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## **Summary and samenvatting**

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## Summary

This thesis, entitled: “Dense Water” and “Fluid Sand” Optical properties and methods for remote sensing of the extremely turbid Wadden Sea’ examines to what extent data of the satellite-instrument MERIS can be used to monitor water quality in the Wadden Sea.

Remote sensing literarily means “detecting from a distance”. This thesis is on measurements and models for optical remote sensing of water quality by means of satellite data (space borne remote sensing). The first chapter describes the principles of optical remote sensing and how sunlight is influenced by the atmosphere and water before it is detected by a remote sensing instrument. Only a small part of the detected light contains information on the substances in the water column. Remote sensing was already applied in the 19<sup>th</sup> century by comparing the water colour with a colour scale, but grew only in the 1960s and 1970s, when water quality gained more attention. The Coastal Zone Scanner was the first water-observation satellite, launched in 1978.

The four substances that have the largest influence on the colour of water are: 1) water itself; 2) phytoplankton, that mostly shows the colour of their main pigment, chlorophyll-a (Chl-a); 3) suspended particulate matter (SPM); and 4) coloured dissolved organic matter (CDOM). As these substances all have their own specific absorption and reflection spectra, their concentrations can in principle be derived from a reflection spectrum (i.e. the colour of the water). This is more difficult in coastal zones, where the specific inherent optical properties (SIOPs) of the various substances can vary substantially, while other factors (e.g. high concentrations, a mixture of substances that are difficult to distinguish, bottom reflection and adjacency effect) also influence the derivation of concentrations from reflection spectra to a great extent.

Nevertheless, remote sensing of coastal water is interesting for several reasons. Firstly, because monitoring of water quality is necessary to maintain the ecological and economical values of coastal zones. Secondly, because remote sensing can add a high frequency and spatial coverage compared to the conventional monitoring methods. This thesis explores two promising models for water quality monitoring with optical remote sensing. The Wadden Sea, an extremely turbid coastal area, was taken as case-study area. The research questions are on the variability of concentrations of optically active substances and the optical properties in the Wadden Sea, and on the two examined models: an inverse bio-optical model and an endmember model.

The Wadden Sea is a heterogeneous area, where tidal flats surface at low tide, and rivers discharge (e.g. the Ems, Jade, Weser, and also the Rhine via the North Sea coast and River IJssel) and their waters mix with the water from the North Sea. Additionally, the Wadden Sea is a nature reserve and has been on the UNESCO World Heritage List since July 2009, making the monitoring of water quality important. At the end of Chapter 1, information on the satellite data used and on the hydrology of the Wadden Sea is given.

Chapter 2 gives an overview of the known information about chlorophyll, SPM, CDOM optical properties, and remote sensing of the area to collect information on which processes influence the optical properties of the Wadden Sea, and to identify what should be taken into account when using

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remote sensing data of this area. Also, algorithms for the Wadden Sea and other extremely turbid areas are examined.

An overview of all processes influencing the optical properties of the Wadden Sea is given in Figure 2.3. There is spatial variability due to the influence of CDOM from various rivers, mixing with relatively clear North Sea water entering via the channels between the islands, and due to the occurrence of shallow areas with tidal flats (on which benthic algae and sometimes macro algae can be found) at the protected locations between the islands and the mainland. On locations where the water is calm, SPM can form flocs, which changes the optical properties of SPM. Sea grass grows at the most sheltered locations in the Wadden Sea. Tidal currents cause resuspension of soil material, which leads to increasing concentrations of SPM, Chl-a (due to the benthic algae) and CDOM (from pore water). The wind also causes resuspension; this effect is stronger in winter, when there are fewer benthic algae that stabilise the sediment with their excretion products. Another important yearly variation is the phytoplankton bloom in spring, during which high concentrations of Chl-a can occur. Such an algae bloom is often followed by elevated CDOM concentrations, as CDOM is an excretion product of algae and is also released as a degradation product after a bloom.

In the Wadden Sea, remote sensing has often been applied to create maps of tidal flats, for example to map sediment types or locations with sea grass. The Wadden Sea has also been used for studies applying radar and laser to detect coastlines. However, there are only a few studies available on optical properties and on remote sensing algorithms that can be applied in the Wadden Sea. Therefore, Chapter 2 also refers to algorithms developed for other extremely turbid areas, such as the Tamar estuary in the United Kingdom and the C2R algorithm which was mainly developed in the German Bight and could therefore probably be applied in the Wadden Sea. Additionally, a list of conditions that should allow remote sensing in areas like the Wadden Sea is given. The required conditions are: a satellite with a high spatial resolution; an atmospheric correction suitable for coastal waters; algorithms tuned for the extremely high concentrations of various substances; a simultaneous detection of water colour and the land-water boundaries or another model that predicts where surfacing tidal flats will be located at the time of image acquisition; enough knowledge on the local circumstances to interpret the results; simultaneous acquisition of satellite data and in situ measurements for validation because of the fast changes; and knowledge of the local optical properties to calibrate an algorithm.

