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Integrated data-modelling approach for suspended sediment transport on a regional scale

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Abstract

This paper discusses an integrated data-modelling concept to monitor the seasonal variability of suspended particulate matter (SPM) patterns in the North Sea. It covers two aspects. First, the use of SPM transport model data to retrieve SPM concentrations from NOAA/AVHRR reflectance imagery by improving the algorithm to convert the reflectance data to SPM concentrations and to generate synoptic SPM images which are consistent in time. Second, the use of these observed SPM concentrations as model output targets to assess the sensitivity of the model performance for various model input parameters in some initial model set-ups, for example, the loads and dumping, the critical shear stress for erosion and sedimentation and settling velocity.

The sensitivity analysis is based on the definition of a so-called Goodness-of-Fit (GoF) criterion (also denoted as cost-function) being a measure to quantify the difference between the model output and the model output targets, which is derived from both synoptic NOAA/AVHRR imagery and in situ concentration data. Key element in this approach is the requirement that a GoF criterion is defined that mimics the main features of the end-user requirements (i.e. the modelling objective) and the associated characteristic length and time scales.

The sensitivity analysis is carried out by means of the adjoint model which is shown to provide a detailed, that is fully spatially and temporally distributed, insight into the model sensitivities.

The objective of this chapter is to describe the components in the integrated use of observations and models as outlined above. This approach is demonstrated in a number of case studies of SPM transport in the Dutch Coastal Zone and in the North Sea. From the case studies, it can be concluded that loads and dumping are a major source of error. Due to the absence of observations over the vertical, the errors in the erosion/sedimentation processes that govern the vertical exchange and the bed sediment load are difficult to assess. As such, concentration profile observations and synoptic remote sensing imagery are considered to provide an ideal and

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necessary combination to monitor the SPM transport on a regional scale.

Keywords: Adjoint modelling; Assimilation; NOAA/AVHRR reflectance imagery; Optimisation; Sensitivity analysis; Suspended sediments

1. Introduction

In the last decade, the ready availability of high-resolution data sets has increased rapidly due to the advent of satellite and airborne remote sensing instruments. With the continuous development of remote sensing technology, a wide range of parameters can be monitored, which are relevant for studying hydrodynamic, water quality and morphodynamic processes in the oceanographic and coastal environment. This implies that a data-oriented approach based on observations and numerical modelling based on the knowledge of the physical processes involved can be recognised as alternative ways to provide information on the physical system under consideration.

In this chapter, the focus is on the transport of suspended particulate matter (SPM). SPM plays an important role in water quality management in coastal zones because it is related to total primary production and fluxes of heavy metals and micropollutants. Since dumping in the coastal zone is quite significant, a sequence of synoptic information on SPM patterns is one of the building stones for adequate national and international coastal zone management.

1.1. Integrated data-modelling approach

Whereas observational data represent the actual state of the system at some fixed points in space and/or time; a mathematical physical model describes the evolution in space and time of the system parameters. Now, recognising the fact that observations and models are indeed both 'alternative' and 'complementary' information sources, the question arises how to integrate observations and models in an optimal way given the user-requirements to monitor the physical system under consideration. This will be referred to as the 'integrated data-modelling approach.'

The present study deals with the SPM transport in the North Sea. The transport of the sediment introduced in the system by erosion/sedimentation, dumping, riverine inputs, etc., is stirred by tidal flow, waves and wind. The erosion/sedimentation fluxes, in turn, are determined by bed stress characteristics and the exchange in the vertical. Therefore, an SPM transport model can be seen as an integrated model consisting of modules that are hierarchically coupled (see Fig. 1). Each of the modules provides input for the modules on the level above.

Within the context of an integrated use of models and observations, especially remote sensing imagery, the focus here is on:

- assessment of the sensitivity of the seasonal variation of SPM patterns to variations in the various modules in the SPM transport model; and

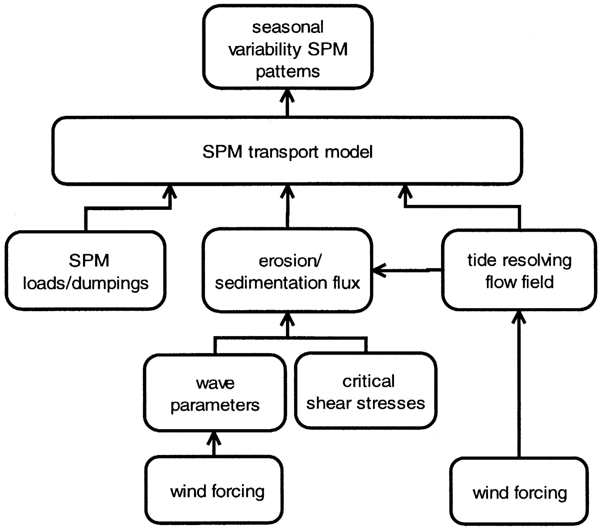


Fig. 1. The SPM transport model.

- the use of model data to retrieve accurate SPM concentration data from remote sensing imagery.

1.2. Modelling objective — Goodness-of-Fit (GoF) criterion

The quantification of the performance of a model obviously depends on the modelling objective. It requires some measure to quantify the differences (or misfit) between some model output target derived from observations and their model equivalents. Such a quantitative measure is referred to as GoF criterion or simply error-function or cost-function. A GoF criterion must reflect the characteristics of the modelling objective, for example, the spatial and temporal scale of the features that are considered to be of primary interest.

1.3. Sensitivity analysis

The presence of model and model input errors makes it possible to improve the model performance by calibration, i.e. tuning of some (empirical) parameters in the model dynamics and/or model forcing. One of the key-issues in model calibration is to establish which parameters are suited to parameterise the model error by means of a sensitivity analysis. A sensitivity analysis can be performed in many different ways. For example, by determining the quantitative effect of single parameter variations (not necessarily small) on the GoF value or by determining those parameters for which the model is most sensitive for in terms of reduction of the GoF value. The latter approach is usually based on the gradient of the GoF criterion. The adjoint model is a very efficient way to determine the gradient of the GoF criterion with respect to any model parameter and model variable (Chavent, 1979). Compared to a finite difference approach, it enables the model's sensitivities to be determined in a fully spatially and temporally distributed way, which is not feasible by other methods. As such, the adjoint model is simply a very efficient way to implement the chain rule to determine the gradient of the GoF criterion with respect to the model input parameters.

In the present study, the interest is in assessing the sensitivity of some suitable GoF criterion to the output parameters of the various modules within the SPM transport model. These sensitivities indicate the required level of accuracy and detail of the computation of these parameters. Parameters with a high spatial and temporal variation obviously require the use of a detailed numerical model, whereas parameters that play a subsidiary role can be determined by means of simple, possibly grey or black box models or can be directly extracted from existing data sets. The value of the approach outlined above is that it focuses on the overall performance of the integrated model given the pre-defined modelling objective instead of the performance of the individual modules. Therefore, this 'top–down' approach avoids the inclusion of detailed and often complex components if they only play a subsidiary role.

1.4. Contents of this chapter

This chapter is organised as follows. In Section 2, an overview is given of the key elements of GoF criteria that reflect the user-defined modelling objective. In Sections 3 and 4, the two-sided relation of observations and models is illustrated; Section 3 deals with the retrieval of information from remote sensing observations using model data, whereas the analysis of an SPM transport model using observations as model target is discussed in Section 4. In Section 5, the results and conclusions are summarised and, finally, in Section 6 some recommendations are given with respect to the rationalisation of the integrated data — modelling concept in operational oceanography and the ways forward.

