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Water quality modelling of the western Scheldt estuary

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Abstract

In 1987 the National Institute for Coastal and Marine Management (the Netherlands) initiated the SAWES project (Systems Analysis WEstern Scheldt). The main goals of the project were to acquire knowledge with respect to the pollution problems in the Scheldt estuary and to apply this knowledge to management issues of the Scheldt on an operational level. The main interest was to understand quantitatively the relation between inputs of polluting substances and effects on the ecosystem. In the framework of the project, a water quality model for the Scheldt estuary was made. In 1995, the model area was expanded to include the Belgian coastal region at the mouth of the estuary.

The model calculates the fate of discharged substances and establishes the relation between pollution inputs and the resulting water quality, including general water quality (oxygen, pH, alkalinity, major ion chemistry and nutrients) as well as pollutant concentrations. The model incorporates all chemical processes which affect these concentrations, including the precipitation/dissolution of metal sulphides which to a large extent controls the fate of trace metals. Based on calibration and verification exercises, it has been shown that the model provides a good representation of the physical and chemical processes taking place within the estuary and can therefore be used to support policy development for the estuary. For example, the model can compute how the water and sediment quality in the estuary will respond to reduced inputs of waste or to such human activities as dredging.

Introduction

The river Scheldt crosses France, Belgium and the Netherlands on its way to the North Sea. It has a length of 355 km and a drainage area of about 22 000 km^2, mostly within Belgium. The average fresh water flow at Rupelmonde is about 100 m^3/s. The estuary of the Scheldt covers a length of 95 km, between the village of Rupelmonde in Belgium and the city of Vlissingen in the Netherlands.

The upper estuary (km 0–40) consists of one channel with a width between 0.4 and 2 km. The lower estuary (km 40–95) is wider, up to 8 km, and consists of deep and shallow parts, with different ebb and flood channels. The average depth is about 11 m, while the maximum depth is 40 m. The tidal motion dominates the water movement in the estuary and significant salt intrusion may be observed over the full 95 km. Normally the estuary is well mixed, except in the upper estuary under high fresh water flow conditions. The main functions of the estuary are shipping, fishing, recreation and sand extraction. The ecological value of the area and the natural landscapes are also of significant importance to the region. However, there are two significant environmental problems in the Scheldt estuary:

(1) In order to maintain the shipping routes to Antwerpen and other smaller harbours, intensive dredging and dumping of (contaminated) sediments is necessary; and

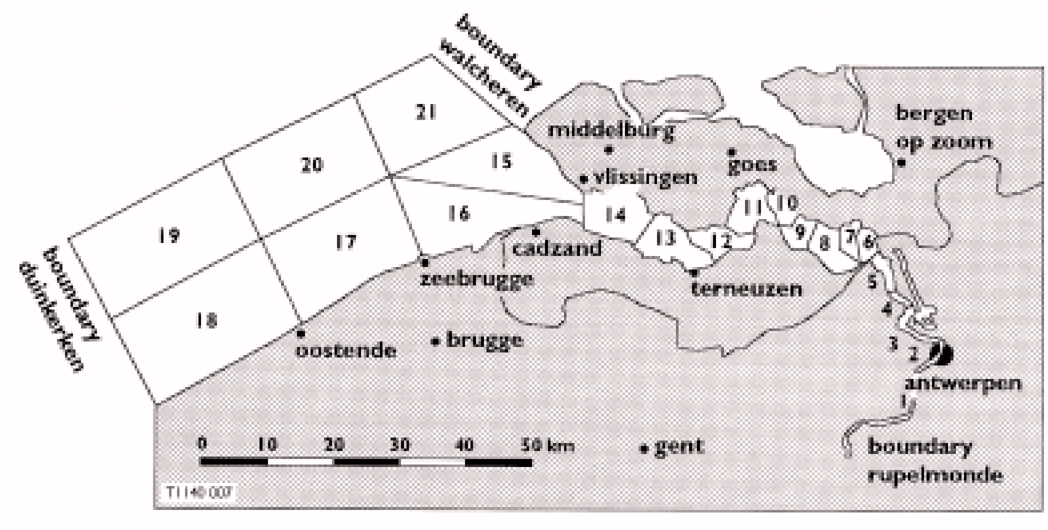

Figure 1. Physical schematisation used in the water quality model.

(2) The area is used to dispose of large amounts of domestic and industrial waste water.

In 1987 the National Institute for Coastal and Marine Management (the Netherlands) initiated the SAWES project (Systems Analysis WEstern Scheldt). The main goals of the project were to acquire knowledge with respect to the pollution problems in the estuary and to apply this knowledge on an operational level. The main interest was to understand the relation between inputs of polluting substances and effects on the ecosystem, with special attention given to heavy metals, specifically cadmium, copper and zinc. A model instrument was created to support policy development and management of the estuary by means of systems analysis. In 1995, the model was expanded to include the Belgian coastal region at the mouth of the estuary. The complete study area is shown in Figure 1.

The systems analysis approach which forms the basis for the present water quality model and its application, has the following main characteristics. The *water system* under consideration is subject to the negative impact of different *human activities*. Consequently, it suffers certain *effects* which may in turn influence the human activities. The systems analysis requires an accurate definition of the relevant impacts from human activities, as well as the changes therein, and the relevant effects. Based on those definitions the design criteria for the water quality model are established.

Description of the model instrument

The water quality model is one component of the complete model instrument, which consists of a self standing data base, the model itself, and a set of post processing, graphical and analysis tools. The entire instrument, also known as a Decision Support System (DSS) runs on an IBM compatible PC. The water and sediment quality calculations have been made using the general water quality model DELWAQ v4.02 (Delft Hydraulics, 1995a and 1995b). This is a deterministic and dynamic model and takes into account relevant polluting substances in the estuary, as well as the main physical, chemical and biological processes affecting the substances of concern.

The most important characteristics of the model are:

- based on mass balance of all modelled substances;
- transport of dissolved substances, calculated on the basis of the water flow (tidally averaged advective transport) and dispersion;
- transport of particulate substances (such as adsorbed metal species), calculated on the basis of suspended sediment transport;
- a number of non-instantaneous, slow kinetic water quality processes, particularly with respect to metal release due to sulphide oxidation, and oxygen and nitrogen processes;
- calculation of chemical equilibrium for instantaneous water quality processes dependent on macro chemistry (oxygen, pH, alkalinity, ma-

jor ion chemistry and nutrients), partitioning and speciation of metals and phosphorous;
- visualisation of substance mass balances in order to see quantitatively the importance of various different processes.