Chapter 3 describes in situ measurements that were carried out to gain more knowledge on optical properties of the Wadden Sea. In May, June, July, August, and September 2006, and May 2007, measurements were carried out on Chl-a, SPM and the inorganic part of SPM, and on CDOM. The total absorption and the beam attenuation were measured with an AC9, and reflection spectra were determined with a TriOS sensor system. Additionally, in May 2007, the specific absorption of the sediments and pigments were determined with the filter pad method. The specific scattering of SPM was derived from the other measurements. The concentrations Chl-a, SPM, and CDOM were indeed very high: 2-67 mg m<sup>-3</sup> for Chl-a; 2-254 g m<sup>-3</sup> for SPM; and 0.15-3.07 m<sup>-1</sup> for CDOM. Variations in these concentrations were seen according to those described in Chapter 2: seasonal variations with particularly high concentrations of Chl-a in spring; tidal variations with the highest concentrations about two hours before high and low tide (during the highest currents); and also with strong wind much

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resuspension and therefore high concentrations of SPM and Chl-a. CDOM concentrations were especially high in the Ems estuary and near Lake IJssel when the locks were open.

It was not yet known that the specific absorption and scattering of SPM in the Wadden Sea were comparable with values of the North Sea, while the specific pigment absorption in the Wadden Sea was found to be much higher. The specific pigment absorption appeared to correlate with the two most dominant phytoplankton species that were present. The spectral slope of the CDOM absorption can be an indication of the type of CDOM. However, no correlations were found between this spectral slope and any other parameter. The specific absorption of SPM also showed no correlation with any other parameter, although the total absorption of SPM correlated with the percentage of mud in the sediment at the measurement location. The total absorption and beam attenuation logically followed the variations in the concentrations of Chl-a, SPM, and CDOM, and therefore also the reflection spectra showed these variations. The reflection spectra could roughly be grouped in classes according to the depth of the sampling location and local extremes in SPM and CDOM concentrations. This data of the in situ measurements can be used to calibrate algorithms for water quality monitoring in the Wadden Sea and to validate the results.

Local calibration is a current topic in the research on remote sensing of coastal zones. Chapter 4 therefore examines a model that can be calibrated with regional (medians) and local (station-specific) SIOPs. The model used is called HYDROPT; it is an inverse bio-optical model as it derives concentrations from a reflectance spectrum (inverse) based on bio-optical properties (the optical properties of pigments, SPM, and CDOM). In a first step the total absorption ( $a$ ) and scattering ( $b$ ) are calculated, and in a second step the concentrations of Chl-a, SPM, and CDOM are derived from these properties. Because the derivation of the total absorption and scattering from a reflection spectrum is completely based on physics, several researchers state that these are theoretically the most precise type of optical models for water quality. Chapter 4 pays much attention to the theory of the HYDROPT model and how it was calibrated. The model contains a lookup-table with possible reflection spectra and the related  $a$  and  $b$ . When a reflectance spectrum is given as input to the model (the input spectrum) the model first chooses the most similar spectrum from the table and what  $a$  and  $b$  belong to this spectrum. Subsequently, it attempts to model this  $a$  and  $b$ , with the SIOPs it is calibrated with and variable concentrations (the sum of the SIOPs  $\times$  concentrations =  $a$  and  $b$ ). When this is achieved, the presented results include: the concentrations, the modelled reflectance spectrum (the one belonging to the modelled  $a$  and  $b$ ), and a measure for the similarity between the modelled spectrum and the input spectrum. This measure is Chi-square ( $\chi^2$ ); the lower the value of  $\chi^2$ , the better the modelling of the spectrum was. An extra option in the HYDROPT model is automatic local calibration. For this option, the model needs to be calibrated with several SIOP sets, after which the model can choose which set leads to the best modelled spectrum. It is examined if this method is valid and if  $\chi^2$  can be used for quality control on the modelled concentrations.

