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Supplement of

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

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Tables

Table S1. 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
PCB008	7.35	-2.06	5.11	4.48E-10	13.72[b]	5500	4200
PCB028	7.86	-1.93	5.66	2.7E-10	13.72	10000	5500
PCB031	7.94	-1.87	5.78	1.4E-11	6.07	10000	5500
PCB052	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 S2. Total emissions of the studied compounds applied in all model simulations.

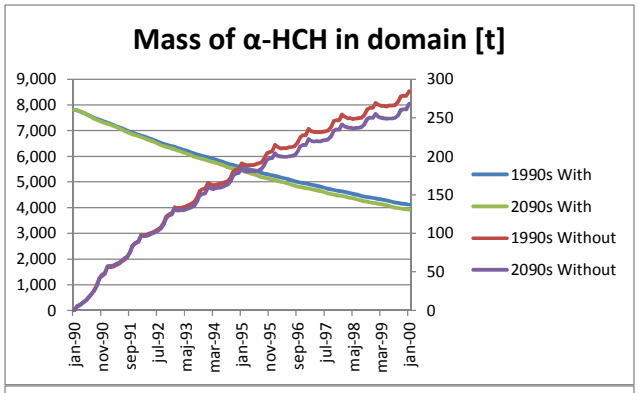
Compound	Emission [t]
α-HCH	1,149.5
β-HCH	191.6
γ-HCH	14,256.3
PCB008	796.7
PCB028	285.7
PCB031	231.9
PCB052	145.3
PCB101	74.7
PCB118	105.1
PCB138	68.9
PCB153	76.0
PCB180	23.7
PCB194	5.3

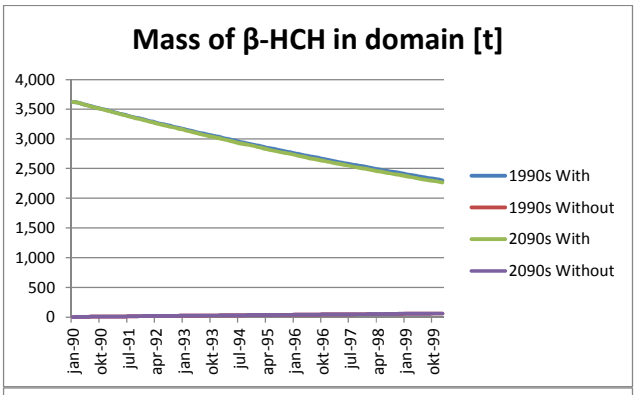
Table S3. t-values according to the Student's t-test and significance level (p). Bold phase show signifance levels lower than 0.01.

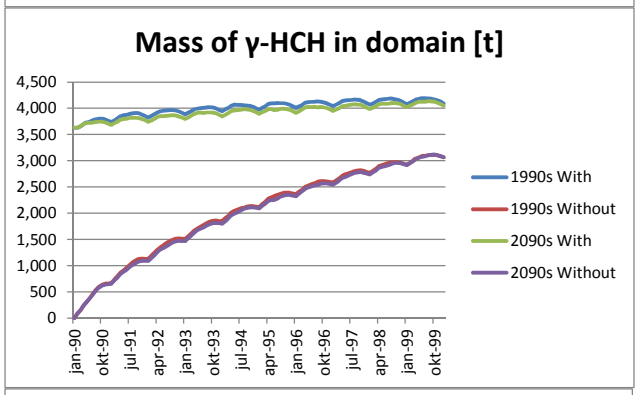
	With spin-up				**Without spin-up**			
	Whole domain t	Whole domain p	Arctic t	Arctic P	Whole domain t	Whole domain p	Arctic t	Arctic P
α-HCH total	-11.06	**3.99E-06**	-21.24	**2.54E-08**	-14.49	**5.03E-07**	21.57	**2.24E-08**
α-HCH air	-6.56	**1.77E-04**	-3.66	**0.006**	2.46	0.039	0.99	0.354
α-HCH sea	-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

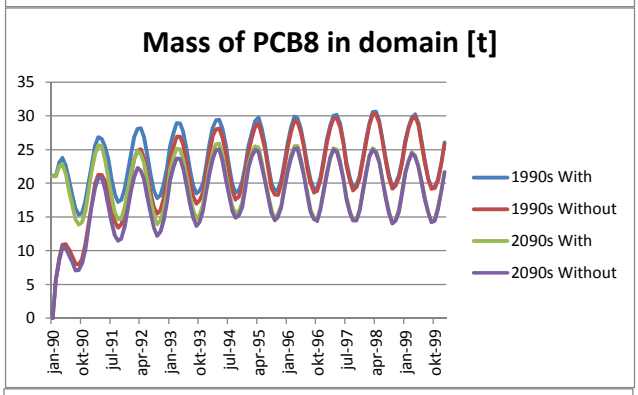
PCB31 air	0.31	0.766	0.27	0.793	0.27	0.792	0.30	0.775
PCB31 sea	-1.62	0.144	-1.62	0.143	-2.54	0.035	-2.82	0.023
PCB31 soil	-11.10	**3.88E-06**	-9.40	**1.34E-05**	-42.57	**1.02E-10**	0.95	0.371
PCB52 total	-12.98	**1.18E-06**	-4.37	**0.002**	-27.28	**3.51E-09**	-0.97	0.360
PCB52 air	0.23	0.821	0.06	0.952	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**

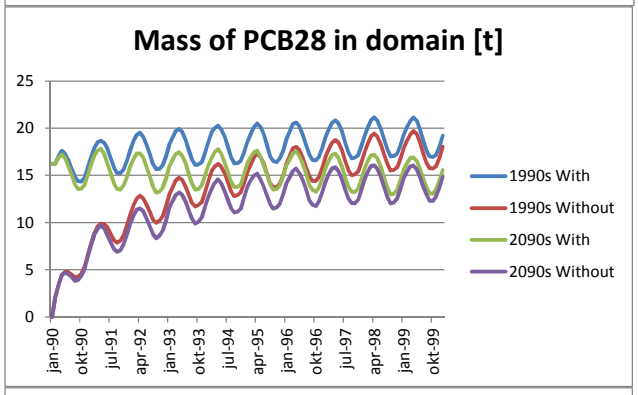
Figures

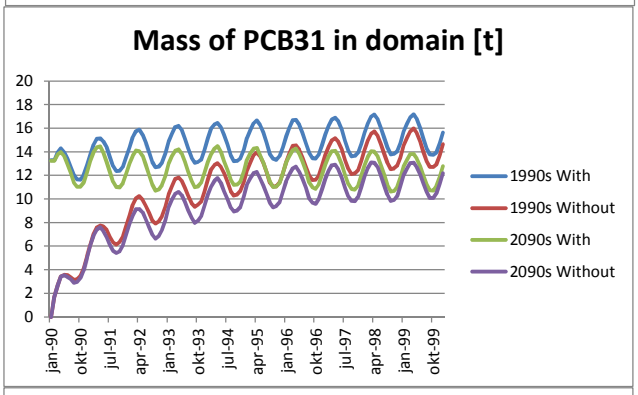

Mass of α-HCH in domain [t]
9,000
8,000
7,000
6,000
5,000
4,000
3,000
2,000
1,000
0
300
250
200
150
100
50
0
jan-90
nov-90
sep-91
jul-92
maj-93
mar-94
jan-95
nov-95
sep-96
jul-97
maj-98
mar-99
jan-00
1990s With
2090s With
1990s Without
2090s Without

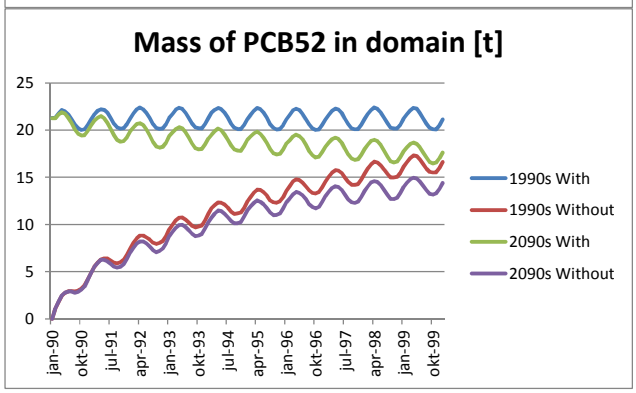

Mass of β-HCH in domain [t]
4,000
3,500
3,000
2,500
2,000
1,500
1,000
500
0
jan-90
okt-90
jul-91
apr-92
jan-93
okt-93
jul-94
apr-95
jan-96
okt-96
jul-97
apr-98
jan-99
okt-99
1990s With
1990s Without
2090s With
2090s Without

