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Dealing with uncertainty in water quality models of the North Sea

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During the last 20 years, several chemical water quality models of the North Sea have been constructed. In general, the available processes, knowledge, data, and parameters have been integrated to describe the distribution, cycling, and fate of metals and organic compounds. Thus, it is possible, from a scientific point of view, to evaluate and identify gaps in knowledge. In some countries, these models have also been used to verify whether emission reduction measures were sufficient to attain water quality objectives. Intercomparisons have demonstrated that various models still show considerable differences in the simulated concentrations of substances. There is still a need for appropriate validation data. The question arises whether further development of North Sea water quality models could benefit from a more systematic approach to uncertainty analysis and from establishing unambiguous quality criteria for evaluating model results. International cooperation is important, to improve both field knowledge as well as models. Better "tuning" of the data necessary for monitoring purposes and model parameterization, initialization, and validation still needs attention. ICES could intensify its coordinating role, using its organizational network and data holdings.

Keywords: North Sea, uncertainty analysis, water quality models.

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Introduction

The cycling, pathways, and fate of substances in marine waters have been studied since the 18th century. Initially, the interest was purely scientific, but since the 1960s, it has been recognized that elevated concentrations of natural and xenobiotic substances cause adverse effects on marine ecosystems (e.g., ICES, 1969; Cole, 1971). This stimulated scientific research with a problem-oriented character. The resultant knowledge was necessary to assess the consequences of political decisions. Sampling cruises were conducted to monitor spatial and temporal distribution of these substances and to study the processes which determine substance behaviour. Models were developed and applied to integrate different disciplines (hydrodynamics, physics, chemistry, biology), interpret observations, compute variables that cannot be measured directly (such as fluxes through a cross-section of the sea), and link sources to concentrations and effects in the field. Some examples of North Sea models are reported in ICES (1988), van

Pagee *et al.* (1988), Prandle *et al.* (1996), Tappin *et al.* (1997), Moll (2000), and Søiland and Skogen (2000).

Model predictions have become increasingly important tools for evaluating policy measures (e.g., Backhaus in ICES, 1988). Models are also being used to screen potentially harmful substances. However, as will be illustrated in this paper, model predictions of the fate and effects of natural and xenobiotic substances in the North Sea still have considerable uncertainties. Some suggestions will be made for dealing with model uncertainty, model and monitoring integration, and the role international organizations like ICES could play.

Uncertainty in water quality models

One objective of water quality models is to simulate concentrations in the environment as a function of loads from different sources (e.g., rivers, atmosphere, adjacent seas, and direct discharges) and of interventions such as dredging or land reclamation. By comparing the calcu-



Figure 1. Calculated mean annual water flows through the English Channel (m3 yr⁻¹). The median is also depicted. References: 1) 1994–1995 (Statham *et al.*, 1999); 2) 1990–1991 (Statham *et al.*, 1999); 3) Tappin *et al.* (1997); 4) Postma *et al.* (1988, cited in Tappin *et al.*, 1997); 5) Zwolsman (1994, cited in Tappin *et al.*, 1997); 6) Prandle *et al.* (1996, cited in Tappin *et al.*, 1997); 7) Jones and Howarth (1995, cited in Tappin *et al.*, 1997).

lated concentration with calculated effect concentrations or water quality objectives, a measure is obtained for the potential effect of the emissions or interventions on the ecosystem.

The concentration of a substance at a certain time and place is the result of (local) inputs, transport to and from adjacent water bodies, and local biological, chemical, and physical processes which affect the substance. This is represented in a mass balance equation (e.g., Schnoor, 1996), which can be expressed in a simplified way as: $C_{x,t} = f(loads, transport, processes)_{x,t}$.

Basically, two types of uncertainty can be distinguished: 1) model concept (formulations, spatial, and temporal definition) and 2) (measurable) input parameters (such as the inputs of substances, water flows, and sorption coefficients). Important sources of uncertainty are spatial or temporal variability of parameters where the model assumes uniform or constant values, steady-state instead of dynamic conditions, and empirical inaccuracy or lack of data (Cowan *et al.*, 1995; Ragas *et al.*, 1999).