Measurements of freshwater balance, sediment balance and pollution loads into the region are part of the self standing data base of the Scheldt estuary, and serve as the input to the water quality model. The model process formulations and parameters are for the most part well accepted equations from the general literature on water quality processes. For a few processes, new formulations were written based on water quality measurements in the Scheldt estuary. The following sections describe the physical schematisation, transport of dissolved and particulate substances, the coupling with external loads, and the water quality processes per group of substances.

Physical Schematisation

The estuary and the coastal region were divided into 21 homogeneous model elements, based on the measured concentration gradients (Figure 1). The estuary is represented by 14 elements, while the coastal region is represented by the remaining 7 elements. The coastal region is schematised in two rows of elements parallel to the coast, the first of which has a width of about 15 km. The second off-shore row is wider, and corresponds to the deeper region of the coast. The division of these two rows into individual elements is based on the location of discharges into the coastal region.

Transport of dissolved and particulate substances

The transport of dissolved substances is calculated by the advection-dispersion equation, which includes terms for loads as well as chemical processes. In one spatial dimension the equation reads:

$$\frac{\partial CA}{\partial t} = -\frac{\partial CUA}{\partial x} + \frac{\partial}{\partial x}\left(DA\frac{\partial C}{\partial x}\right) + A(W+P) \quad (1)$$

with:
A = wet cross section (m^2)
C = concentration in the water phase ($g\ m^{-3}$)
D = longitudinal dispersion coefficient (m^2)
P = source and sink terms from water quality processes ($g\ m^{-3}\ s^{-1}$)
t = time (s)
U = flow velocity, averaged over the cross section ($m\ s^{-1}$)
W = pollution loads ($g\ m^{-3}\ s^{-1}$)
x = longitudinal distance (m)

The hydrodynamic coefficients in the equation are based on tidally averaged flow. The water depth in the model is constant, and is taken to be the average water depth for each segment. The exchange between model elements in the estuary is based on the mass balance of fresh water inflow into the estuary. The total fresh water discharge into the coastal region is further transported along the coast based on principles of continuity, using certain assumptions about the direction of transport, e.g. water inflow to the estuary occurs through a northern channel along the coast of Walcheren, and water outflow from the estuary occurs through a southern channel, along the coast of Zeeuws-Vlaanderen. The tidally averaged transport is based on the average measured chloride concentrations and the chloride balance per element. In the coastal zone, the advective and dispersion terms are coupled in one overall transport term. This approach is possible due to the fact that the largest tidal mixing occurs in the direction of the smallest observed concentration gradient (i.e. along the coast).

The approach for suspended sediment is similar to that for dissolved substances, with the difference that the advective term in equation (1) is replaced by a term that contains the net transport of suspended solids. The time and space dependent net transport of suspended solids is an input item to the model. It is supplied on a seasonally integrated basis, so that the effects of high discharges or storm events are included. In the coastal region, this approach could not be used, due to a lack of data. In that area the transport of suspended sediment is modelled identically to that of dissolved substances.

Additional attention has been given to the accumulation of toxic substances in the bottom sediment. This is an important process affecting the fate of these substances in the environment, specifically with the adaptation of the system to changes in the pollution loads. In the model, the bottom sediment has a thickness of 0.5 meter. The exchange between this layer and the overlying water column is determined by the presence of so-called ‘mega ripples’ which are influenced by the tidal flow over the migrating bottom ripples. The exchange between these sand dunes and the water column results in a residence time of 0.5 years for the bottom sediment at any one point. The mass of sediment in the bottom is the reason that the water quality in the model area needs approximately 15 years to come into equilibrium with the decreasing loads from upstream. Figure 2 provides an overview of the modelling of the transport of suspended solids and adsorbed pollutants.

Loads of substances

The substance loads into the estuary and coastal region are given in the SAWES data base. Since there are no measurements available, assumptions had to be made concerning the concentrations at the boundaries of the model area:

- the inflow of metals at the southern boundary of the modelled coastal region was estimated based on the available measurements of bottom concentrations;
- for the open ocean boundaries, the concentrations of sulphate, sodium, potassium, calcium and magnesium were based on measured chloride concentrations and a fixed ratio of each of the ions in sea water;
- for the upstream boundary in the estuary by Rupelmonde, as well as for the open sea boundary, the algae concentrations are based on measured chlorophyll concentrations and the assumption that half the algae are diatoms and the other half are non-diatoms;
- the CO_2 concentration at the upstream boundary in the estuary (Rupelmonde) is estimated based on the measured pH and alkalinity, and the relation between pH, alkalinity and CO_2 concentration.

Water quality processes for oxygen and nitrogen

The water quality model includes a number of water quality processes that contribute to the oxygen balance and to the nitrogen cycle. All these processes including the exchange of oxygen and carbon dioxide with the atmosphere, the mineralization of carbonaceous organic waste (BOD) and organic nitrogen, nitrification and denitrification are incorporated in the source/sink term of the model equation. The formulations used are conventional and have been derived from textbooks on water quality modelling and aquatic chemistry, such as Crank (1973), DiToro et al. (1987) and Stumm & Morgan (1981). However, due to the special character of the Scheldt estuary with a very low oxygen concentration during summer, an extra factor was added to account for the change in the reaction rates with a decreasing oxygen concentration. A complete definition of the model formulations is given by Van Gils et al. (1993).

The presence of algae affects the oxygen balance, the nutrient cycles as well as the adsorption of trace metals through the pH. Therefore algae were also included in the water and sediment quality model. The model distinguishes between diatoms and all other non-diatom species. In the present study the mortality was increased in the area with the highest salinity gradient, to account for the effect of salt stress on algae. Van Gils et al. (1993) provide a detailed description of the algae model.

The exchange of oxygen and CO_2 between the water and atmosphere is calculated based on their over or undersaturation in water relative to the atmosphere. Decay reactions are based on first order reactions including a temperature function as well as an oxygen concentration function. The pH in the system is calculated by the thermodynamic equilibrium model CHARON as a function of the alkalinity and the CO_2 concentration. This same model is also used to calculate metal speciation (Smits et al., 1985). Figure 3 shows a schematic overview of the general water quality model.

