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

Supporting Information

for

Introducing a Nested Multimedia Fate and Transport Model for Organic Contaminants (NEM)

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Total 20 pages: Tables S1-S2 and Figures S1-S16.

Table S1: Stations, station coordinates, years covered (ebas.nilu.no) and selected references [*)].

Station	Coordinates	Years covered	References (selected)
Andøya (Norway)	69°16'N, 16°00'E	2010-2017	[1]
Birkenes (Norway)	58°23'N, 08°15'E	2004-2019	[2, 3]
Košetice (Czech Republic)	49°34'N, 15°04'E	1999-2014	[4, 5]
Pallas (Finland)	68°00'N, 24°15'E	1996-2018	[6]
Aspvreten (Finland)	58°48'N, 17°23'E	1995-2018	[7]
Rörvik (Sweden)	57°25'N, 11°56'E	1994-2001	
Råö (Sweden)	57°23'N, 11°54'E	2002-2018	[6]
Stórhöfði (Iceland)	63°24'N, 20°17'W	1995-2018	[8]
Zeppelin (Spitsbergen)	78°54'N, 11°53'E	1998-2019	[9]

[*)] Data from four additional stations with more limited time-series were available from ebas.nilu.no. These stations are High Muffles in Great Britain (54°20'N, 00°48'W: 2004-2008), Schauinsland (47°54'N, 07°54'E: 2007-2010), Westerland (54°55'N, 08°18'E: 2007-2010) and Zingst in Germany (54°26'N, 12°43'E: 2009-2010). These data were only included for the initial model evaluation for the sake of completeness (Figure S5).

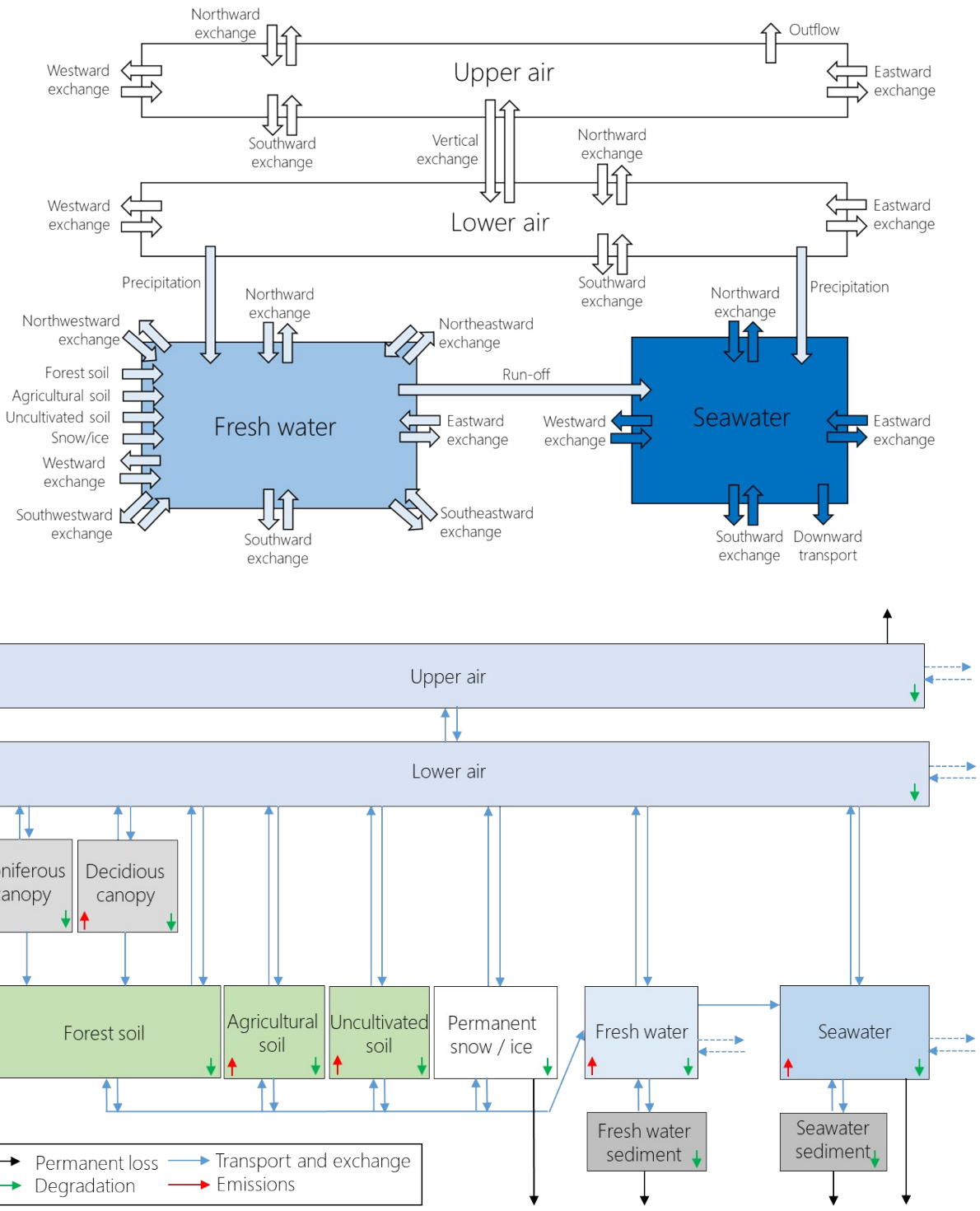


Figure S1: Transport of air, fresh water and seawater in the air-fresh water-seawater system (top) and chemical transport and fate processes included for each compartment (bottom) that are included within each grid cell.