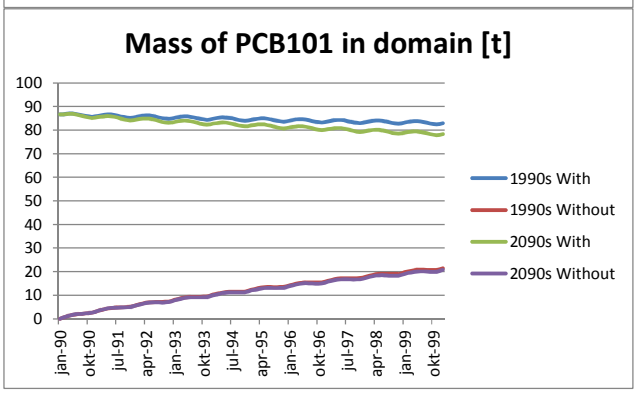

Mass of γ-HCH in domain [t]
4,500
4,000
3,500
3,000
2,500
2,000
1,500
1,000
500
0
jan-90
okt-90
jul-91
apr-92
jan-93
okt-93
jul-94
apr-95
jan-96
okt-96
jul-97
apr-98
jan-99
okt-99
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB8 in domain [t]
35
30
25
20
15
10
5
0
jan-90
okt-90
jul-91
apr-92
jan-93
okt-93
jul-94
apr-95
jan-96
okt-96
jul-97
apr-98
jan-99
okt-99
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB28 in domain [t]
25
20
15
10
5
0
jan-90
okt-90
jul-91
apr-92
jan-93
okt-93
jul-94
apr-95
jan-96
okt-96
jul-97
apr-98
jan-99
okt-99
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB31 in domain [t]
20
18
16
14
12
10
8
6
4
2
0
jan-90
okt-90
jul-91
apr-92
jan-93
okt-93
jul-94
apr-95
jan-96
okt-96
jul-97
apr-98
jan-99
okt-99
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB52 in domain [t]
25
20
15
10
5
0
jan-90
okt-90
jul-91
apr-92
jan-93
okt-93
jul-94
apr-95
jan-96
okt-96
jul-97
apr-98
jan-99
okt-99
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB101 in domain [t]
100
90
80
70
60
50
40
30
20
10
0
jan-90
okt-90
jul-91
apr-92
jan-93
okt-93
jul-94
apr-95
jan-96
okt-96
jul-97
apr-98
jan-99
okt-99
1990s With
1990s Without
2090s With
2090s Without

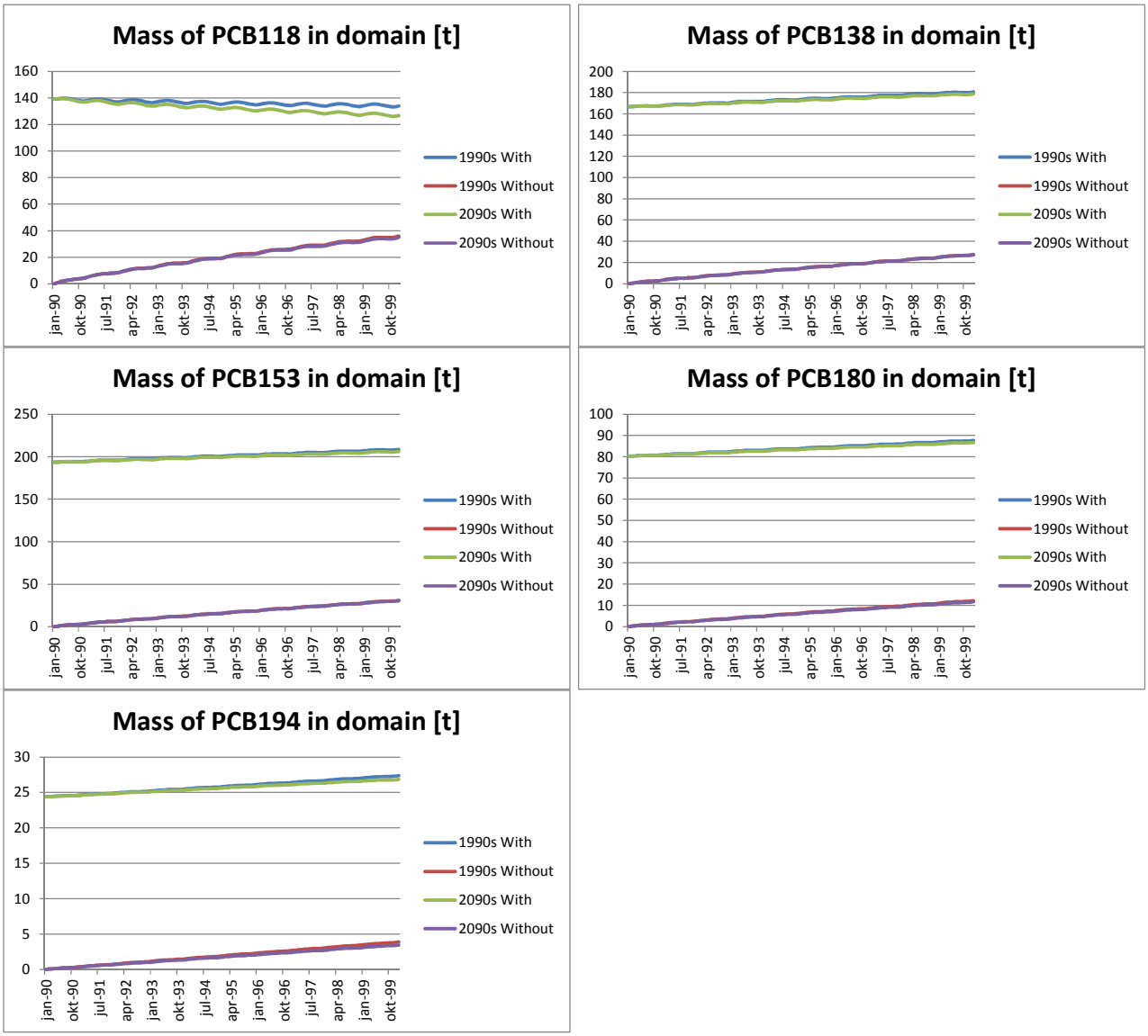
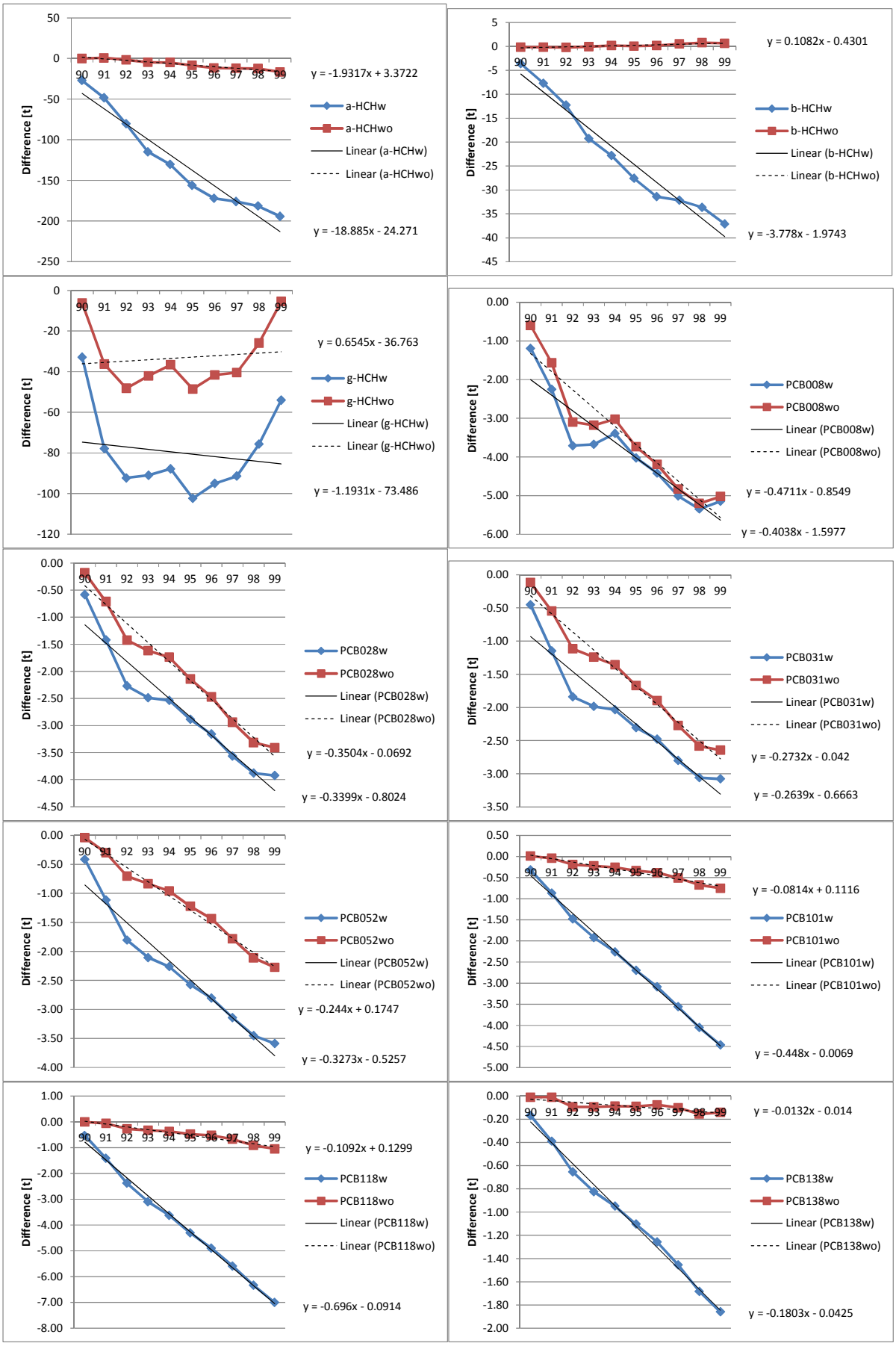


Figure S1. Monthly averaged total mass of all compounds in the model domain for the 'W19' (blue), the 'W20' (green), the 'WO19' (red) and the 'WO20' (purple) simulations. Note that the masses of α-HCH for the simulation without initial environmental concentrations are plotted on the secondary axis.