2. Modelling objective — GoF criterion

2.1. Introduction

In the present work, the seasonal variability of the transport of SPM on a regional scale was chosen as the modelling objective. This implies that the focus is on processes and features on: (i) a characteristic time scale of, say, 1 month; and (ii) a characteristic length scale of 100–200 km. Although in principle an SPM transport model computes the SPM concentration per grid cell, evaluating and interpreting of the model results will be carried out after aggregation of the model results up to the characteristic spatial and temporal scales according to the modelling objective. Consequently, the spatial model domain is divided into non-overlapping (geographical) zones, the simulation interval into so-called time-windows.

2.2. GoF criterion

In order to measure the performance of a model in a quantitative way, some GoF criterion must be defined. Within the present context such a GoF criterion is defined in least squares sense according to Eq. (1) and is based on

- a residual SPM concentration, i.e. the difference between the computed and observed SPM concentration,
- a representativity factor denoting the representativity of the observed SPM concentration, and
- weight factors for each residual SPM concentration based on (i) the expected error in the SPM concentration residual and (ii) user preferences.

The general form of the GoF criterion that is considered here is

$$\mathrm{GoF}(p) = \sum_{\substack{\text{zones}\\ i}} \sum_{\substack{\text{time windows}\\ k}} w_{i,k}^{\text{user}} \left[\frac{w_{i,k}^{\text{outlier}}}{\sigma_{\text{RS}}^{2}(c_{\text{RS}}, c_{\text{model}}, c_{\text{sat}})} \left(\Delta_{i,k}^{\text{RS}}\right)^{2} + \frac{R_{i,k}(c_{\text{in situ}}, c_{\text{model}})}{\sigma_{\text{in situ}}^{2}(c_{\text{in situ}}, c_{\text{model}})} \left(\Delta_{i,k}^{\text{in situ}}\right)^{2} \right], \tag{1}$$

where $w_{i,k}^{\text{user}}$, user-defined weight factor for zone i and time-window k; $w_{i,k}^{\text{outlier}}$, weight factor for zone i and time-window k, to penalise large residuals that are due to high SPM model concentrations in combination with observed SPM concentrations at saturation level; $R_{i,k}$, representativity factor (for in situ data only); $\Delta_{i,k}^{\text{RS}}$, $\Delta_{i,k}^{\text{in situ}}$, residual SPM concentration for zone i, time-window k; σ_{RS}, $\sigma_{\text{in situ}}$, standard deviation; c_{RS}, $c_{\text{in situ}}$, remote sensing/in situ SPM concentration; c_{model}, modelled SPM concentration; and c_{sat} saturation value for SPM concentration.

2.2.1. SPM concentration residual

Since the quantification of the performance of a model is application dependent, the GoF criterion used must be consistent with the characteristics of the modelling objective. For the modelling objective outlined above, emphasising the seasonal variations of SPM patterns, the residual SPM concentration is defined as

$$\Delta_{i,k}^{\text{obs}} = \max\left\{ |\bar{c}_{i,k}^{\text{obs}} - \bar{c}_{i,k}^{\text{model}}| - \Delta c_{\text{threshold}}, 0 \right\}, \tag{2}$$

where $\bar{c}_{i,k}^{\text{obs}}$, the remote sensing or in situ SPM concentration c^{obs} averaged over zone i and time-window k; $\bar{c}_{i,k}^{\text{model}}$, the modelled SPM concentration c^{model} averaged over zone i and time-window k; and $\Delta c_{\text{threshold}}$, a threshold for the SPM concentration residual.

2.2.2. Spatial aggregation — zonal partitioning

Aggregation in space and time can be particularly important in order to reduce the large natural variability that is often noted in SPM observations. The areas over which the aggregation in space is performed may be consist of, for example, erosion areas, deposition areas and coastal zones. In the presently reported case studies, the Dutch Coastal zone model and the North Sea model, a partition of 18 zones is introduced, see Fig. 2.

2.2.3. Temporal aggregation

The seasonal variability of SPM patterns is manifest on a characteristic time scale of, say, 1 month. The temporal aggregation is performed over all data samples (computed, remote sensing and in situ SPM concentrations) that lie within time-windows covering periods of 1 month.

2.2.4. Representativity factor

Due to the synoptic character of the remote sensing data the SPM concentration, averaged over a zone and time-window, can be assumed to be representative for that particular zone and time-window. On the other hand, given the natural variability of in situ data samples and the limited spatial and temporal coverage of data samples, the average of the distributed in situ samples may not be assumed to be representative for the entire zone and time-window. To account for this difference in 'representativity' of the average in situ concentration compared to the average remote sensing concentration, a representativity factor $R_{i,k}$ is introduced in the in situ term of the GoF criterion. For a single in situ data sample, $R_{i,k}$ is defined as the ratio of (i) a cube in the space–time domain for which this particular data sample is representative and (ii) the volume of the cube of the ith zone and kth time-window. The representativity of the average of the in situ samples is assumed to increase linearly with the number of in situ data samples in this zone and time-window. For synoptic remotely sensed (RS) concentrations, the representativity factor is equal to unity. From the limited representativity of in situ concentration residuals, it may not be concluded that in situ measurements cannot be

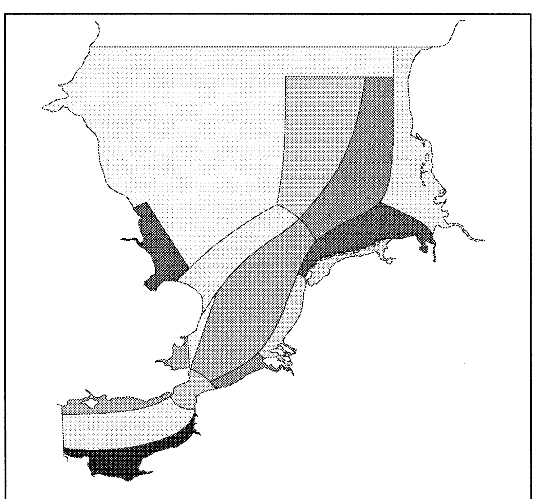


Fig. 2. The partitioning in zones used for the North Sea model (see Section 4).

used at all. However, with modelling objective as the seasonal variability of SPM on a regional scale, the amount of information that can be extracted from in situ data will be limited.

2.2.5. User-defined weight factor

In order to allow for the preferences of the user with respect to the presumed relevance of a particular zone/time-window, a weight factor $w_{i,k}^{\mathrm{user}}$ is introduced. This factor is assumed to be independent of the type of observations.

2.2.6. Accuracy of concentration residuals

In order to guarantee the usefulness of an SPM concentration residual as an appropriate measure for the misfit between model and observations, the effect of errors introduced by the conversion of reflectance data to SPM concentrations has to be taken into account. First, it is known that the accuracy of the necessary pre-processing to convert the raw reflectance data registered by optical remote sensors into SPM concentrations is concentration dependent. The relation between reflectance and SPM concentration, as given by Gordon and Brown (1975), saturates. The saturation value for NOAA/AVHRR reflectance images obtained with standard atmospheric correction procedures (Roozekrans and Prangsma, 1992) is 20 g m^{-3}. This implies that the errors in RS concentrations above the saturation level are rather large compared to the error in RS concentrations in the unsaturated range. This increased error (or reduced accuracy) is accounted for in the standard deviation σ_{RS}. Here, σ_{RS} is defined as the reciprocal of a smooth damping function with prescribed Gauss-width (see Fig. 3).

