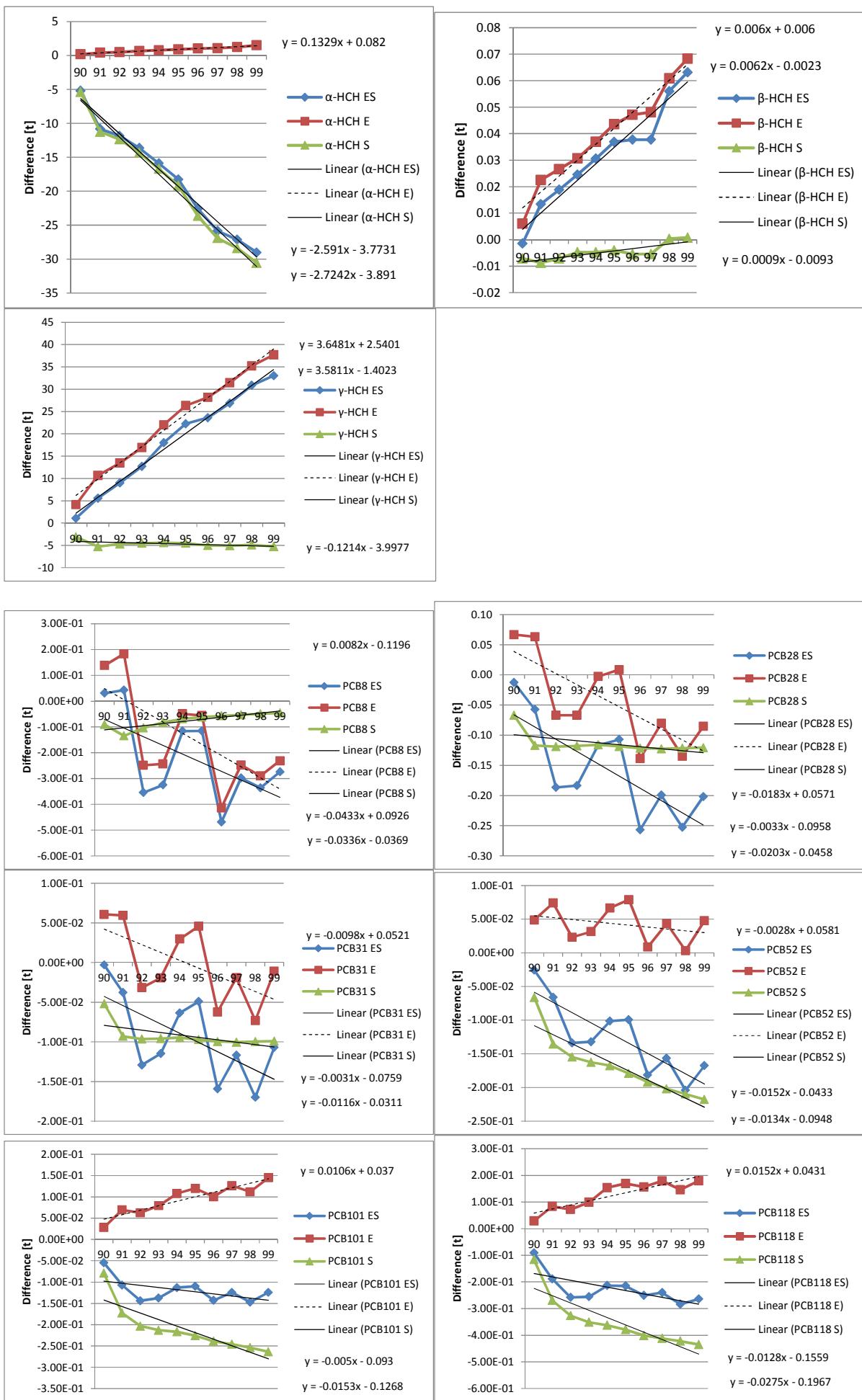


Figure S1. Difference in annual average mass in the entire model domain for the simulation with (blue diamonds) and without (red squares) initial environmental concentrations as well as fitted linear regressions.



