Water Quality modelling of the Southern North sea using TELEMAC-3D coupled with AED2

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Abstract – **The increased number of marine works occurring in the North Sea, such as for offshore renewables infrastructure and aquaculture, gave rise to more frequent Environment Impact Studies in the area. Activities with impact on turbidity or light penetration might have secondary impact on water quality and other aquatic parameters such as primary production and nutrient levels.**

To study such phenomena, IMDC has recently started the implementation of water quality simulations in TELEMAC-3D. As a basis, the three-dimensional hydrodynamic model of the Southern North Sea and English Channel has been chosen (KaZNo model). TELEMAC-3D was applied coupled to the AED2 library to determine the nutrient cycle, primary production, and zooplankton grazing. The coupling allows to solve the interactions between hydrodynamics (transport, diffusion) and the aquatic ecodynamics. Assumptions were made for river inflow nutrient conditions. This step resulted, after calibrating a number of parameters, in a satisfactory comparison of modelled and in situ monitored seasonal patterns of Chl-a levels.

Keywords: Water quality; TELEMAC-3D; North Sea, English Channel, AED2

I. Introduction

Eutrophication and algae blooms has been one of the major environmental issues in the North Sea for decades, enhanced by anthropogenic stressors. More specifically, eutrophication is driven by the continuous increase of nutrient concentration, especially the increased availability of nitrogen and phosphorous. The North Sea is considered a nutrient-enriched coastal zone where nutrient loads primarily arrive by riverine sources (such as rivers Scheldt, Rhine and Seine). High nutrient concentration drives intense phytoplankton blooms with large phytoplankton biomass. Along the continental coast line of the North Sea, dominant phytoplankton are diatoms that are characterised by early spring blooms, followed by an important development of Phaeocystis colonies [1].

Climate change plays an important role on the expansion of biomass production by affecting the temperature of the area. It is expected that the following years the North Sea will become warmer. For this reason, an increasing interest is observed into managing the biochemical pollution observed in the area. Numerical models that allow to predict the aquatic ecodynamics of the system accurately under different meteorological and eutrophication scenarios, are proven to be useful tools for understanding and managing these issues. However, a crucial parameter for the proper use of the numerical models is the availability and accessibility of monitoring data (for calibration and validation). For the moment, available data is limited despite the great deal of scientific research has been carried out in this region [3].

In the framework of an OSPAR initiative six ecosystem models (MIRO&CO-3D BE, ECO_MARS3D FR, ECOHAM4 DE, Delft3D-GEM NL, Cefas GETM-BFM UK, POL POLCOMS-ERSEM UK-POL) have been developed to investigate the influence of the riverine nutrient loads on the North Sea system. In this project, it was concluded that the winter sea nutrient concentration has a high response with the reduction of the riverine nutrient inputs. However no similar behaviour was observed for chlorophyll or net primary production [2]. In addition, it was proven that models could be applied to support the assessment process and predict the future eutrophication status of specific water bodies.

The goal of this paper is to use the aquatic ecodynamics library AED2 coupled to TELEMAC-3D to calculate the temporal evolution of nutrients and chlorophyll-a (chl-a) in the Southern North Sea. The performance of the model was tested against available measurement data in the area of interest. The long-term objective of this work is that the developed model will be used for environment impact assessment studies in the area.

The present text is organised as follow: Initially, the setup of a model of the Southern North Sea is presented in section II and in section III the required changes made to the TELEMAC code are described. Since the water quality variables depend strongly on the water temperature, the calibration of the water temperature is described in detail in section IV. Preliminary results of the water quality model in terms of nutrient and chlorophyll-a concentration for a full year simulation are reported and compared to observations in section V. Finally, the paper ends with some conclusions.

II. Model Setup

The water quality modelling is performed with the in-housed developed TELEMAC-3D model of the Southern North Sea (KaZNo model), coupled with AED2 library see Figure 1.