The usefulness of a particular remote sensing concentration residual is also hampered by a possible dominant contribution of outliers, which emerge whenever the modelled concentration far exceeds the saturation level c_{sat} and the observed concentration is at

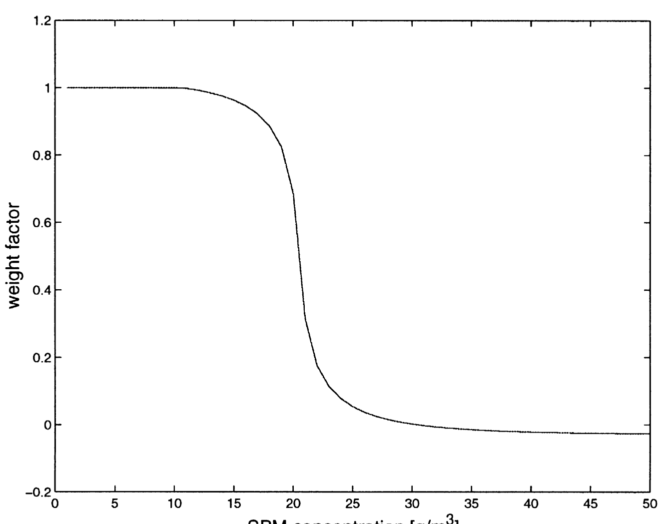


Fig. 3. The normalised $\sigma_{\mathrm{RS}}^{-2}$ as a function of the (remotely sensed) RS concentration.

saturation level. In the present framework of GoF criteria, this is accounted for by introducing an additional weight factor $w_{i,k}^{\text{outlier}}$, which depends on the modelled concentration instead of the observed concentration. The shape of this weight factor is similar to the reciprocal of σ_{RS}^2, which is a smooth damping function with specified Gauss-width. However, the saturation-dependent accuracy might give rise to numerical problems due to additional local minima. In order to check the occurrence of this artefact, the weight $w_{i,k}^{\text{outlier}}$ factors should be monitored.

The concept of zonal and temporal partitioning is especially suited to synoptic observations. This is reflected in the limited representativity of in situ data. However, by defining a zonal partitioning consisting of small and distributed neighbourhoods of the in situ data points, the dominant impact of the synoptic observations is lost. Such a GoF criterion closely resembles the ‘standard’ output least squares approach for distributed data samples, see Vos and ten Brummelhuis (1997).

3. Retrieval of SPM concentrations from reflectance imagery using model data

3.1. Introduction

Reflectance is the standard product that results after atmospheric correction of the remotely sensed observed signal aboard the NOAA/AVHRR satellite. Conversion algorithms are needed to convert the reflectance into SPM concentrations. In this section, a conversion algorithm is outlined that ensures the consistency between the SPM concentrations derived from reflectance data that partially circumvents the problems due to (i) saturation of the relation between reflectance and SPM concentrations and (ii) cloud cover. The use of model data will prove to be a crucial factor in this conversion algorithm.

3.2. Conversion of the reflectance data

Reflectance percentages of the North Sea are registered by the NOAA/AVHRR satellite (in particular NOAA-12 and NOAA-14). The channel 1 data are atmospherically corrected by KNMI (Roozekrans and Prangsma, 1992) using the near infrared data of channel 2. The following problems have been observed with NOAA/AVHRR data.

- The reflectance percentage[2] strongly depends on the sun angle. Saunders and Kriebel (1988) state that for sun angles larger than 60° no reliable satellite measurements can be made due to an unknown contribution from diffusive skylight (see also Peters and Roozekrans (1998)). Even for sun angles between 50° and 60°, the absolute value of the reflectance percentage is less accurate. For the North Sea with sun angles in this critical region this ambiguity is reflected in a (much) lower average reflectance percentage than images at noon (NOAA-14) and/or images for spring and summer. However, the SPM patterns in the images do not change significantly from morning to

[2] Reflectance values may be negative due to a slow, continuous degradation of the AVHRR sensor. New calibration factors are available for NOAA-14, however, KNMI have yet to use them. This error, although disturbing, is much less significant than others mentioned here.

afternoon (Boon and Baart, 1996; Vos et al., 1998a) or within a series of consecutive images over a few days (Vos and Schuttelaar, 1997). Therefore, it was concluded that the patterns in the images contain relevant and useful information with respect to the large scale (seasonal) variation of SPM patterns.

• Although, saturation of the relation between reflectance and SPM concentration theoretically should occur at approximately 100 g m^{-3} (Althuis and Shimwell, 1994), in practice, saturation in the reflectance data observed by the AVHRR sensor is already found at the much lower level of 20 g m^{-3}. Recently, it was shown that the low saturation threshold of 20 g m^{-3} is caused by a contribution of SPM in channel 2, which is used for atmospheric correction (Peters and Roozekrans, 1998). For conversion algorithms for SPOT-XS and Landsat TM satellites, similar problems have been encountered (Vos et al., 1998b) but there the saturation is found at an SPM concentration level above 50 g m^{-3}.

The abovementioned problems have made many oceanographers reluctant to use AVHRR imagery.

Gordon and Brown's quasi-single scattering approximation of the reflectance percentage R in terms of the SPM concentration c. The inherent optical properties can be expressed using two coefficients a and $R(0+,c=0)$ to account for the linear part and two parameters δ and c^* to account for the non-linear effects (Gordon and Brown, 1975)

$$R(0+,c) = R(0+,c=0) + ac\frac{\delta + c^*}{\delta + c}, \quad (3)$$

where $R(0+,c)$, percent reflectance just above the water surface in channel 1 of NOAA/AVHRR, corrected for atmospheric disturbances observed in channel 2; c, SPM concentration (g m^{-3}); a, parameter (slope) in linear scaling with model results; δ, half

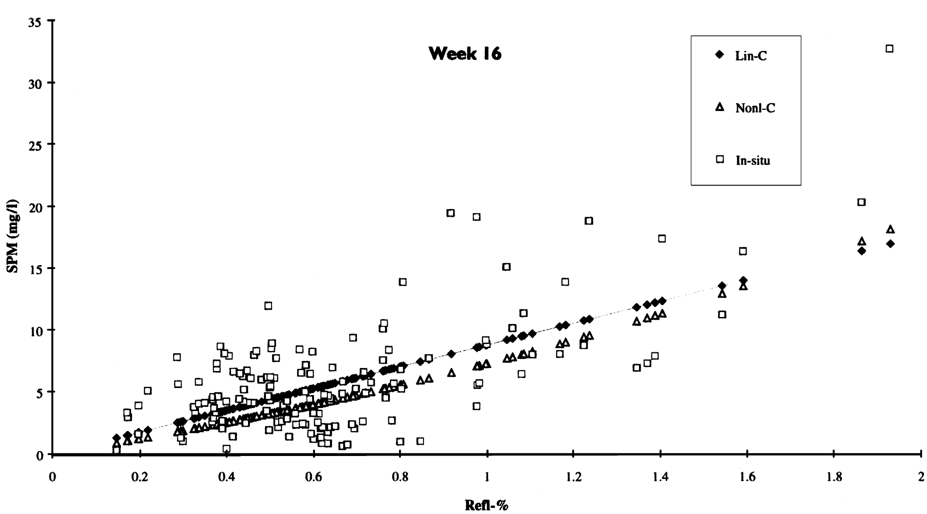


Fig. 4. Correlation between NOAA/AVHRR weekly composite (percent reflectance) and North Sea Project in situ concentrations (g m^{-3}) for the 16th week of 1990 (from Vos et al, 1998a).

saturation concentration (g m^{-3}); and c^*, cross point (g m^{-3}) between linear fit and non-linear fit.