Difference [t]
y = -1.9317x + 3.3722
a-HCHw
a-HCHwo
Linear (a-HCHw)
Linear (a-HCHwo)
y = -18.885x - 24.271
y = 0.1082x - 0.4301
b-HCHw
b-HCHwo
Linear (b-HCHw)
Linear (b-HCHwo)
y = -3.778x - 1.9743
y = 0.6545x - 36.763
g-HCHw
g-HCHwo
Linear (g-HCHw)
Linear (g-HCHwo)
y = -1.1931x - 73.486
PCB008w
PCB008wo
Linear (PCB008w)
Linear (PCB008wo)
y = -0.4711x - 0.8549
y = -0.4038x - 1.5977
PCB028w
PCB028wo
Linear (PCB028w)
Linear (PCB028wo)
y = -0.3504x - 0.0692
y = -0.3399x - 0.8024
PCB031w
PCB031wo
Linear (PCB031w)
Linear (PCB031wo)
y = -0.2732x - 0.042
y = -0.2639x - 0.6663
PCB052w
PCB052wo
Linear (PCB052w)
Linear (PCB052wo)
y = -0.244x + 0.1747
y = -0.3273x - 0.5257
y = -0.0814x + 0.1116
PCB101w
PCB101wo
Linear (PCB101w)
Linear (PCB101wo)
y = -0.448x - 0.0069
y = -0.1092x + 0.1299
PCB118w
PCB118wo
Linear (PCB118w)
Linear (PCB118wo)
y = -0.696x - 0.0914
y = -0.0132x - 0.014
PCB138w
PCB138wo
Linear (PCB138w)
Linear (PCB138wo)
y = -0.1803x - 0.0425

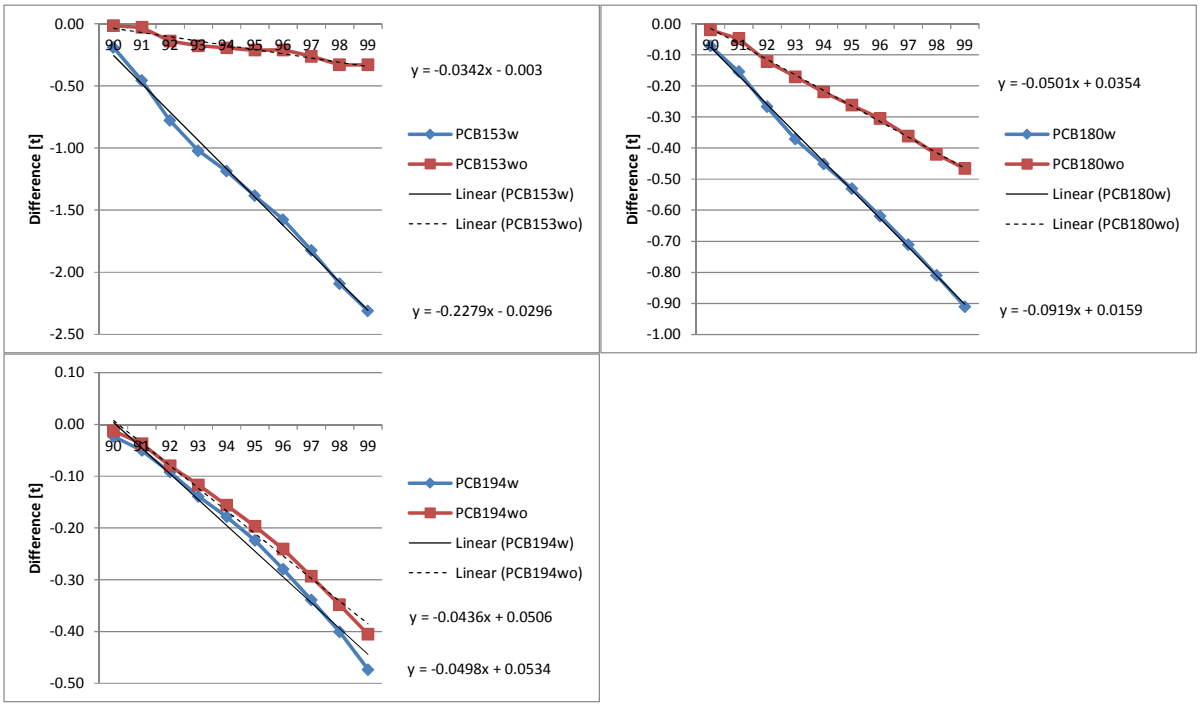
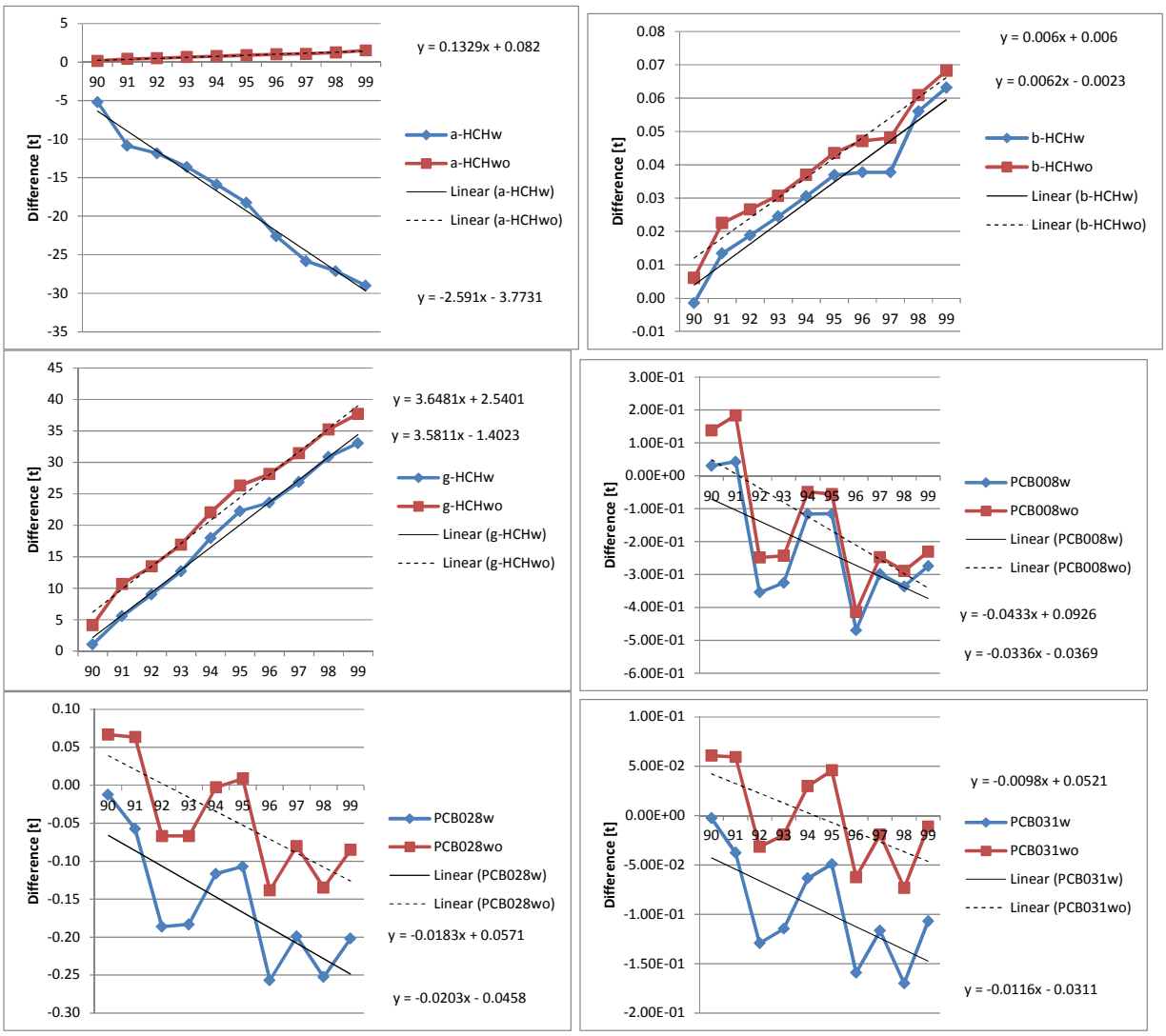


Figure S2. Difference in annual average mass in the entire model domain for the simulation with (blue diamonds) and without (red squares) initial environmental concentrations as well as fitted linear regressions.



