DATA ASSIMILATION OF SATELLITE DATA OF SUSPENDED PARTICULATE MATTER IN DELFT3D-WAQ FOR THE NORTH SEA

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Abstract

The role and value of data assimilation techniques have been verified in many engineering areas. In this paper, the data assimilation technique, Ensemble Kalman Filter (EnKF), is used to assimilate the remote sensing data of Suspended particulate matter (SPM) from the MEdium Resolution Imaging Spectrometer instrument (MERIS) sensor on ESA's ENVISAT in the computational water quality model, Delft3D-WAQ. The objective is to determine SPM concentrations and calculate the flux of marine silt along the Dutch coast. The first results are demonstrated together with the new aspects and challenges.

INTRODUCTION

Suspended particulate matter (SPM) is small organic and inorganic particles that are in suspension form in the water column. Those particles play an important role in the ecology. They influence the underwater light climate, and in turn have an important effect on the plankton growth. Due to future extension of the present Maasvlakte land reclamation at the mouth of the Rhine outflow as shown in *Figure 1*, mining of about 300 million cubic meters of sand from the sea bed just offshore of the reclamation site is proposed. The mining of the sand will cause additional resuspension of silt fractions present in the upper layers of the sea bed.

In order to enhance our knowledge on possible effects of turbidity in the water for environmental assessment, the SPM transport system has to be modelled to identify the highly variable concentrations in time and space. The transport system is described in Blaas et al. (2007).

Any sophisticated modelling system is always based on assumptions and simplifications that may result in errors in the model's predictions. The system has to be also monitored to identify the flaws and/or errors that are present within the modelling system.

Figure 1 **The Southern North Sea with the Maasvlakte at the mouth of the river Rhine; MODIS (Terra) recording of the southern North Sea, March 26, 2007, illustrating spatial distribution of suspended matter in the surface water. (Image courtesy MODIS Rapid Response Project NASA/GSFC)**

The measurements, on the other hand are often sampled with a low spatial and/or temporal resolution. Remote sensing data however are often available with high spatial resolution. The recent synoptic mapping products of sea surface SPM retrieved from ocean colour of the ESA's MERIS sensor as explained in Eleveld et al. (2007) are used to monitor the turbidity. However, the lack of temporal resolution is still an issue. Combining those two sources of information (i.e. numerical models and remote sensing data) through data assimilation techniques would yield more accurate synoptic information on SPM in the North Sea coastal waters. The new sources of information from remote sensing data available of Dutch coastal waters, were also exploited and/or combined in Gerritsen et al. 2000, De Boer et al, 2007, and Allen et al, 2007, for example to further describe and understand the coastal system.

In this paper, the generic data assimilation technique, the Ensemble Kalman Filter (EnKF) as introduced by Evensen (1994) and described in Evensen (2003) is used to reduce the model errors and to significantly improve the accuracy of the predictions and operational forecasts. The objectives of this research are to calculate fluxes of SPM and to obtain information in space and time including the vertical distribution of SPM over the entire Dutch coastal zone that are not available from measurements alone.

SEDIMENT TRANSPORT-WATER QUALITY MODEL SETUP

The numerical model description is given in Blaas et al, 2007. The sediment transport and water quality model Delft3D-WAQ (Los et al 2006) is applied on a domain covering the southern North Sea. The sediment transport is driven by the Delft3D Flow hydrodynamic model (Lesser et al, 2004) and the surface wave model SWAN (Booij et al 1999). The modelled domain is covered by an orthogonal grid of 65 x 134 in the horizontal with a resolution that varies between 2x2 kms to 20x20 kms.