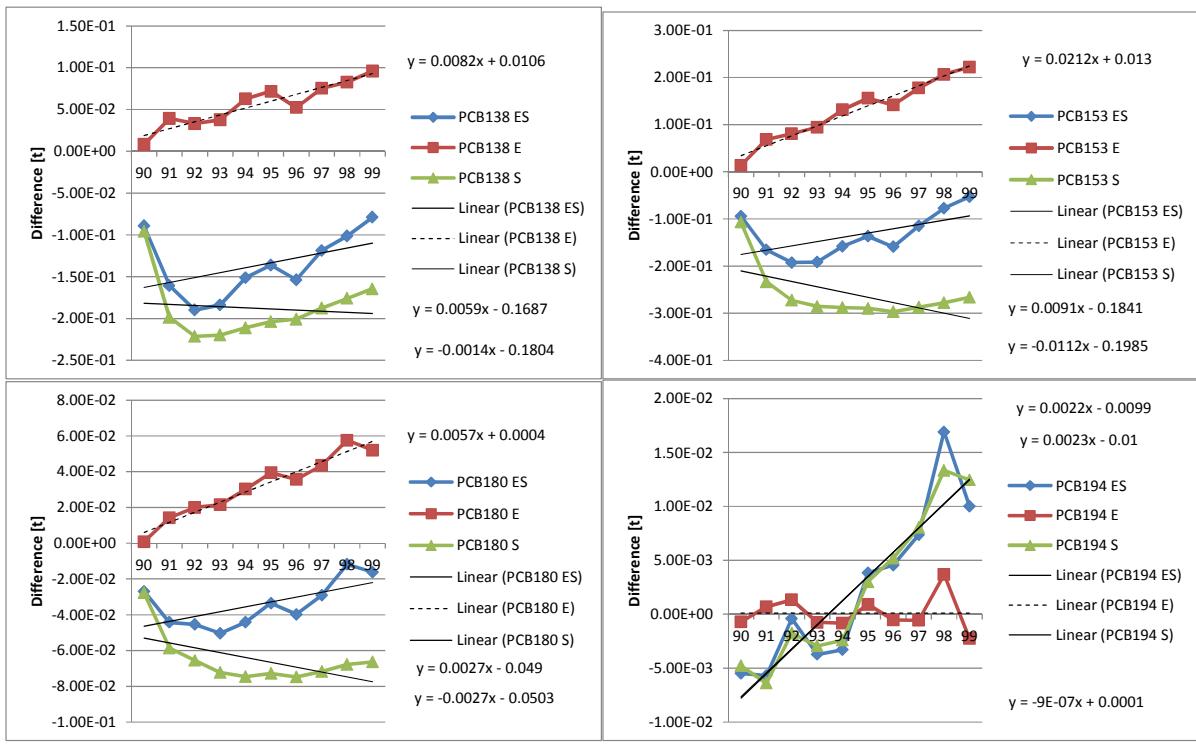
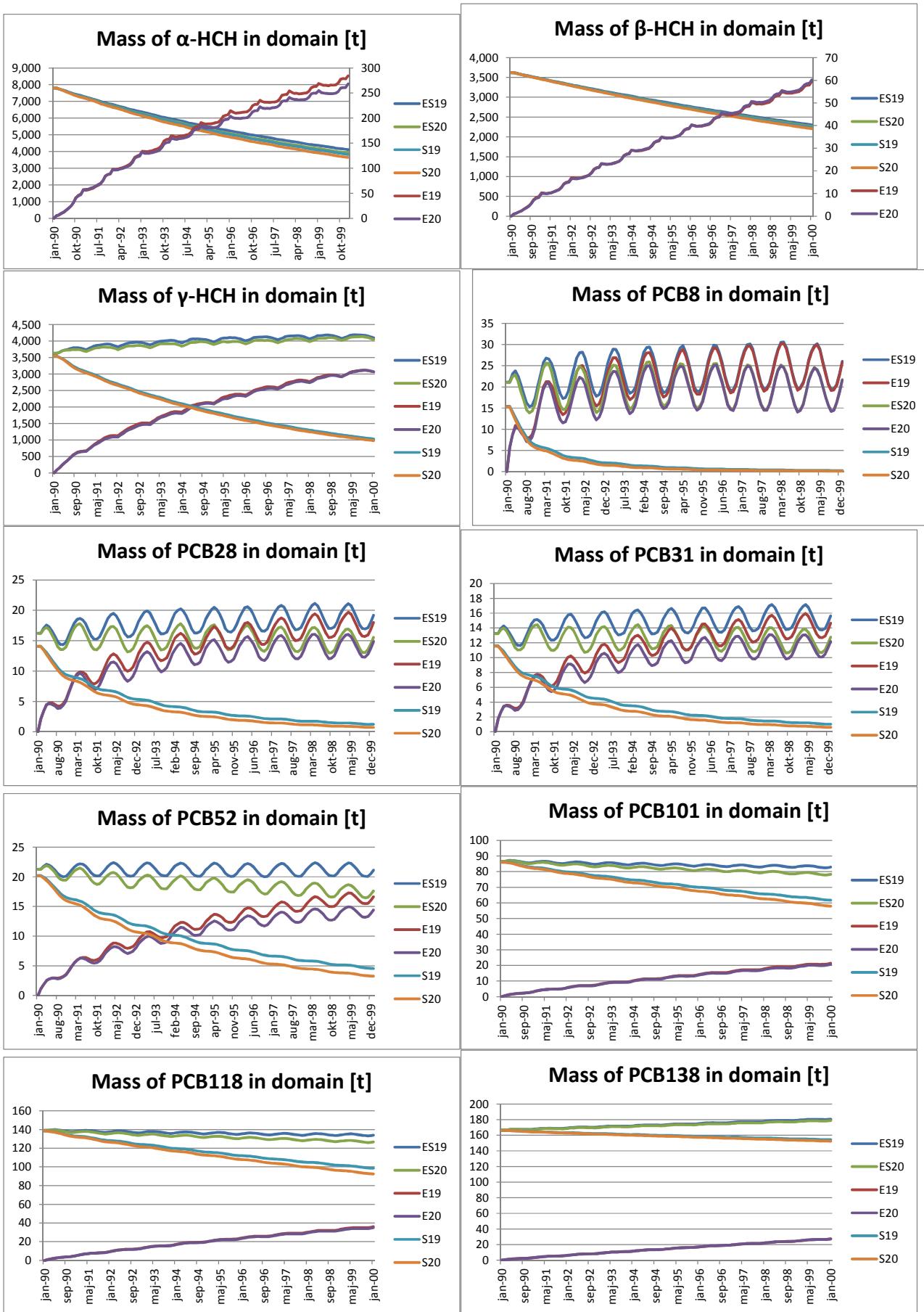


Figure S2. Difference in annual average mass in the Arctic for the simulation with (blue diamonds) and without (red squares) initial environmental concentrations as well as fitted linear regressions.