The disturbing effect of sun angles leads to retrieved SPM data that are inconsistent in time. In Vos and Schuttelaar (1997), a pragmatic approach is introduced to establish a

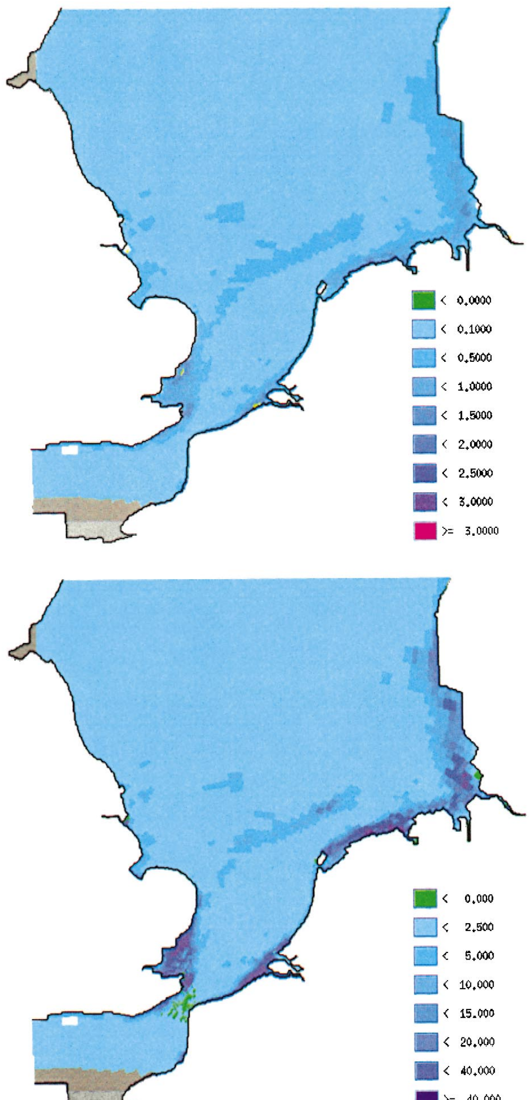


Fig. 5. Upper frame: reflectances (NOAA/AVHRR weekly composite), lower frame: corresponding suspended sediment concentration for week 25 starting at 20th June 1994. The original data were transformed onto the curvilinear model grid and scaled by a non-linear extrapolation method. Maximum concentrations are in the Thames estuary and Flemish Banks. The average concentration in the image is 1.7 g m^{-3}. The concentration in the plume that crosses the North Sea varies from 5 to 15 g m^{-3}.

time-consistent series of SPM concentration patterns derived from reflectance data. This approach is based on enforcing the total amount of mass in the upper layer according to the observed SPM concentration to be equal to the total amount of mass in the upper layer according to the SPM transport model. This is achieved by tuning the parameters a and $R(0+, c=0)$ in the linear part of Eq. (3), assuming that the variation in time of the total amount of mass is small; enforcing the consistency of the amount of sediment in the upper layer will give rise to a series of observed SPM concentrations, which is consistent in time.

Furthermore, a concentration-independent correlation will lead to an incorrect conversion of the normalised reflectance for SPM concentrations above the saturation threshold. Therefore, a non-linear extrapolation method is included in the conversion algorithm to account for the saturation above 20 g m^{-3} parameterised by the curvature parameters c^* and δ. The latter is calibrated based on a comparison of the NOAA/AVHRR images and in situ data from 1994–1995 from the DONAR data base of the National Institute for Marine and Coastal Zone Management (RIKZ, 1998). The calibrated values for 1994–1995 are $c^* = 15$ g m^{-3} and $\delta = 30$ g m^{-3}. Although, in principle, these curvature parameters should be calibrated for every image separately, due to the lack of sufficient in situ data, this is usually impossible to accomplish. Consequently, c^* and δ are fixed at the above mentioned values of 15 and 30 g m^{-3}, respectively. In Fig. 4, an example is given of the correlation between the weekly composite of the NOAA/AVHRR data (percent reflectance) and in situ concentration samples for the 16th week of 1990.

Despite its simplicity, this approach has been shown to be effective to retrieve relevant information with respect to large scale and seasonal variation of SPM patterns. In Vos and Schuttelaar (1997), it was concluded that the linear relation was valid for the North Sea for concentrations up to 15 g m^{-3} and sometimes 20 g m^{-3} (Vos and Schuttelaar, 1997). For higher concentrations, it was shown that the non-linearity has to be accounted for. In both the latter study and the present study, the seasonal variability was calculated using monthly composite SPM concentrations. The absolute values in SPM in these monthly composites show deviations with in situ data up to 25% below 25 g m^{-3}, while for SPM concentrations above 25 g m^{-3} the deviations might be somewhat larger (Fig. 5).

4. Sensitivity analysis SPM transport models

4.1. Introduction

The integrated SPM transport model with all its contributing modules is shown in Fig. 6. These modules can be seen as (non-linear) input–output relations. Insight into the model's sensitivity can be assessed in two different ways: first, by considering the quantitative effect of variations of individual input parameters in one of the modules (to what extent does the variation of a particular input parameter affect the GoF value?); second, by assessing the sensitivity in a qualitative way by determining the relative impact of all possible model parameters variations simultaneously (for which input parameter is the GoF criterion most sensitive?). The qualitative top–down analysis and

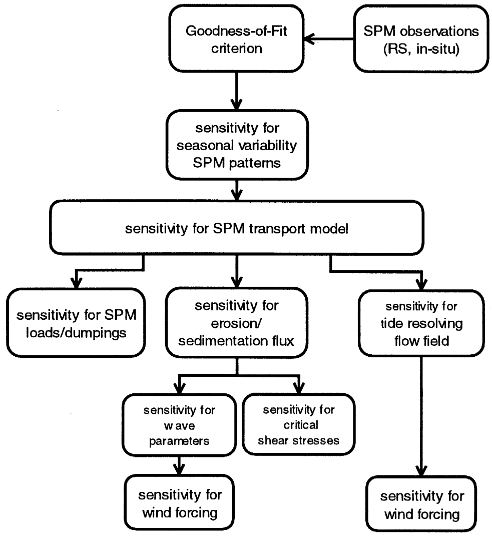


Fig. 6. Top–down sensitivity analysis of the SPM transport model.

the quantitative forward analysis form the two basic ingredients of any model calibration procedure. Model calibration is simply a repeated application of (i) a qualitative analysis to determine for which parameters the model performance is most sensitive, and (ii) a quantitative (forward) analysis to determine the actual improvement of the model in terms of a reduction of the GoF criterion.

In principle, the sensitivity analysis of the SPM transport model can be easily extended to the input parameters of the hydrodynamic module such as the air–sea interaction coefficient, bottom friction, boundary forcing, etc. However, as this chapter focuses on the concept of sensitivity analysis and the methodology, the analysis is restricted to a limited set of parameters distributed over the modules of the SPM transport model that may be assumed to account for the major part of the error in the transport part of the model.

4.2. Example 1 — the model of the Dutch Coastal Zone

The SPM transport model of the Dutch Coastal zone is run on a curvilinear boundary fitted 2D horizontal grid with along-shore orientation and increased resolution in on-shore direction. The model is stirred by a tidally averaged flow under mean wind conditions (Lander et al., 1996) and wind-induced wave action based on daily averaged wind data at station K-13 provided by the Royal Netherlands Meteorological Institute (KNMI). Here, only one fraction of sediment is taken into account and the erosion/sedimentation processes are represented by means of the Partheniades–Krone formulation (Partheniades, 1962; Krone, 1962). At the Southern open boundary, the multi-year average derived from in situ observations was imposed, whereas in situ data from Noordwijk and Terschelling were used to represent the Western open boundary (Boon and Baart, 1996). The simulation of SPM transport in the Dutch Coastal zone covers a

2-year period, 1994–1995. The hydrodynamic forcing was based on previous modelling (De Kok and Salden, 1994).

