Supplement: Importance of high resolution nitrogen deposition data for biogeochemical modeling in the western Baltic Sea and the contribution of the shipping sector

Figure S.1 contains four vertical salinity profiles at the station TF113. Sub-figures (a) and (b) indicate differences between measurement and model in the timing of the onset of the stratification in the beginning of 2012. The stratification develops earlier in the model than in the reality. Sub-figures (c) and (d) indicate differences between measurement and model in the timing of the decline of the stratification in autumn. The mixing starts earlier in the model than in reality.



Figure S.1: Measured (black cross) and modeled (blue line) vertical salinity profiles at the stations TF113 during four different time periods.

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Figure S.2a shows the contribution of shipping-related and total atmospheric (shipping + everything else) nitrogen deposition to the nitrate $(NO_3^-; top)$ and particulate organic nitrogen (PON; bottom) concentrations at the station DB2. These results are based on the CMAQ16mod simulation. Additionally, the total nitrate concentrations of the CMAQ16mod and CMAQ04mod simulations are plotted. One clearly sees that nitrogen from atmospheric deposition (red) dominates the nitrate concentrations (total is plotted in blue). Figure S.2b shows the same but for particulate organic nitrogen (PON).



Figure S.2: Nitrate (NO₃⁻; top, (a)) and particulate organic nitrogen (PON; bottom, (b)) concentrations at the station DB2 (station in the Grabow). Total (blue), total atmospheric (red), and atmospheric shipping-related (magenta) nitrate/PON of the CMAQ16mod simulation and total nitrate/PON of the CMAQ04mod simulation (green) are plotted.



Figure S.3: Like left side of Fig. 8 but showing the monthly mean data of June 2012 instead of annual mean data of 2012.



Figure S.4: Modeled surface layer concentrations of dissolved inorganic nitrogen (DIN, top row) and chlorophyll-a (bottom row) at five stations in four consecutive model years (four colors; see legend top left). The upper five model layers (0 m to ≈ 12 m depth) are considered as surface layer.



Figure S.5: Similar to Fig. 6 but showing only the shipping contribution at the five considered stations.



Figure S.6: left column: atmospheric nitrogen deposition, dissilved inorganic nitrogen (DIN), and particulate organic nitrogen (PON) with nitrogen from atmospheric deposition (top to bottom); center column: full atmospheric nitrogen deposition, DIN, and PON; right column: relative ratio left column to center column in percent (quotient of left column divided by center column times 100). CMAQ16dep deposition and CMAQ16mod simulation results are plotted.

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Table S.1:	List of	abbreviations	and	acronyms	part A	(continued on	next page)
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Abbreviation	Full Name			
AIS	Automatic Identification System (sends position and travel information			
	of ships)			
BSAP	Baltic Sea Action Plan (programme of HELCOM – and member states			
	- to restore the good ecological status of the Baltic marine environment)			
BSH	German Federal Maritime and Hydrographic Agency (Bundeamt für			
_ /	Seeschiffahrt und Hydrographie)			
BMBF	Federal Ministry of Education and Research (Bundesministerium fr Bil-			
	dung und Forschung)			
BMVI	Federal Ministry of Transport and Digital Infrastructure (Bundesminis-			
	terium fr Verkehr und digitale Infrastruktur)			
BOOS	Baltic Operational Oceanographic System			
CCLM	COSMO-CLM (a regional meteorological climate model)			
cdo	Climate Data Operators (a command line program to process NetCDF			
	and GRIB files)			
CEIP	Center for Emission Inventories and Projections			
CMAQ	Community Multiscale Air Quality (a chemistry transport model by the			
	US EPA)			
COSMO	COnsortium for SMall scale MOdeling (a regional meteorological fore-			
	cast model)			
COSMO-CLM	COSMO model in CLimate Mode (a regional meteorological climate			
	model)			
CTM	chemistry transport model			
DIN	dissolved inorganic nitrogen			
DIP	dissovled inorgnic phosphorus			
DKRZ	German Climate Computing Center (Deutsches Klimarechenzentrum)			
DMI	Danish Meteorological Institute			
DWD	German Weather Service (Deutscher Wetterdienst)			
ECMWF	European Centre for Medium-Range Forecast			
EMEP	European Measurement and Evaluation Programme			
ERA-Interim	ECMWF ReAnalysis (a global meteorological reanalysis) – Interim			
	Product (interim between ERA-40 and ERA5)			
ERGOM	Ecological ReGional Ocean Model (a marine biogeochemical model)			
EU	European Union			
GES	Good Environmental Status (a defined)			
GMT	Generic Mapping Tools (a set of command line programes to create			
	vector graphic plots, particularly maps)			
GRIB	General Regularly-distributed Information in Binary form (a binary data			
	format mainly used for meteorological data)			
HBM	HIROMB-BOOS-Model (an ocean physics model)			
HELCOM	Helcom Commission (Baltic Marine Environment Protection Commis-			
	sion – governing body of the Convention on the Protection of the Marine			
	Environment of the Baltic Sea Area)			
HIROMB	High Resolution Operational Model for the Baltic Sea			
HNO_3	nitric acid			
HONO	nitrous acid			
HZG	Helmholtz-Zentrum Geesthacht			
ICES	International Council for the Exploration of the Seas			
IFS	Integrated Forecasting System			
IMO	International Maritime Organization (an UN body responsible for inter-			
	national shipping traffic)			
IMO Number	unique id number of an ocean-going vessel given by the IMO			