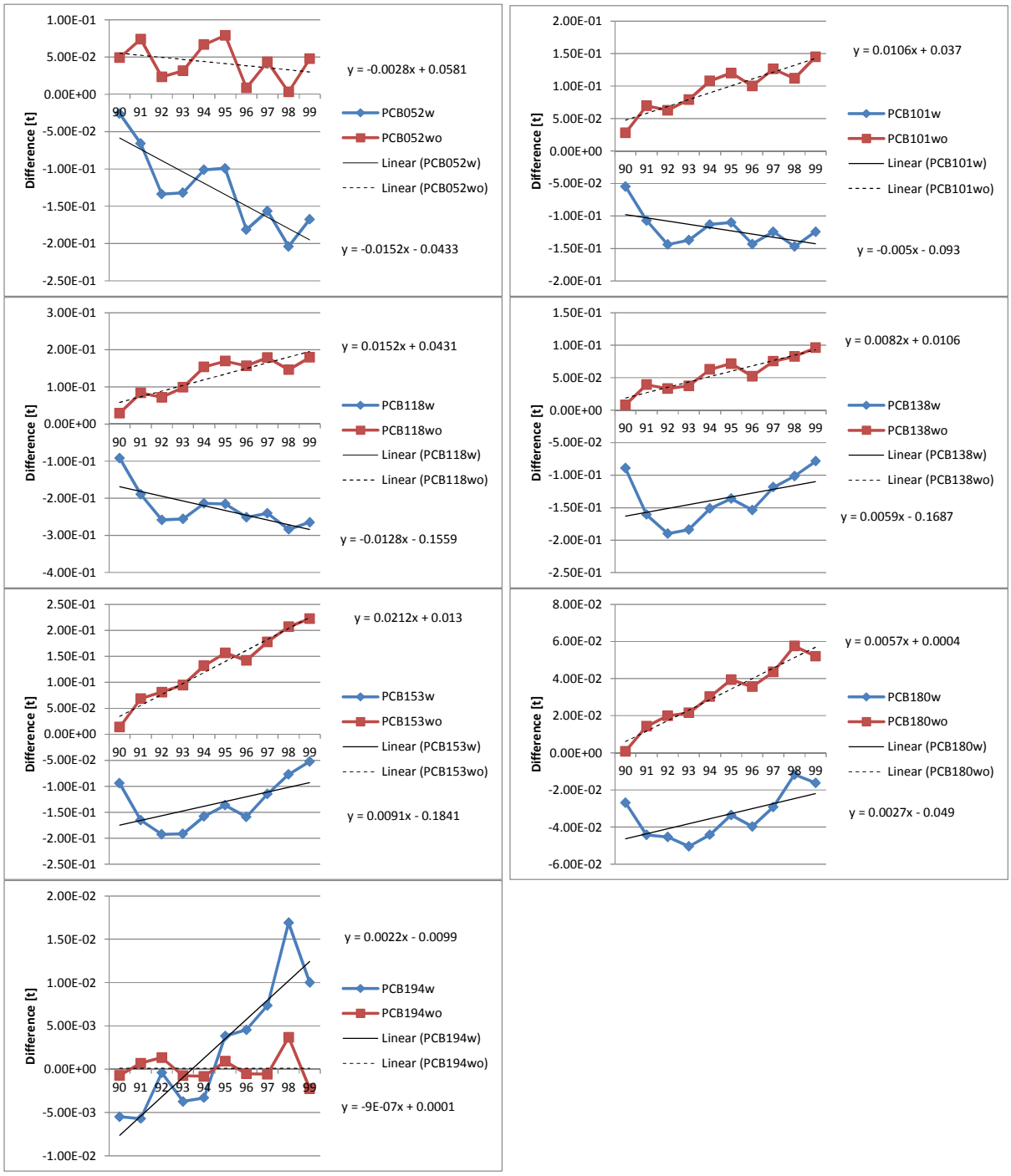


Figure S3. Difference in annual average mass in the Arctic for the simulation with (blue diamonds) and without (red squares) initial environmental concentrations as well as fitted linear regressions.

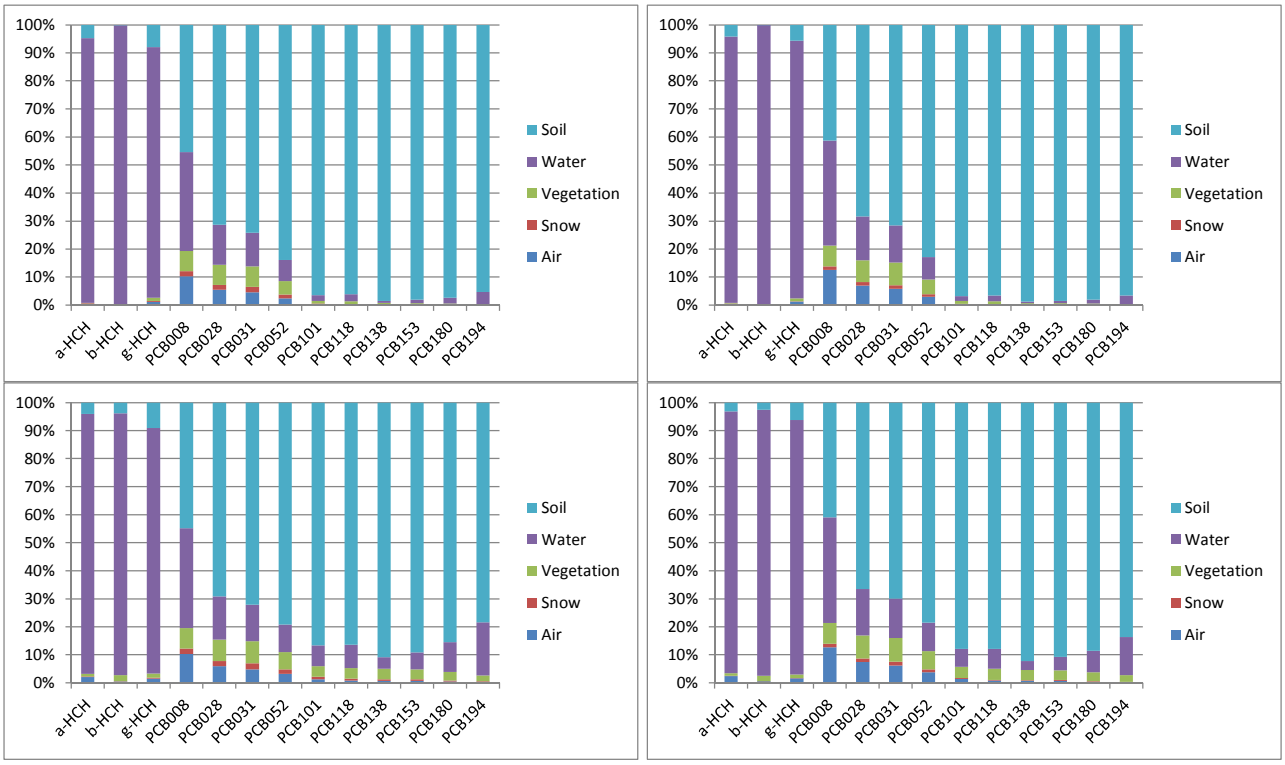


Figure S4. The distribution of the studied compounds between the five media in the entire model domain in the end of the 1990s (left column) and the 2090s (right column) for the simulations with (top row) and without (bottom row) initial environmental concentrations.