• In the initial model set, the settling velocity w_s was assumed constant in time, i.e. $w_s = V_0$. However, in some of the runs that are carried out as part of the sensitivity analysis the settling velocity in waters with a depth less than 20 m was defined as a function of the day-number:

$$w_s(t) = V_0\left[1 + 0.5\cos\left(\frac{2\pi(t+\varphi)}{365}\right)\right], \tag{4}$$

where V_0 and φ the amplitude (m day^{-1}) and phase lag (days), respectively, and t the Julian day number. A time-dependent formulation mimics the presence of stratification in a 2D model. Stratification effectively modulates the sedimentation flux in spring and summer. This effect is lumped into the cosine function where the phase lag φ is tuned to adjust the moment of maximum settling velocity over the year.

• The erosion rate E_0 is assumed to be constant and fixed at 0.2 kg m^{-2} s^{-1}.

• The critical bed shear stress for sedimentation and erosion are $\tau_{c,sed} = 0.10$ Pa and $\tau_{c,ero} = 0.75$ Pa, respectively.

• Information on the bed load in the Dutch Coastal zone suggests that the sea bed is rather clean (Dronkers et al., 1990), which is not fully consistent with the initial bottom assumption employed in this model where the bed load is overestimated and the initial erodibility condition of the sea bed in the model is inaccurate.

4.2.1. Set-up of the sensitivity analysis

For the Dutch Coastal zone model, six uncertain parameters were varied in the sensitivity analysis, namely, the magnitude and phase of the settling velocity (V_0, φ), the erosion rate (E_0), retention factors for the dumping at Loswal Noord (R_L), for the river discharge from Rotterdam Water Way (R_{NW}) and the fetch length for wave stirring by wind (F_w). In the experiments, only the wind fetch in the Wadden Sea area was varied. In some simulations, the dumping at Loswal Noord is made time-varying (dynamic load) over the years 1994–1995 according to figures supplied by the local authorities (see Fig. 2.5 in Vos et al., 1998a). The geographical zones over which the spatial aggregation is carried out consist of zones oriented alongshore to the Dutch coast.

4.2.2. Results

The analysis shows the following.

• The main parameters to improve the model performance are the amplitude and seasonal variability of the settling velocity, the erosion rate, the fetch and the loads at Loswal Noord. However, the reduction of the GoF criterion for individual parameter variations does not add up, which confirms the large uncertainty in the SPM transport model, especially concerning the exchange in the vertical.

• All variations of the parameters that imply a removal of mass of the suspended sediment from the system lead to a reduction of the GoF criterion. Since the total amount of sediment in the upper layer according to the model was made equal to the amount of sediment observed in the SPM concentration, it must be concluded that the distribution of sediment is in error.

· Inspection of the contribution per month reveals that approximately 55% of the reduction of the GoF value is found in July–August. The stratification in summer (see Fig. 7) induces a large sensitivity for the parameter settings that determine the net erosion/sedimentation flux and shows up as large sensitivity for time-dependence and magnitude of the settling velocity (runs 3 and 10) and the erosion rate and fetch length (runs 8 and 6) (Fig. 8).

· Optimisation of the settling velocity (using a time-dependent description) alone gives already satisfactory results. Based on these experiences, it is expected that the present data mainly allow for optimisation of the seasonal variability of SPM. Time-dependent data on the sea bed are required for a more accurate initialisation of the bottom and to estimate the erosion rate.

· The trends in the adjustment of the GoF criterion for various parameter variations that are observed for in situ data are similar to those for the remote sensing data. It demonstrates that for sensitivity analysis remote sensing data are equally useful as in situ data.

4.3. Example 2 — the SPM transport model of the North Sea (2D mode)

In the contribution to the PROMISE study, the transport of SPM was modelled on a boundary fitted curvilinear grid (see Gerritsen et al., 2000) covering the North Sea area from 2°W to 57°N. The grid has an increased resolution in Dover Strait and the coastal areas of England, Belgium and the Netherlands. Wind and pressure fields were obtained from the Norwegian Meteorological Institute (DNMI) and used to drive the tide resolving hydrodynamic model. The wave action on erosion is included through the bottom shear stress. The significant wave height and wave period are enhancements of the WASA wave model results (WASA group, 1995).

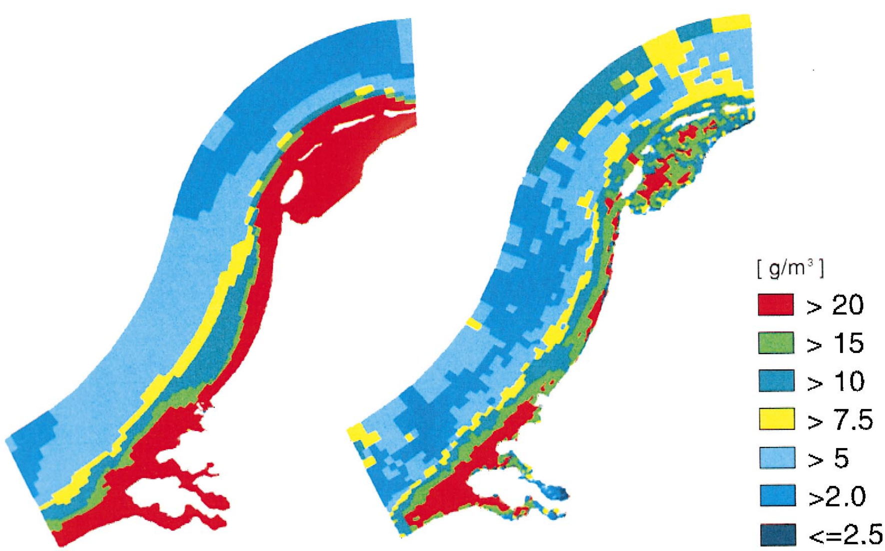
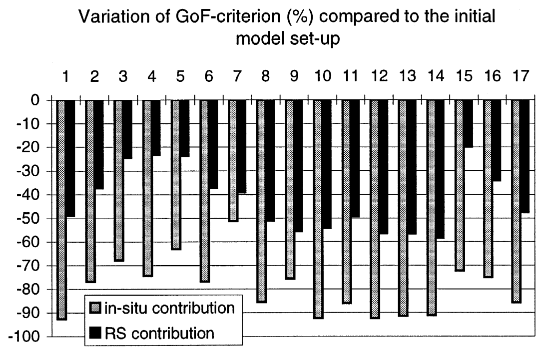


Fig. 7. The SPM concentration according to the calibrated model of the Dutch Coastal Zone (left) and the NOAA/AVHRR monthly composite for March 1995.



Run ID	Description
	Initial model set up (reference run)
1	No dumping at Loswal
2	Reduced Load at Rotterdam Water Way
3	Seasonal varying settling velocity, Eqn. (4)
4	as 3 but with reduced loads at Loswal
5	as 3 but increased fetch
6	as 4 but reduced fetch
7	as 6 but dynamic loads
8	as 4 but reduced erosion rate
9	as 4 but adjusted phase lag
10	as 4 but doubled settling velocity
11	as 10 but dynamic load and reduced fetch
12	as 11 but reduced erosion rate
13	as 10 but different phase lag
14	as 12 but different phase lag
15	10% reduced loads at Loswal
16	as 15 but reduced fetch
17	as 16 but reduced erosion rate

Fig. 8. Contribution of remote sensing and in situ data in the reduction of the GoF criterion compared to the reference run.