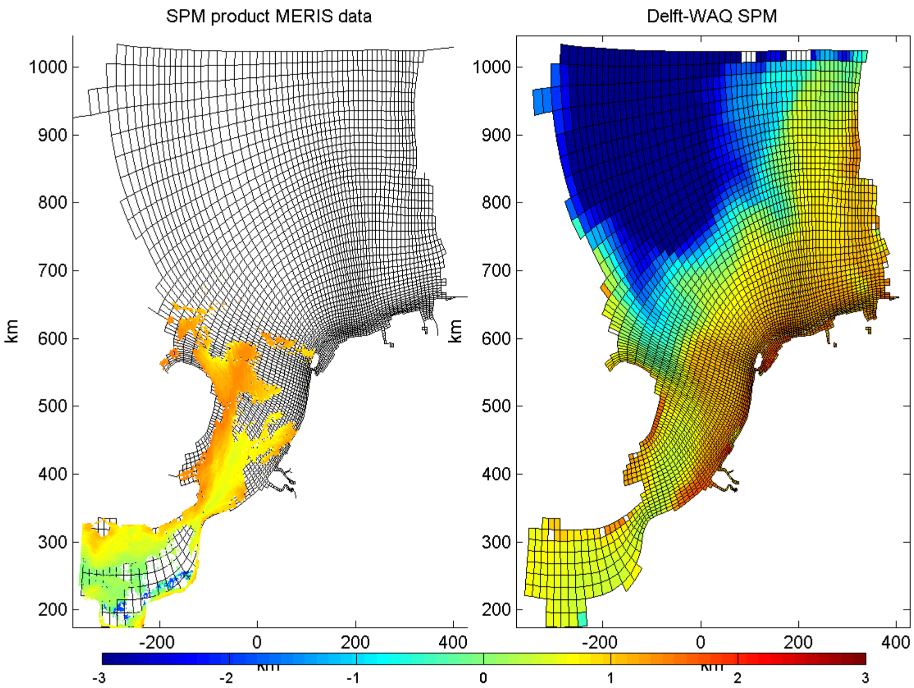

Figure 2 **SPM product from Meris data (left) and the SPM predicted by the sediment transport water quality model of Delft3D-WAQ (right) on the 17th of December 2003.**

The water depth is modelled by sigma layers to capture the variability of the water level caused by the tidal influence in the domain. Moreover, the sigma layers are of a variable thickness to allow for increased resolution near sea bed. The water motion is governed by tidal, wind and density currents. Astronomic tides have been prescribed at the open boundaries and meteorological forcing has been derived from meteorological hindcasts (HIRLAM, KNMI, see also http://hirlam.org). In addition, point sources of rivers discharge fresh water have been prescribed from gauge data. The surface waves have been accurately described through the combination of wave buoy observations with the SWAN wave model results (Booij et al. 1999). Finally, Delft3D-WAQ has been extended with an improved parameterization of the resuspension and buffering of silt fractions from and in a predominantly sandy sea bed (Van Kessel et al., 2007). This parameterization enables a realistic description of the relatively limited resuspension during the tidal cycle and the massive resuspension during high wave events. An example of the comparison between the model results and the MERIS SPM monitored data is shown in *Figure 2* for the 17th of December 2003. Other examples are given in Blaas et al (2007).

MERIS REMOTE SENSING SPM

The remote sensing SPM in the North Sea is retrieved from the MEdium Resolution Imaging Spectrometer instrument (MERIS), an imaging spectrometer on board ESA's ENVISAT spacecraft. The atmospherically corrected data (ESA, 2007) were processed using HYDROPT (Pasterkamp and van der Woerd, 2007). The full description of HYDROPT is given in Eleveld et al., (2007). The inverse model not only estimates the so-called retrieved SPM but also gives a measure of the error in the estimate (i.e. standard errors (σ) with the retrieved SPM). Additional information on the optical depth is also calculated as a first approximation (inverse of the complementary vertical diffuse attenuation coefficient K_{D560}). Example of the SPM product MERIS data and its measure of error for a large coverage day and a low coverage day, the SPM product of MERIS data are given in *Figure 3* and *Figure 4* respectively. Note that the model grid is only used as a location reference and is thus not related to the retrieval of the data here explained.