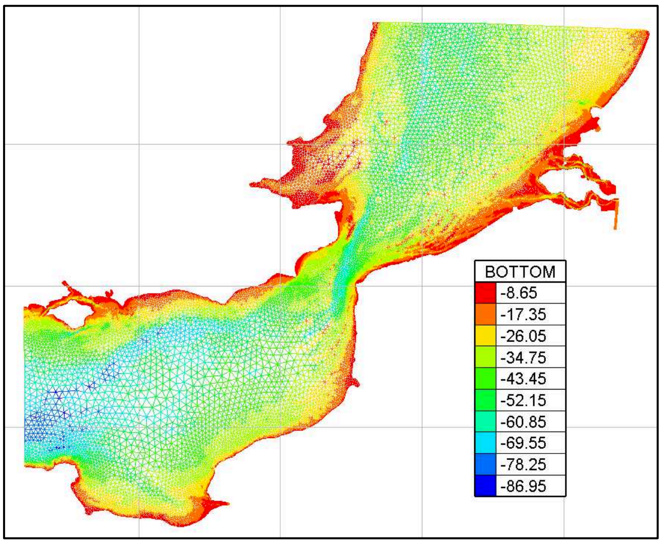

Figure 1. Figure II-1: Mesh and bathymetry of the Kazno Model (bathymetry is relative to m MSL).

The total number of computational nodes is 22,941, with 43,156 triangular elements. To better represent the water quality process, the KaZNo model runs in 3-D mode with 12 vertical nodes (11 layers) using equivalent sigma coordinates (0, 0.1, 0.2…0.9 and 1.0 from bottom to top). The mesh resolution varies from 500 m near the coast to maximum 10 km in deep waters. The model bathymetry is adopted from the EMODNET 2018 dataset with a spatial resolution of 1/16 × 1/16 arc minutes (circa 115 × 115 meters).

The hydrodynamic condition (water level and velocity) at the northern and western offshore boundary sections are computed by the in-house 2D barotropic model continental shelf model iCSM [4, 5] The hourly salinity and temperature data at the offshore boundary are provided by Copernicus Marine (https://resources.marine.copernicus.eu/product-detail/NWSHELF_MULTIYEAR_PHY_004_009/INFORMATION). Daily data of river discharge and nutrient concentration (NH4, etc) [8] are imposed at the river boundaries of Rhine, Scheldt and Seine.

The meteorological surface forcing includes the space- and time varying wind (at 10-meter height), air pressure at MSL, 2-meter air temperature, relative humidity and cloud cover, which are provided by the ERA5 hourly dataset of European Centre for Medium-range Weather Forecasting (ECMWF).

The model runs for the entire year of 2015. The initial condition of salinity and temperature are also taken from data by Copernicus Marine.

The hydrodynamic parameter settings of the KaZNo model are summarized in Table I.

Table I Model parameters.

Parameter	**Description**
Time Step	120 s
Number of vertical levels	10
Version TELEMAC	v8.1goblinshark
Salt transport	On
Wind	On
Roughness formula	Nikuradse law
Bed roughness value	Space varying roughness field
Option for the treatment of tidal flats	1: equations solved everywhere with correction on tidal flats
Treatment of negative depths	2: flux control
Free surface gradient compatibility	0.9
Vertical turbulence model	2: MIXING LENGTH
Minxing length model	3: Bakhmetev distribution
Horizontal turbulence model	4: Smagorinski
Scheme for advection of velocities	1: characteristic method
Scheme for advection of tracers	13: Leo Postma for tidal flats
Solver for Propagation	7: GMRES
Scheme for diffusion of tracers	0: No diffusion (see section III.D) + set_dif.f for vertical diffusion.

III. CODE CHANGES TO RUN AED-2

A couple of changes were implemented to TELEMAC-#D in order to be able to perform the study.

A. Meteorlogical input

In TELEMAC, there are two different models for the atmospheric exchange, a linearized model, which uses the water temperature at the surface and the air temperature (at an elevation of 2m above the sea), and a full energy balance, which uses air temperature, air pressure, nebulosity and relative humidity as input parameters. The model domain in the current study is quite large, meaning that it is likely that substantial spatial variation occurs in these parameters. However, for nebulosity and relative humidity, it is currently only possible to use a time series without spatial variation. Therefore, some code was added to allow these variables to be read. Also, a modification was made to the source code, because the atmospheric pressure in TELEMAC uses a different unit in different modules: Pa is used for the hydrodynamic calculation in TELEMAC-2D and TELEMAC-3D, whereas hPa is used for the atmospheric exchange modelling in WAQTEL.