Water quality processes for heavy metals

The behaviour of trace metals in aquatic systems is influenced strongly by adsorption to organic and inorganic particles. The dissolved fraction of the metals are transported by water, while the adsorbed fraction is transported by sediment. The distribution of a trace metal into adsorbed or dissolved fractions depends on the trace metal itself, the adsorption characteristics of the particles and the local environmental conditions (e.g. temperature, pH, redox state, salinity and ionic strength). The distribution can be described by a mineral equilibrium and/or adsorption to a particulate surface. This phenomenon was included in the water and sediment model as an equilibrium computed by a chemical sub-model CHARON.

In the Belgian part of the estuary, the metals Cd, Cu and Zn often exist as precipitated sulphides (Zwolsman et al., 1990, Zwolsman & Van Eck, 1992). The field data suggest that these sulphides are present where the oxygen concentration is low. Because these sulphide minerals have a low solubility, a large fraction of the metals are in particulate form. In a seaward direction, as the oxygen concentration increases, the sulphides become oxidised. However, the field data

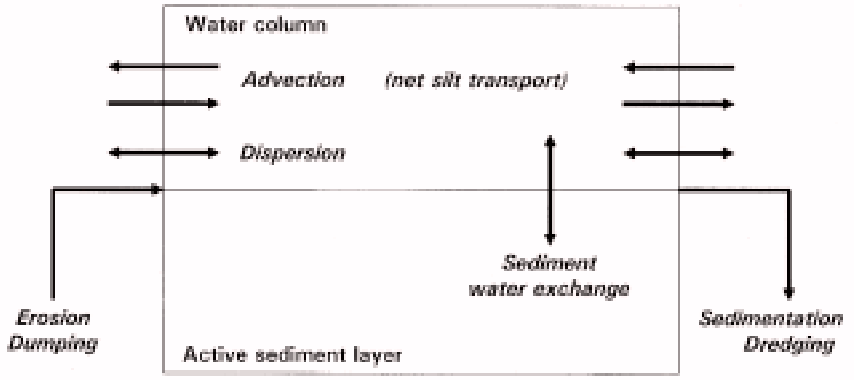

Figure 2. Schematic overview of the transport processes for particulate matter (suspended solids and adsorbed pollutants) which were incorporated in the model.

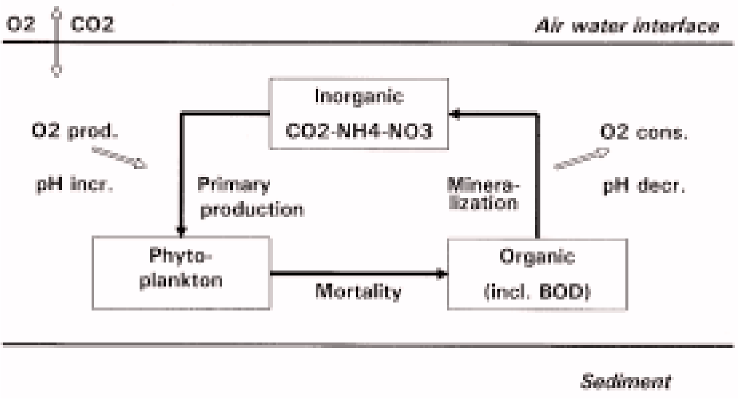

Figure 3. Schematic overview of the general water quality model.

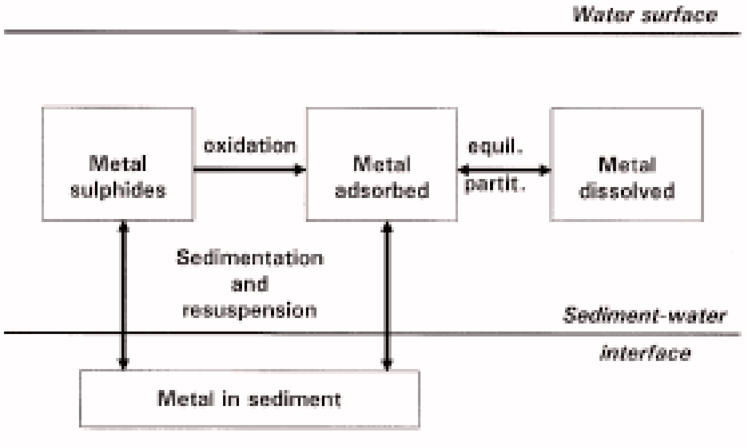

Figure 4. Schematic overview of the model for the behaviour of trace metals.