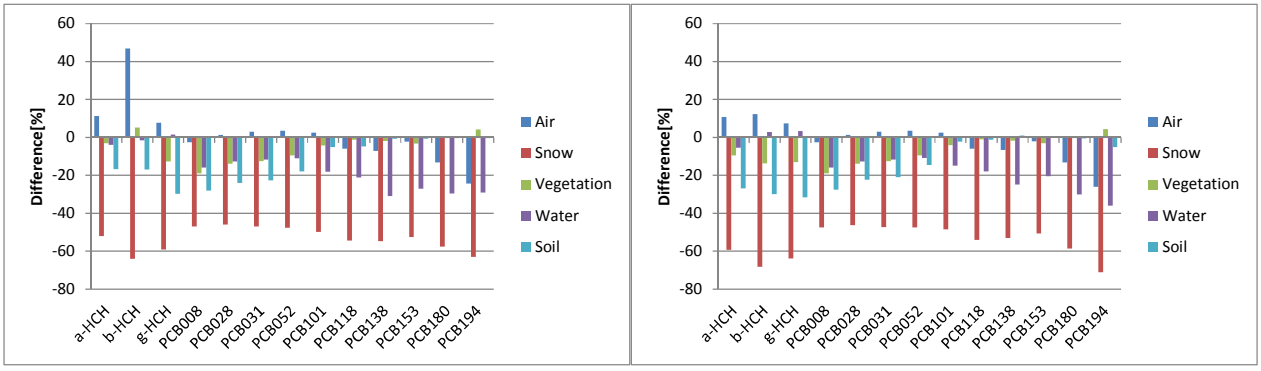
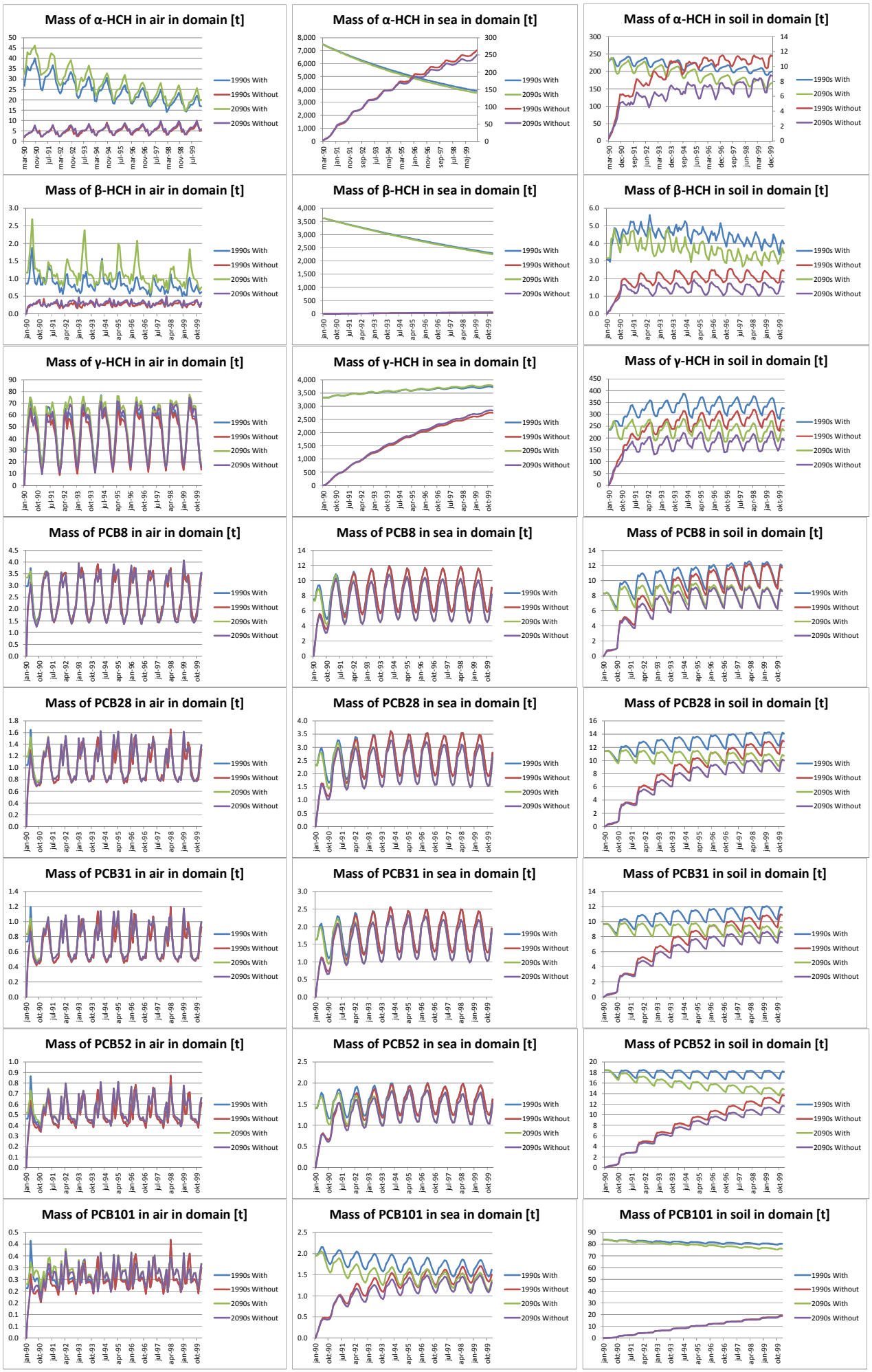


Figure S5. Relative differences in total mass in the five media within the model domain between the 1990s and the 2090s for the simulation with (left) and without (right) initial environmental concentrations.


Mass of α-HCH in air in domain [t]
Mass of α-HCH in sea in domain [t]
Mass of α-HCH in soil in domain [t]
Mass of β-HCH in air in domain [t]
Mass of β-HCH in sea in domain [t]
Mass of β-HCH in soil in domain [t]
Mass of γ-HCH in air in domain [t]
Mass of γ-HCH in sea in domain [t]
Mass of γ-HCH in soil in domain [t]
Mass of PCB8 in air in domain [t]
Mass of PCB8 in sea in domain [t]
Mass of PCB8 in soil in domain [t]
Mass of PCB28 in air in domain [t]
Mass of PCB28 in sea in domain [t]
Mass of PCB28 in soil in domain [t]
Mass of PCB31 in air in domain [t]
Mass of PCB31 in sea in domain [t]
Mass of PCB31 in soil in domain [t]
Mass of PCB52 in air in domain [t]
Mass of PCB52 in sea in domain [t]
Mass of PCB52 in soil in domain [t]
Mass of PCB101 in air in domain [t]
Mass of PCB101 in sea in domain [t]
Mass of PCB101 in soil in domain [t]
1990s With
1990s Without
2090s With
2090s Without

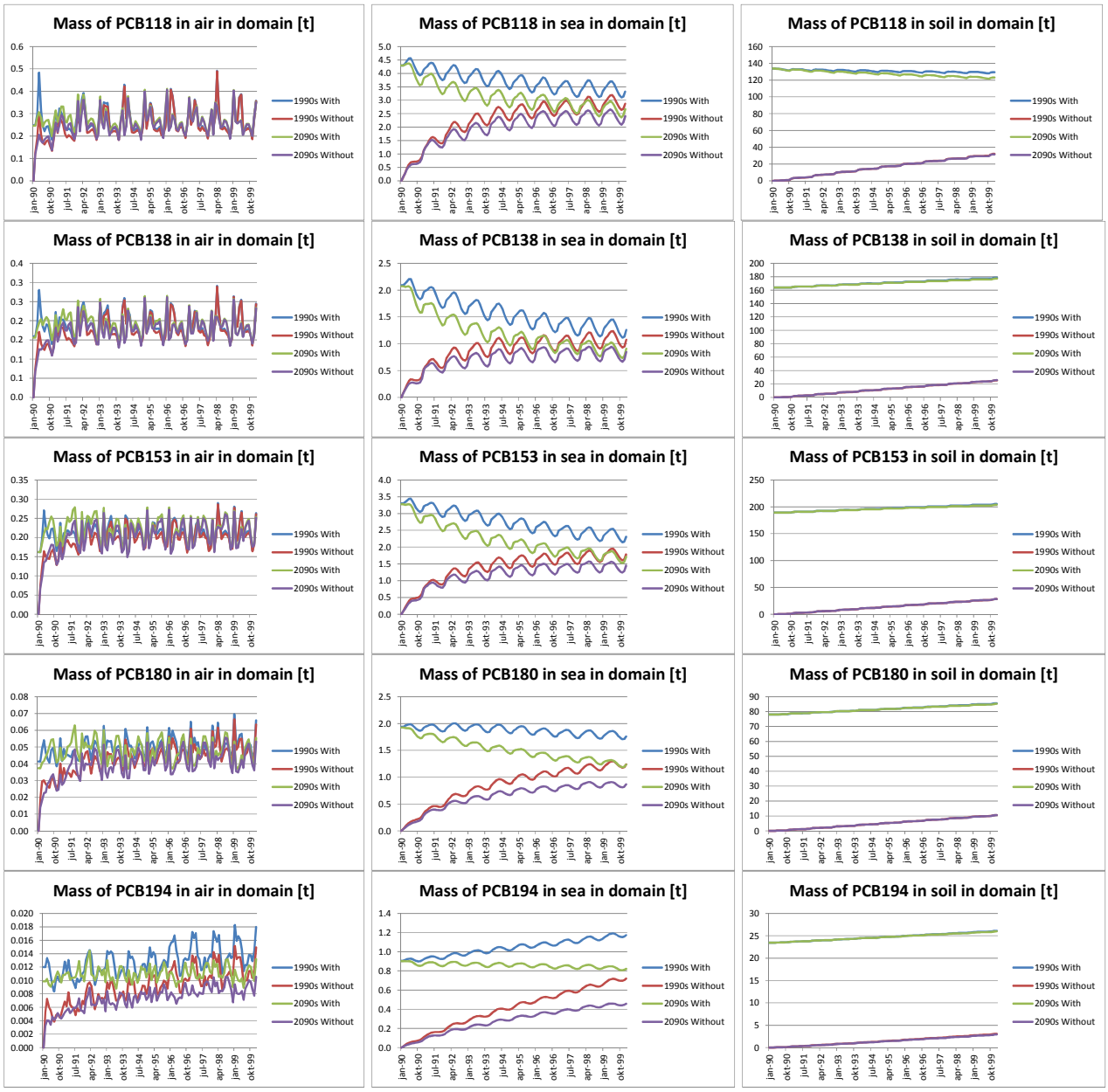
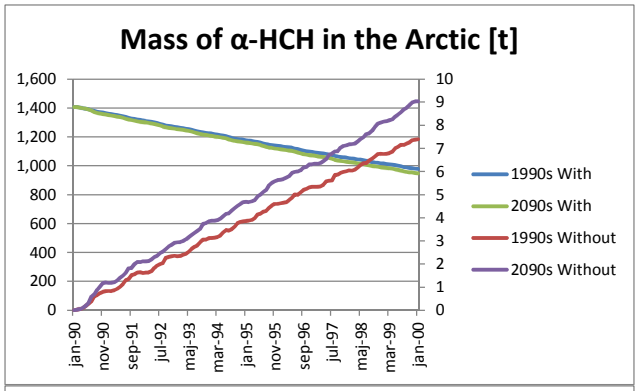
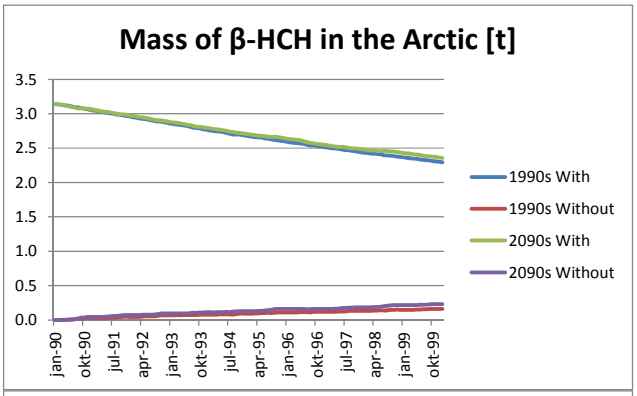
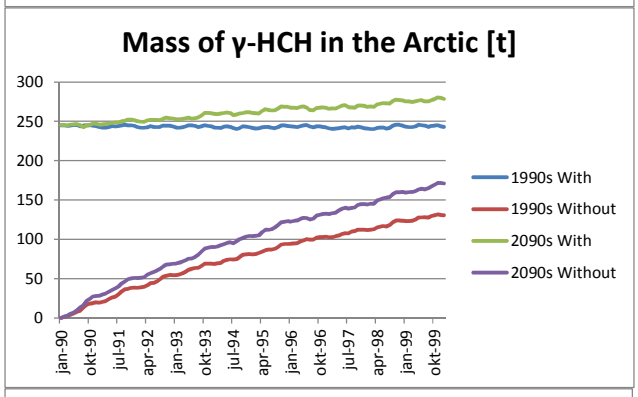
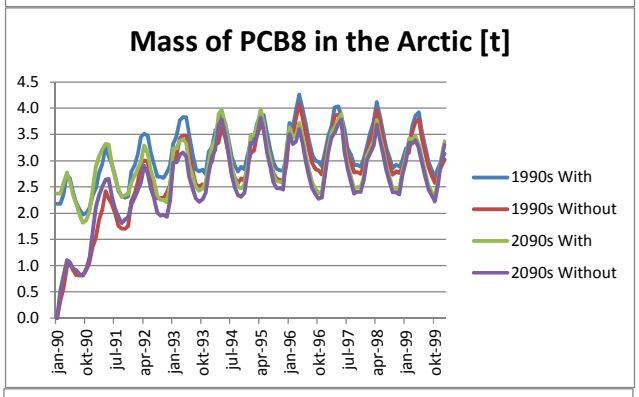