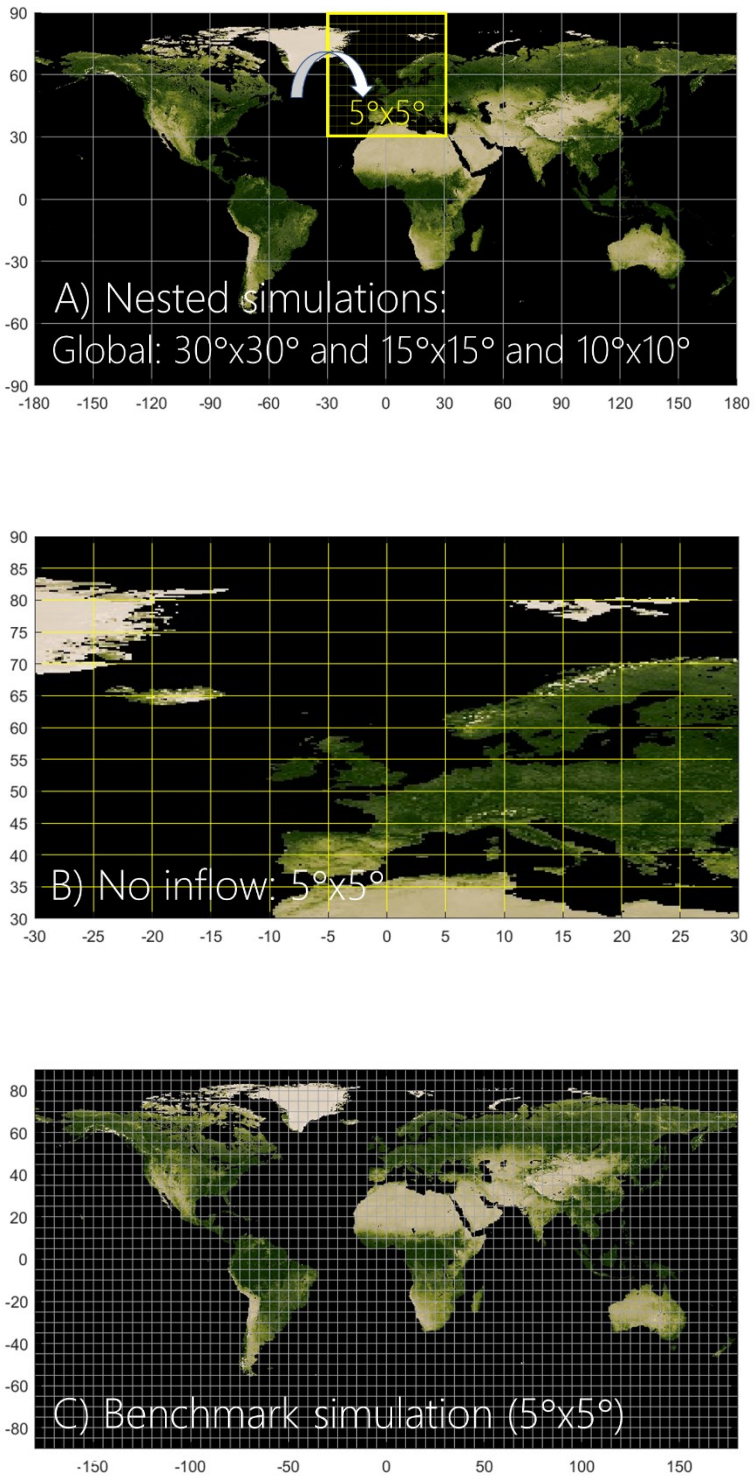


Figure S2: Illustration of the modelling approach used to explore the impact of the spatial resolution of the external global domain on the predicted concentrations of PCB-153 within a nested European region (90°N, 30°W to 30°N, 30°E) with a 5°x5° resolution.

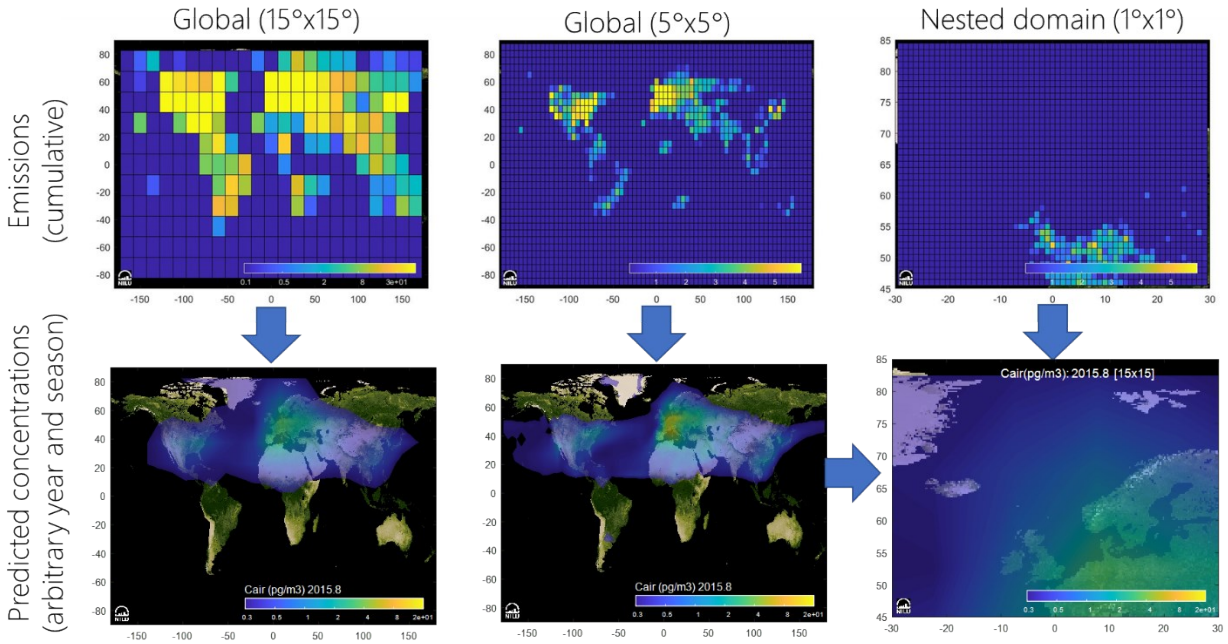


Figure S3: Illustration of the modelling approach used for the model evaluation and application for the Northern European domain (85°N, 30°W to 45°N, 30°E).

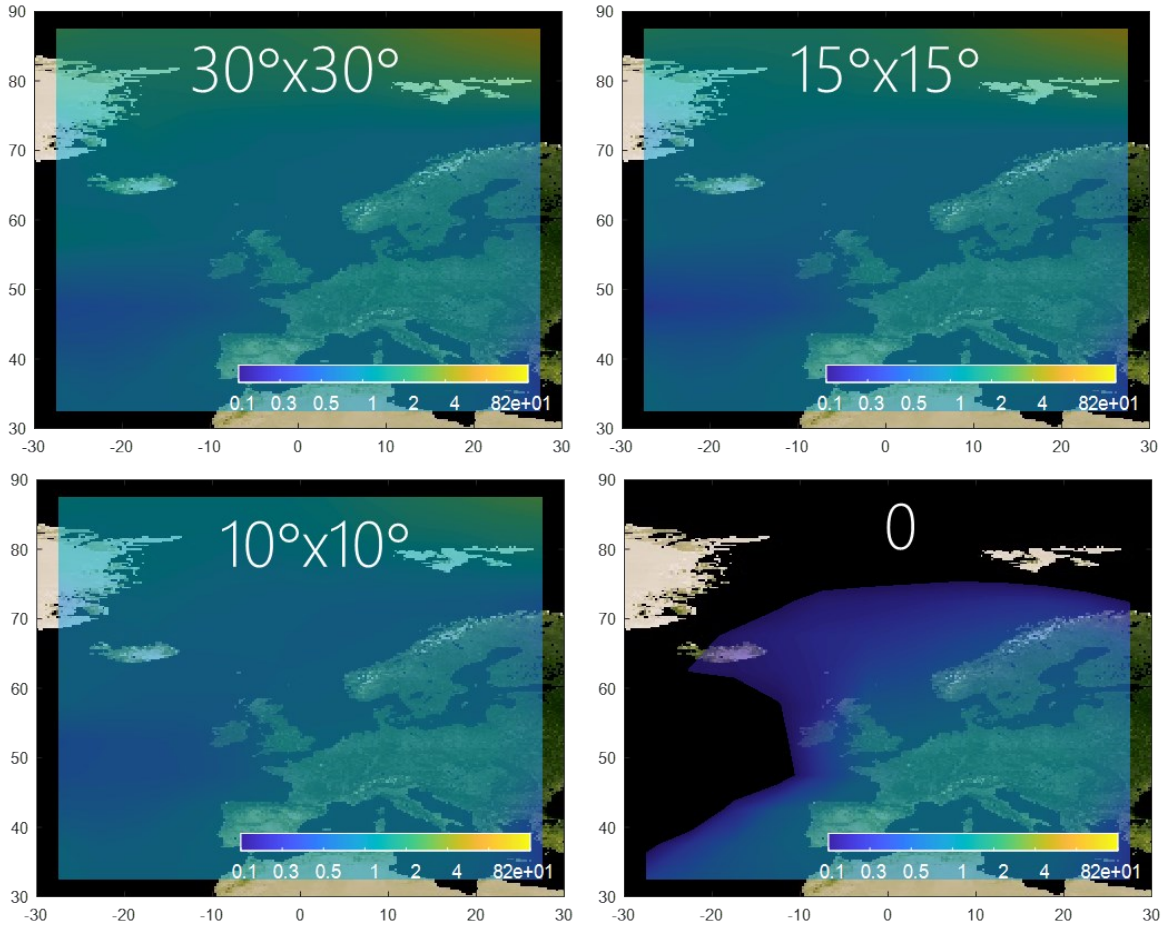


Figure S4: Impact of variable resolutions outside a nested domain on predictions within a nested domain (90°N, 30°W to 30°N, 30°E). The maps show the predicted concentration in air from three nested simulations at 5°x5°, relying on outputs from global simulations (30°x30°; 15°x15° and 10°x10°) as input, divided by the predicted concentrations from the global reference simulation at 5°x5° during late summer, 2015. The lower panel to the right shows the results from the scenario without any inflow of PCB-153 into the nested domain.