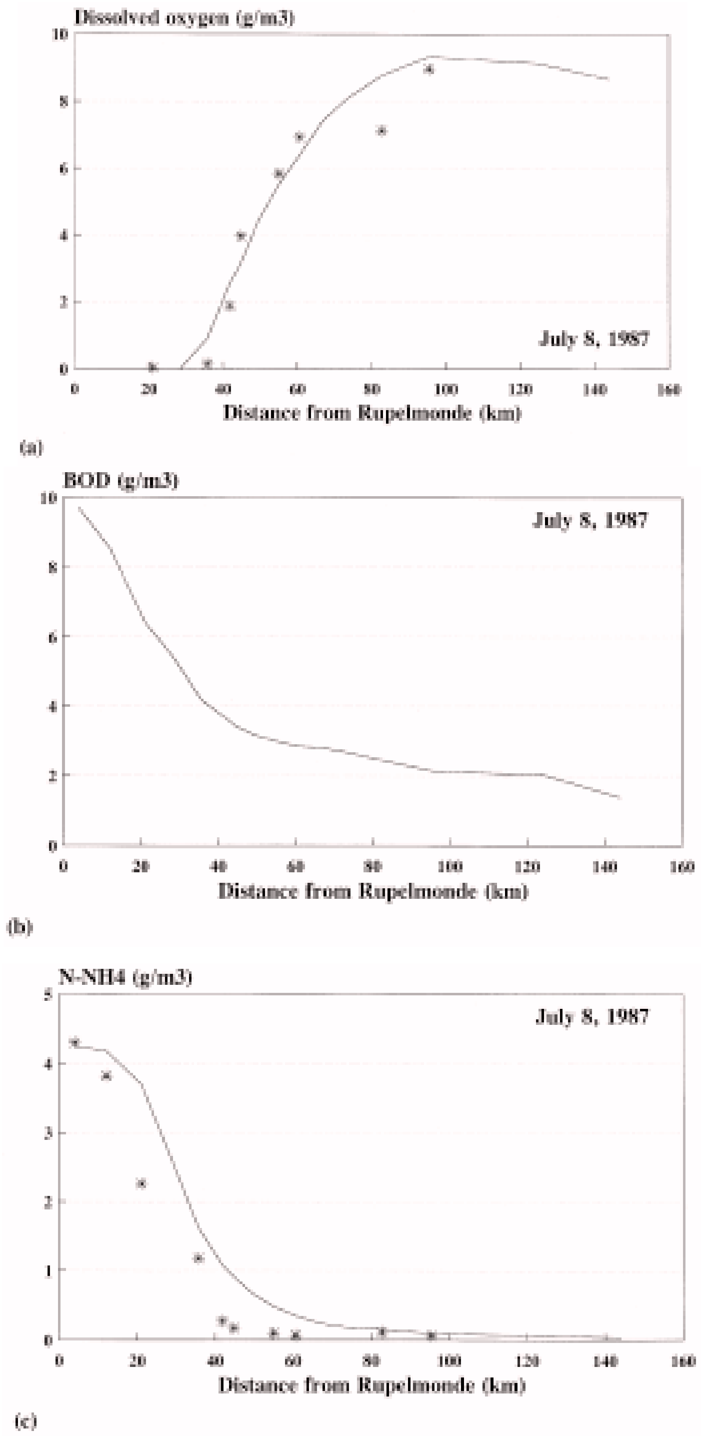

Figure 5. Calculated concentrations of oxygen (a), BOD (b) and ammonium (c), compared to measured concentrations (*) on July 8 1987, as a function of the distance from Rupelmonde.

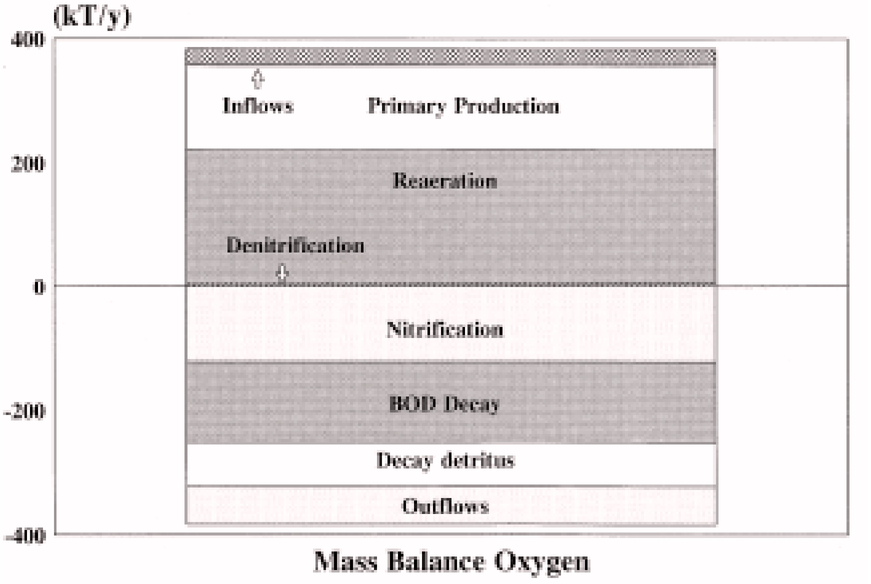

Figure 6. Oxygen balance for the total model area during the final model calibration run: positive terms are above x-axis, negative terms are below the x-axis.

also show that the oxidation is a slow process, dependant on the temperature and oxygen concentration. Therefore oxidation can not be modelled as an equilibrium process and a kinetic formulation for the oxidation of metal sulphides had to be developed. In the water quality model, the trace metals enter the estuary as sulphides and thus are not incorporated in the sorption equilibrium system. This happens only after the oxidation of the sulphides. Figure 4 shows a schematic overview of the model for the behaviour of trace metals.

Calibration of the water quality model

Measurements used for calibration

For calibration of the model, the consistency of the loads to the system, the transport and other processes within the system, and the measured concentrations within the system must be assessed. For calibration of the general water quality model and the model of the behaviour of metals and phosphate, two years are relevant. In 1987, the results of 8 specific monitoring campaigns were available from the SAWES project, providing detailed longitudinal profiles of a wide variety of water quality parameters over a range of seasons. As part of the SAWES project, water quality measurements were also gathered from the standard water quality monitoring program for a more recent year, namely 1991. This year contrasts to 1987 with regard to discharges and large scale dredging in the harbours of Antwerp. Both years are modelled using the same process formulations and process coefficients.

Steps in the calibration process

The model calibration took place in three steps:

- calibration of the dispersion coefficient by fitting to the average chloride profile in the estuary;
- calibration of the parameters in the oxygen and nitrogen related processes, including the algae model; and
- calibration of the parameters in the heavy metal related processes.

The first two steps are important primarily to determine the general water chemistry which affects metal partitioning. They were executed by iteratively running the model and adjusting the coefficients by hand until sufficient similarity between the model results and field data was achieved. A postprocessing facility supported this procedure, enabling the user to observe the magnitude and the spatial and temporal variability of all modelled processes. In this process, the known ranges of the process coefficients as given in the literature were taken into account.