Sources of uncertainty

Inputs of substances

Sources of substances to the North Sea include direct discharges (e.g., from shipping and offshore activities,



Figure 2. Calculations of the net annual input of suspended particulate matter into the southern North Sea through the English Channel (Mtonne yr⁻¹). The median is also given. Data from Velegrakis *et al.* (1999).

outfalls), disposal of dredged materials, rivers and estuaries, atmospheric deposition, and imports through open sea boundaries such as the English Channel (e.g., Salomons *et al.*, 1989; Wulffraat *et al.*, 1993; Tappin *et al.*, 1997). The latter three will be discussed here.

The basic formulation to compute a substance load or flux is: water flow (volume/time) times concentration $(Q \times C)$. Q may be measured (e.g., a river discharge, or precipitation) or computed by a model (e.g., flow through a cross-section of the North Sea). Q as well as C vary in time and space. Several methods are available to calculate annually averaged loads from time-series of Q and C (de Vries and Klavers, 1994).

Discharge and concentrations in rivers are variable, which causes temporal variations in the load. Especially for rain-fed rivers, discharge peaks may contribute a major part of the annual load, e.g., for the River Meuse, 80% of the suspended matter load is transported in 20% of the time (de Vries and Klavers, 1994). Sampling that is too infrequent causes poor accuracy and precision of calculated loads. Another important factor which affects riverine inputs to the North Sea is estuarine retention (Zwolsman, 1994). The filtering capacity for estuarine substances depends on physical and (bio)chemical properties of the estuary and the substance under consideration. For instance, in the Scheldt estuary (freshwater residence time 60 d, fluvial SPM retention 80%), the calculated filtering capacity varies between 54% and 77%



Figure 3. Calculated net annual inputs of cadmium (Cd), copper (Cu), lead (Pb), and zinc (Zn) into the southern North Sea through the English Channel (tonne yr⁻¹). References: 1) Statham *et al.* (1999); 2) Statham *et al.* (1993, cited in Statham *et al.*, 1999); 3) Tappin *et al.* (1997, low estimate); 4) Tappin *et al.* (1997, high estimate).

for metals and 76% to 97% for PCBs (Zwolsman, 1994). For the Rhine-Meuse estuary (residence time 4 d, fluvial SPM retention 45%), the author reports filtering capacities of 20–42% for metals and 26–32% for PCBs. Thus, using data from monitoring stations at the riverine end of the estuary may lead to a considerable overestimation of loads to the sea.

At the open sea boundaries, it is difficult to determine Q and C. Estimates of the mean annual flow through the English Channel into the North Sea differ by a factor of 2 (Figure 1, data from or cited in Statham et al., 1999; Tappin et al., 1997; Prandle et al., 1996; Zwolsman, 1994). Concentrations can be highly variable in time, for instance, as a result of wind-induced resuspension of sediments and primary production. Most estimates of the net annual input of suspended sediment through the English Channel into the North Sea vary by a factor of 3, between 10 and 30 Mtonne yr⁻¹ (Figure 2, data from compilation in Velegrakis et al., 1999), but extreme estimated values differ by one order of magnitude. Estimates of the net annual input of metals into the North Sea through the English Channel vary from a factor of 2 for copper to a factor of over 10 for lead (Figure 3, data from Statham et al., 1993, 1999; Tappin et al., 1997).

Routine measurements of atmospheric deposition at sea are difficult. One of the reasons is disturbance of measurements by sea spray (Baart *et al.*, 1995). Further, it is difficult to set up an appropriate sampling grid at sea. Estimates are often based on extrapolation of measurements at coastal stations or calculated by an emission-based model (Wulffraat *et al.*, 1993). The computed total annual deposition in the North Sea for some heavy metals differs considerably for direct measurements at sea, extrapolation of coastal measurements, and model calculations, up to a factor of over 10 for cadmium and copper (Wulffraat *et al.*, 1993). For emissionbased model calculations of the annual average atmospheric deposition, Baart *et al.* (1995) reported estimated uncertainties of factors of 1.5–2.5 for metals, 2–5 for PCBs, and 2–3 for PAHs.