Figure S5: Observed long-term trends of PCB-153 in air for four additional monitoring sites versus model predictions based on different spatial resolutions (15°x15°, 5°x5°, 1°x1°).

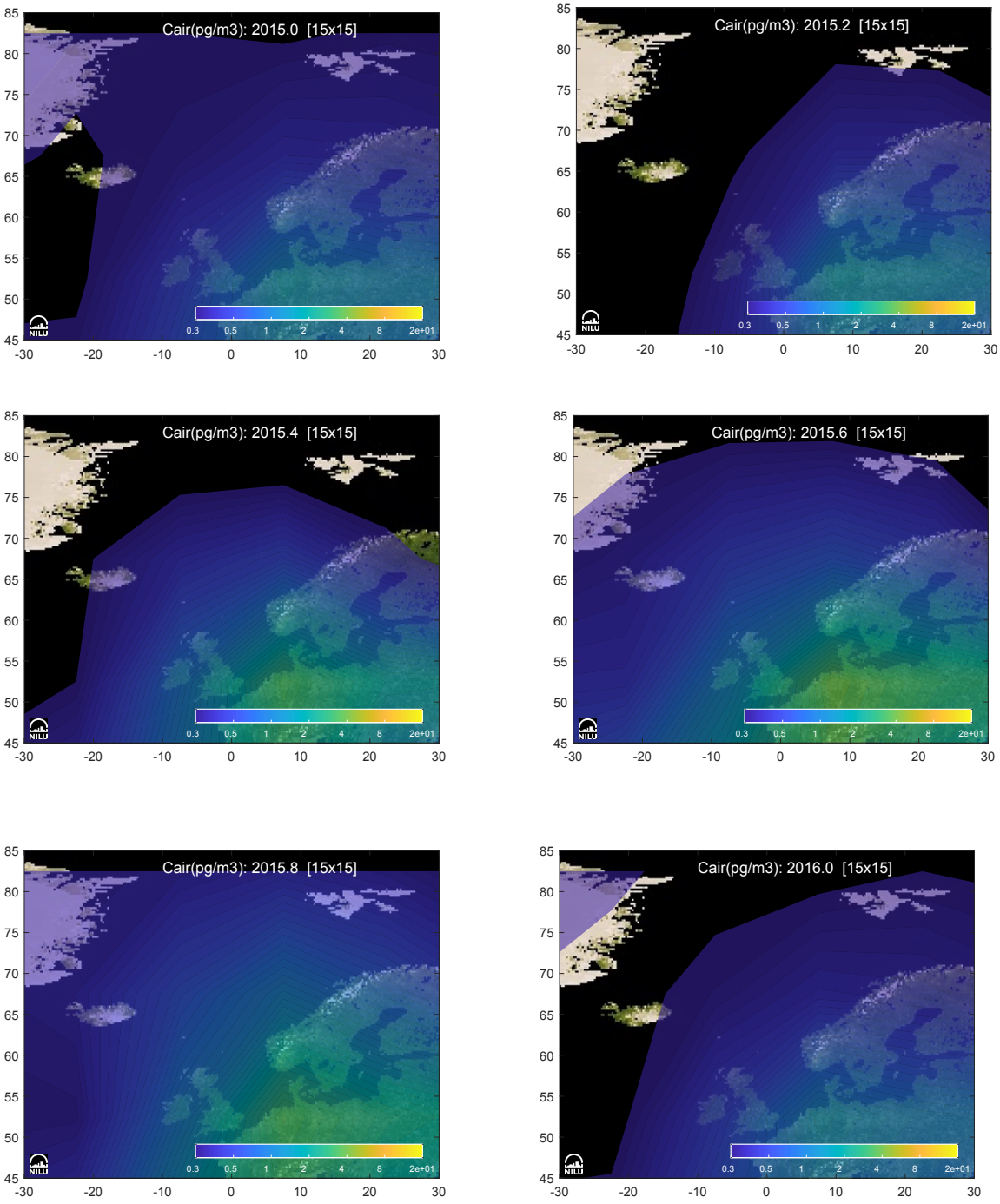


Figure S6: Predicted concentrations of PCB-153 in air during 2015 at 15°x15°.