The concentrations modelled by HYDROPT were good when manually measured reflection spectra were used as input. Differences between modelled and in situ concentrations were given as the root mean squared error (RMSE), and these values were 0.15-0.52  $\text{mg m}^{-3}$  for Chl-a, 0.27-0.46  $\text{mg m}^{-3}$  for SPM, and 0.17-0.34  $\text{g m}^{-3}$  for CDOM. The results varied per calibration, from which it can be concluded that local calibration influenced the results. However, 70 % of the reflection spectra appeared to be ambiguous:

these spectra could be modelled well with different combinations of SIOPs and concentrations. Hence, the calibration leading to the best  $\chi^2$  did not necessarily give the best solutions. Therefore, the automatic calibration and the quality control did not function well. This became problematic when satellite data were used as model input. Maps of modelled concentrations resulting from these input data appeared to be correct (Figure 4.7). However, when the concentrations were compared with simultaneous in situ measurements the results were poor, although not worse than those of other satellite processors. As  $\chi^2$  could be used for quality control it was unclear for which pixels the results were good and for which they were not. It seemed that the satellite results were mainly poor for the stations near to tidal flats or land. It was likely that the flats of the land influenced the reflectance. However, the database with simultaneous satellite and in situ measurements (matchups) was too small to give confidence to this assumption. More research is needed on what is the minimal distance required from land or tidal flats in order to be able to trust the results of the model.

The last part of Chapter 4 is on the modelling of water types. When HYDROPT chooses which SIOP set leads to the lowest  $\chi^2$ , it gives as output not only the concentrations and  $\chi^2$ , but also which SIOP set was chosen. When the chosen SIOP sets per pixel are plotted, maps like those in Figure 4.11 are the output (each colour stands for an SIOP set). The water at locations for which the model chooses one SIOP set apparently had similar optical properties; probably the same type of phytoplankton was present, or the SPM or CDOM was similar. Waters with similar SIOPs are here defined as “water type”. The water types modelled with HYDROPT could logically be explained with knowledge on water currents in the Wadden Sea and the German Bight. For example, a different water type could be seen in the North Sea than in the Wadden Sea (Figure 4.11). With low tide (Figure 11.4a), a third water type was visible in (and to the north of) the large German rivers; this was probably river water following the residual current. With high tide (Figure 4.11b) this river water apparently had less influence; the North Sea water was seen much closer to the coast. We believe that the results of the water type detection can be enhanced with more and better SIOP sets. SIOP are difficult to determine because they comprise of a series of measurements, and the errors of these accumulate in an SIOP set. However, the results showed that water type modelling with an inverse bio-optical model, such as HYDROPT, is possible.

Chapter 5 continues on the subject of water masses. Monitoring water masses can be interesting in areas where monitoring of precise concentrations with remote sensing data is difficult. It should be taken in account that some substances in a water mass disappear (for example SPM finally sinks to the bottom and CDOM degrades), while other substances, such as salt, are “conservative” and stay in the water mass. Therefore, it matters whether a water mass is defined as water in which the SIOPs are similar while the concentrations might change, or whether the water mass is defined as water in which the total optical properties are similar, so that it becomes another water mass when the concentrations change. Therefore, we define water in which the SIOPs are similar as the same “water type”, and water in which the total optical properties are similar as a “water class”.

Subsequently, two methods to identify water masses are compared: one based on water types (HYDROPT, as in Chapter 4) and another based on water classes (with an endmember method). The endmember method is new for monitoring water masses. The method is often used in remote sensing of land to assign percentages of typical land cover to pixels. Water masses do not have such crisp boundaries as land coverages; however, water at one location can be a mixture of different water

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masses. That is why a similar endmember model as on land can be applied on water. Various ways to determine the necessary endmembers were listed. The Gordon model, combined with the SIOPs of the Wadden Sea, as described in Chapter 3, was used for the generation. In total, there were 9 endmembers: one for pure water; one generated with low concentrations of SPM, Chl-a, and CDOM; one with high concentrations for the three substances; and subsequently one for each option with high concentrations for one or two of the substances, and low concentrations for the others.

The advantage of the endmember model is that transitions and mixing of water classes is clearly visible; most other classification methods lead to crisp boundaries. A disadvantage of such a model occurs with changing concentrations. For example, when SPM sinks to the bottom while the water mass is moving horizontally forward, the water will be classified as another water class, which makes it impossible to monitor the water mass. In the results derived from the two methods, a clear difference was seen in the North Sea. Almost the whole area outside the Wadden Islands was labelled as one water type with HYDROPT, while the water in the same area was classified with the endmember model with both the low-concentrations endmember and the Chl-dominated endmember. Probably the same phytoplankton species were common in the whole German Bight, while the total concentrations changed drastically. This explained the differences between the results using the two methods. The best water mass monitoring will be obtained by combining the two methods. Another possibility is to use the endmember model to determine the locations in which calibration of the inverse bio-optical model would be the best choice to achieve a local calibration and to derive concentrations. Some researchers have already obtained positive results with comparable methods.