A large number of meteorological variables for a full year, leads model to large input files when the data is interpolated to the mesh. However, the resolution of the meteorological input data (from ERA-5) is substantially coarser than the mesh resolution of the TELEMAC model. Reading the meteo data at the original mesh, rather than on the TELEMAC mesh, can reduce the file size of the meteorological data substantially. Therefore, a modification was implemented to the find_variable.f subroutine that is used in TELEMAC to read data from Selafin files, which allows the use of input data with a mesh that is different from the computational mesh. Data from the meteo file are automatically interpolated to the computational mesh using linear interpolation. In order to ease the implementation, and in order to prevent the large time loss during partitioning input files in PARTEL, the full meteorological mesh is read by all parallel processors.

Finally, the code was adapted to read a spatially varying Secchi depth from the WACGEO file, which is then used in the energy balance for calculating the water temperature. For the moment, the spatially varying Secchi depth is only used in the calculation of the water temperature, and not yet for the water quality calculation in AED2. In the later case, changes in the light penetration due to the presence of algae are taken into account is combination with a spatially constant background turbidity. It is planned to include the spatial variation of the background Secchi depth on the water quality calculations in a later stage. It is also planned to couple the calculation of the Secchi depth to the calculation of cohesive sediment concentrations that are calculated using GAIA.

B. *Implicitation of the source terms*

In the original implementation of TELEMAC-3D coupled to AED2, all source terms were discretised explicitly in time:

$$\frac{c^{n+1}-c^{n}}{\Delta t}+ADV+DIFF=S(c^{n})$$

Here, c^{n+1} and c^{n} are the concentrations of the water quality variables at time steps n+1 and n respectively, Δt is the time step, ADV and $DIFF$ are the advection and diffusion terms, which we will not consider here, and $S(c^{n})$ is the source term. This method is conditionally stable, but with a time step criterion, which is roughly given by:

$$\Delta T < -c^{n}/S(c^{n})$$

It is easy to show that larger time steps lead to the occurrence of negative concentrations, which then will lead to problems in the calculation of the sources in AED2 in the next time step. In order to prevent instabilities, the numerical discretisation was changed to an implicit discretisation using Patankar's [9] method:

$$\frac{c^{n+1}-c^{n}}{\Delta t}+ADV+DIFF=\frac{S(c^{n})}{c^{n}}c^{n+1},$$

which is based on the assumption that $\frac{c^{n+1}}{c^{n}}\approx 1$. Using this method, it was found that the stringent time step limit that were found with the original implementation indeed disappeared, thus allowing for time steps of the order of minutes (they are now limited by the hydrodynamic processes), whereas previously the maximum time step was of the order of seconds. This code change has been included in the official TELEMAC release v8p3.

C. *Drying-flooding*

When the first test runs were performed, the model crashed rapidly. After investigating the instabilities, it appeared that these are related to the calculation of source terms and surface boundary conditions for water quality and temperature on cells with small water depths. Therefore, a threshold water depth was implemented, currently set to 0.1 m, below which, no water quality calculations are calculated using AED2, and below which surface boundary conditions and source terms are not applied in the tracer equation in TELEMAC-3D. An additional change was made to the code of the NERD scheme, as still some crashes occurred, related to tracer transport on areas with very small water depths ($O(10^{-3}$ m)), where concentrations of tracers (like dissolved oxygen) all of a sudden increased rapidly. In order to overcome this issue, the code of cvdf3d.f was changed, such that for nodes with a water depth lower than 0.01 m, the tracer concentration does not change due to advection[8]. After these modifications, the water quality model could be run for a full year period, without any crashes.