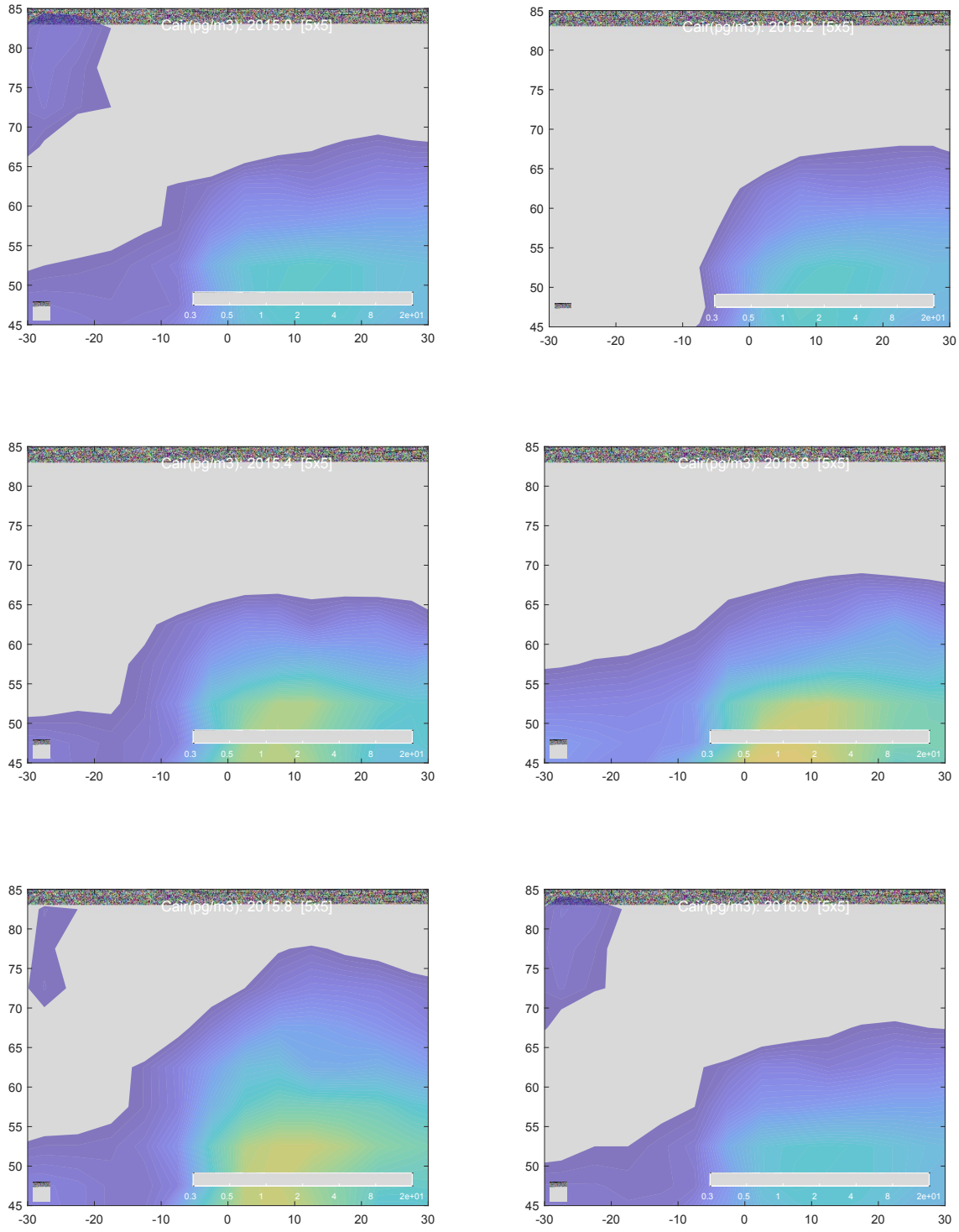


Figure S7: Predicted concentrations of PCB-153 in air during 2015 at 5°x5°.

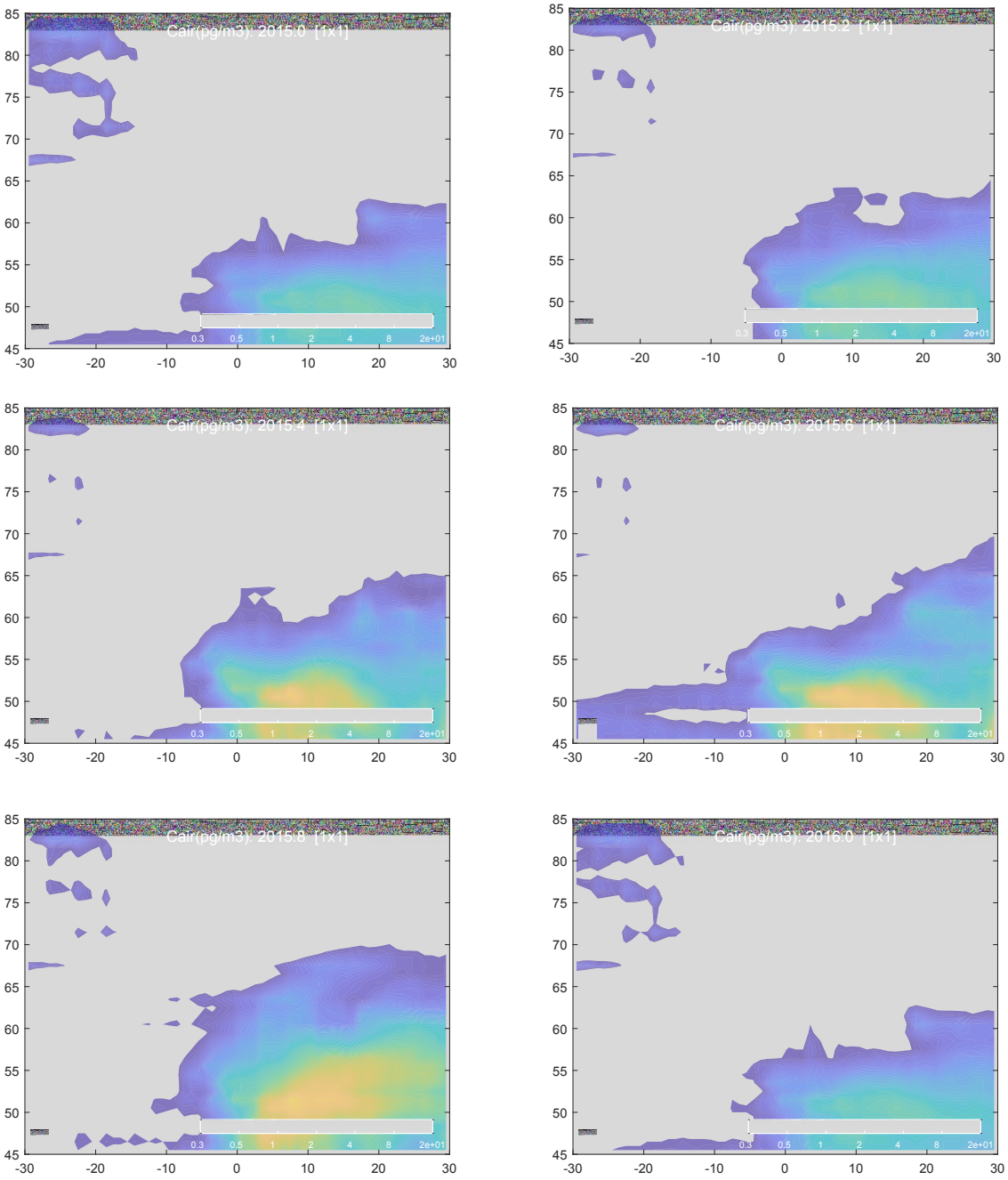
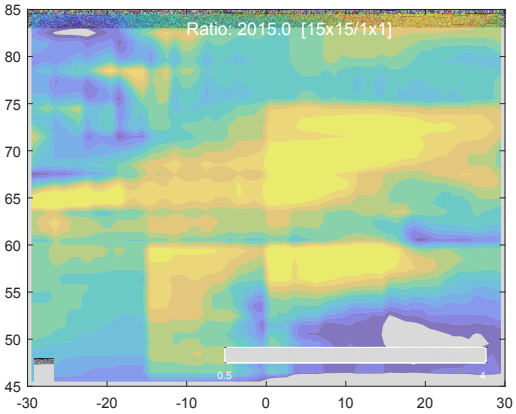
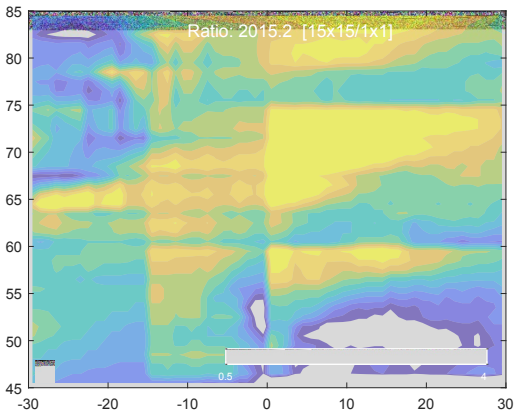


Figure S8: Predicted concentrations of PCB-153 in air during 2015 at 1°x1°.