In the present 2D mode SPM transport model, only one fraction of sediment is taken into account and the erosion/sedimentation processes are represented by means of the well-known Partheniades–Krone formulation (Partheniades, 1962; Krone, 1962) with the following parameter values:

- concentration dependent settling velocity, $w_s = V_0 c_n$, $V_0 = 5.13 \times 10^{-4}$ s^{-1} m^{3m+1} kg^{-m}, $m = 1.29$;
- erosion rate, $E_0 = 0.2$ kg m^{-2} s^{-1} (see Boon and Baart, 1996);
- critical shear stress for sedimentation, $\tau_{c,sed} = 0.10$ Pa;
- critical shear stress for erosion, $\tau_{c,ero} = 0.75$ Pa (see van Alphen, 1987).

The sediment inputs (dumping and riverine inputs) were derived from known budgets for the main estuaries and a constant concentration of 2 g m^{-3} was imposed at the western open boundary. The values used for the dumping at Holderness, Loswal Noord and Zeebrugge, coastal erosion at Holderness, Suffolk and Norfolk are described in detail in Gerritsen et al. (2000). All model parameters listed above are assumed to be constant in space and time. The model was spun up for a period of 12 months to initialise the horizontal salinity distribution and the bed surface sediment distribution, the simulation period was 1st March–1st October, 1994 (Fig. 9).

As interest is in SPM patterns and their variation in time, in the North Sea application it was decided to focus on remote sensing data considering the fact that the contribution of the limited set of in situ data available for the coastal areas was expected to be small. Moreover, the case study on the Dutch Coastal zone model already demonstrated that in situ data give similar information as the remote sensing data. Therefore, the analysis of the North Sea model is carried out using only the GoF criterion for remote sensing data.

4.3.1. Set-up of the sensitivity analysis

The sensitivity analysis of the SPM transport model of the Dutch coastal zone showed that the SPM transport on a local scale was most sensitive for the magnitude of

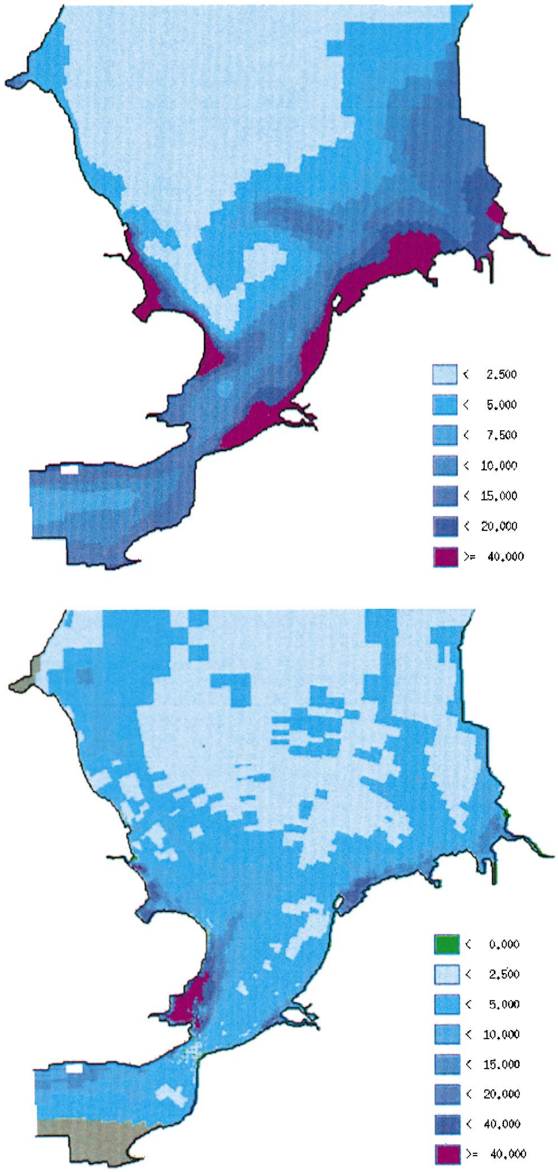


Fig. 9. SPM concentration according to the initial model set-up (upper frame) and the observed SPM concentration retrieved from NOAA/AVHRR images (lower frame) for July 1994.

the dumping at Loswal and the magnitude of the settling velocity and the erosion rate. With this result in mind, the following parameters are taken into account in the sensitivity analysis of the North Sea model: the critical bed shear stress for erosion, the critical bed shear stress for sedimentation, the erosion rate, the magnitude and the exponent of the concentration in the settling velocity. For the zonal partitioning, see Fig. 2.

4.3.2. Results

With the North Sea model, 23 runs were carried out, each being a single parameter variation. In order to scan the sensitivity of each of these parameters over the parameter space, variations of −50% and +100% were applied. The effect of parameter variations on the GoF criterion is shown in Fig. 10.

In general, the average reduction of the GoF criterion is much smaller than found for the analysis of the Dutch Coastal Zone model. This is due to the fact that on a North Sea scale the impact of the horizontal transport is much larger than for the model of the Dutch coastal zone where the processes in the vertical dominate the horizontal transport. A detailed discussion of the sensitivity analysis can be found in (Gerritsen et al., 2000).

Fig. 10 shows that, considering the relatively limited variation of the GoF criterion over the considered parameter space, the chosen parameterisation of the model error does not have sufficient degrees of freedom to enable a substantial improvement of the SPM transport model. The assumed uniformity in space and time may form a severe constraint for the model sensitivity, although this cannot be deduced directly from Fig. 10. Removing the uniformity assumption leads to a high-dimensional parameterisation of the model uncertainty and the single parameter variation approach will show its computational burden. An alternative in assessing the spatially and temporally distributed sensitivity is to use the adjoint model (Chavent, 1979), see Section 4.4.

4.4. Adjoint modelling

In this section, the sensitivity of some model output c_{out} with respect to a variation in the model input p_{input} is determined as $\partial c_{out}/\partial p_{input}$. Now, starting at the top level of the 'pyramid' shown in Fig. 6, the sensitivity of the GoF criterion for model parameters on

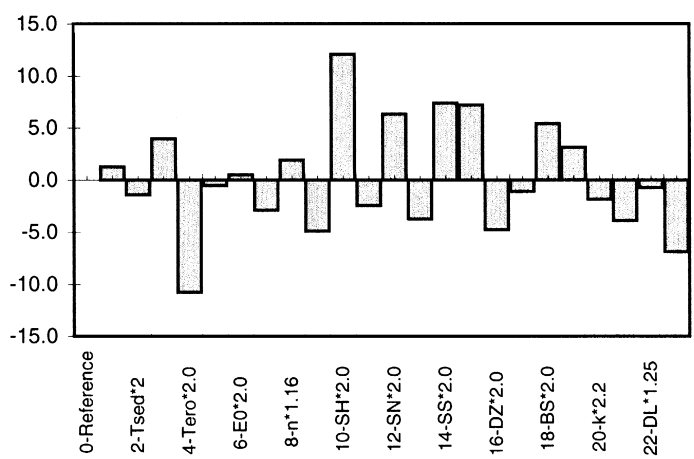


Fig. 10. Relative difference (%) in GoF criterion for the SPM simulations in 2D mode compared to the initial model set-up (for details see Gerritsen et al., 2000).

the lower levels can be found by applying the chain rule of differentiation. For example, the sensitivity of the GoF criterion for the bed shear stress τ is found according to

$$\frac{\partial \mathrm{GoF}}{\partial \tau} = \frac{\partial \mathrm{GoF}}{\partial \bar{c}}\left[\frac{\partial \bar{c}}{\partial \phi_{\mathrm{ero}}}\frac{\partial \phi_{\mathrm{ero}}}{\partial \tau} + \frac{\partial \bar{c}}{\partial \phi_{\mathrm{sed}}}\frac{\partial \phi_{\mathrm{sed}}}{\partial \tau}\right], \tag{5}$$

where ϕ_{ero}, ϕ_{sed} are the erosion and sedimentation fluxes, respectively. The adjoint model is simply an implementation of the chain rule of differentiation of a function (here, the GoF criterion) that is defined in coded statements, see Chavent (1979). It is a computationally very efficient procedure to determine the sensitivity of all model parameters simultaneously as the computation time is independent of the number of model input parameters that are included in the sensitivity analysis.