D. *Settling velocity improvements*

In the original implementation of the coupling, a separate settling routine (called SETTLING) was included in the module t3d_aed2.F90. However, it appeared that the changes in the concentrations due to the settling of water quality constituents, where later overwritten in the advection diffusion module. Instead of debugging this routine, it was chosen to use the existing settling functionalities (developed for sediment) in TELEMAC-3D. The code was modified, such that the settling velocities coming from AED2 are copied to the variable containing the settling velocities in TELEMAC-3D (called WCHU), which has a default value of 0.0 m/s (no settling). In this way, the set_dif.f subroutine, for which a version including source terms and surface boundaries was previously developed [10], can be used to calculate the vertical settling and vertical diffusion of the water quality variables. When then the horizontal diffusion is switched off, which typically leads to very limited changes in the results, because the used advection schemes in TELEMAC are rather diffusive, the simulations are speedup substantially.

IV. WATER TEMPERATURE CALIBRATION

Knowing the importance of sea water temperature on driving water quality processes, an accurate representation of sea water temperature is necessary prior to perform water quality modelling. The measureddata of sea water temperature collected at a number of stations at the Belgian Coastal Zone (Figure 2) from Meetnet Vlaamse Banken, are used for the sea water temperature calibration.

[8] Additionally, tests were performed setting the fluxes to and from dry nodes (defined as cells with a water depth lower than 1 cm) to zero. The advantage of this approach is that the tracer mass is fully conserved. It appeared that in these simulations the maximum occurring tracer values decreased, leading to an improved model stability. However, the decrease was substantially less, and very high tracer values were still encountered on dry areas. Therefore, this method was not used further.

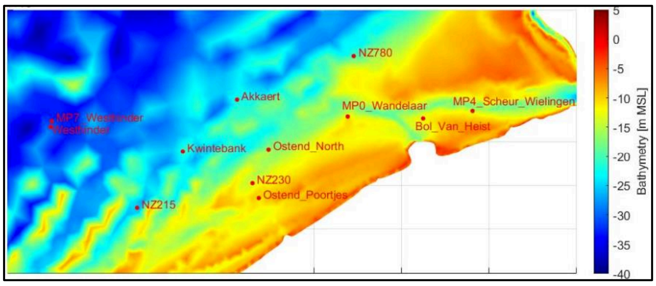

Figure 2. Figure IV-1: Measurement stations of sea water temperature in the Belgian coastal zone.

The calibration is firstly carried out for ATMOSPHERE-WATER EXCHANGE MODEL = 1 (linearised formula at the free surface), for which the optimal calibration parameter C_ATMOS (coefficient to calibrate the atmosphere-water exchange model) is found to be 0.0035.

For ATMOSPHERE-WATER EXCHANGE MODEL = 2 (model with complete energy balance), the most sensitive parameter is found to be the Secchi depth. Other parameters such as coefficients of aeration formula, coefficients for calibrating atmospheric radiation, coefficients for calibrating surface water radiation, coefficient of clouding rate etc are found to have a limited impact on the sea water temperature. The space varying Secchi depth map are adopted from [6] and is implemented in the KaZNo model.

After calibration, the KaZNo model reproduces sea water temperature in the North Sea reasonably well, with an average root mean square error (RMSE) for the sea water temperature of 0.8° C with both ATMOSPHERE-WATER EXCHANGE MODEL of 1 and 2 (Figure 3 and Table II). Time series plots are shown for the measurement station at Akkaert and Westhinder (Figure 4 and Figure 5). The yearly patterns of the sea water temperate variations are well captured by the KaZNo model.

It is also noticeable that with ATMOSPHERE-WATER EXCHANGE MODEL = 2, the daily variation of sea water temperature is better simulated, which might be important for the sea water quality modelling. Therefore, the water quality modelling will proceed with ATMOSPHERE-WATER EXCHANGE MODEL = 2.