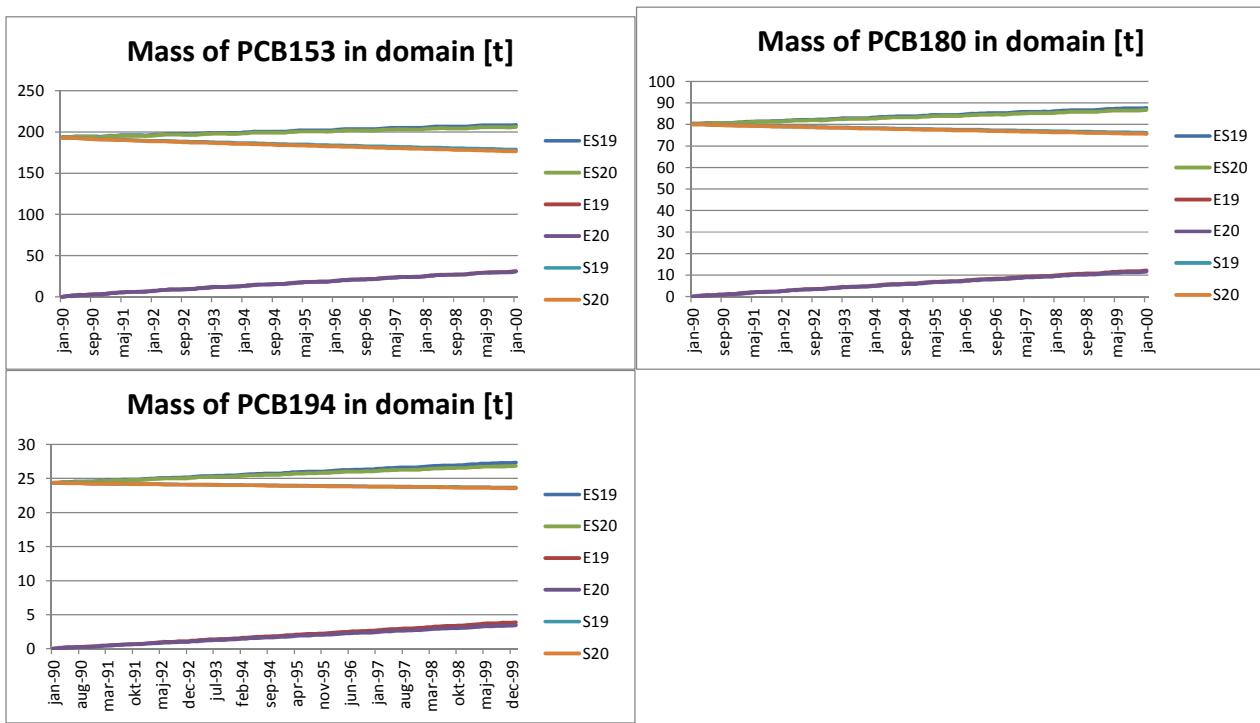
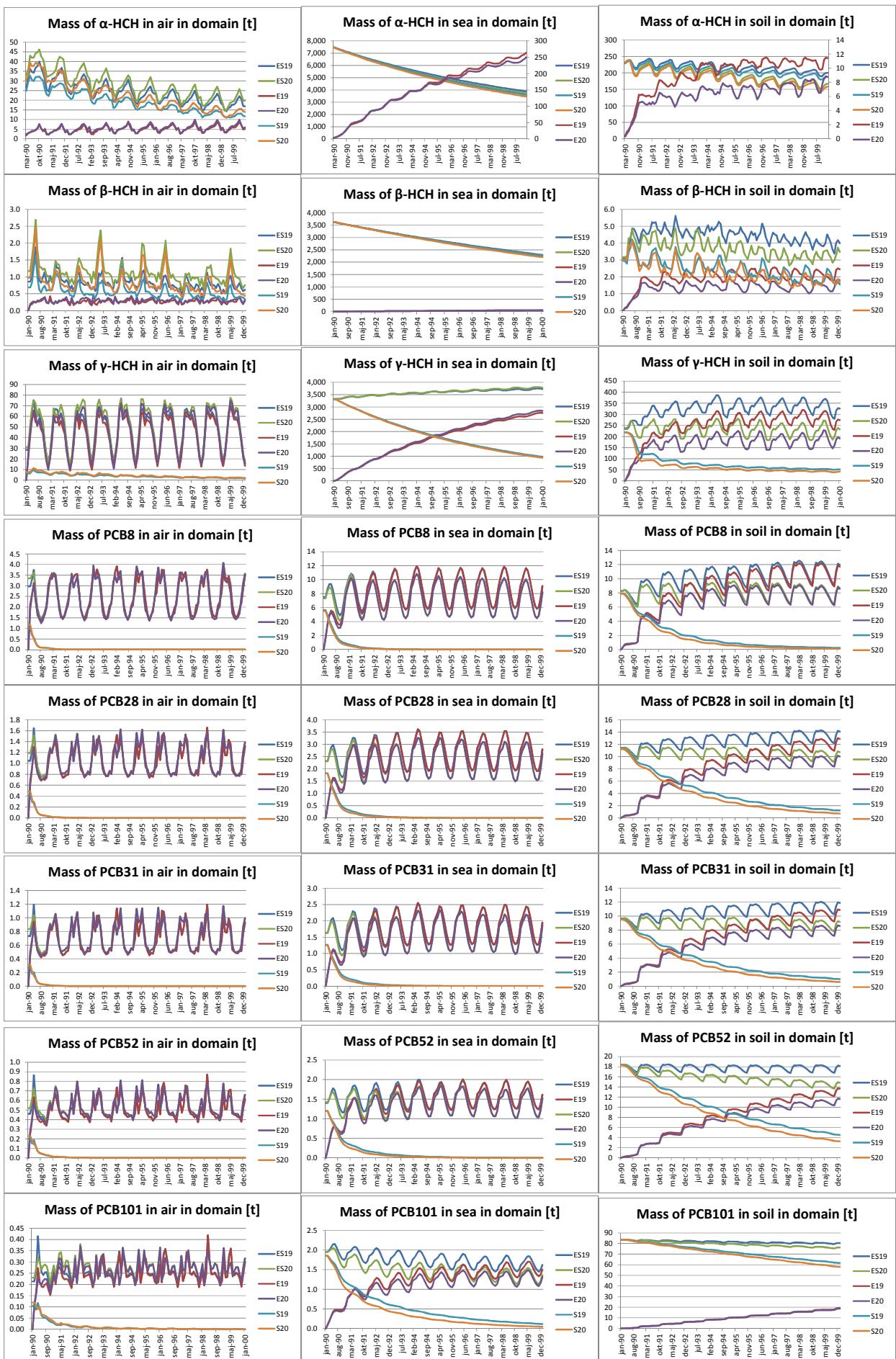


Figure S3. Monthly averaged total mass of all compounds in the model domain for the ‘ES19’ (blue), the ‘ES20’ (green), the ‘E19’ (red), the ‘E20’ (purple), the ‘S19’ (turquois), and the ‘S20’ (orange) simulations. Note that the masses of α -HCH and β -HCH for the simulation without initial environmental concentrations are plotted on the secondary axis.