Ratio: 2015.0 [15x15/1x1]
85
80
75
70
65
60
55
50
45
-30
-20
-10
0
10
20
30
0.5
4


Ratio: 2015.2 [15x15/1x1]
85
80
75
70
65
60
55
50
45
-30
-20
-10
0
10
20
30
0.5
4

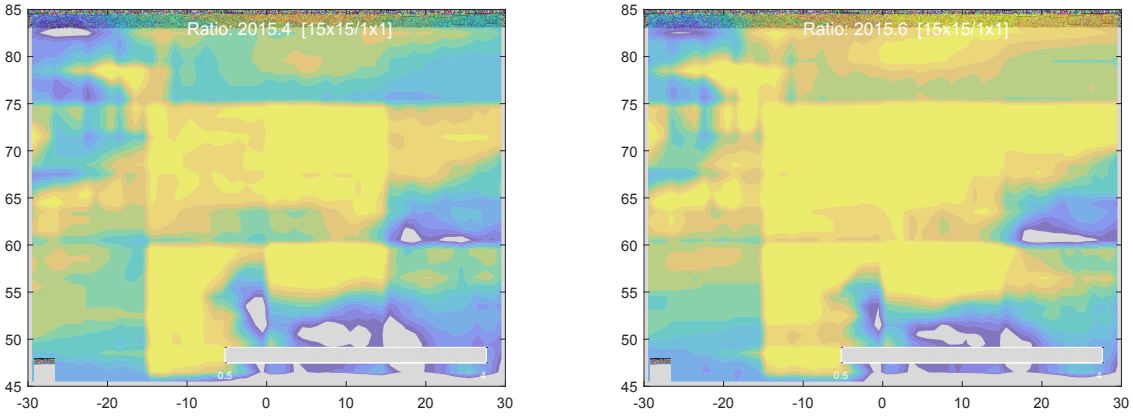
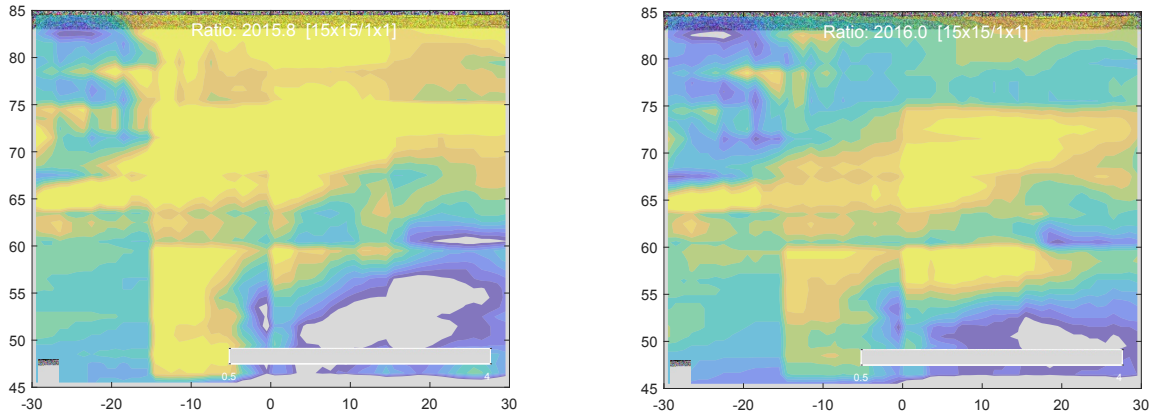


Figure S9: Predicted concentrations of PCB-153 in air during 2015 at 15°x15°, divided by predictions obtained at 1°x1°.



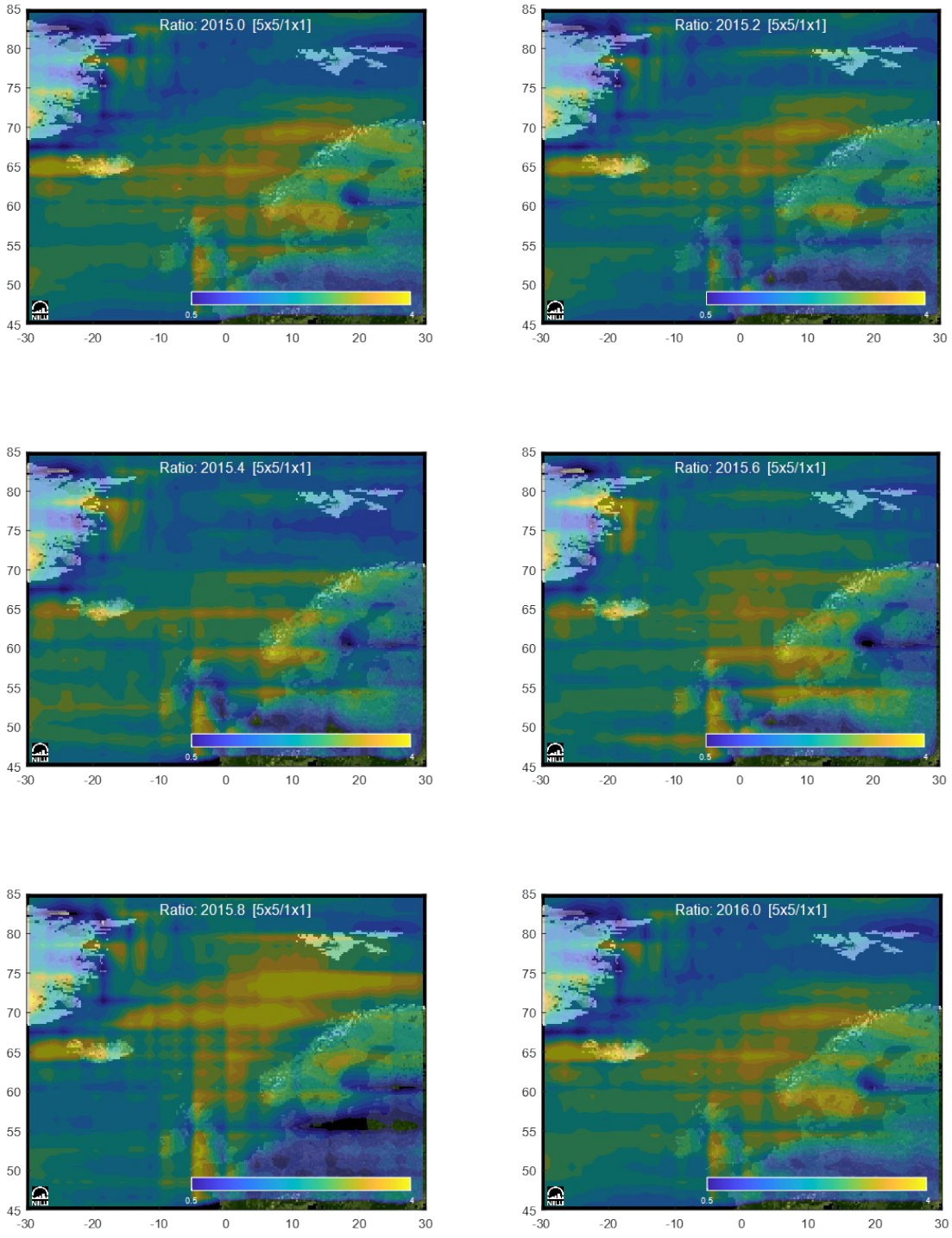


Figure S10: Predicted concentrations of PCB-153 in air during 2015 at 5°x5°, divided by predictions obtained at 1°x1°.