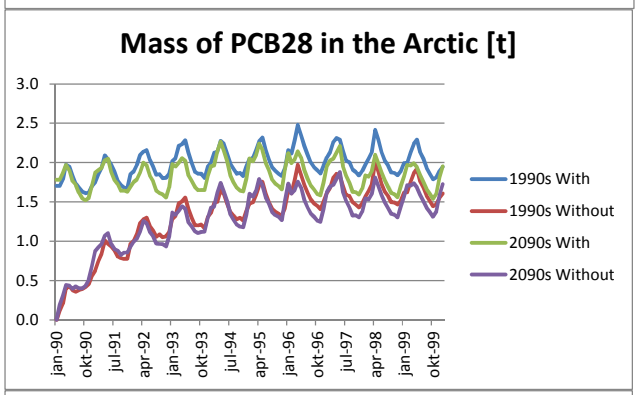
Figure S6. Monthly averaged mass in air (left column), sea water (middle column) and soil (right column) of all compounds in the entire model domain for the 'W19' (blue), the 'W20' (green), the 'WO19' (red) and the 'WO20' (purple) simulations. Note that the masses of α-HCH in sea water and soil are plotted on the secondary axis for the simulation without initial environmental concentrations.

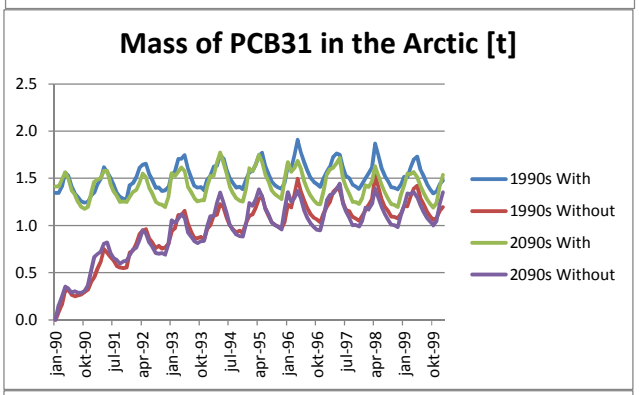

Mass of α-HCH in the Arctic [t]
1990s With
2090s With
1990s Without
2090s Without

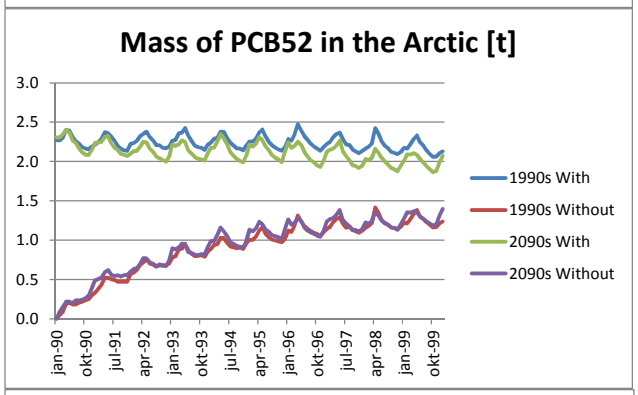

Mass of β-HCH in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without

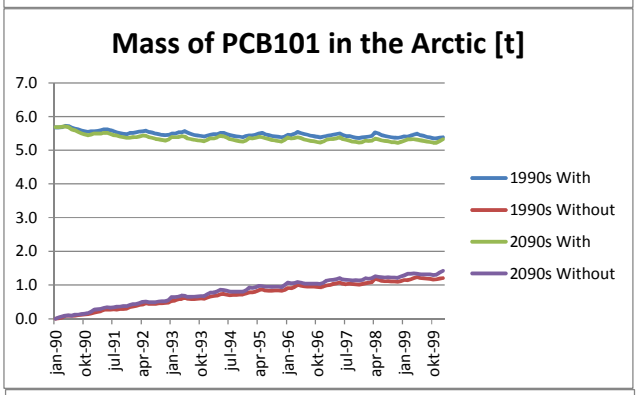

Mass of γ-HCH in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without

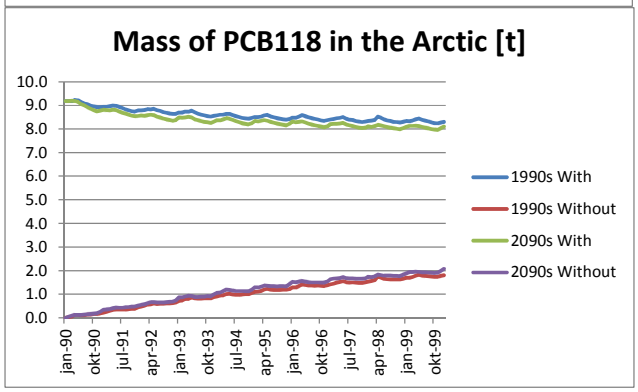

Mass of PCB8 in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without

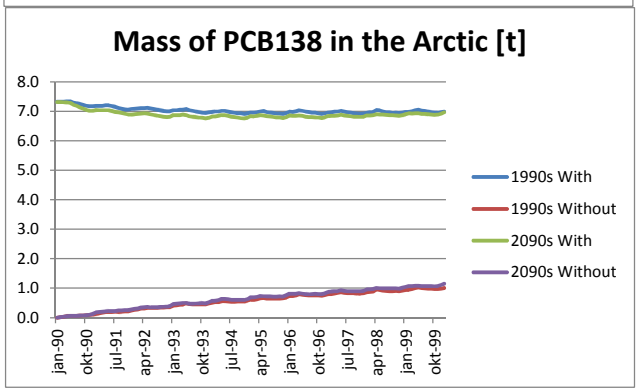

Mass of PCB28 in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB31 in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB52 in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB101 in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB118 in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without