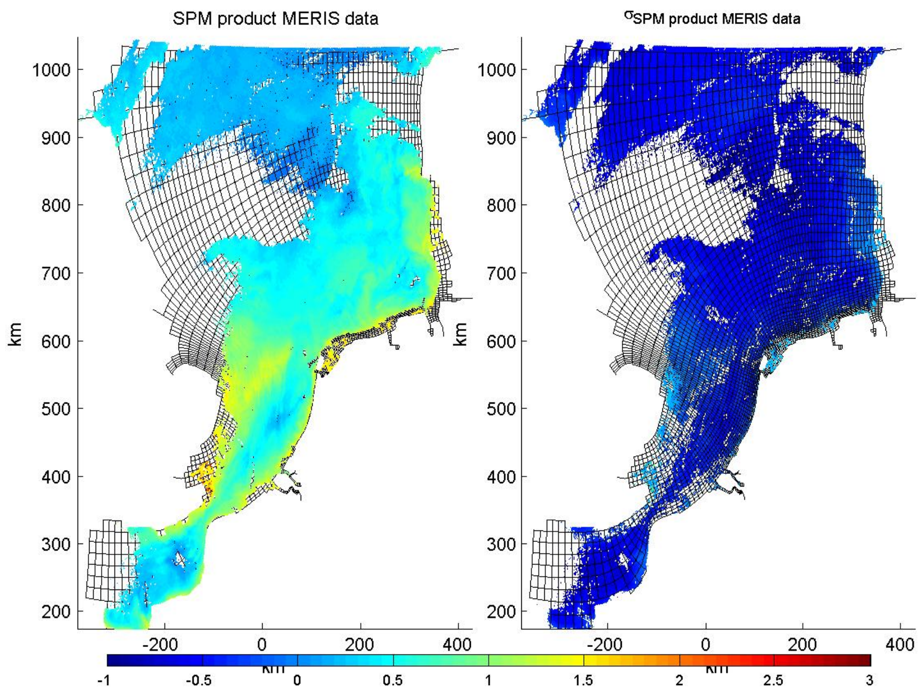

Figure 3 **Retrieved SPM observed by MERIS (left) and standard deviation (σ) of the retrieved SPM on 17th February, 2003 (large coverage).**

With large data coverage (*Figure 3*), the error in the estimate of SPM (i.e. standard deviation of the left panel) is small while at low coverage (*Figure 4*) and due to the presence of clouds and other obstacles for the retrieval process the error in the estimate is high as expected. This would confirm the fact that the SPM product MERIS data used in the assimilation is to be trusted since it reflects possible errors in the estimated retrieved SPM. The SPM data is available at least once and maximum twice a day during the year 2003. This data is used in the assimilation present in this paper.