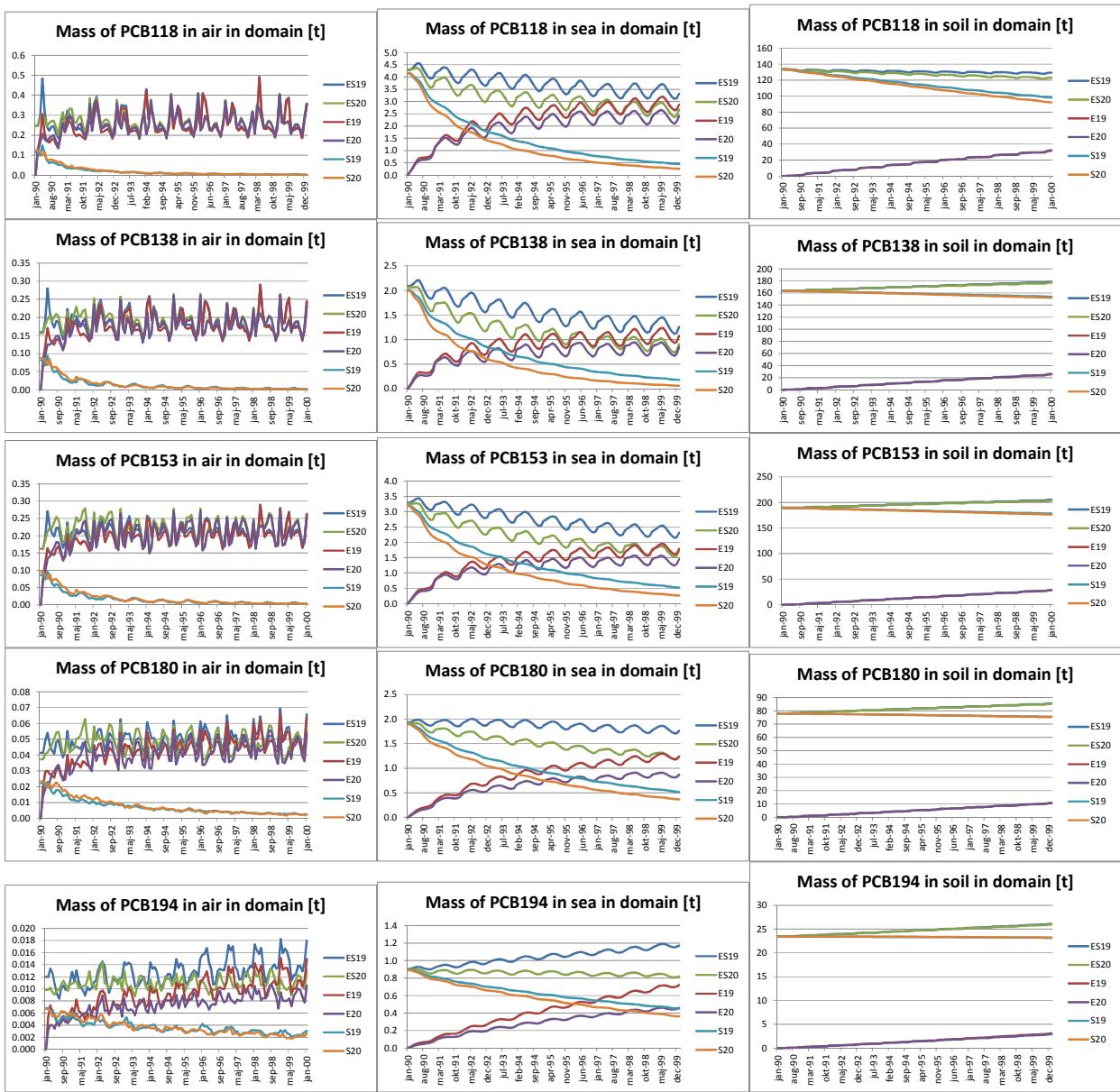


Figure S4. Monthly averaged mass in air (left column), sea water (middle column) and soil (right column) of all compounds in the entire model domain for the ‘ES19’ (blue), the ‘ES20’ (green), the ‘E19’ (red), the ‘E20’ (purple), the ‘S19’ (turquoise), and the ‘S20’ (orange) simulations. Note that the masses of α-HCH in sea water and soil are plotted on the secondary axis for the ‘E’ simulations.

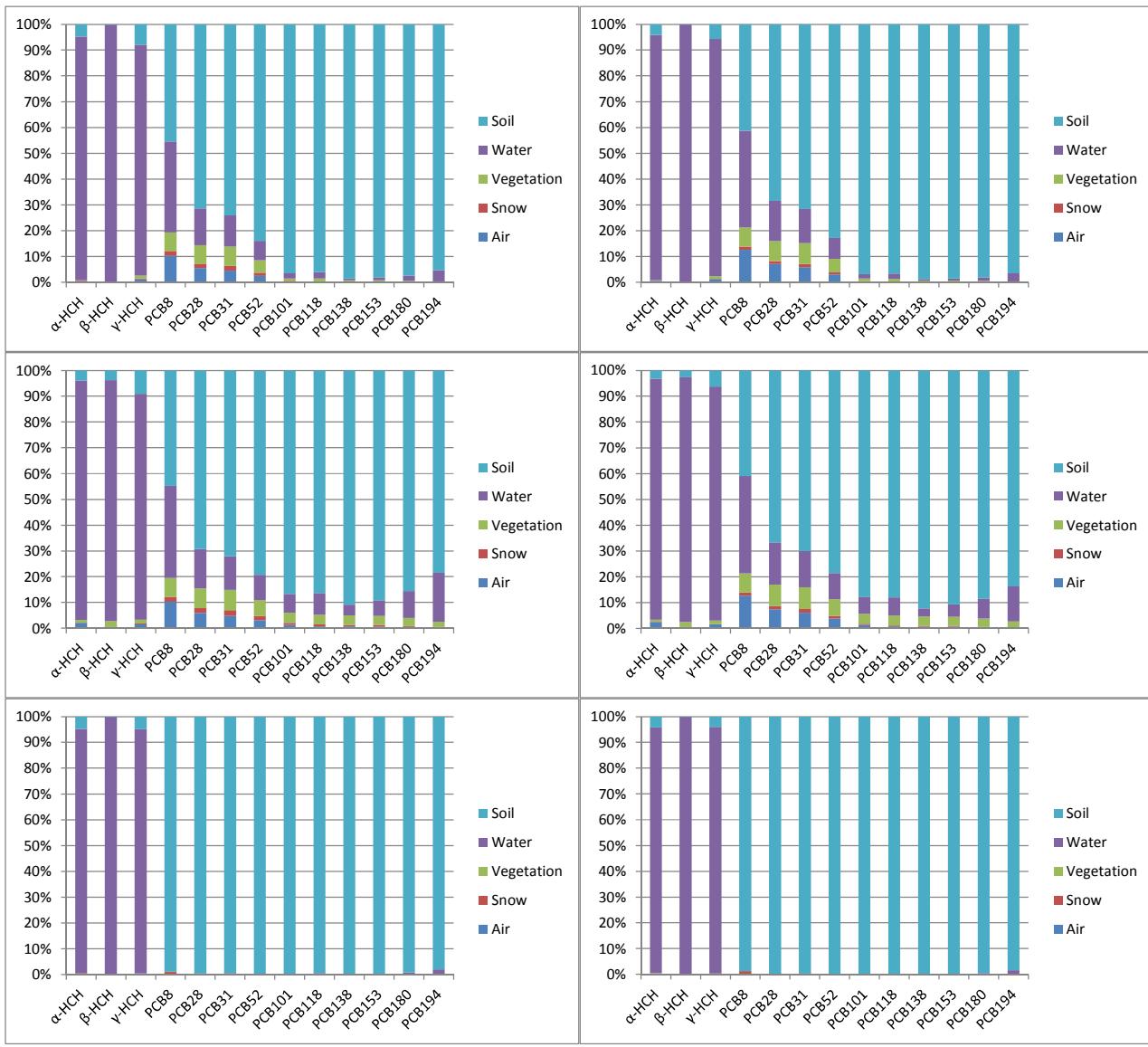


Figure S5. The distribution of the studied compounds between the five media in the entire model domain in the end of the 1990s (left column) and the 2000s (right column) for the ‘ES’ simulations (top row), the ‘E’ simulations (middle row), and the ‘S’ simulations (bottom row).