4.4.1. The adjoint formalism

Suppose that in state-space form, the SPM transport model is represented as:

$$f_{\mathrm{im}}(p, c_t, c_{t+1}) = f_{\mathrm{ex}}(p, c_t) + b(p, u_{t+1}). \tag{6}$$

Eq. (6) describes the evolution of the SPM concentration c_t in time (for $t = 0, \ldots N-1$). u_t represents the external model forcing (wind, waves) and p represents some (empirical) model parameters. The functions f_{im}, f_{ex} denote the implicit and the explicit part of the numerical model, respectively.

Assume the GoF criterion is defined as by Eq. (1), the gradient $\nabla_{\bar{p}}\mathrm{GoF}$ is found as

$$\nabla_{\bar{p}}\mathrm{GoF} = \sum_{t=0}^{N-1}\left\{\left[\frac{\partial f_{\mathrm{im}}}{\partial p}(c_t, c_{t+1})\right]^T - \left[\frac{\partial f_{\mathrm{ex}}}{\partial p}(c_t)\right]^T - \left[\frac{\partial b}{\partial p}(u_{t+1})\right]^T\right\} v_{t+1}, \tag{7}$$

if the adjoint variables $\{v_t | t = 0, \ldots, N\}$ satisfy the following equation:

$$\begin{aligned}\left[\frac{\partial f_{\mathrm{im}}}{\partial c_t}(c_{t-1}, c_t)\right]^T V_t = &\left\{\left[\frac{\partial f_{\mathrm{ex}}}{\partial c_t}(c_t)\right]^T - \left[\frac{\partial f_{\mathrm{im}}}{\partial c_t}(c_t, c_{t+1})\right]^T\right\} v_{t+1} \\ &- \frac{\partial}{\partial c_t}\left\{\sum_{\substack{\text{zone} \\ i}} \sum_{\substack{\text{time windows} \\ k}} w_{i,k}^{\mathrm{user}}\left\{w_{i,k}^{\mathrm{outlier}}\left[\frac{\Delta_{i,k}^{\mathrm{RS}}}{\sigma^{\mathrm{RS}}}\right]^2\right.\right. \\ &\left.\left. + R_{i,k}\left[\frac{\Delta_{i,k}^{\mathrm{in\ situ}}}{\sigma_{\mathrm{in\ situ}}}\right]^2\right\}\right\},\end{aligned} \tag{8}$$

with an 'initial' condition $v_{N+1} = 0$ at the final time t_{N+1}.

The adjoint model, Eq. (8), is integrated backward in time, from t to $t-1$. The adjoint model is again an advection–diffusion equation, not driven by sediment fluxes but driven by sources, which are a linear function of the SPM concentration residuals $\Delta_{i,k}^{\mathrm{RS}}$, $\Delta_{i,k}^{\mathrm{in\ situ}}$.

The sensitivity analysis by means of adjoint modelling has the following advantages over an analysis based on single parameter variations:

- the spatial and temporal variation of the sensitivity of each individual model variable and model input parameters is easily assessed;

- once the adjoint solution is determined, the partial derivative of the GoF criterion with respect to virtually any model parameter is given by Eq. (7). This implies that
- the computational time to determine $\nabla_{\bar{p}}$GoF is independent of the dimension of p.

Adjoint modelling has become one of the basic ingredients of oceanographic data assimilation. Although its application in the field of transport modelling is new, its concept and application in oceanographic (as well as in meteorological) applications are reviewed in numerous textbooks, see for example Daley (1991)).

4.4.2. Adjoint analysis

From Eq. (7), it is seen that the summand is a function in space and time representing the spatially and temporally distributed sensitivity. For a number of parameters this spatial and temporal variability of the sensitivity is illustrated in Figs. 11 and 12. The spatial and temporal variability of the model sensitivities as determined by the adjoint analysis allow a detailed insight and more balanced conclusions compared to the analysis based on single parameter variations. Fig. 11 demonstrates the temporal variability of the sensitivity of the GoF criterion with respect to the loads in the Southern coast of England, the Thames estuary and the Flemish Banks, Fig. 12 represents the spatial variability of the GoF criterion with respect to the west–east flow and the settling velocity, respectively. The use of a spatially uniform scale factor for the settling velocity is obviously sub-optimal as it has opposite effects in the Dutch coastal area and the Wadden Sea. A similar argument holds for a time-invariant scale factor for the loads.

The sensitivity with respect to the input due to dumping in, for example, Holderness and the German Bight are rather persistent in time, which marks the presence of a systematic model input error. The spatially fully distributed sensitivity for the loads, dumping and coastal erosion shows areas where the sediment influx is overestimated (Holderness, Norfolk, German Bight) as well as areas where it is underestimated (Flemish Banks, Thames). Therefore, the adjoint analysis substantiates the conjecture that the spatial distribution of the sediment is found to be in error although the total amount of sediment according to the model is equal to the observed SPM concentration as the result of the reinforced consistency in amount of sediment in the conversion algorithm outlined in Section 3.

The model sensitivities, expressed in terms of the sensitivity of the GoF criterion for variations of scale factors for dumping, the loads, the bottom shear stress, critical bottom shear stress, etc., lead to the following ranking of sensitivities (in decreasing order):

1. sensitivity for the prescribed dumping and coastal loads,
2. sensitivity for the shear stress and the critical shear stress for sedimentation,
3. sensitivity for the residual flow driving the transport, and
4. sensitivity for the settling velocity.

If interpreted in terms of the sensitivity for scale factors for dumping, coastal loads, etc., the (indicative) ratio of these sensitivities is 10^2:10^0–10^1:10^{-1}:10^{-3}. On the level of sediment budgets, no distinction can be made between errors in the loads, errors in

