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A novel modeling tool with multi-stressor functionality for organic contaminant transport and fate in the Baltic Sea

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HIGHLIGHTS

- A new model for organic chemical transport and fate in the Baltic Sea is presented.
- Physical and biogeochemical processes are linked to organic contaminant transport.
- The model is evaluated for PCBs, HCB and PCDD/Fs.
- The model can predict dissolved concentrations within a factor of ca 2–4.
- Predictions for concentrations in particulate matter and sediment are less accurate.

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ABSTRACT

The coupled physical–biogeochemical model BALTSEM, previously used to assess nutrient/carbon cycles and eutrophication in the Baltic Sea, has been expanded to include algorithms for calculations of organic contaminant environmental transport and fate. This novel model version (BALTSEM-POP) is evaluated for polychlorinated biphenyls (PCBs), polychlorinated dibenzo-p-dioxins/dibenzofurans (PCDD/Fs) and hexachlorobenzene (HCB) in Baltic Sea surface water and sediment. Modeled dissolved concentrations are usually within a factor of 2–4 of observed concentrations, however with larger deviations for furans. Calculated concentrations in particulate organic matter are less accurate (within factors of 1–700), likely due to errors in estimated pelagic biomass, particulate matter–water partitioning, and large natural variability in field data. Concentrations in sediments are usually predicted within a factor of 6. The good performance of the model illustrates its usefulness for exploration of contaminant fate in response to variations in nutrient input and climatic conditions in the Baltic Sea marine environment.

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1. Introduction

Several environmental problems threaten the ecological status of the Baltic Sea and its catchment. Alongside eutrophication and loss of biodiversity, pollution by organic contaminants and other potentially hazardous chemical substances is recognized as one of the major stressors in this environment (HELCOM, 2007). Organic contaminants are emitted within the Baltic Sea catchment, or transported to this region via air masses from far distances. A multitude of physical and biological processes in the environment influence the subsequent distribution and ultimate fate of the contaminants. Several multimedia transport and fate models have been developed during the past decades for the purpose of identifying and describing the dominant processes that determine the fate of organic chemicals as functions of various physical–chemical properties in order to better understand and predict chemical pollution (Arnot, 2009; Mackay, 2001; Wania and Mackay, 1999).

A handful of models have been developed and/or parameterized specifically for predicting the fate of chemicals in the environment of the Baltic Sea region (e.g. Breivik et al., 2010; Czub and McLachlan, 2004), with the dynamic POPCYCLING-Baltic being state-of-the-art and also the only model covering the entire region, including the marine environment, the catchment and the atmospheric compartment (Wania et al., 2000). This model has successfully reproduced historical concentrations of a number of chemicals measured in the Baltic Sea environment including hexachlorocyclohexanes, polychlorinated biphenyls (PCBs), polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs) and hexachlorobenzene (HCB) (Armitage et al., 2009; Breivik and Wania, 2002; Wiberg et al., 2009), lending confidence to the process descriptions and model assumptions applied.

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The rather static description of certain key environmental parameters, however, makes POPCYCLING-Baltic less suitable for assessing the future distribution of organic chemicals in the Baltic Sea: a) water fluxes (rain rates, river discharge, inter- and intra-basin exchange) and b) fluxes and production of particulate organic matter (POM) in rivers and in the marine environment, as well as between basins in the Baltic Sea, are given as long time averages based on data from the early 1990's, with no seasonal or inter-annual variation and without vertical resolution in the sea basins. Also, fixed monthly values for air temperatures, wind speeds and water temperatures (independent of air temperature) are applied and repeated each year of the simulation. Hence, there is no dynamic link between contaminant fate and variations in external forcing such as changing meteorology, hydrology and loads of carbon and nutrients from land and air. The lack of a modeling tool with such capacity impedes studies of potential future impact of multiple environmental factors and assessment of the complex interactions between e.g. climate change, eutrophication and contaminant fate. In this study we introduce a novel tool for modeling transport and fate of organic contaminants in the Baltic Sea, BALTSEM-POP, developed to meet these deficits. BALTSEM-POP is an extended version of the coupled physical–biogeochemical model BALTSEM (the BAltic sea Long-Term large Scale Eutrophication Model) (Gustafsson, 2000a, 2000b, 2003; Gustafsson et al., 2014; Savchuk, 2002; Savchuk et al., 2012). BALTSEM has previously been used to model nutrient flows, primary production and carbon cycling in the Baltic Sea (e.g. Eilola et al., 2011; Gustafsson et al., 2012; Meier et al., 2011) and is a key module of the Baltic Nest system (Wulff et al., 2001), a decision support system applied by the Helsinki convention to allocate country-wise nutrient emission reduction goals for the Baltic Sea Action Plan (HELCOM, 2013b).

We here describe the implementation of algorithms in BALTSEM for contaminant transport and transformation that enables the model to mechanistically calculate time-dependent concentrations of organic chemicals in water, suspended particulate organic matter and sediment. The accuracy of the extended model is evaluated by comparing simulated concentrations of PCBs, PCDD/Fs and HCB in these matrices with empirical observations, and deviations between measurements and model results are discussed. The overall goal is to provide and build confidence in a modeling tool that in a consistent manner integrates physical and biogeochemical dynamic processes with contaminant fate in the entire Baltic Sea, and facilitates the understanding of these complex interactions.