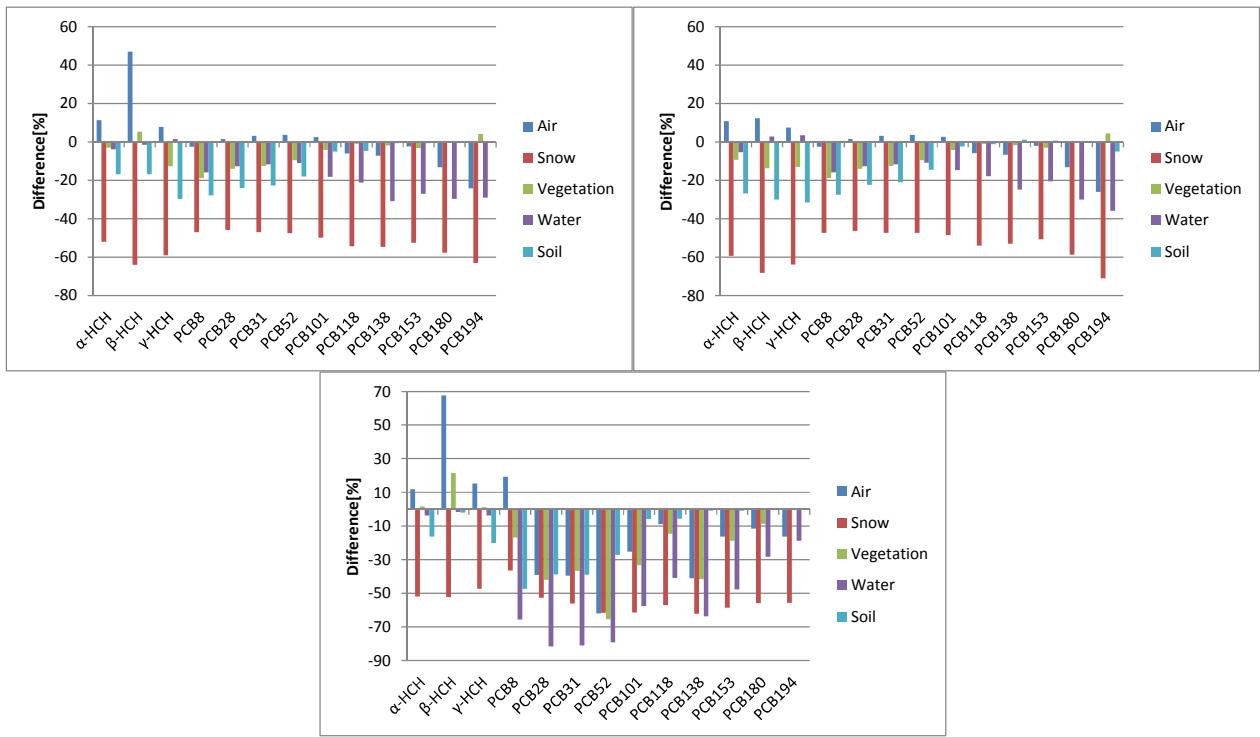
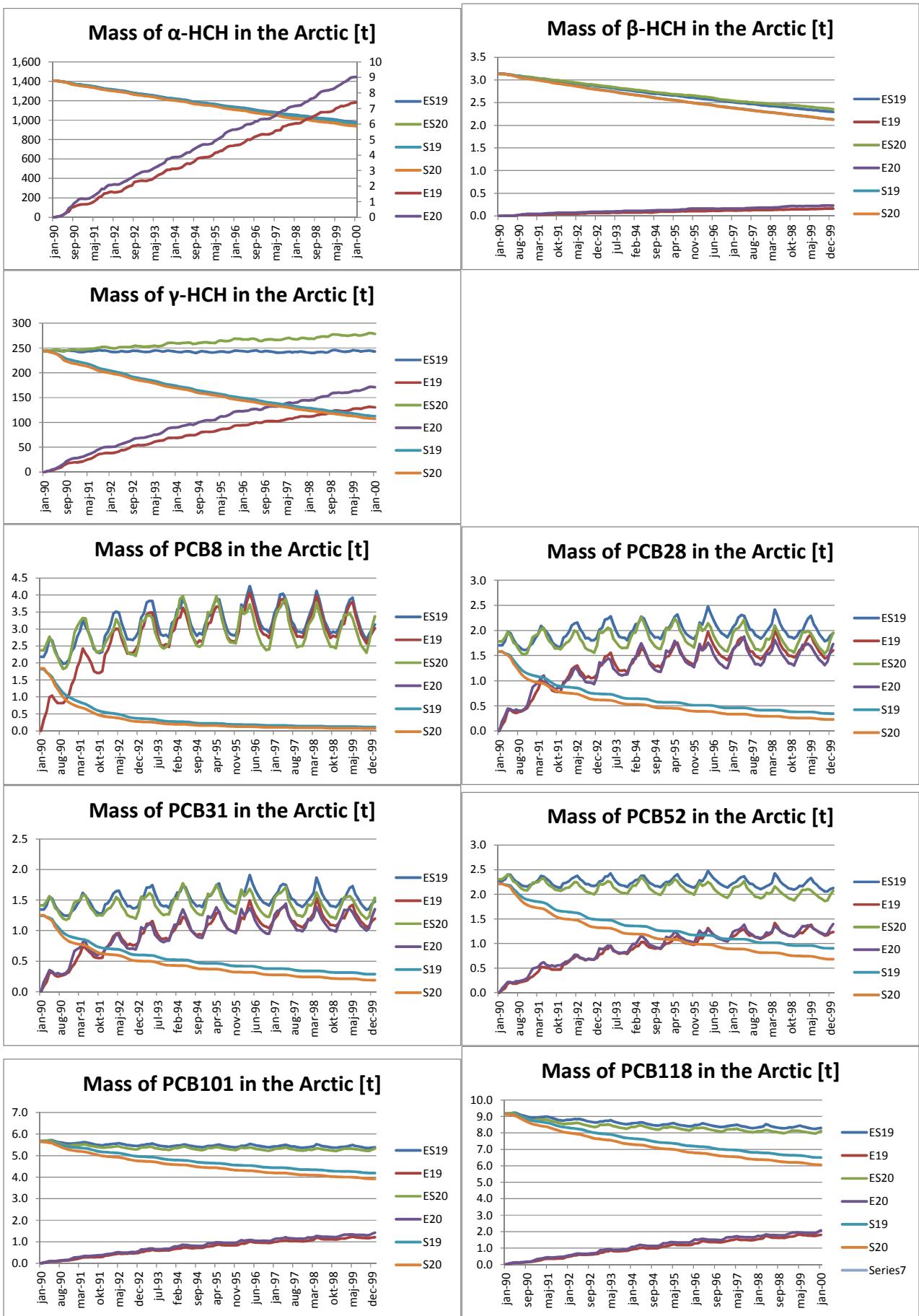


Figure S6. Relative differences in total mass in the five media within the model domain between the 1990s and the 2090s for the ‘ES’ simulation (top left), the ‘E’ simulation (top right), and the ‘S’ simulation (bottom).