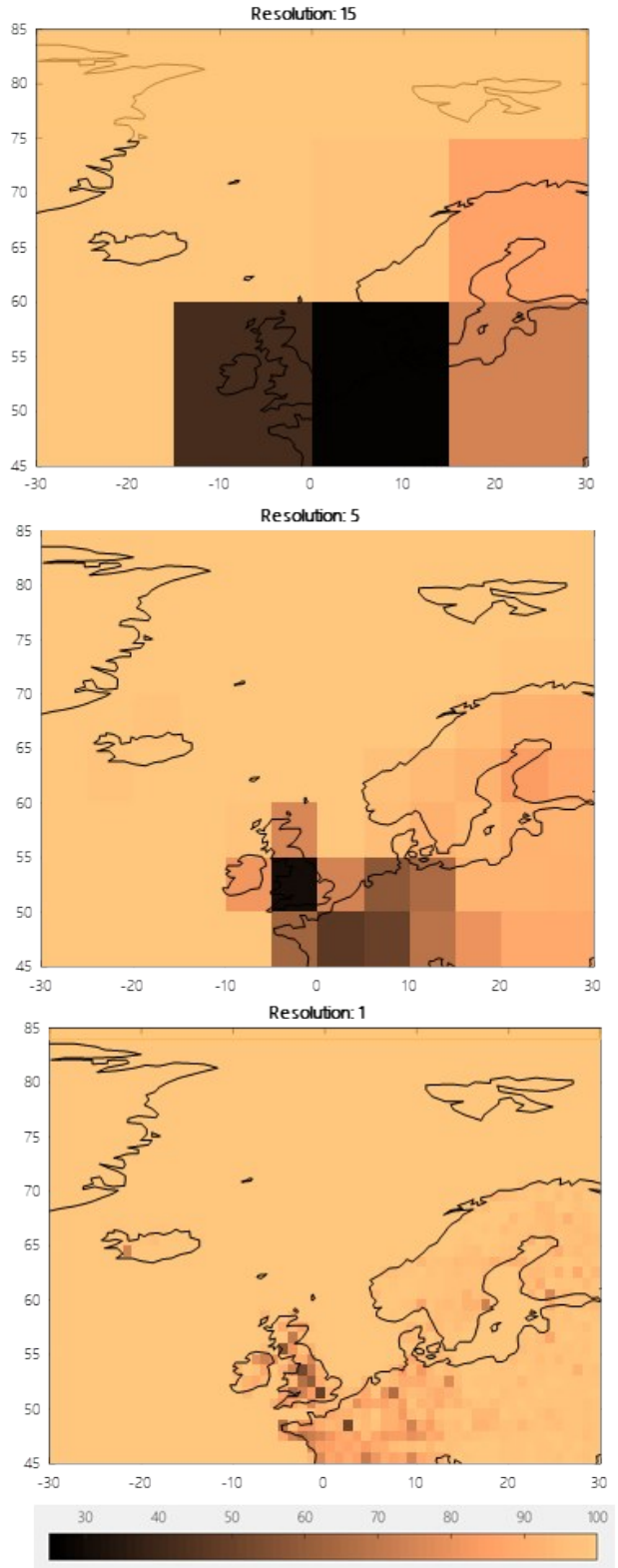


Figure S11: Relative significance of atmospheric inflow to the sum of atmospheric inflow plus emissions, simulated using three different spatial resolutions, 1930-2020 (15°x15°, 5°x5°, 1°x1°).

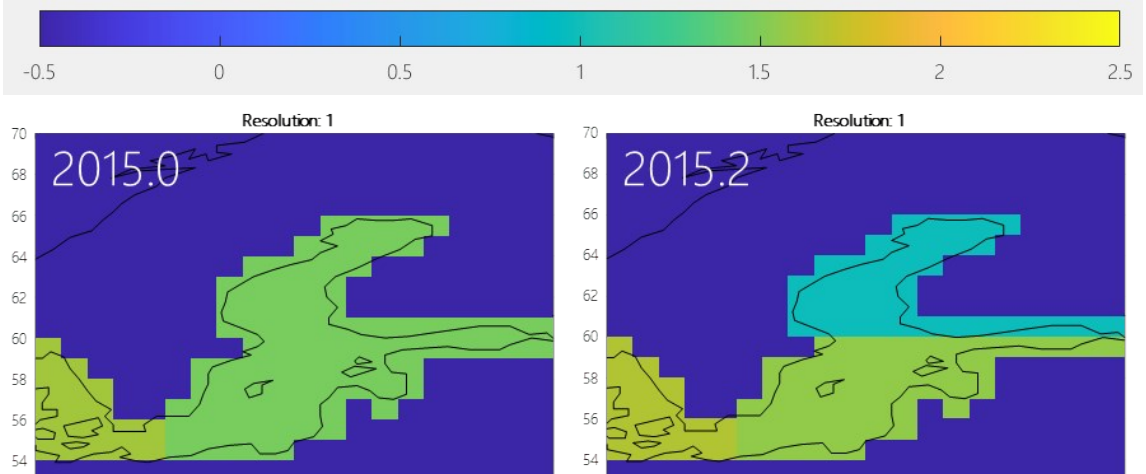

-0.5
0
0.5
1
1.5
2
2.5
Resolution: 1
2015.0
Resolution: 1
2015.2
70
68
66
64
62
60
58
56
54

Figure S12: Predicted atmospheric deposition of PCB-153 to the Baltic Sea during 2015 at 15°x15° in ng m^{-2} h^{-1} (log_{10}). The Baltic Sea is defined at a 1°x1° degree resolution.

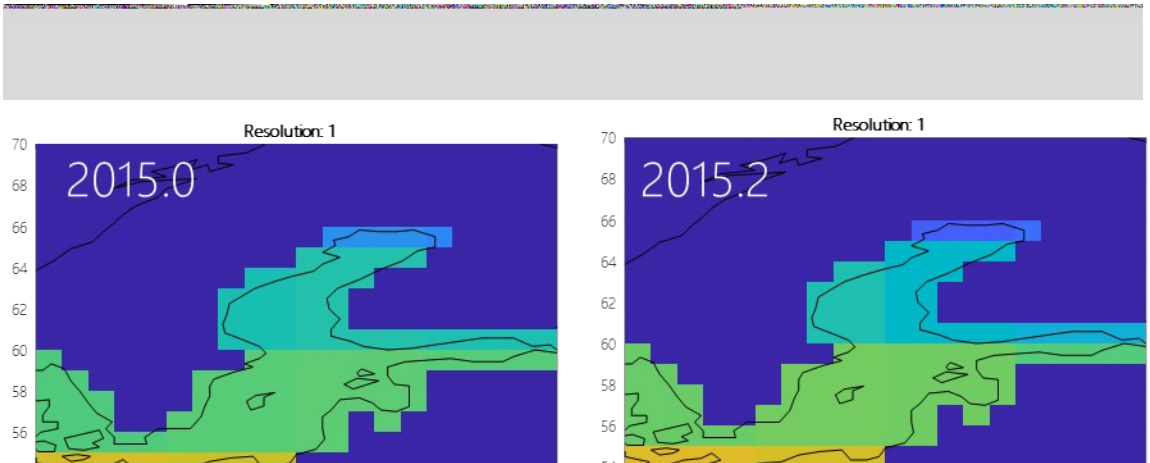

Resolution: 1
2015.0
70
68
66
64
62
60
58
56
Resolution: 1
2015.2
70
68
66
64
62
60
58
56

Figure S13: Predicted atmospheric deposition of PCB-153 to the Baltic Sea during 2015 at 5°x5° in ng m^{-2} h^{-1} (log_{10}). The Baltic Sea is defined at a 1°x1° degree resolution.