Chapter 6 describes the practical application of the endmember method introduced in Chapter 5. First, the in situ measured reflectance spectra were used as model input. The percentages (“abundances”) for each endmember derived from the model were compared with the concentrations of Chl-a, SPM, and CDOM measured at the stations. The low-concentrations endmember was seen in relatively high abundances in almost every result. Additionally, in each reflection spectrum one or two other endmembers with relatively high abundances were found, showing the dominance of one or two substances on the shape of the reflectance spectrum. When the concentrations were relatively similar, SPM had the highest influence on the reflectance spectrum; this finding agreed with earlier knowledge.

Because the endmember model seemed to work well, it was applied to satellite images. The reflectances in images of various seasons, various moments in the tidal cycle, and situations with and without wind, as well as with differences in wind direction, were unmixed in abundances of endmembers in order to examine whether the model could visualise expected variations (as described in Chapter 2). The processes influencing the concentrations of Chl-a, SPM, and CDOM - examined in Chapter 2 - became visible in the results of the endmember model. Variations over the area with relatively clear North Sea water in the deep channels between the islands, and very turbid water in the Dollard near the Ems, were visible in the abundances of the low-concentrations endmember, the SPM dominated endmember, and the SPM-chlorophyll dominated endmember (for example in Figure 6.6). The SPM-Chl-dominated endmember was least abundant at high tide (Figure 6.7), when a lot of clear North Sea water was present, while it was most abundant two hours before high tide, when the tidal currents were strongest and there was most resuspension. During low tide, many tidal flats were visible. However, the abundances of the SPM-Chl-dominated endmember were relatively low during low tide,

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probably because the sediment sinks to the bottom in the shallow, calm water. With the use of images of spring 2007, the appearance and movement of an algae bloom could be followed (Figure 6.5). Finally, Figures 6.9 and 6.10 show the effect of strong wind with high abundances of the SPM-Chl dominated endmember and the SPM-dominated endmember, compared to the abundances during calm periods (Figures 6.3 and 8b). The wind-direction influenced where the highest abundances could be found.

“Novelty spectra”, which are exceptional spectra outside the limits of the endmembers, could also be detected with the endmember method. In one image a patch was seen with a much higher error than in the surrounding pixels. From in situ data and the shape of the patch it was concluded that this was most probably a bloom of coccoliths, a certain phytoplankton species with high scattering effect. A special endmember should be generated to directly detect such blooms. A disadvantage of the endmember method is that it does not directly deliver values for concentrations, but information on high or low concentrations and the dominance of several optically active substances on the reflectance spectrum. However, the results for the monitoring of water classes are positive. Therefore, more research to examine the possibilities of this method is recommended.

Chapter 7 gives the synthesis of the results in the preceding chapters as well as recommendations for application of optical remote sensing in the Wadden Sea and other extremely turbid areas. Referring to the necessary issues that should be taken in account for optical remote sensing of these areas (Chapter 2), Chapter 7 discusses which issues were dealt with in this thesis, and which issues need further research or other materials or techniques.

The new WorldView2 satellite is expected to give better results for the entire Wadden Sea area, especially during low tide, than MERIS due to its smaller pixel size. Determining land-water boundaries, with or in combination with optical remote sensing, will remain to be an important issue and needs more research. The C2R algorithm applied to MERIS data gave much better reflectance spectra than the standard MERIS algorithm. However, also with this algorithm more research is needed on the required distance from land or tidal flats that leads to high-quality reflectance data. Although this thesis largely increased the amount of optical data available for the Wadden Sea, more matchup (simultaneously measured) in situ data for calibration and validation is needed, and more data will increase the accuracy of algorithms. Measurement poles can attribute significant amounts of this type of data, which should be gathered simultaneously (without a time lag) with the satellite overpass. The algorithms examined in the thesis were tuned for the extreme concentrations in the Wadden Sea and the modelled concentrations on in situ reflectances were good. However, for HYDROPT concentration data a valid quality control was lacking when MERIS data were used as input.

Water mass identification shows promising results in this thesis. Water type results from HYDROPT can be improved by determining more SIOP sets and improving their quality, for example by measuring multiple times at each location and using the median SIOP set per location. Monitoring water classes with the endmember model is new and gives good preliminary results. Therefore, more research on the use of this method is recommended, for example on specific endmembers to detect, for example, coccoliths. The best water mass tracing is expected by a combination of both models.