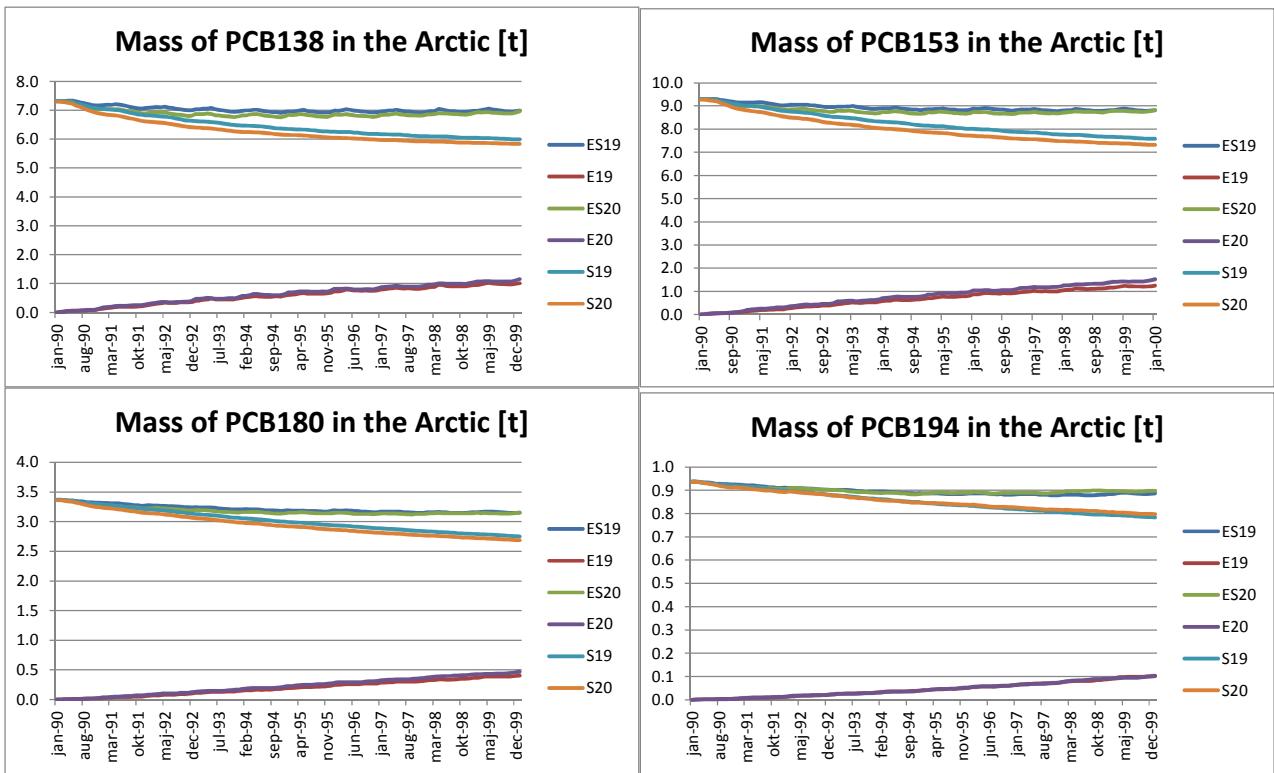
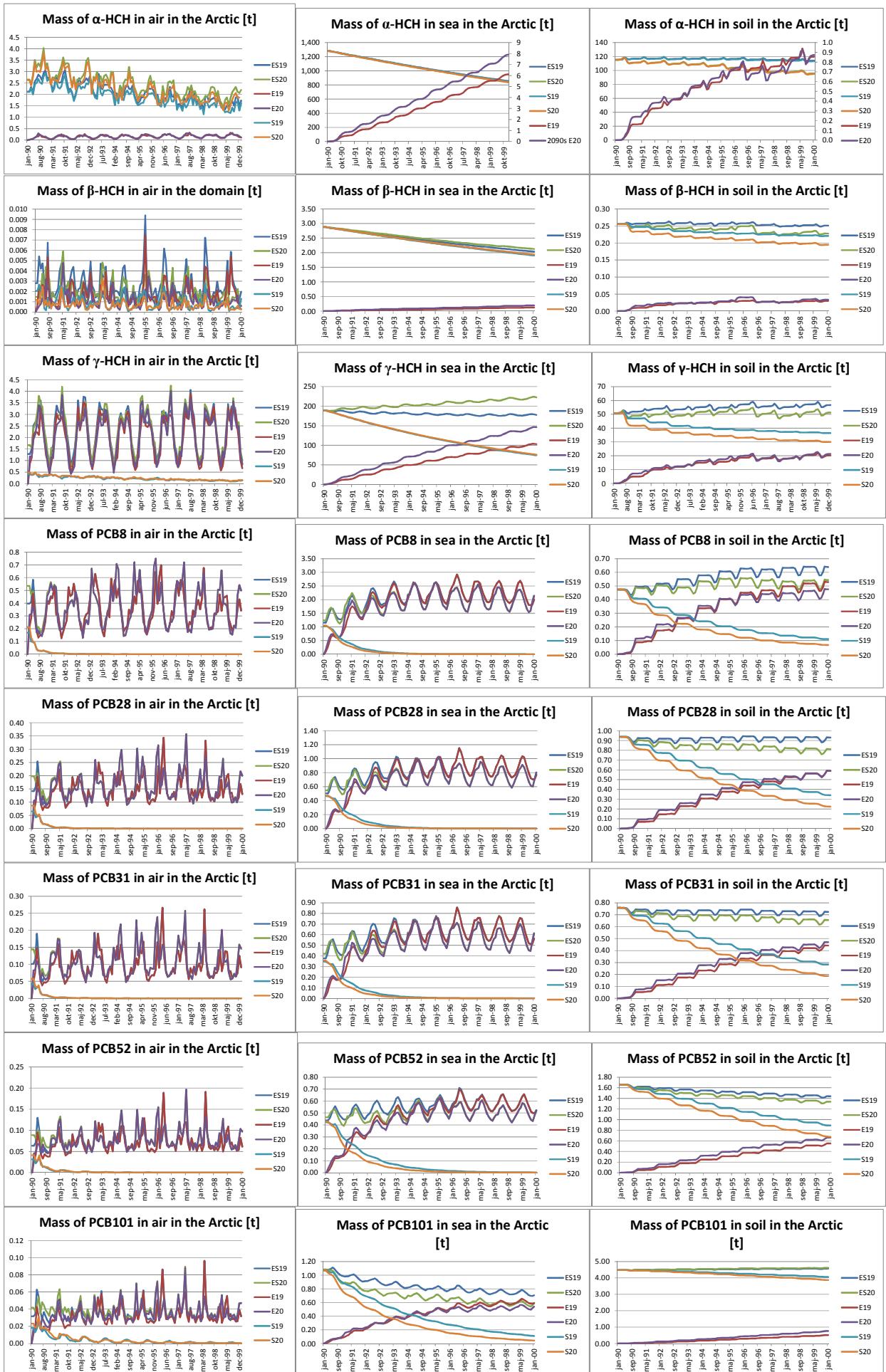