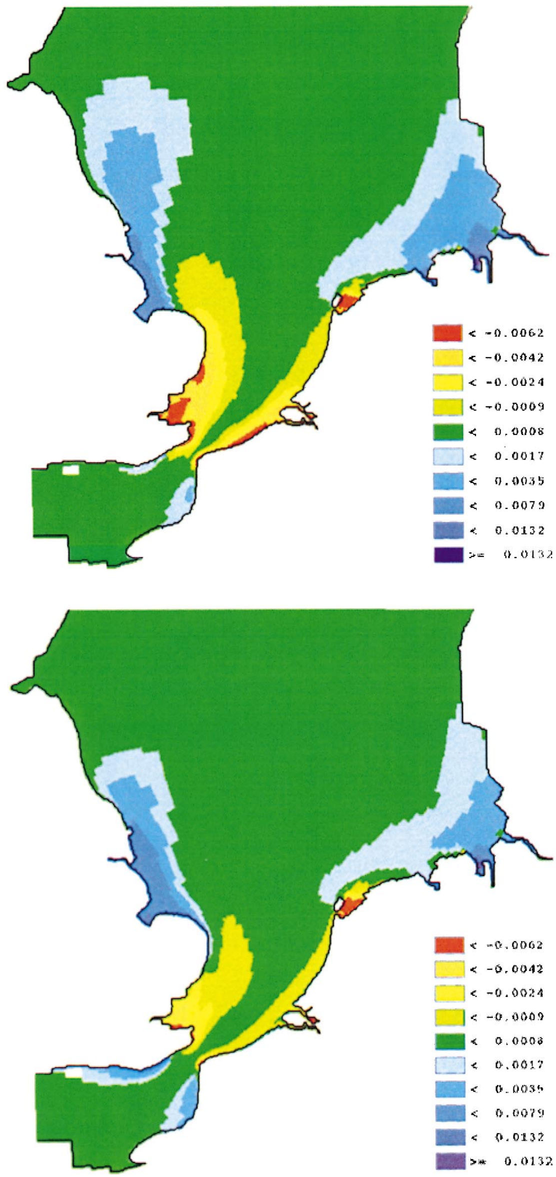


Fig. 11. The sensitivity for the loads (expressed as the gradient of the GoF criterion to the loads) in April (upper panel) and June (lower panel) 1994.

dumping and errors in the net erosion/sedimentation flux, only their cumulative effect can be assessed. Here, site-specific information is required to assign these sensitivities to specific loads, dumping or net erosion/sedimentation flux.

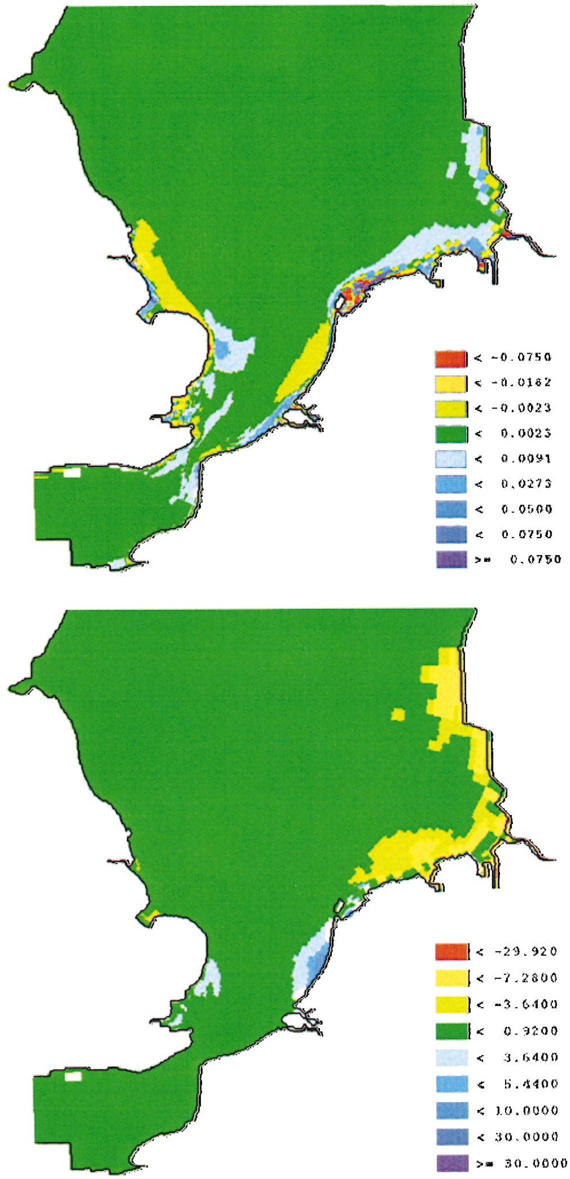


Fig. 12. The sensitivity for the flow (upper panel) and the settling velocity (lower panel) in May 1994. The sensitivity is expressed as the gradient of the GoF criterion to the flow and settling velocity, respectively.

Besides a ranking of sensitivities, comparison of the sensitivity plots may reveal a possible causal relation between sensitivities on different levels in the hierarchy of modules (see Figs. 1 and 6). By comparing the sensitivity for parameters on different hierarchical levels (for example the loads and the settling velocity) one can estimate the ratio of errors on a higher level that can be explained by errors on a lower level. For example, in the present application, it is found that the error in the Holderness area with respect to the sediment input cannot be explained by an erroneous settling velocity or sedimentation flux and must therefore be assigned to an erroneously prescribed coastal load.

5. Summary of results and conclusions

The integrated data-modelling concept and the two examples of sensitivity analysis discussed in this study are built upon the following key-issues: (i) the current set-up of the SPM transport model, (ii) the definition of a GoF criterion that reflects the modelling objective and (iii) the model reference derived from remote sensing and/or in situ observations. With respect to the latter, the expected observation error, representativity, concentration threshold, etc., need to be taken into account to assess the accuracy of the model reference in relation to the pre-defined modelling objective.

The GoF criterion has been shown to be a powerful tool in quantifying the model performance. It facilitates the evaluation of the model in a quantitative, objective and reproducible way. Nevertheless, it is not a fully objective method as it also reflects some user-preferences. Its main advantage is that it supports explicit testing and substantiation (validation) of (i) the simulation results, (ii) the modelling objective and (iii) the model output reference. By comparing the sensitivity for parameters on different hierarchical levels, one can determine the ratio of errors on a higher level (expressed by the sensitivity for the loads) that can be explained by errors on a lower level (expressed by the sensitivity for the settling velocity).

In 2D mode, the performance of SPM transport models seems to be largely determined by the correctness of the local sediment budgets and/or estimate of the loads. In this way, modelling the large-scale variability of SPM is primarily a matter of bookkeeping of the sediment budgets. Considering the limited sensitivity for, e.g. the settling velocity, the required level of detail in the formulation of the erosion/sedimentation processes used in this and likely any 2D model is limited.

6. Recommendations and ways forward

In the present study, an integrated data-modelling concept has been described to assess the performance of a model for the seasonal variability of SPM patterns in the North Sea. Besides the results discussed in the previous sections, some general recommendations can be formulated with respect to future research and application in operational oceanography.

A major source of error in SPM modelling is the sediment budget. More site-specific data is required to establish accurate estimates for the loads, dumping data and erosion/sedimentation fluxes. Here, the combined use of in situ and remote sensing data is likely to be very powerful. Whereas the synoptic remote sensing image based concentrations adequately represent the large scale horizontal variability of SPM, in situ data can provide information on more detailed aspects of the (erosion/sedimentation) processes that determine the SPM transport and the variability over the vertical.

Retrieval of information from data requires consistency and cross-correlation analyses. Given the problems of retrieving SPM concentration data from reflectance imagery, the use of models is shown to be very powerful. Still, it is expected that new and improved sensors like SeaWiFS, MODIS and MERIS will allow the use of simpler and more accurate conversion algorithms.

At the moment, the winter period may be considered as a ‘grey area’ in our knowledge and understanding of the SPM transport related processes in the North Sea. Dedicated measurement and monitoring campaigns to fill this ‘winter gap’ is one of the challenges for the coming years.

Summarising, the integrated data-modelling concept that is illustrated in this chapter is demonstrated to be well suited as a framework to support the modelling practice, both with respect to the model and the data requirements. As such, this concept undoubtedly contributes to an integrated and application-oriented use of models and observations to monitor physical processes in an operational setting.

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