The third step of the calibration procedure was dedicated to the trace metal behaviour. The metal

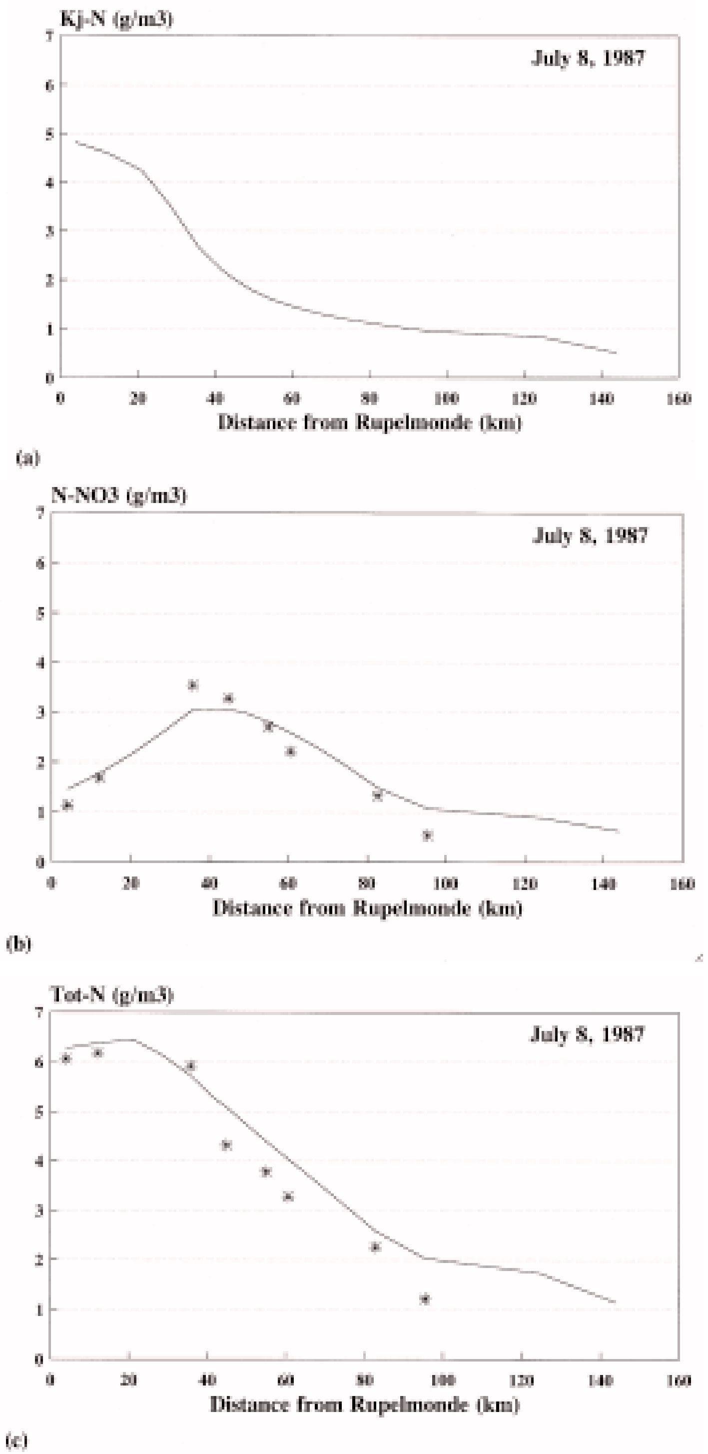

Figure 7. Calculated concentrations of Kjeldahl nitrogen (a), nitrogen in nitrates (b) and total nitrogen (c), compared to measured concentrations (*) on July 8 1987, as a function of the distance from Rupelmonde.

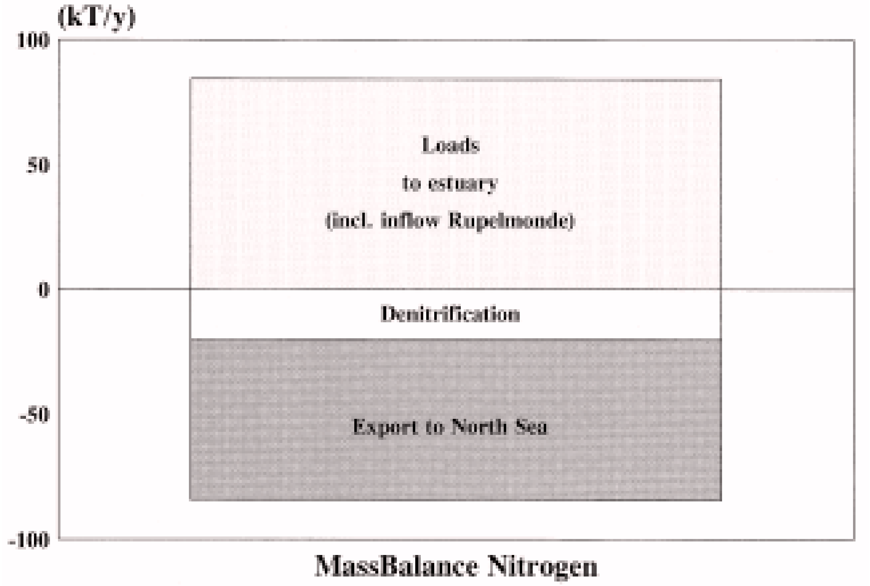

Figure 8. Nitrogen balance for the total model area during the final model calibration run: positive terms are above the x-axis, negative terms are below the x-axis

sulphides of Cd, Cu and Zn have a very poor solubility and their occurrence can be recognised by an extremely high partition coefficient. Lower partition coefficients indicate a ‘normal’ reversible partition between adsorbed and dissolved metal species.

All samples from the monitoring campaigns in 1987 were divided in samples with and samples without sulphides, based on the magnitude of the partition coefficient. The samples without sulphides were used to calibrate the Gibbs parameters of the adsorbed metal species in the chemical equilibrium model representing the adsorption characteristics of the particles present. For this purpose an automatic calibration procedure was used (Ouboter & De Rooij, 1990). The adsorption of trace metals to fine particles differs between different water systems, due to the different characteristics of the particles. In the Western Scheldt estuary the adsorption is relatively strong, possibly due to the strong adsorption to reactive iron hydroxide FeOOH, which forms at the oxic-anoxic interface in the estuary.

The samples with sulphides were used to calibrate the kinetics of sulphide oxidation. Based on the calibrated equilibrium model, the adsorbed fraction excluding sulphides was calculated and subtracted from the measured particulate fraction in the sample. The difference was assumed to consist of sulphides and thus the sulphide concentration in the samples was estimated. A kinetic formulation for the oxidation of sulphides, dependent on the oxygen concentration and the water temperature was derived from the measurements. Both a high temperature and a high oxygen concentration stimulate the oxidation process.