Figure S7. Monthly averaged total mass of all compounds in the Arctic (North of 66.5°N) for the ‘ES19’ (blue), the ‘ES20’ (green), the ‘E19’ (red), the ‘E20’ (purple), the ‘S19’ (turquois), and the ‘S20’ (orange) simulations. Note that the masses of α-HCH for the ‘E’ simulations are plotted on the secondary axis.



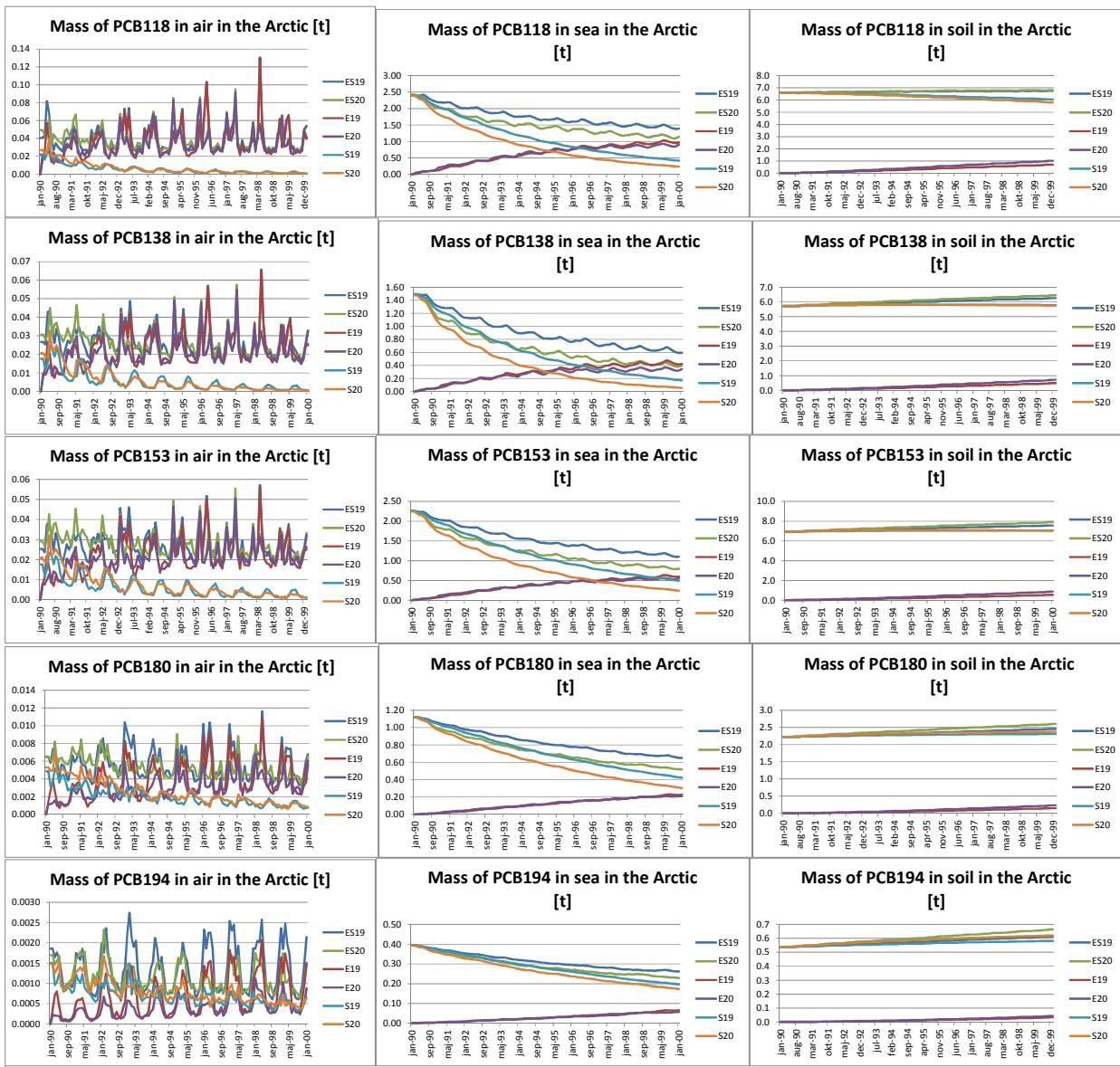


Figure S8. Monthly averaged mass in air (left column), sea water (middle column) and soil (right column) of all studied compounds in the Arctic (North of 66.5°N) for the ‘ES19’ (blue), the ‘ES20’ (green), the ‘E19’ (red), the ‘E20’ (purple), the ‘S19’ (turquoise), and the ‘S20’ (orange) simulations. Note that the masses of α -HCH in sea water and soil are plotted on the secondary axis for the ‘E’ simulations.