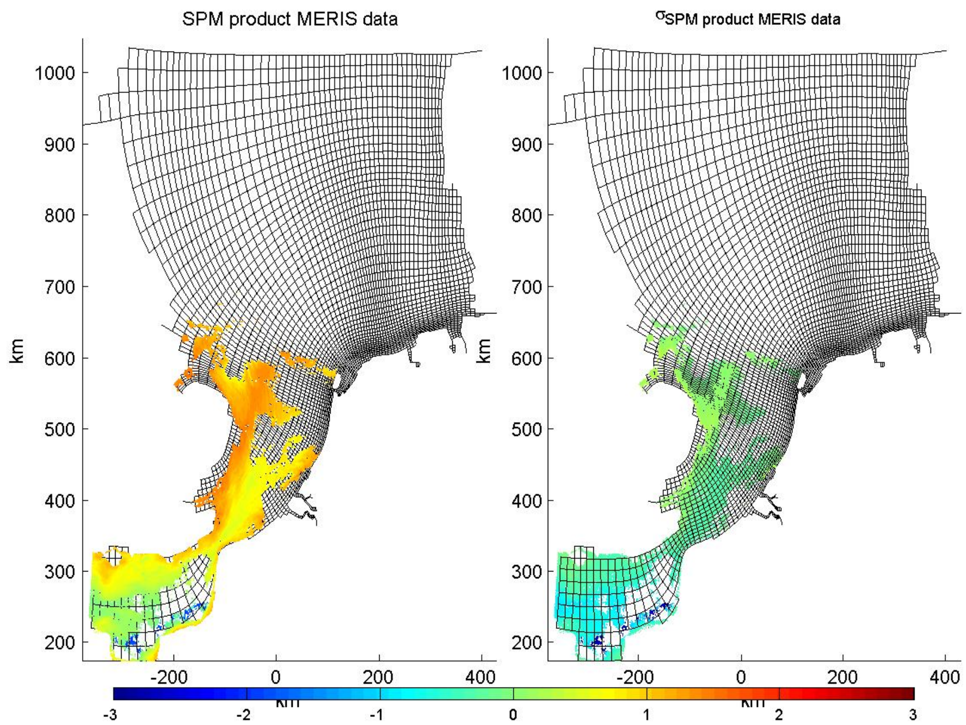

Figure 4 **Retrieved SPM observed by MERIS (left) and standard deviation (σ) of the retrieved SPM on 17th December, 2003 (limited coverage).**

ENSEMBLE KALMAN FILTERING (ENKF)

Hydrodynamic and transport models often contain several sources of uncertainty, which can occur at several stages during operation of the model. The governing equations may contain inaccuracies due to lack of knowledge about the complex physical processes and their interaction. Also, simplifications often must be made to avoid high computation times. These simplifications will increase the model's uncertainty. Uncertainties can also occur due to incorrect or incomplete input data of the model, such as boundary conditions, meteorological data, wave data and bathymetry. To reduce those uncertainties in the model output and improve its predictions, data assimilation techniques such as Kalman filter techniques can be applied. Those techniques combine the model forecast with recent measurement data, using the information on the uncertainties in the model and the measurements to give a better estimate of the model output. The Ensemble Kalman filter algorithm is here summarized as follows:

The non-linear sediment transport model propagates the system space state vector, SPM, in time. At initial time, t_k, an ensemble of size N is generated on the state vector. The ensemble is generated with a mean representing the initial condition of the state vector and with a covariance matrix that represents the uncertainty in the estimate of the initial condition. At every time step, t_k, each ensemble member, i, with its state vector forced by model errors is propagated in time through the model. The model errors are randomly drawn from a predefined distribution with zero mean and a covariance matrix, Q_k. This covariance matrix represents the structure of the uncertainties in the model (also addressed as model errors). The estimate of the time update of the state vector can be calculated, at any time step, through the mean of the ensemble. The error covariance matrix in the estimate of the time update of the state vector, $P_{k|k-1}$, is calculated from the statistics of the ensemble. Moreover, random perturbations are added to the measurements. An ensemble of size N of possible observations is generated on the actual observations, using measurement errors. The measurement errors are also randomly generated from a predefined distribution with zero mean and covariance matrix, R_k, representing the uncertainties in the measurements or measurement errors. The Kalman gain matrix that acts as a weighting factor is then calculated using the measurement operator that maps the state vector to measurement domain. Finally, the state vector for every ensemble is then updated using the information on the uncertainties assumed. The full EnKF formulation is to be found in (Evensen 2003). The advantage of the ensemble Kalman filter is the feasibility of fast implementation in complex and high non-linear models. In this paper, the EnKF is applied to assimilate SPM Remote Sensing data in Delft3D-WAQ sediment transport model, where the uncertainties in both the model and observations and model are used to sequentially update the model.

SPATIAL MAPPING

In order to assimilate the data into the model, spatial mapping has to be done to be enable consistent comparison of two different domains (i.e. measured domain and modelled domain). Within the data assimilation technique, it is the model state that is normally mapped to the data. However, in the present aaplication that would involve too many linear interpolations between the grid centres and the measured SPM at pixel level. This will introduce far too much complication in the data assimilation scheme. This might also lead to redundancy in the information, since two adjacent pixels most likely contain the same information. To avoid these complications, the data of the MERIS was mapped to model grid. There are several choices of mapping. The use of the error information in the averaging is most likely to be the best choice. For simplicity, a regular spatial averaging procedure was used as a first choice for the first tests of assimilation as here presented.