Transport

The accuracy of model-calculated concentrations and spatial distribution of substances transported by advective and dispersive processes is first and foremost dependent on whether the dominant advection and mixing processes have been properly captured in the model.

Transport of dissolved substances that behave conservatively, e.g., S, can be calculated accurately once inside a system, but transport across open boundaries is very sensitive to even minute errors in the boundary condition, as the transport flux is C_b (Q_b , with Q_b being of the order of 7–14 (10^9 m³ d⁻¹ for the net daily inflow into the North Sea through the Strait of Dover (Tappin *et al.*, 1997).

The transport of particulates (and the adsorbed contaminants) is even more uncertain, as the particulates are subject to gravity and thus have a tendency to settle out as soon as turbulent mixing is insufficient to keep them suspended. As turbulence levels are both temporally (wind) and spatially (depth, topography) highly variable, 2D transport models with simple turbulent mixing parameterizations cannot be expected to provide much more than very coarse estimates of the transport.

In the North Sea model advection-dispersion study (NOMADS), the majority of the available 2D and 3D models for the North Sea were intercompared (Proctor, 1997). This study only considered the transport of water and salt and did not address the transport of particulates. One conclusion was that all the models reproduced the generally accepted features of circulation, advection, and dispersion within the southern North Sea, but there are differences between the results of the different models.

The models agreed on the direction of travel of particles released, but disagreed by up to a factor of 4 as to the distance travelled. The calculated spread of a contaminant was shown to be dependent on the proportion between advective and diffusive transport, and the model grid size, with large grid models being more dispersive.

The authors conclude that the variability in the underlying hydrodynamics is the single largest factor in the variation seen in the results from the various models, but that the methodology adopted in the analysis has not been able to separate the causes of the differences. Before the effects of advection and dispersion can be considered quantitatively, differences in the underlying



Figure 4. Modelled dissolved cadmium concentration (mg l^{-1}) in the Dutch coastal zone for different observed values of Kd (log[l kg⁻¹]) as a function of the distance to the coast (km). From Stolwijk *et al.* (2000).

hydrodynamics need to be removed. Alternatively, the models might have been validated by comparison with observations. However, for most substances of interest, a suitable data set probably does not exist, and compiling it is not a trivial exercise.

The uncertainties in calculated transport will only be reduced with the use of models that demonstrably (by hindcasting) reproduce observed spatial and temporal concentration patterns in the substances of interest. This almost certainly requires major improvements in the treatment of resuspension/deposition processes and most likely requires full 3D models with advanced turbulence closure schemes.

Process formulations and process parameters

Metals and organic substances in the marine environment are subject to complex (bio)chemical processes (Schwarzenbach *et al.*, 1993; Stumm and Morgan, 1996). Both types of substances become associated with solid matrices such as particulate organic carbon (POC) and mineral surfaces. Dissolved organic substances also associate with dissolved organic carbon (DOC), while metals may form various complexes in solution, depending on such factors as pH, redox potential, and salinity. Organics are subject to transformation reactions (such as hydrolysis, biodegradation, and photolysis). Vertical transport processes (such as volatilization, bottom-water exchange) are also important.

Despite the complexity of the behaviour of substances, it is often highly simplified in water quality models because detailed process formulations or accurate values of process parameters are not yet available. Some models even assume conservative behaviour of substances (Stolwijk *et al.*, 1998). The uncertainty associated with the use of simplified formulations will be illustrated with a case for the partitioning coefficient.

The partitioning coefficient (Kd) represents all sorption and complexation reactions which lead to the (observed) distribution between particulate matter and the (total) dissolved phase. Because of the complexity of the underlying processes, values of Kd, as observed in the field, are highly variable in space and time (e.g., Balls, 1989; Stolwijk et al., 2000). For example, the Kd for cadmium in the Dutch coastal zone during 1983-1988 varied considerably between summer (log Kd 5.1-6.0 log[1.kg⁻¹]) and winter (log Kd 3.7-5.6 log[l.kg⁻¹]) (Stolwijk et al., 2000). The difference was attributed to phytoplankton growth in the summer. A water quality model for the Dutch coastal zone, which assumes a constant value of Kd, appeared to be quite sensitive to the Kd value. The simulated dissolved cadmium concentration in the coastal zone varied up to a factor of 7 for the different Kd values (Figure 4, data from Stolwijk et al., 2000).

