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Predicting the impact of seasonal fluctuations on the potential ecotoxicological risk of multiple contaminants in the River Scheldt discharge into the Western Scheldt estuary

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ABSTRACT

The study site, Land van Saeftinghe, is an area within the Western Scheldt estuary with Special Protection Area (SPA) status for the EU Birds directive. We used a combination of hydrodynamic and water quality monitoring, hydrodynamic and water quality and modeling, ecotoxicity modeling and observations on the ecological status to correlate the water quality to the observed ecological status of the study site.
The monitoring and modeling results show that the copper concentrations are elevated above the Maximum Tolerable Concentration (MTR) during the whole year, while zinc and cadmium show a spring peak (>MTR). Other metals, and all the measured organic contaminants where below the MTR.
The peak in the three metals during springtime translates into an increase in the ecotoxicity, as expressed by the calculated multi-substance Potentially Affected Fraction (ms-PAF). The ms-PAF peaked at 25% for all organisms, and 30% for benthic invertebrates. The observed ecological status for the study site at the time of monitoring (2000) was Maximum Ecological Potential (MEP). This result seems to be in contradiction with the exceedance of the MTR for three metals during spring time. However the calculated ms-PAF during the spring peak of 25% is deemed acceptable based on current policy, therefore potential ecotoxic stress is within acceptable boundaries. The ms-PAF results therefore do not contradict the MEP status.
The evaluation of the ecological status versus the water quality within the EU Water Framework Directive (WFD) can be improved by using the calculated ecotoxicity (ms-PAF) instead of the water quality. We propose an additional step for water bodies which are currently 'at risk', based on their chemical status. In this additional step, the ms-PAF is calculated for all contaminants in the water phase, not discriminating between priority and non-priority substances. The outcome of this calculation defines if the water body is at risk.

1. Introduction

The Western Scheldt (WS) estuary is an important ecosystem with mudflats, sandbanks and raised saltmarshes, and has a special protected status within the European Union (EU) Habitat Conservation and Protection Guidelines, Birds directive (Directive 2009/147/EC). Protection of the estuary is based on both ecological and chemical status, which refers to a number of specified toxic substances in the context of the Water Framework Directive (WFD) (Directive 2000/60/EC). The discharge and sedimentation of contaminants by densely populated and industrialized areas of Belgium, the Netherlands and France are major sources of pollution (Ouboter et al., 1998). Since there are still challenges in maintaining the chemical status of the estuary, attempts to restore the ecological status of the estuary might be adversely impacted (Escaravage et al., 2004). We focused on a small part of the Western Scheldt area, the Land van Saeftinghe. The Land van Saeftinghe saltmarsh is considered a Special Protection Area (SPA) and is located close to the harbor of Antwerp and the Scheldt River. The questions addressed in this case study are three folded.

1) Can we use monitoring data, which is limited in time and space, to predict the daily (tidal) and seasonal (river discharge) water quality differences in the estuary.
2) If we can predict the water quality on spatial and time scale for the estuary, can we then correlate the chemical status, as defined by the WFD water quality standards, to a potential ecotoxicological risk?
3) Does the calculated potential ecotoxicological risk give a better match with the observed ecological quality state (as defined by the WFD) of the estuary?

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By answering these three questions successively, we drafted an addendum to the current WFD chemical status classification by introducing an extra evaluation step; the calculation of the multi-substance Potentially Affected Fraction (ms-PAF). The ms-PAF calculates the potential ecotoxicological risk for all contaminants in the water phase.

2. Material and methods

2.1. General description on the approach

To derive the potential ecotoxicological risk for the study site "Land van Saeftinghe", and compare the potential ecotoxicological risk with the observed ecological status a number of steps were taken:

1. Setting up a hydrodynamic model (SOBEK 1D/2D) for the Western Scheldt (including the suspended sediment transport), based on tidal derived exchange (calibrated on water surface elevation), and varying river discharge (calibrated on the daily discharge).
2. Setting up a water quality model (D-water Quality) based on measurements of the water concentrations of WFD priority substances at different locations within the Western Scheldt estuary. Also, taking into account the suspended sediment concentration and the partitioning of contaminants between the dissolved water phase and suspended matter.
3. Calculations of the potential effected fraction for multiple contaminants (the ms-PAF) within the study site were based on the resulting water quality predictions using the OMEGA model.
4. Comparison of the ms-PAF with the ecotope quality status for the study site to determine if toxic stress can be correlated to the observed ecological status.