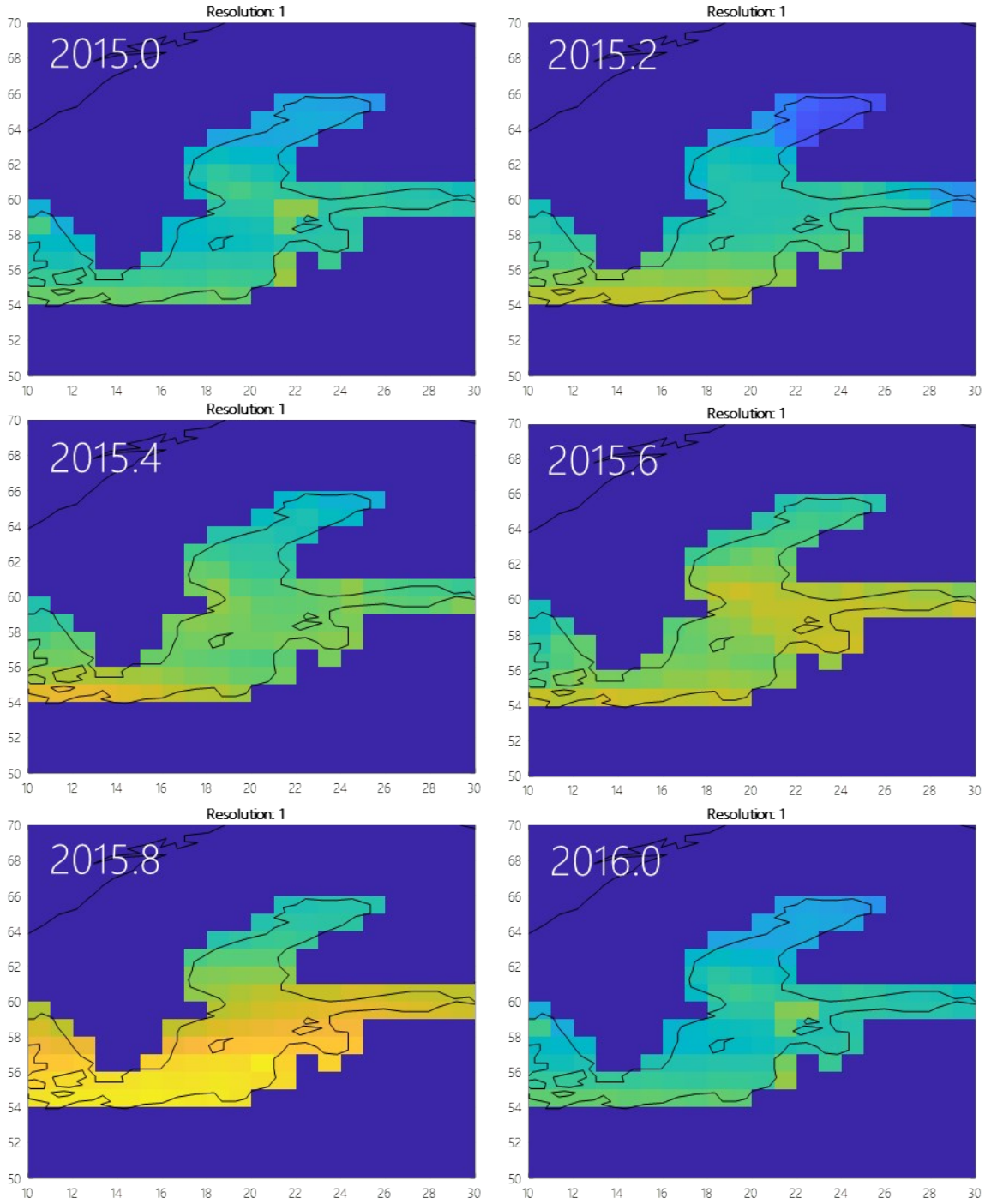


Figure S14: Predicted atmospheric deposition of PCB-153 to the Baltic Sea during 2015 at 1°x1° in ng m^{-2} h^{-1} (log_{10}). The Baltic Sea is defined at a 1°x1° degree resolution.

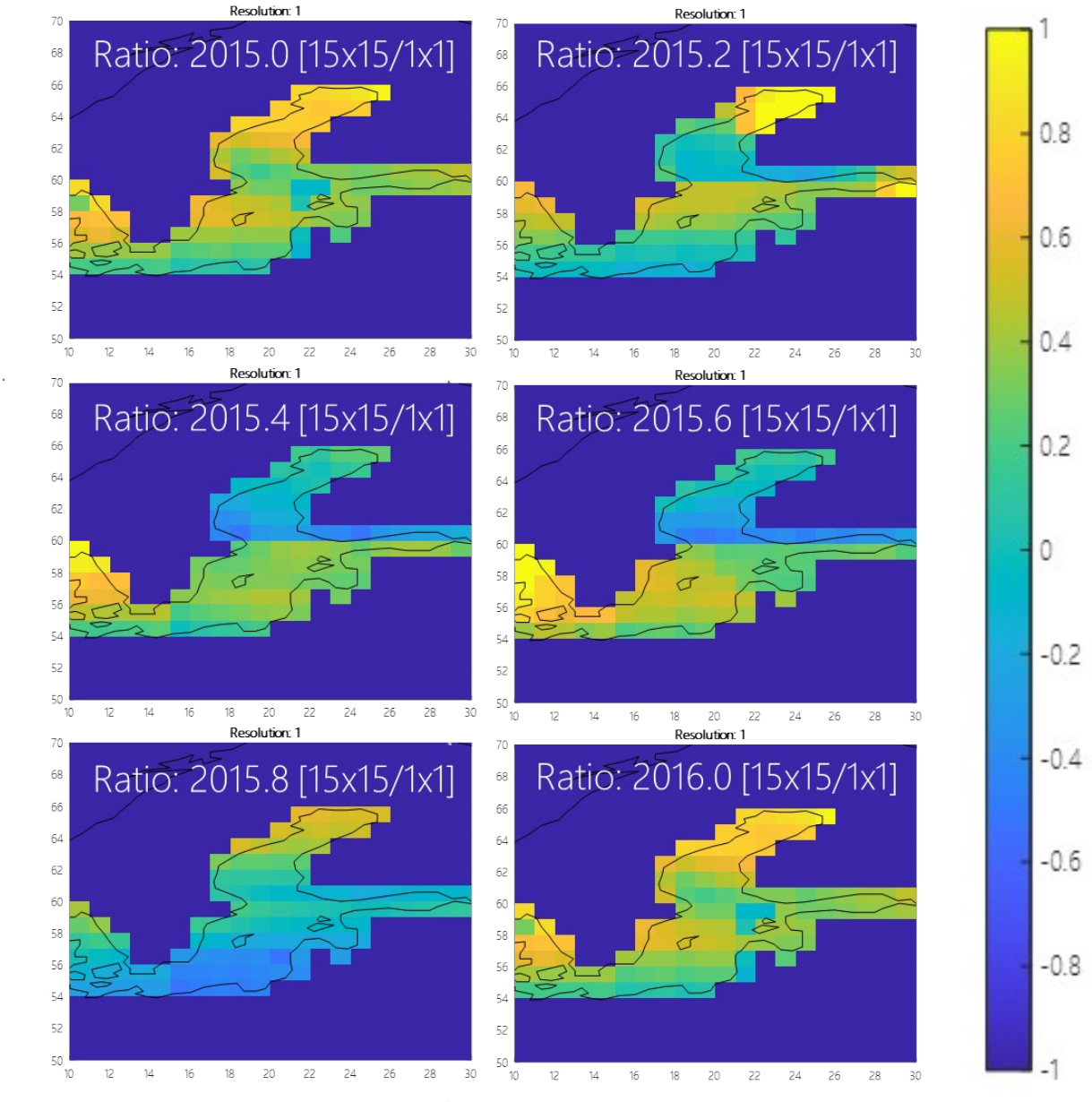


Figure S15: Logarithm of the ratio of 2015 atmospheric deposition flux of PCB-153 to the Baltic Sea predicted with NEM at a resolution of 15°x15°and 1°x1°. A value of 0 indicates the same predicted deposition, positive values (yellow) indicate higher deposition at coarser resolution and negative values (blue) designate lower deposition at coarser resolution. A value of 1

corresponds to differences in deposition by one order of magnitude. The Baltic Sea is defined at a 1°x1° degree resolution.