Environmental standards

An important objective of water quality models is to evaluate whether environmental quality values (EQVs) will be met for different management (load reduction) scenarios. Environmental standards are enforced in national laws and thus are accurate from a legal point of view. However, several recent publications discuss the scientific value of EQVs.

A recent summary shows that sediment quality values (SQVs) from more than 30 countries vary over orders of magnitude and are sometimes below background values (Chapman *et al.*, 1999). Augustijn *et al.* (in press) report the uncertainty in the "chemical yardstick" applied in the Netherlands. For cadmium and benzo(a)pyrene, the maximum permissible concentration appears to be quite uncertain, which causes different sediment quality classes to overlap (for instance, in the Western Scheldt in 1987). Long *et al.* (1998) found that SQGs (sediment quality guidelines) provided reasonably accurate estimates of extreme concentrations that are either clearly toxic or clearly non-toxic in laboratory bioassays. However, for intermediate concentrations, the use of SQGs should be accompanied by other tools.

Several factors contribute to the uncertainty in EQVs. The actual toxicity of a certain total sediment concentration is very dependent on highly variable environmental factors such as hardness of water, pH, pe, temperature, organic carbon content, etc. (Chapman *et al.*, 1999). Also, the derivation of no-effect concentrations (NOECs) is debatable (Augustijn *et al.*, in press). NOECs should be representative for the ecosystem under consideration (Chapman *et al.*, 1999).

Sensitivity analyses and validation of North Sea water quality models

Although uncertainty and sensitivity analyses are important steps during model development (Cowan et al.,



Figure 5. Comparison of simulated and annual averaged dissolved cadmium concentrations calculated from observations at different locations in the North Sea. Concentrations are shown relative (%) to the field data (which were set at 100%). Field data from 1985 (ICES); simulations by four models (from Stolwijk *et al.*, 1998).

1995; Schnoor, 1996), they are not reported for all published water quality models for the North Sea. Some examples are reported in Tappin *et al.* (1997), Stolwijk *et al.* (2000), and Sonneveldt and Laane (2001). Tappin *et al.* (1997) reported a factor of 2 in uncertainty in the estimated total input of metals to the southern North Sea (except a factor of 5 for Pb). This range was reflected in their modelling results. A comparable range in uncertainty of inputs (\pm 50% for particulate metals and \pm 60% for particulate PCBs and PAHs) is reported for the Dutch coastal zone by Sonneveldt and Laane (2001). This range appeared to be a major source of uncertainty which, in the case of lead and PCBs in bottom sediments, dominated over uncertainty in process parameters. The example for Kd was discussed above.

Another way to assess the performance of water quality models is through model intercomparisons such as the NOMADS project (see above). Within the framework of the Environmental Assessment and Monitoring Committee (ASMO) of the Oslo and Paris Commissions (OSPAR), intercomparisons were carried out for accidental spill models (OSPAR/ASMO, 1997), eutrophication models, and contaminant models (OSPAR/ASMO, 1998; Stolwijk et al., 1998). The latter compared the performance of five water quality models for the North Sea. The simulated yearly averaged dissolved cadmium concentration for 1985 deviated considerably between the models and with ICES data (Figure 5, Stolwijk et al., 1998). The model approaches appeared to be quite different. The representation of physics ranged from 2D with steady state residual flow to 3D with actual wind forcing. The chemical processes included in the models ranged from none (conservative transport) to detailed formulations for sorption, sediment-water exchange, etc. Further, validation of the model results appeared to be difficult because of a lack of (quality-controlled) field data (Stolwijk *et al.*, 1998).