Mass of PCB138 in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without

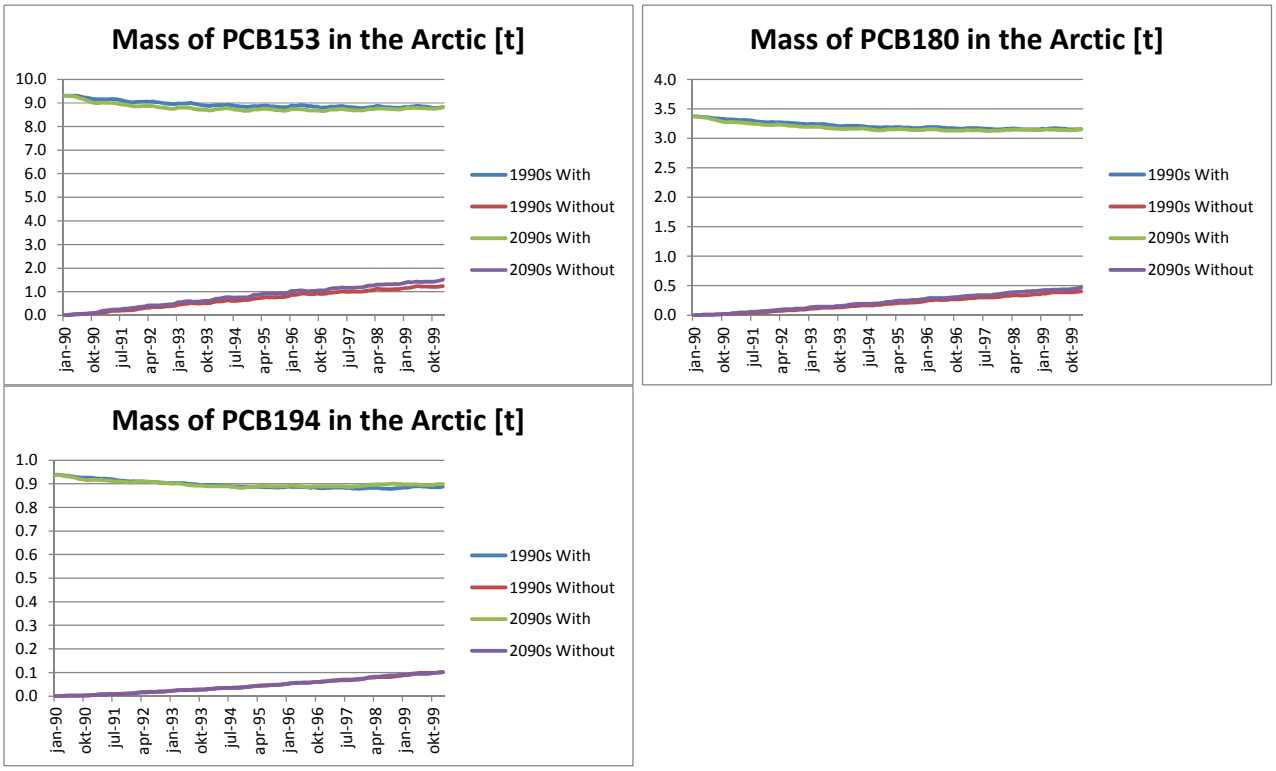


Figure S7. Monthly averaged total mass of all compounds in the Arctic (North of 66.5°N) for the 'W19' (blue), the 'W20' (green), the 'WO19' (red) and the 'WO20' (purple) simulations. Note that the masses of α-HCH for the simulation without initial environmental concentrations are plotted on the secondary axis.

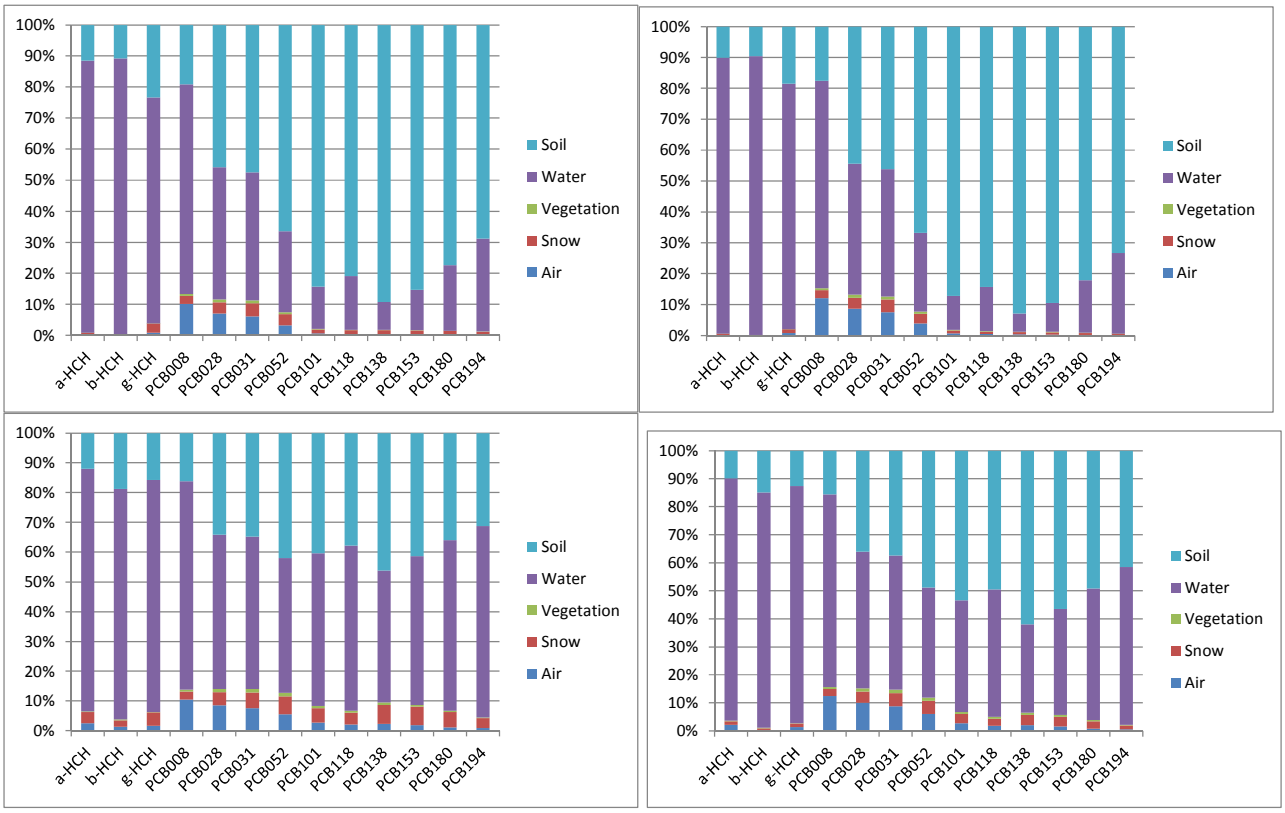


Figure S8. The distribution of the studied compounds between the five media in the Arctic (North of 66.5°N) in the end of the 1990s (left column) and 2090s (right column) for the simulations with (top row) and without (bottom row) initial environmental concentrations.