2. Materials and methods

2.1. Model development

BALTSEM-POP is a mechanistic non-steady state environmental model that simulates water fluxes, salinity, temperature, concentrations of oxygen, silica, nitrogen, phosphorous, carbon, plankton, detritus and organic pollutants in the Baltic Sea. The model builds upon the BALTSEM model, which combines a hydrodynamic (Gustafsson, 2000a, 2000b, 2003) and a biogeochemical module (Savchuk, 2002; Savchuk et al., 2012) as well as a recently developed module for carbon cycling (Gustafsson et al., 2014). BALTSEM-POP is an extended version of the latter version of the model with algorithms for transport and degradation of organic chemicals implemented in the original code. The model divides the Baltic Sea into 13 basins assumed horizontally homogenous but vertically highly resolved with variable number of layers in each basin (up to 250 layers) created by inflows of water with differing density (see Fig. 1). Water, nutrient and organic contaminant loads from rivers (monthly averages), point sources (yearly load) and the atmosphere (daily concentrations) are given as forcing for each basin, and the subsequent mixing and cycling via hydrodynamic and biogeochemical processes are calculated by the model. Other forcing data (3 hour resolution) are wind, cloudiness, precipitation, air temperature and relative humidity.

2.1.1. Hydrodynamic module

Water exchange between the basins and through the boundary to northern Kattegat is simulated by the hydrodynamic module as a function of wind, varying sea level and density differences between basins, and is also controlled by frictional resistance and dynamical flow contraction due to Bernoulli and Coriolis effects. Vertical mixing, stratification, sea-ice, heating/cooling and evaporation at the sea surface, and deep-water inflows are modeled dynamically (Gustafsson, 2000a, 2000b, 2003).

2.1.2. Biogeochemical module

Internal pelagic and benthic oxygen and nutrient dynamics (including nitrate, ammonia and phosphate) in each basin are driven by a number of biogeochemical processes. Functional groups of the pelagic system are phytoplankton (diatoms, cyanobacteria, other autotrophs) and zooplankton (heterotrophs), which together with dead organic matter (detritus) constitute the particulate organic matter (POM). In addition, a number of new state variables were recently added to the original BALTSEM version, enabling modeling of detrital carbon, dissolved organic carbon and nutrients, dissolved inorganic carbon and total alkalinity (Gustafsson et al., 2014). Detritus and phytoplankton sink and enter the model sediment compartment as benthic carbon, silica, nitrogen and phosphorous. Temperature dependent mineralization of organic matter is coupled to oxygen consumption and occurs in the water column and in the sediments. A fraction of the nitrate produced by mineralization and nitrification under aerobic conditions is released to the overlying water and the remainder is denitrified. Anaerobic conditions result in the release of mineralized nitrogen as ammonium. Phosphorous produced by mineralization in aerobic conditions is partly retained in the sediments and partly released to the water column, whereas anaerobic conditions result in the release of all phosphorous to the overlying water. Nutrients and carbon are lost from the system via export to the North Sea, burial in bottom sediments and denitrification. Carbon may in addition be lost to the atmosphere as the result of CO_2 outgassing.

2.1.3. Contaminant module

Organic contaminants enter the BALTSEM-POP Baltic basins via rivers, point sources and deposition from the atmosphere. Once transferred to the sea water, instantaneous horizontal mixing is assumed, and the physical module of BALTSEM-POP calculates diapycnal mixing and lateral transports between sub-basins. The descriptions of the additional physical fate processes relevant for organic contaminants in the pelagic and benthic systems are taken from previously published multi-media fate and transport models, mainly the POPCYCLING-Baltic model (Wania et al., 2000) and CoZMo-POP 2 (Wania et al., 2005).

For clarity, the equations for phase partitioning, intermedia transport and degradation are here, as in POPCYCLING-Baltic, expressed in fugacity terms (Mackay, 2001), i.e. based on D-values (chemical transport capacity of a pathway, mol h^{-1} Pa^{-1}) and Z-values (fugacity capacity of a phase, mol m^{-3} Pa^{-1}) as conventional in fugacity modeling, although the final mass balance is formulated in terms of concentrations to follow the original BALTSEM calculation scheme. Fugacity f (Pa) is related to concentration via the fugacity capacity of a phase ($C = f \cdot Z$) and Z is calculated for all relevant environmental media from equilibrium partition coefficients K_{xy} (m^3_y m^{-3}_x) of the corresponding environmental phase pairs (Mackay, 2001). The physical chemical properties and environmental characteristics (other than those already specified or calculated in the original BALTSEM model) which are required for the descriptions of contaminant transport and transformation are listed in Tables S1 and S2.

2.1.4. Description of chemical processes

BALTSEM-POP calculates concentrations of 7 state variables in addition to the 32 that are calculated by the original model: contaminant concentrations in detritus (subscript “detr” used in all equations),

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