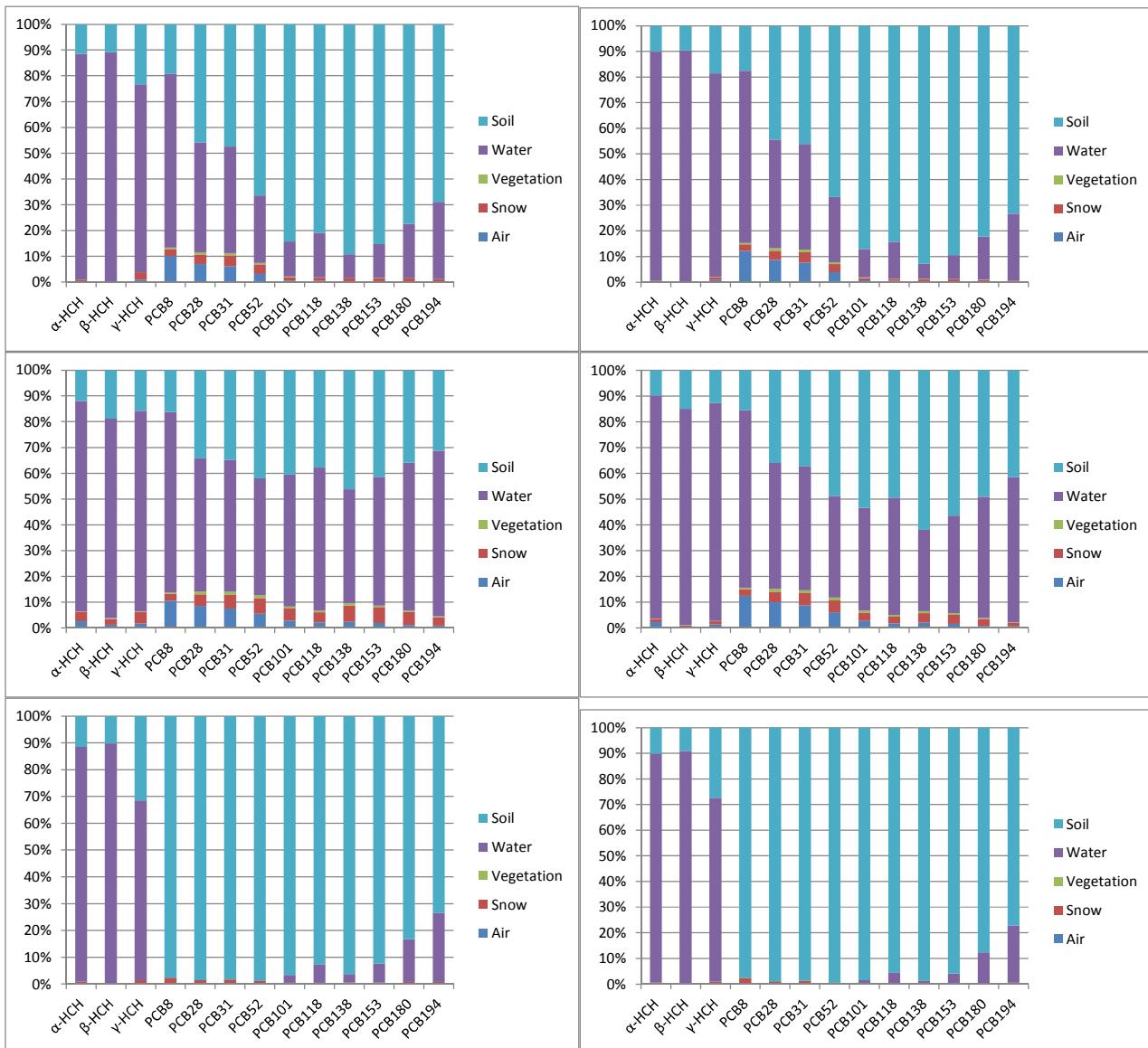


Figure S9. The distribution of the studied compounds between the five media in the Arctic (North of 66.5°N) in the end of the 1990s (left column) and 2090s (right column) for the ‘ES’ simulations (top row), the ‘E’ simulations (middle row) and the ‘S’ simulations (bottom row).

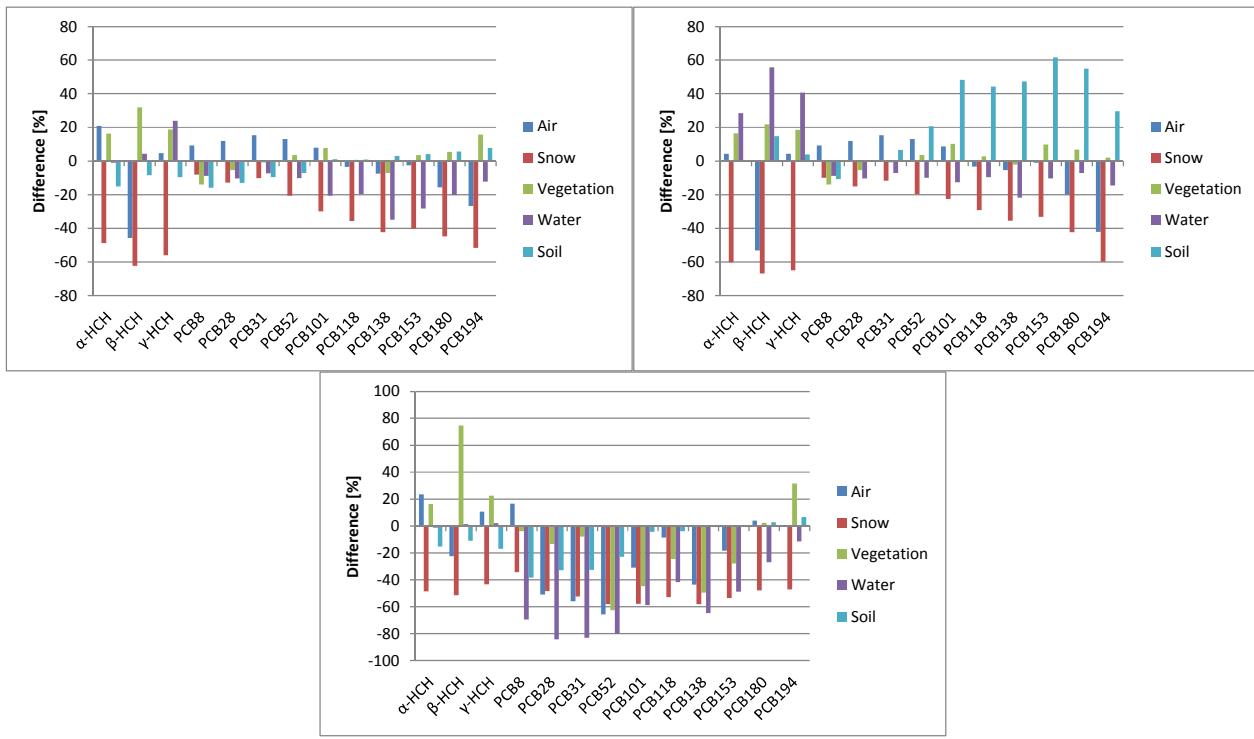


Figure S10. Relative differences in total mass in the five media within the Arctic domain (North of 66.5°N) between the 1990s and the 2090s for the ‘ES’ simulation (top left), the ‘E’ simulation (top right), and the ‘S’ simulation (bottom).