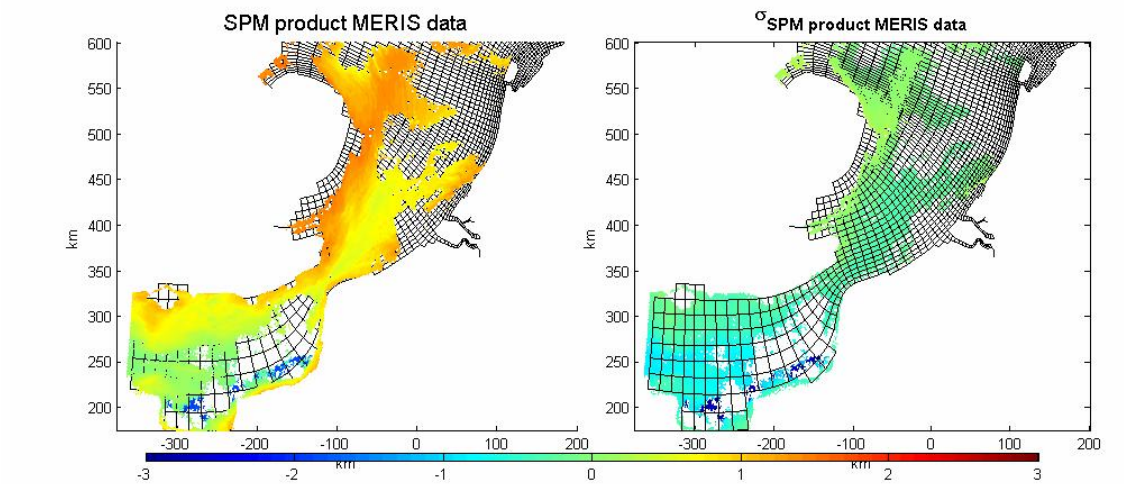

Figure 5 **SPM product MERIS data and its standard deviation "zoomed" into the area of interest on the 17th December 2003 (Addressed in the text as RAW data)**

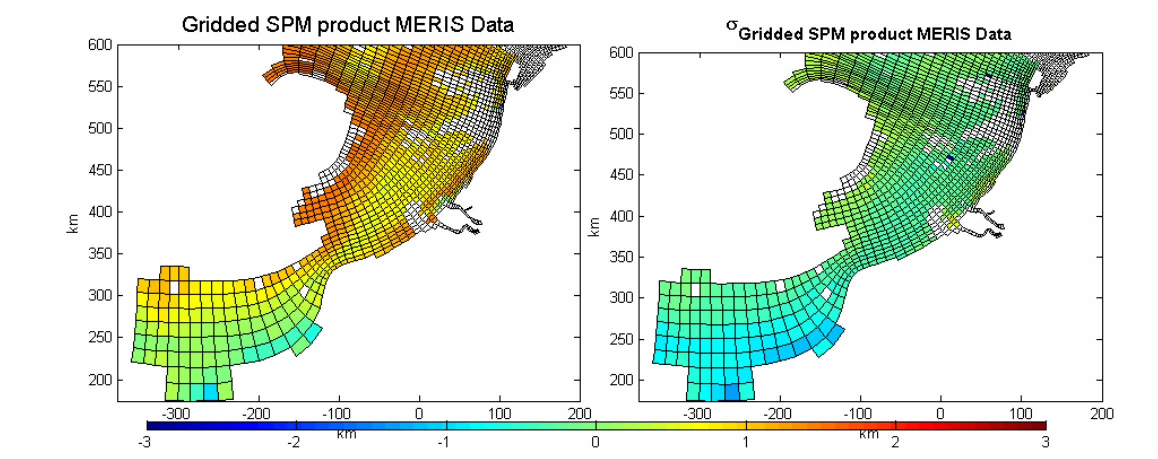

Figure 6 **Gridded SPM product from MERIS data and the standard deviation of the gridded SPM on the 17th December 2003 used in the assimilation. Only the area of interest is shown in the figure.**

. In *Figure 5* and *Figure 6*, the difference between SPM product MERIS data (raw) and gridded data can be seen. From comparing the SPM shown in the figures, it is clear that all contained information in the pixel data is actually present in the gridded data. However, meanders and eddies resolved in the original, reduced resolution MERIS data are lost upon girding. This indicates that a reasonable aggregation level has been achieved even with a simple spatial averaging procedure. However, when very few pixels are present within a grid cell of the model, some unrealistic results of SPM can be interpreted. By comparing the SPM product MERIS raw data (left panel of *Figure 5*) to the SPM gridded data (left panel of *Figure 6*) some unrealistic data coverage are present in the cloudy areas. This is due to the presence of one or two pixels in the grid cell. To avoid such artefacts, more sophisticated averaging including the number of pixels present in the cell, the error information and spatial interpolation would be recommended.