Discussion of the calibration results

The results of the model calibration give a clear understanding of the functioning of the water quality processes in the Scheldt estuary and coastal zone system. It must be noted that many more measurements of loadings and water quality concentrations were available for the estuary than for the coastal region. The description of the system is thus focused primarily on the estuary and the mouth up to the region of Cadzand.

The loadings with BOD and ammonium cause low oxygen concentrations in the upstream regions of the estuary, especially during the summer (Figure 5). The mass balance of oxygen (Figure 6) shows that consumption of oxygen occurs due to the decay of organic material (mostly anthropogenic of origin) and nitrification. The concentration profiles in the estuary show where the different oxygen consuming processes are dominant. A detailed analysis of the model results shows that in the upper estuary oxygen consumption is mainly due to nitrification, whereas in the lower estuary oxygen is consumed mainly by the decay of BOD. Therefore, nitrification is the main cause of anoxia in the upstream part of the estuary.

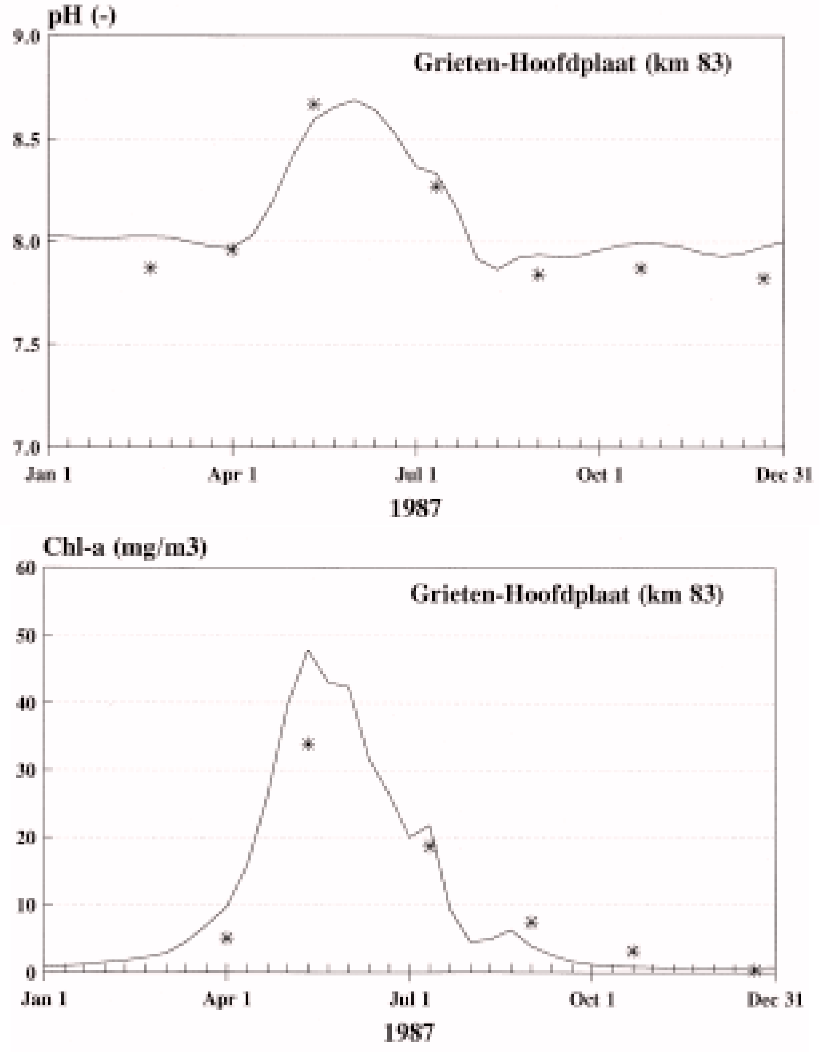

Figure 9. Calculated pH (a) and chlorophyll concentration (b), compared to measured values (*) at the location Grieten-Hoodplaat (83 km downstream of Rupelmonde) for 1987.

The total nitrogen concentration is controlled by waste loads in the river Scheldt and in the upper Scheldt estuary (Figure 7). In the seaward direction the concentration drops, mainly due to dilution with sea water. The overall mass balance for nitrogen shows that about 25% of the total nitrogen load is removed by denitrification (Figure 8). With a method of parameter analysis, it can be determined within which flux ranges the measurements can be reproduced with the model. From this analysis, it is shown that between 15–30% of the nitrogen is denitrified in the estuary.

Looking at the different nitrogen forms, it can be seen that the loads to the system are primarily in the form of Kjeldahl nitrogen, which is the sum of organic nitrogen and ammonium. However, almost all of the organic nitrogen and the ammonium is mineralised and nitrified, especially in the upstream part of the estuary. To illustrate this, Figure 7 shows the Kjeldahl nitrogen profile. The nitrification reaction produces nitrates, and together with the dilution from the sea, this results in a typical maximum in the nitrate concentration.

The transport and concentrations of the trace metals are dominated by the transport of silt in the longitudinal direction in the water column, and in the vertical direction between the active bottom layer and the water column. The dissolved concentration, which is important for bioaccumulation, depends on the sul-

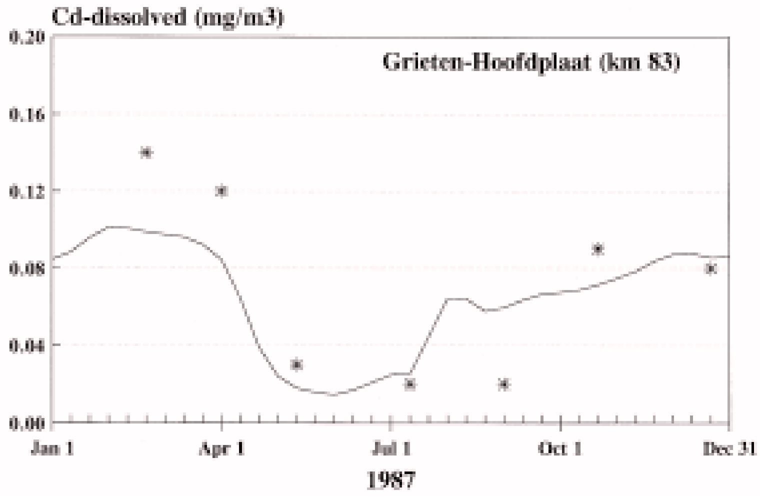

Figure 10. Calculated and measured concentrations of dissolved cadmium at the location Grieten-Hoofdplaat (83 km downstream of Rupelmonde) for 1987.

phide oxidation and after oxidation on the pH, alkalinity, temperature and salinity. The pH is determined by the acid forming processes (nitrification and decay of organic material), and the exchange of CO_2 with the atmosphere. An another important influence on the pH is the production of organic material during an algae bloom. This occurs primarily between mid April and mid July in the mouth of the estuary. Different amounts of production occur in different years, usually due to the turbidity conditions. In 1987 there was a significant amount of production (Figure 9), which was coupled to a noticeable increase in the pH. By high pH, heavy metals are more strongly adsorbed to particulate material. As a result, the concentration of dissolved metals (e.g. cadmium) decreases (Figure 10).