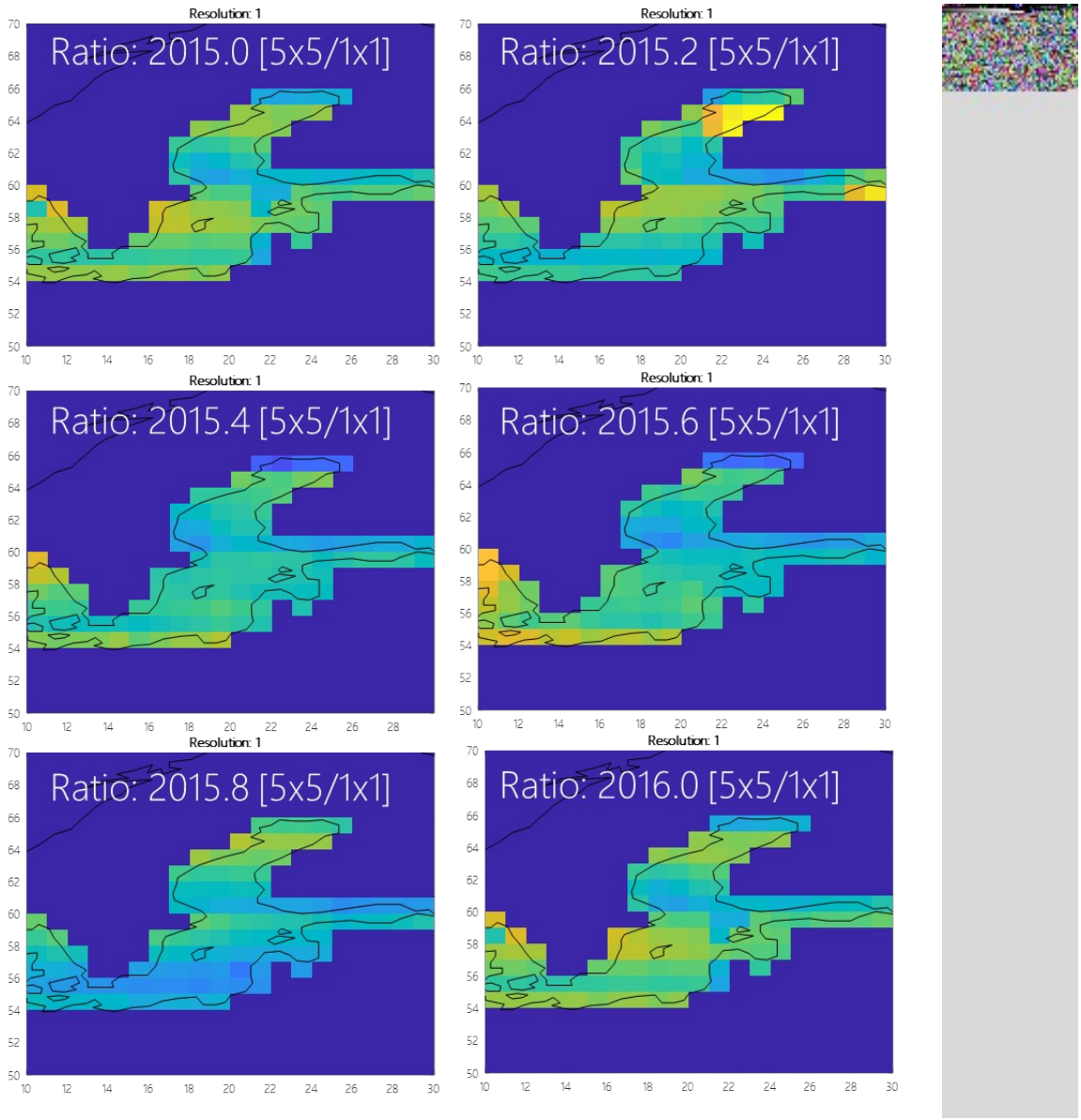


Figure S16: Logarithm of the ratio of 2015 atmospheric deposition flux of PCB-153 to the Baltic Sea predicted with NEM at a resolution of 5°x5°and 1°x1°. A value of 0 indicates the same predicted deposition, positive values (yellow) indicate higher deposition at coarser resolution and negative values (blue) designate lower deposition at coarser resolution. A value of 1 corresponds to differences in deposition by one order of magnitude. The Baltic Sea is defined at a 1°x1° degree resolution.

Table S2: Seasonal atmospheric deposition flux of PCB-153 to the Baltic Sea predicted with NEM at a resolution of 15°x15°, 5°x5° and 1°x1° (Kg/Year). The Baltic Sea is defined at a 1°x1° degree resolution, and the three different basins at 15°x15° are defined as in the main text and as illustrated in Figure S13.

Time	Resolution	Kattegat/ Skagerrak	Baltic Proper	Bothnian Sea	Baltic Sea (Total)
2015.0	15°x15°	3.2	6.5	3.5	13.2
	5°x5°	2.7	5.7	1.2	9.6
	1°x1°	1.4	3.5	1.2	6.0
2015.2	15°x15°	3.6	7.8	1.1	12.6
	5°x5°	3.2	6.7	1.0	10.9
	1°x1°	2.4	4.9	0.9	8.2
2015.4	15°x15°	9.0	13.3	1.3	23.7
	5°x5°	6.3	8.7	1.7	16.8
	1°x1°	3.4	6.6	2.0	12.0
2015.6	15°x15°	11.0	20.5	2.2	33.6
	5°x5°	7.3	11.7	2.7	21.7
	1°x1°	2.5	8.8	3.7	15.0
2015.8	15°x15°	9.0	16.6	4.9	30.5
	5°x5°	9.4	18.9	3.5	31.8
	1°x1°	12.2	29.5	3.5	45.2
2016.0	15°x15°	3.0	6.1	3.3	12.5
	5°x5°	2.6	5.3	1.1	9.0
	1°x1°	1.3	3.3	1.1	5.6

References

1. Wong, F.; Shoeib, M.; Katsoyiannis, A.; Eckhardt, S.; Stohl, A.; Bohlin-Nizzetto, P.; Li, H.; Fellin, P.; Su, Y.; Hung, H., Assessing temporal trends and source regions of per- and polyfluoroalkyl substances (PFASs) in air under the Arctic Monitoring and Assessment Programme (AMAP). *Atmospheric Environment* **2018,** *172*, 65-73.
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9. Eckhardt, S.; Breivik, K.; Manø, S.; Stohl, A., Record high peaks in PCB concentrations in the Arctic atmosphere due to long-range transport of biomass burning emissions. *Atmospheric Chemistry and Physics* **2007,** *7*, (17), 4527-4536.