FIRST RESULTS

In this section, the application of the EnKF as the data assimilation technique applied to Delft3D-WAQ water quality model is described. A key aspect in the application of data assimilation is the use of known or assumed uncertainties or errors in both measurements and process model. The uncertainties in the measurements are provided as a measure of the retrieved value (i.e. standard deviation) as explained in Eleveld et al (2007). The structure of the uncertainties in the model and typical correlation scales however is indirectly assumed based on the experience with the model itself during the calibration and validation of the model setup (Blaas et al 2007). For the water quality model (Delft3D-WAQ), the uncertainties are assigned only to the water column suspended particulate matter (i.e. independent variables in the filtering sense). The bed sediment load was considered to be a “certain” source and/or sink. At present, all other variables such as hydrodynamic variables and wave variables are considered to be considerably accurate driving forces for the sediment transport model and thus are not part of the state vector. It was also assumed that the observed SPM is equivalent to the modelled SPM within the surface layer of the model.

The experiment is carried out by assimilating the gridded SPM shown in figure into the model results on the 17^{th} December 2003. An ensemble of only 30 members is used perturbed with the noise generated with the statistical assumptions made on the model error. It is assumed that the errors in the model are normally distributed with correlation scales of 100 kms. The assimilated field is shown in *Figure 7*. From the figure, it is seen that only slight improvements in the model results are obtained in the (stretch part) of the sea due to the lack of information in this area. Deterioration has been also encountered in the SPM values in the open sea, presumably due to the large assumed correlation scales. Noticeable improvements are observed along the Dutch shore line, the high SPM values are improved to resemble those monitored by MERIS. Though the improvements in the model prediction appear not remarkably large, the results are very acceptable as a first preliminary results of the research, since they do point out the steps for future improvements. They also agree with sound reasonable explanations the results. Besides, they do point out steps for future improvements.

For example, having the correlation scales assumed to be 100 kms may be reasonable in the area around the Maasvlakte; however in the open sea this might be considered a too high correlation scale of errors, and vice versa in the stretch along the Belgian and French coast. The assumptions on the uncertainty structure of the model errors are to be considered as rough first estimates. Uncertainty analysis should be thoroughly carried out as a follow up. It is expected that this will enhance the results of the assimilation. Comparison of assimilation results due to different assumptions is also recommended as a verification step for the assumption on the uncertainties structure.