The concentration profile of dissolved cadmium along the estuary is determined by the oxidation of sulphide in the area of the Belgian-Dutch border and from the dilution with sea water. The two processes determine a profile for dissolved metals with a maximum in the central part of the estuary (Figure 11). This maximum is further enhanced by the desorption of cadmium due to the influence of chloride in the sea water.

Following the calibration and verification of the model, a sensitivity analysis has been executed. This analysis focused on about 10 important input parameters. The sensitivity analysis was the last step in a modeling exercise aimed at a better understanding of the water system under consideration. It is also led to a general understanding of the reliability of the model as a decision support tool. This understanding was communicated to decision-makers using the model (DELFT HYDRAULICS et al., 1995).

Model application for policy analysis

Based on the ability of the model to accurately reproduce the most important transport and chemical processes occurring in the estuary and coastal region, it is possible to use the model to assess different management policies and scenarios. One such evaluation can be made of the effect of the large scale dredging in the harbours of Antwerp.

According to international agreements between the Netherlands and Belgium, a large amount of sediment has been removed from the estuaries since 1990 (approximately 300 000 tons per year). Rijkswaterstaat in the Netherlands has made a calculation of the sediment balance in the estuary, in which this amount is taken into account (Vereeke, 1994). The model has been used to calculate the effects of the dredging on the discharge of cadmium from the Scheldt estuary to the North Sea. Two calculations have been made, based on the sediment balances with and without dredging activities in the harbours (as calculated by Vereeke, and Van Maldegem, respectively). Both calculations use the meteorological conditions and loads for 1987. For substances which are adsorbed to particulates, the reaction time of the water quality system is on the order of 10–20 years. This is due to the large amount of material in the bottom sediment, which changes slowly due to kinetics. Therefore, both calculations

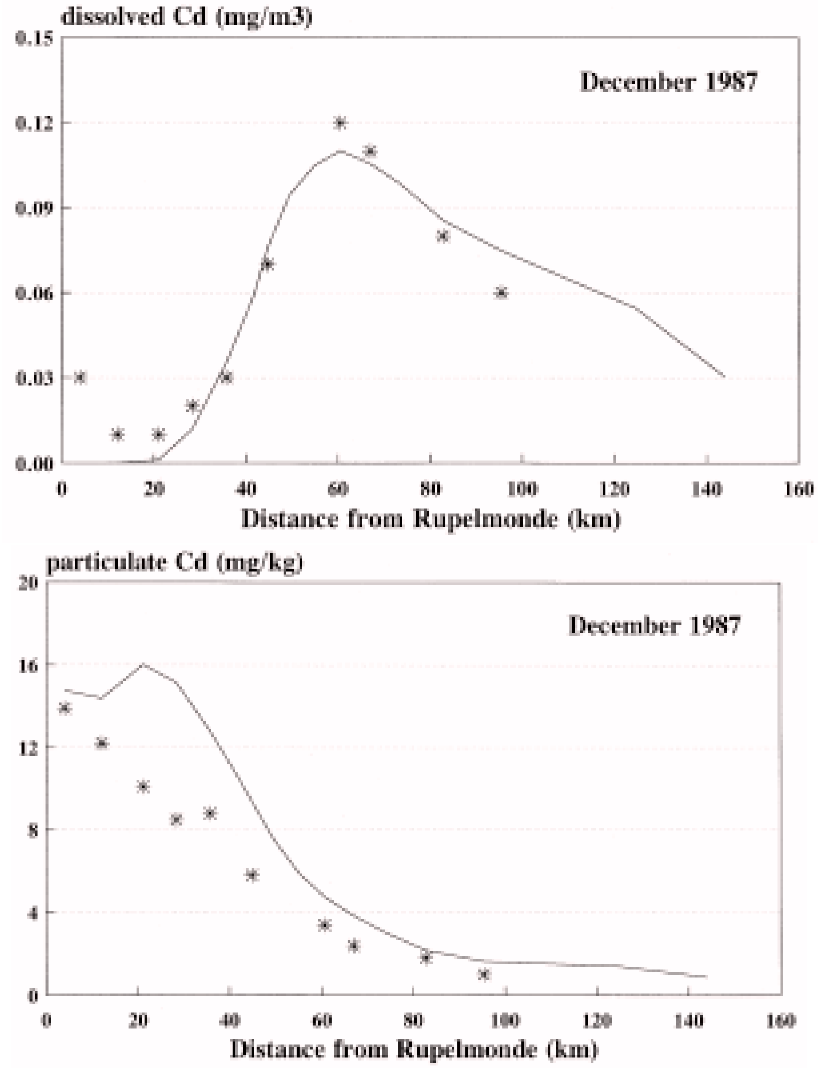

Figure 11. Calculated concentrations of dissolved (a) and particulate (b) cadmium, compared to measured concentrations (*) in December 1987, as a function of the distance from Rupelmonde.

have been made for a period of 10 years. The results for the last year are presented.

Near Vlissingen, the dredging activities are expected to resulted in a 25% decrease in the total cadmium concentration (Figure 12). This decrease implies that approximately 33% of the cadmium enters the North Sea, where as prior to dredging this fraction is computed as 50% (Figure 13). These values are based on the equilibrium between the water column and bottom.

