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The effects of global climate change on the cycling and processes of persistent organic pollutants (POPs) in the North Sea

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Supplementary materia

Table S1. List of physicochemical, physical and chemical parameter values used with the simulations.

Physical-chemical property	unit	γ-HCH value (with source)	PCB 153 value (with source)
partitioning coefficient: K_{OW} (octanol-water)	-	$3.98 \cdot 10^6$ [S1]	$5.62 \cdot 10^6$ [S2]
K_{OC} (organic carbon-water)	-	$K_{OC} = 0.411 \cdot K_{OW}$ [S3]	$K_{OC} = 0.411 \cdot K_{OW}$ [S3]
Temperature dependent Henry's Law constant: slope	-	-3208 [S4]	-3662 [S5]
intercept	K	10.14 [S4]	14.05 [S5]
Half-life in: ocean water	hours	10350 [S6]	120000 [S8]
sediment	hours	14230 [S7]	165000 [S8]
Settling velocity of SPM	m/s	$5 \cdot 10^{-6}$ [S9]	$5 \cdot 10^{-6}$ [S9]
Threshold shear velocity for erosion of SPM	m/s	0.028 [S10]	0.028 [S10]
Threshold shear velocity for deposition of SPM	m/s	0.01 [S10]	0.01 [S10]

S2. Summary of FANTOM model processes

Air-Sea gas exchange

For the FANTOM, gas exchange processes at the air-sea interface are based on the stagnant two-film theory formulated by [S11, S12]. A fugacity formulation is included as described by [S13]. The chemical equilibrium of the POP between the air and water is controlled by the following parameters: temperature, wind speed, and the physical-chemical properties of the compound and its abundance in the environment. See [S9] for further details.

Fugacity capacities in air, Z_a, and water, Z_w, (mol m^{-3} Pa^{-1}) are calculated as

$$Z_a = \frac{1}{RT_a}$$

and

$$Z_w = \frac{1}{H_c T_w}$$

respectively, where *R* is the ideal gas constant, T_a and $T_w$are air and water temperatures, respectively, and H_c is Henry's law constant at T_w. The overall volatilisational exchange rate, D_{wa} (mol Pa^{-1} s^{-1})is calculated according to [S13] and [S14]:

$$D_{wa} = \frac{A_w}{\frac{1}{u_1 Z_a} + \frac{1}{u_2 Z_w}}$$

where A_w is water surface area and u_1, u_2, (m/s) are mass transfer coefficients, which are functions of wind speed [S15].

Other processes
Advection-diffusion: the total concentration of a POP is calculated at a fixed point with a simple Eulerian, advective–diffusive model with sources and sinks. Phase distribution and flux from water into sediment: the amount of the POP either freely dissolved or bound to suspended particulate matter (SPM) in seawater is calculated using the organic carbon–water equilibrium partition coefficient, dependent on the substance, and the sinking rate is calculated using a settling velocity. Degradation rates are calculated using 1st order rate decay coefficients in water and sediment. Water–sediment exchange occurs due to sinking and resuspension. Resuspension occurs when strong friction velocities are found close to the bottom, particularly in shallow water and during storms and high tides. A full description of these processes is found in [S9].

References for supplementary material

S1. Klöpffer, W., and Schmidt, E.: A multimedia load model for the Baltic Sea. Environ. Sci. Pollut. Res. Int., 8, 180–188, 2001.

S2. Beyer, A., Matthies, M.: Long-range Transport Potential of Semivolatile Organic Chemicals in Coupled Air-Water Systems. Environ. Sci. Poll. Res., 8, 173-179, 2001.

S3. Karickhoff, S.W.,: Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. Chemosphere, 10, 833–846, 1981.

S4. Sahsuvar, L., Helm, P., Jantunen, L., Bidleman, T.F.: Henry's law constants for α-, β-, and γ-hexachlorocyclohexanes (HCHs) as a function of temperature and revised estimates of gas exchange in Arctic regions. Atmos. Environ., 37, 983–992, 2003.

S5. Paasivirta, J., Sinkkonen, S., Mikkelson, M., Raantio, T., Wania, F.,: Estimation of vapor pressures, solubilities and Henry's law constants of selected persistent organic pollutants as functions of temperature. Chemosphere 39, 811–832, 1999.

S6. Ngabe, B., Bidleman, T.F., and Falconer, R. L.: Base Hydrolysis of alpha- and gamma- Hexachlorocyclohexanes, Environ. Sci. Technol., 27, 1930-1933, 1993.

S7. Hornsby, A. G., Wauchope, R. D., and Herner, A. E.: Pesticide Properties in the Environment, Springer-Verlag, New York, 1996.

S8. Sinkkonen, S. and Paasivirta, J.: Degradation half-life times of PCDDs, PCDFs and PCBs for environmental fate modeling, Chemosphere, 40, 943--949, 2000.

S9. O'Driscoll, K., Mayer, B., Ilyina, T., and Pohlmann, T.: Modelling the cycling of persistent organic pollutants (POPs) in the North Sea system: fluxes, loading, seasonality, trends, Journal of Marine Systems, 111-112, 69–82, doi:10.1016/j.jmarsys.2012.09.011, 2013.

S10. Pohlmann, T., and Puls, W.: Currents and transport in water. In: Sündermann, J. (Ed.), Circulation and contaminant fluxes in the North Sea. Springer, Berlin, pp. 345–402, 1994.

S11. Whitman, W. G.: The two-film theory of gas absorption, Chem. Metall. Eng., 29, 146–150, 1923.

S12. Liss, P. S. and Slater, P. G.: Flux of gases across the air–sea interface, Nature, 247, 181–184, 1974.

S13. Mackay, D.: Multimedia Environmental Models: The Fugacity Approach, Lewis, Boca Raton, 2nd edition, 2001.

S14. Wania, F., Persson, J., di Guardo, A., and McLachlan, M. S.: The POPCYCLING-Baltic Model. A non-steady state multicompartment mass balance model of the fate of persistent organic pollutants in the Baltic Sea environment, Norwegian Inst. Air Research, OR 10/2000, U-96069, Kjeller, Norway, 2000.

S15. Schwarzenbach, R. E., Gschwend, P. M., and Imboden, D. M.: Environmental Organic Chemistry, Wiley, New York, First ed, 1993.