Table 5.2. List of al	bileviations and actonyms part B (continuation from previous page)		
Abbreviation	Full Name		
IOW	Leibniz Institute for Baltic Sea Research Warnemünde		
ISORROPIA	a heterogeneous (= gas-particle phase) chemistry mechanism used		
	CTMs		
LLUR-SH	State Agency for Agriculture, Environment and Rural Areas Schleswig-		
	Holstein (Landesamt fr Landwirtschaft, Umwelt und Indliche Rume		
	Schleswig-Holstein)		
LUNG-MV	State Agency for the Environment, Nature Conservation and Geology		
	of Mecklenburg-Western Pomerania (Landesamt fr Umwelt, Naturschutz		
	und Geologie Mecklenburg-Vorpommern)		
MACC	Monitoring Atmospheric Composition and Climate (an atmospheric		
	chemistry data set)		
MARPOL	International Convention for the Prevention of Pollution from Ships		
	(convention focussing on environmental impacts by ships such as re-		
	lease of sewage, garbage, and harmful substances as well as atmospheric		
	emissions of selected air pollutants)		
MeRamo	Untersttzung der mit der Umsetzung der EU Meeresstrategie-		
	B ahmenrichtlinie befassten Behrden mittels eines a ssimilativen kosys-		
	tem mo dells (a research project)		
MOSSCO	Modular System for Shelves and Coasts (a research project)		
MSFD	Marine Strategy Framework Directive (an EU directive)		
N ₂ O ₅	dipitrogen pentoxide (an gaseous atmospheric compounds)		
NCO	NetCDF Operators (a set of command line programes to process		
1000	NetCDF files)		
NECA	Nitrogen Oxyde emission control area		
NetCDF	Network Common Data Format (a binary file format to store array-		
NetODI	ariented scientific data: the corresponding library to read NotCDE files		
	also is denoted as NotCDE)		
\mathbf{NH}^+	and is denoted as NetODF		
NH ₄	ammonia (as gaseous atmospheric compound)		
NO	nitrogen ovide (an gascous atmospheric compound)		
NO-	nitrogen dioxide (an gaseous atmospheric compound)		
NO_2 NO^-	nitrogen dioxide (an gaseous atmospheric compound)		
NO ₃	nitrate		
NO ₃	nitrate radical (an gaseous atmospheric compound)		
	introgen oxides (NO and NO_2); it does not mean oxidized nitrogen		
1 AIN DNA	peroxyacetyr intrate		
I INA DON	peroxymenic acid		
	Particulate organic introgen		
SHEDA	Sustainable Shipping and Environment of the Baltic Sea region (an EU		
SMOKE	Donus project) Sparce Matrix Operator Kernel Emissione Medeline Contem (cont		
SMOKE	sparse Matrix Operator Kernel Emissions <i>Modeling System</i> (an atmo-		
CMOVE (E	SMOKE - Just - Engen - 1 ((
SMOKE for Europe	SMOKE adapter to European data sets		
SILAM	Ship frame Emission Assessment Model (a model to calculate ship emis-		
TNO	Sions from AIS data)		
INO	Netnerlands Organisation for Applied Scientific Research (Nederlandse		
	Organisatie voor toegepast-natuurwetenschappelijk onderzoek)		
THREDDS	Thematic Real-time Environmental Distributed Data Services (service		
TINI	to provide access to datasets)		
UN	United Nations		
US EPA	U.S. Environmental Protection Agency		

Table S.2: List of abbreviations and acronyms part B (continuation from previous page)