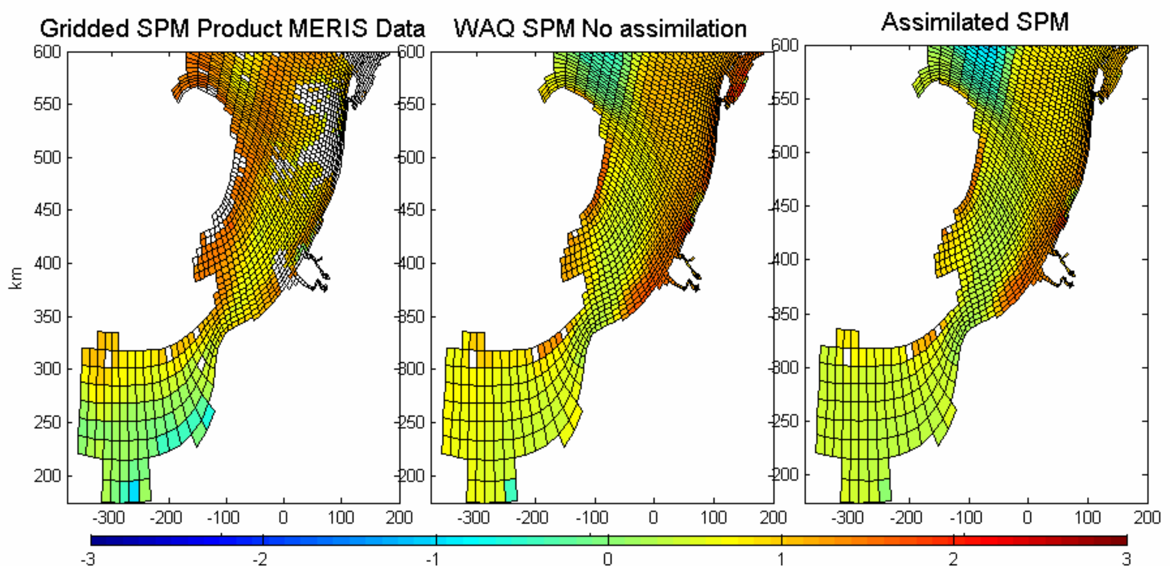

Figure 7 **Gridded SPM Product of MERIS (left), Delft3D-WAQ predicted SPM without any assimilation (middle) and the SPM Estimate due to assimilation (right) on the 17th December 2003.**

Moreover, the remote sensing data is observed from space and is limited to the surface layer (i.e. within the visible depth of the instrument) while the numerical model deals with the suspended particulate matter concentration within the upper sigma layers of variable depth. The water quality model also has a physical visible depth based on the concentration predicted. To be able to compare and/or to assimilate the observed SPM concentration into the model, one has to calculate and use the equivalent depths. In this experiment, this was not taken into consideration, only the first sigma layer of the model is assumed to be the optical depth observed. In other word, it is thus assumed that the SPM concentration observed by the instrument is equivalent to the predicted SPM concentration by the numerical model in the surface layer of the model. This can create horizontally inconsistent mismatch between the observation SPM mass within the visible depth and that of the model within the corresponding depth. Optical depth information needs to be incorporated in the assimilation to eliminate and/or decrease this mismatch.

Finally, the results here shown are a one-time assimilation at an individual date. By incorporating more data every day, the difference between the model SPM prediction and the observed data will decrease resulting in a better results of the EnKF. In other words, there is no prior information in the ensemble through the propagation of errors of the model in time at first applications, except the prior on initial conditions. It is expected that the EnKF results improve by incorporating measurements in time.

It has to be emphasised that the results here are preliminary results and will be improved by taking into consideration those aspects mentioned such as corresponding observed optical depth to the optical (visible depth) for the model, other averaging procedure including error information, and the assimilation of data for a period of time longer than one day.

CONCLUSIONS, CHALLENGES AND OUTLOOK

In this paper, the deterministic DELFT3D-WAQ sediment transport and water quality model is extended with an Ensemble Kalman filter (EnKF) technique that enables assimilation of recent observational data of different nature one of which is the remote sensing data from the MERIS imaging spectrometer on board ESA's ENVISAT spacecraft. This improves the forecasting capability of the SPM predicting system. The techniques are demonstrated for SPM prediction in the southern North sea, with particular application for the Maasvlakte area. From the first results, it is concluded that the assimilation of MERIS derived SPM into a sediment transport model is technically feasible. It improves the prediction of the concentration distribution. Many new aspects related to the assimilation of SPM remote sensing data in numerical models such as the spatial mapping, the uncertainty

definition, the definition of the optical depth, is identified during this research. Those issues have to be included as improvements in the present system.
The use of satellite optical depth information should be included in the assimilation scheme to eliminate any possible inconsistency between the observation SPM mass within the visible depth and that of the model within the corresponding depth. Moreover, applying physical constraints on the updated vertical distribution of suspended particulate matter (SPM concentrations) can be investigated. To be able to assimilate the remote sensing data into a numerical model, a special type of aggregation or spatial mapping is required. Mapping of the remote sensing data to model grid and vice versa to include error information and spatial interpolation is recommended. Finally, since the assumption on the uncertainty structure of the model errors used here are rough first estimates, more thorough uncertainity analysis should be carried out as a follow up. This would enhance the results of the assimilation. Comparison of assimilation results due to different assumptions is also recommended as a verification step for the assumption on the uncertainties structure.

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