2.2. Hydrodynamic model

Elskens et al. (2014) has published a 3D model for the WS estuary to carry out environmental simulations based on a flexible resolution model (SLIM) for the hydrodynamics (including the salinity, cohesive suspended sediment and metal partitioning based partially on equilibrium equations and empirical relations). We have chosen to apply a 1D/2D approach for the WS estuary. The hydrodynamic model applied is part of the Deltares model system design and analysis tools (SOBEK Suite, 2014). The SOBEK 1D/2D model is based on the national grid for the Dutch River systems (the South-West Delta model), taking into account the bathometry and variation in bottom roughness (friction values) of the Western Scheldt, the discharge on the River Scheldt, and the tidal influence of the North Sea Boundary (Meijers and Groot, 2007). A 1D/2D model describes effectively the situation at this case study site, the Land van Saeftinghe, near the eastern River Scheldt boundary. Typical processes which require a 3D design, like density driven stratification and predicting channel development are of importance on the middle and western part of the estuary, not the currently modeled eastern part.

Water quality is calculated with the D-water quality module within the Deltares systems design and analysis tools (SOBEK Suite). The SOBEK 1D/2D and D-water Quality models include the transport and sedimentation of suspended matter and the distribution of contaminants between the dissolved phase and suspended matter as expressed by partition coefficients. SOBEK is used for a broad spectrum of water quantity and quality related questions in mainly one dimensional (1D) network systems (e.g., rivers, channels, sewers) and two-dimensional systems (2D) systems based on a horizontal grid (e.g., floodplains and estuaries) [5]. The advantage of using a 1D based system is that the calibrated national South-West Delta model (Meijers and Groot, 2007) can be used. By including the additional 2D layer with a cross section of the bathymetry for the cells, the overall approach can split the 1D model into spatial depended friction maps (outside the main channel) for the bottom roughness. This results in varying flow velocities and therefore spatial differences in water residence time and the sedimentation of suspended matter.

The South West Delta model is a 1D Sobek model with two channels for the Western Scheldt. The total channel flow was therefore divided over the cross section of the Western Scheldt (latitude dependent) with an average water depth of 5 m (Van Gils, 2005). For the water quantity calculation, the tidal influence (western model boundary) and river discharge (eastern model boundary) of the River Scheldt was calculated using a 2 h time step based on input from the Sobek model South West Delta for the year 2000 (Meijers and Groot, 2007). For the 2D grid of the Western Scheldt, a size of 1 × 1 km was used for each cell.

2.3. Water quality and suspended sediment modeling

Water quality data was collected by the Dutch Directorate–General of Public Works and Water Management (Rijkswaterstaat/RWS) and stored in the on line database 'Waterbase' (Waterbase, 2014). We used concentration data for the year 2000 for the WFD priority contaminants concentrations at "Schaar van Oude Doel" (near the eastern model boundary) and for background, the North Sea concentrations (western model boundary). Water quality was measured on a two weekly base. Water quality measurements also include the suspended sediment concentration. Suspended sediment transport is important since many contaminants are in part bound to the solid phase. The process of partitioning between dissolved and solid phase is well described (Langmuir, 1979; Stumm and Morgan, 1981).

2.3.1. Eq. (1) partition coefficient

$$Kp = \frac{C_{(suspended\ \ solid)}}{C_{(dissolved)}}\left(\frac{l}{kg}\right) \tag{1}$$

$K_p = partition\ coefficient\ (-)$
$C_{suspended\ solid} = concentration\ contaminant\ bound\ to\ suspend\ solid\ (mg/kg)$
$C_{dissolved} = concentration\ contaminant\ dissolved\ in\ water\ (mg/l)$

For organic contaminants the partition coefficient was normalized by the organic carbon content of the suspended sediment (POC), resulting in the K_{OC}. The K_p (metals) and K_{OC} (organic contaminants) partition coefficients are based on the default Dutch values for suspended sediments (Commissie Integraal Waterbeheer, 2000). The contaminants Cd, Cu, Zn, naphthalene, hexachlorobenzene (HCB) and α,β,γ hexachlorocyclohexane (HCH) were selected based on their presence above detection limit in the Dutch on-line water quality database (Waterbase, 2014) for the location "Schaar van Oude Doel". Table 1 lists the resulting partition coefficients for the modeled contaminants.

Sediment transport was modeled with a resuspension - sedimentation approach. The bed shear stress is the primary parameter for resuspension and sedimentation. The bed shear stress is a function of the flow velocity,

Table 1
Calculated partition coefficients for modeled pollutants.

		log Kp (l/kg)
Metals	Cadmium	4.93
	Copper	4.53
	Zinc	4.86
		log Koc (l/kg)
PAH's	Naphtalene	2.85
Chlorobenzenes	Hexachlorobenzene (HCB)	4.61
Hexachlorocyclohexane	Alpha-HCH	3.39
	Beta-HCH	3.36
	Gamma-HCH (lindane)	3.37