Evaluation and recommendations

The analysis of Western Scheldt estuary by means of a mathematical model was possible due to the availability of a large set of waste load and water quality data. The model system that has been developed seems to match its main objectives. Its set up as an integrated tool, based on available knowledge about the system, increased the understanding of the water system with respect to the relation between waste disposal and water quality. With the calibration, verification, sensitivity analysis and application of the water quality model to the Scheldt estuary it has been shown

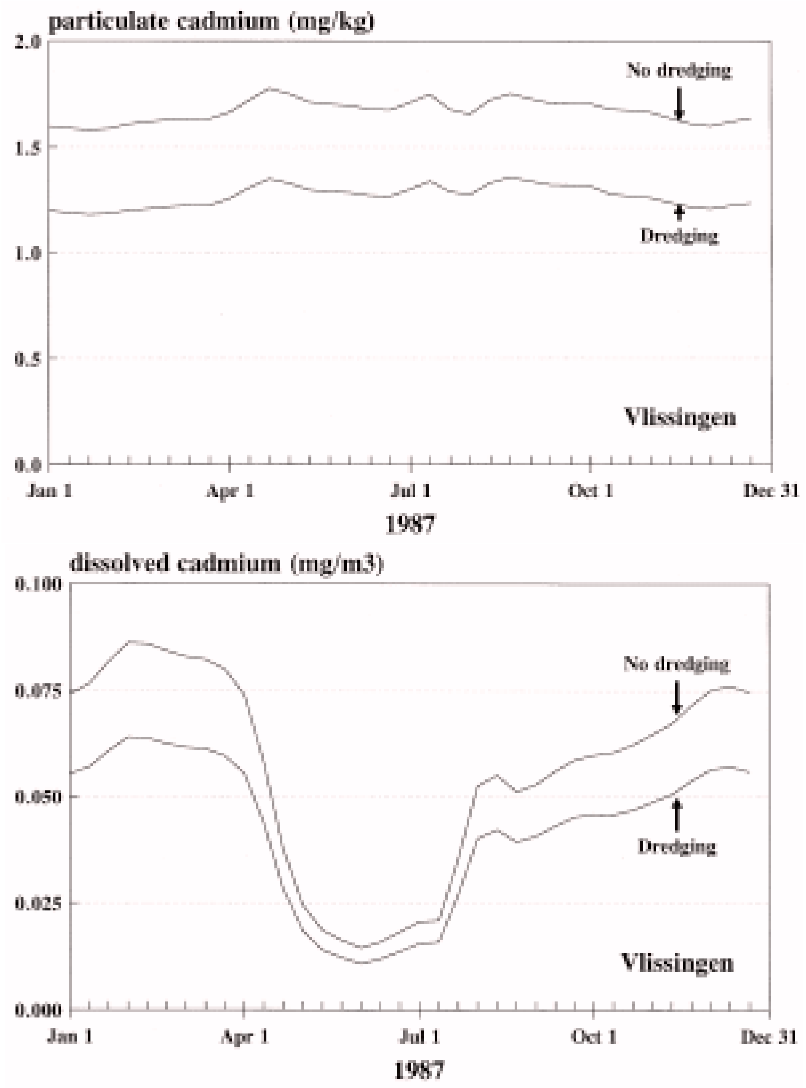

Figure 12. Effect of dredging (starting in 1990) on the concentrations of particulate cadmium (a) and dissolved cadmiuim (b) at the location Vlissingen (pollution loads from 1987).

that a model for the combined eastuary and coastal region can be an important aid for the management of such a system. The use of the model indicated clearly which processes are the most important in this particular estuary. The model also proved to be an important tool to decide about the necessities and the priorities for further investigations. For the estuary, a large set of measurements were available, for both the loads to the system as well as for the water quality in the system. For the coastal region, fewer measurements were available. Especially for the Belgian region of the coast, data availability was the limiting factor in the model development. In this region, the model is based only on large scale transport features, process dynamics in the estuary, on a limited nuumber of nutrient, oxygen, and on some measurements of bottom sediment concentrations of metals.

Further investigations may be aimed at two aspects in particular. Firstly, it is necessary to have more insight on the adsorption characteristics of suspended matter. It must be verified if it is actually iron precipitates that have a high affinity for metals. It must also be checked what is the influence of the loss of the redox boundary caused by a reduction in the loads. This aspect is important in order to make a good estimate of the effect of large scale load reductions on the metal

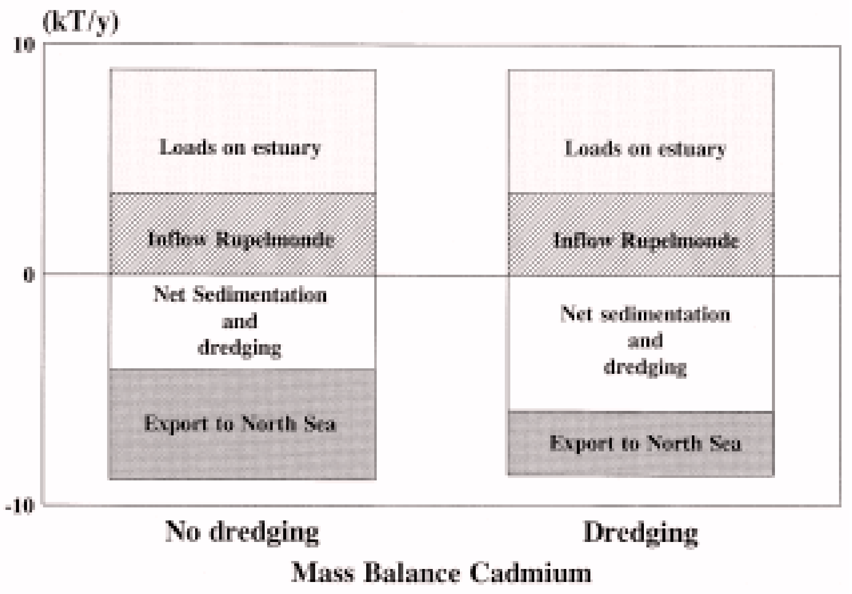

Figure 13. Comparison of cadmium, balances for the total model area, with and without dredging (dredging started in 1990, pollution loads from 1987).

concentrations. In the second place further work may be dedicated to establish more accurate data about the net transport of suspended solids through the estuary, for example by multidimensional modelling.

Acknowledgements

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