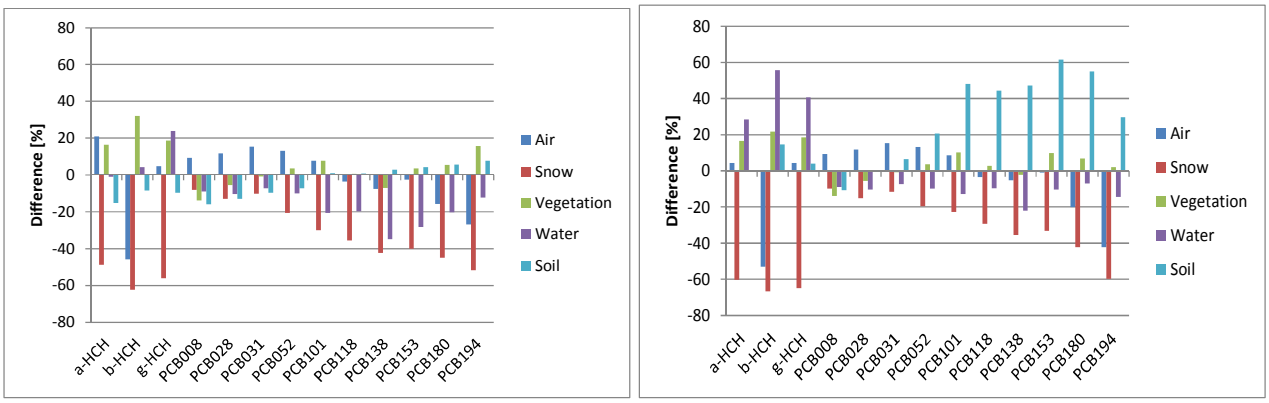
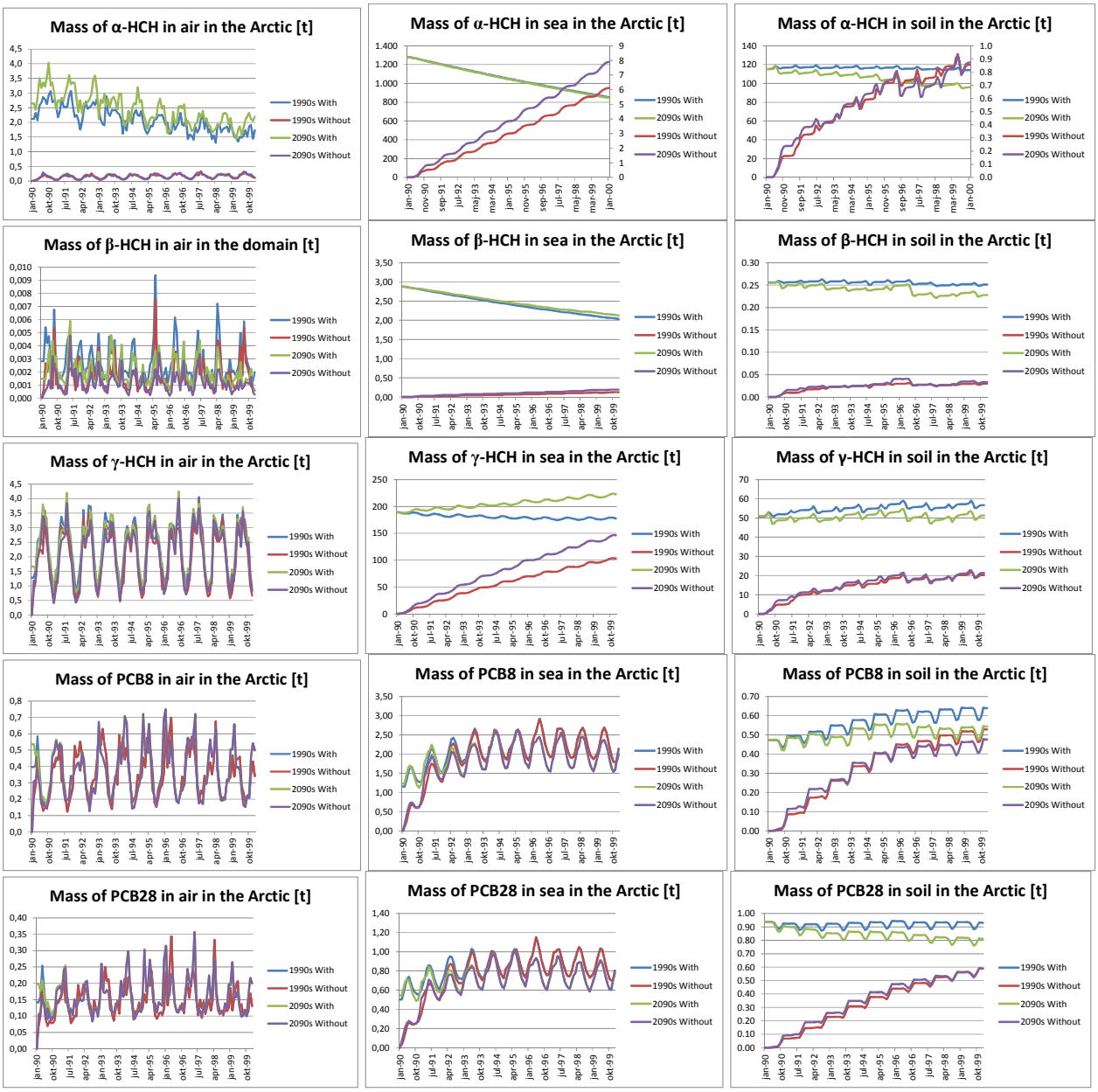


Figure S9. Relative differences in total mass in the five media within the Arctic domain (North of 66.5°N) between the 1990s and the 2090s for the simulation with (left) and without (right) initial environmental concentrations.



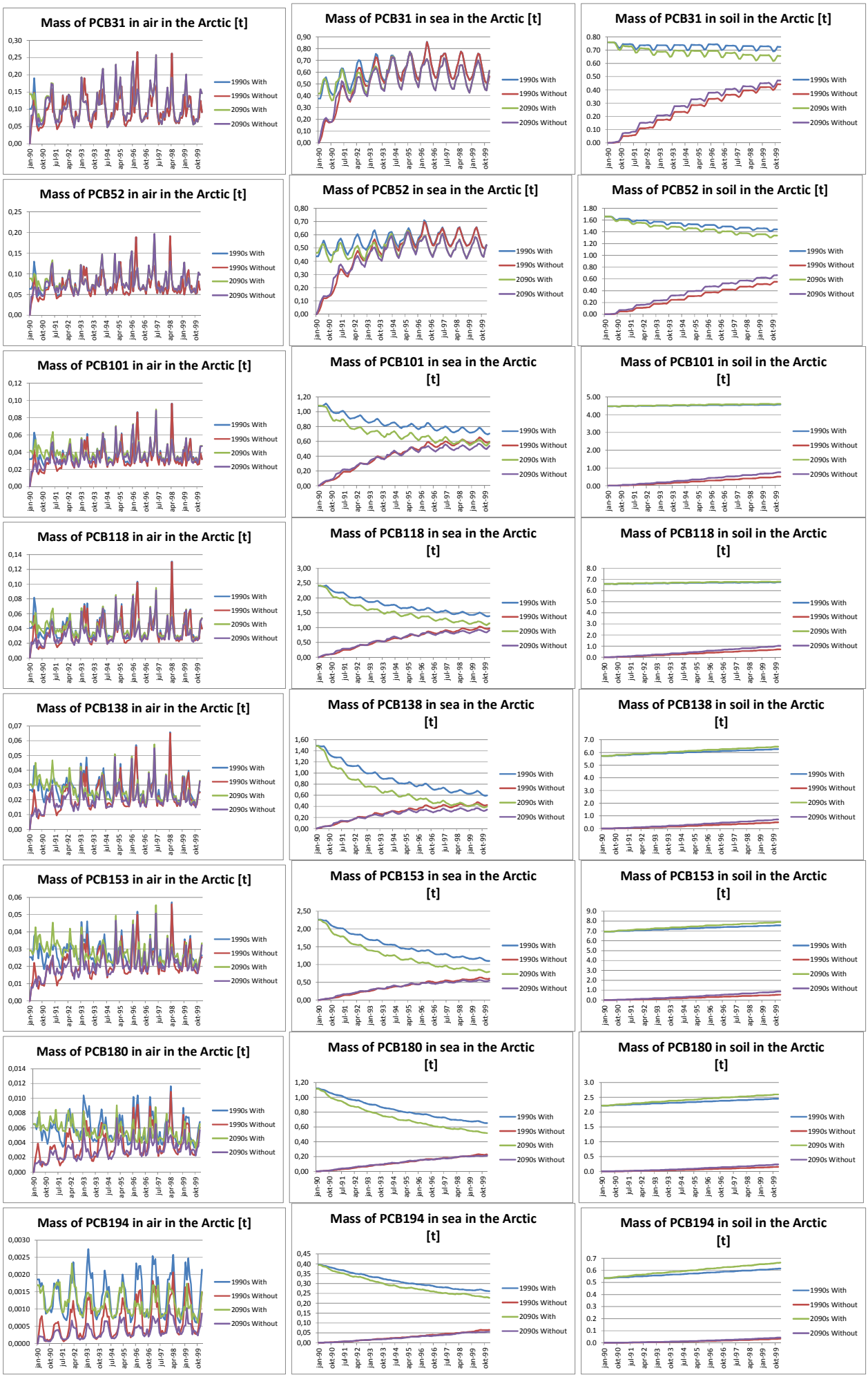

Mass of PCB31 in air in the Arctic [t]
Mass of PCB31 in sea in the Arctic [t]
Mass of PCB31 in soil in the Arctic [t]
Mass of PCB52 in air in the Arctic [t]
Mass of PCB52 in sea in the Arctic [t]
Mass of PCB52 in soil in the Arctic [t]
Mass of PCB101 in air in the Arctic [t]
Mass of PCB101 in sea in the Arctic [t]
Mass of PCB101 in soil in the Arctic [t]
Mass of PCB118 in air in the Arctic [t]
Mass of PCB118 in sea in the Arctic [t]
Mass of PCB118 in soil in the Arctic [t]
Mass of PCB138 in air in the Arctic [t]
Mass of PCB138 in sea in the Arctic [t]
Mass of PCB138 in soil in the Arctic [t]
Mass of PCB153 in air in the Arctic [t]
Mass of PCB153 in sea in the Arctic [t]
Mass of PCB153 in soil in the Arctic [t]
Mass of PCB180 in air in the Arctic [t]
Mass of PCB180 in sea in the Arctic [t]
Mass of PCB180 in soil in the Arctic [t]
Mass of PCB194 in air in the Arctic [t]
Mass of PCB194 in sea in the Arctic [t]
Mass of PCB194 in soil in the Arctic [t]
1990s With
1990s Without
2090s With
2090s Without

Figure S10. 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^{o}N) for the 'W19' (blue), the 'W20' (green), the 'WO19' (red) and the 'WO20' (purple) simulations. Note that the masses of α-HCH in sea water and soil are plotted on the secondary axis for the simulation without initial environmental concentrations.