Supporting material

## Methane dynamics in the Baltic Sea: investigating concentration, flux and isotopic composition patterns using the coupled physical-biogeochemical model BALTSEM-CH<sub>4</sub> v1.0

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Figure S1: Sub-basin division of the Baltic Sea in BALTSEM: 1. Northern Kattegat (NK), 2. Central Kattegat (CK), 3. Southern Kattegat (SK), 4. Samsø Belt (SB), 5. Fehmarn Belt (FB), 6. Öresund (OS), 7. Arkona Basin (AR), 8. Bornholm Basin (BN), 9. Gotland Sea (GS), 10. Bothnian Sea (BS), 11. Bothnian Bay (BB), 12. Gulf of Riga (GR), 13. Gulf of Finland (GF).



Figure S2: Global mean atmospheric CH<sub>4</sub> level (ppb) expressed as mole fraction of dry air (data available at <u>https://gml.noaa.gov/dv/data/</u> (observed) and <u>https://tntcat.iiasa.ac.at/RcpDb/dsd?Action=htmlpage&page=download</u> (RCP), respectively).



Figure S3: Model output from the standard model run, showing simulated monthly mean profiles of S, T (°C), O<sub>2</sub> ( $\mu$ M), CH<sub>4</sub> (nM),  $\delta^{13}$ C-CH<sub>4</sub> (‰), and aerobic oxidation rates (nM d<sup>-1</sup>) from 0 to 65 m in the Gotland Sea sub-basin (cf. Figure S1) year 2015 (January to June).



Figure S4: Model output from the standard model run, showing simulated monthly mean profiles of S, T (°C), O<sub>2</sub> ( $\mu$ M), CH<sub>4</sub> (nM),  $\delta^{13}$ C-CH<sub>4</sub> (‰), and aerobic oxidation rates (nM d<sup>-1</sup>) from 0 to 65 m in the Gotland Sea sub-basin (cf. Figure S1) year 2015 (July to December).



Figure S5: Simulated surface water CH<sub>4</sub> concentration (nM; full line) and equilibrium concentration  $CH_{4eq} = K_0 * pCH_{4a}$  (nM; dots) in the Gotland Sea sub-basin (upper panel), as well as surface water CH<sub>4</sub> saturation level (%) (lower panel).



Figure S6: Monthly mean profiles of CH<sub>4</sub> (nM),  $\delta^{13}$ C-CH<sub>4</sub> (‰), and MOX (nM d<sup>-1</sup>) in the Gotland Sea sub-basin (see Figure S1) in February (blue) and August (red) in year 2015: comparison between the standard (full lines), test 1 ( $v_{WCH4_{-}02}$  -50%; dashes), and test 2 ( $v_{WCH4_{-}02}$  +50%; dots) runs, respectively (see Table 3 in main article).



Figure S7: Monthly mean profiles of CH<sub>4</sub> (nM),  $\delta^{13}$ C-CH<sub>4</sub> (‰), and MOX (nM d<sup>-1</sup>) in the Gotland Sea sub-basin (see Figure S1) in February (blue) and August (red) in year 2015: comparison between the standard (full lines), test 3 ( $h_{CH4}$  -50%; dashes), and test 4 ( $h_{CH4}$  +50%; dots) runs, respectively (see Table 3 in main article).



Figure S8: Monthly mean profiles of CH<sub>4</sub> (nM),  $\delta^{13}$ C-CH<sub>4</sub> (‰), and MOX (nM d<sup>-1</sup>) in the Gotland Sea sub-basin (see Figure S1) in February (blue) and August (red) in year 2015: comparison between the standard (full lines), test 5 ( $h_{02}$  -50%; dashes), and test 6 ( $h_{02}$  +50%; dots) runs, respectively (see Table 3 in main article).



Figure S9: Monthly mean profiles of CH<sub>4</sub> (nM),  $\delta^{13}$ C-CH<sub>4</sub> (‰), and MOX (nM d<sup>-1</sup>) in the Gotland Sea sub-basin (see Figure S1) in February (blue) and August (red) in year 2015: comparison between the standard (full lines), test 7 ( $a_{oxi}$  -4‰; dashes), and test 8 ( $a_{oxi}$  +4‰; dots) runs, respectively (see Table 3 in main article).



Figure S10: Monthly mean profiles of CH<sub>4</sub> (nM),  $\delta^{13}$ C-CH<sub>4</sub> (‰), and MOX (nM d<sup>-1</sup>) in the Gotland Sea sub-basin (see Figure S1) in February (blue) and August (red) in year 2015: comparison between the standard (full lines), test 9 ( $\delta^{13}$ C-CH<sub>4sed</sub> -10‰; dashes), and test 10 ( $\delta^{13}$ C-CH<sub>4sed</sub> +10‰; dots) runs, respectively (see Table 3 in main article).



Figure S11: Monthly mean profiles of CH<sub>4</sub> (nM),  $\delta^{13}$ C-CH<sub>4</sub> (‰), and MOX (nM d<sup>-1</sup>) in the Gotland Sea sub-basin (see Figure S1) in February (blue) and August (red) in year 2015: comparison between the standard (full lines), test 11 ( $r_{sed}$  -50%, oxic water; dashes), and test 12 ( $r_{sed}$  +50%, oxic water; dots) runs, respectively (see Table 3 in main article).