A systematic approach to uncertainty analysis (supported by statistical techniques, such as Monte Carlo simulation) is not common practice yet for North Sea water quality models. Recently, the cost-function approach has been suggested as a step forward towards a standardized and objective method for the validation of North Sea models and model intercomparison (Søiland and Skogen, 2000; Stolwijk *et al.*, 1998). In other disciplines (ecology, risk analysis of substances, life-cycle analysis), statistical techniques are already being applied frequently (e.g., Omlin and Reichert, 1999; Witting, 1999; Hertwich *et al.*, 1999; Huijbrechts *et al.*, 2000).

Another issue is how to decide when a water quality model for the North Sea is "good enough". Despite the uncertainties which have been discussed above, models have already been able, in some cases (for some substances in specific areas), to reproduce field data (ranges overlap), e.g., Tappin *et al.* (1997), Sonneveldt and Laane (2001), Søiland and Skogen (2000), and Moll (2000).

However, generally accepted quality criteria for North Sea water quality models do not exist yet.

Loague (2000) stresses the importance of rigorous, non-subjective, model performance criteria and simulation protocols which include uncertainty impacts when models are used for decision support.

The question arises whether the development of North Sea water quality models would benefit from a systematic approach to uncertainty analysis and from establishing unambiguous criteria for evaluating model results.

Conclusions

Intercomparisons demonstrated that various models still show substantial differences in simulated concentrations of substances. This is not surprising in view of the considerable uncertainties in the input parameters of the models and gaps in (field) knowledge.

Sufficient data for validation and parameterization are crucial for improvement of models. Still, a lack of appropriate data is often mentioned as a major problem (e.g., Radach in ICES, 1988; Stolwijk *et al.*, 1998), despite efforts to combine existing data sets (e.g., the North West European Shelf Project NOWESP, Berlamont *et al.*, 1996). Therefore, better "tuning" of the data necessary for monitoring purposes and for model parameterization, initialization, and validation still needs attention.

It should be realized that, besides models and data, water quality objectives also are often ill defined from a scientific point of view. Comparing model results with such uncertain water quality objectives will add uncertainty to the decision-making process.

Most authors of water quality models discuss the major weaknesses of their models. A more realistic representation of the hydrodynamics (appropiate spatial and temporal schematization, actual wind forcing) would be a major improvement of most models (e.g., Proctor, 1997). Also, more accurate and precise data on the inputs of substances is often identified as a major uncertainty (e.g., Sonneveldt and Laane, 2001; Søiland and Skogen, 2000). With respect to water quality processes, several authors mention the interaction between water column and bottom sediments as an important knowledge gap in their models (e.g., Tappin *et al.*, 1997; Søiland and Skogen, 2000; Moll, 2000).

However, priorities for improvement of models will depend on the objective and scope of the models. The bottom sediment quality of the Dutch coastal zone could be represented accurately without a detailed hydrodynamical model (Sonneveldt and Laane, 2001). In contrast, the accurate prediction of, for example, phytoplankton blooms will require detailed modelling of the underlying physical, chemical, and biochemical processes.

Although some uncertainty analyses of water quality models for the North Sea have already been carried out, a systematic approach is not yet common practice. There are also no generally accepted criteria yet to decide whether a model is good enough for a certain purpose. For environmental monitoring data, quality criteria have been established for acceptance of analytical results (e.g. Wells and Cofino, 1997). Similar criteria for acceptance of model results would be very useful (if not necessary) when models are being used for decision support and policy-making.

Substantial progress in the development and quality assurance of North Sea water quality models cannot be achieved without intensive international cooperation.

ICES had already taken initiatives more than a decade ago to stimulate scientific cooperation with respect to the development and validation of water quality models (e.g., ICES, 1988), and in recent years, this topic has attracted the attention of the ICES Working Group on Shelf Seas Oceanography. However, the international cooperation with respect to model improvement is still not as intensive as the cooperation with respect to the quality assurance of monitoring, the latter being institutionalized in organizations like QUASIMEME (Wells and Cofino, 1997) and ICES. Given the possible role of water quality models in decision-making, it is advisable that international cooperation for the further improvement and quality assurance of water quality models is intensified. ICES could strengthen its role here, using its organizational network and data holdings.

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