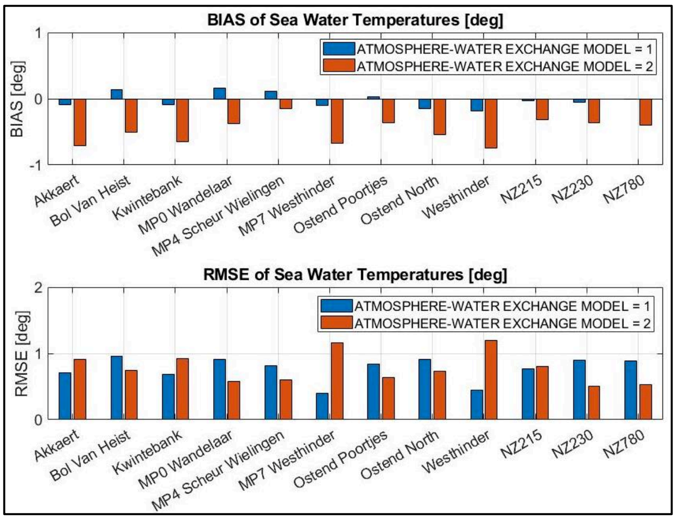

Figure 3. Figure IV-2: Bias and RMSE of the sea water temperature with ATMOSPHERE - WATER EXCHANGE MODEL = 1 and 2.

Table II RMSE of sea water temperature [deg C] with atmosphere - water exchange model = 1 and 2.

Stations	**atmosphere - water exchange model = 1**	**atmosphere - water exchange model = 2**
Akkaert	0.7	0.9
Bol Van Heist	1.0	0.7
Kwintebank	0.7	0.9
MP0 Wandelaar	0.9	0.6
MP4 Scheur Wielingen	0.8	0.6
MP7 Westhinder	0.4	1.2
Ostend Poortjes	0.8	0.6
Ostend North	0.9	0.7
Westhinder	0.4	1.2
NZ215	0.8	0.8
NZ230	0.9	0.5
NZ780	0.9	0.5
Average	**0.8**	**0.8**

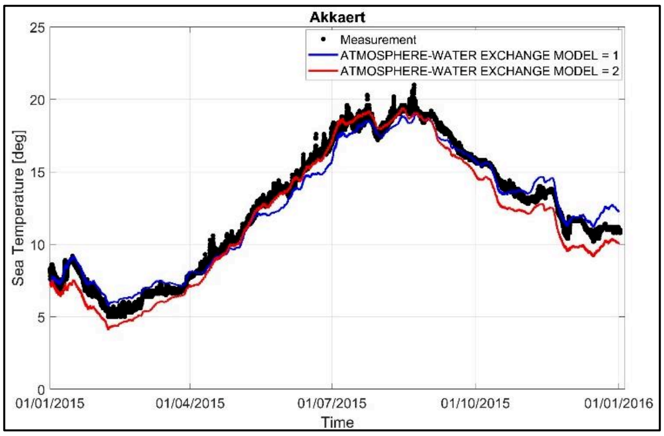

Figure 4. Figure IV-3: Comparison of measured and modelled sea water temperature at Akkaert

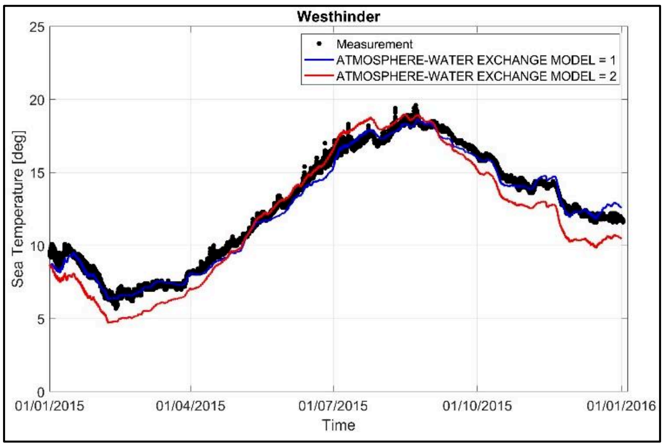

Figure IV-4: Comparison of measured and modelled sea water temperature at Westhinder .

V. PRELIMINARY RESULTS WATER QUALITY MODELLING

To numerically reproduce the nutrient cycle and primary production in the North Sea the Aquatic EcoDynamics (AED2) model was used [7]. AED2 is a biochemical library that consists of various modules that allow to simulate different processes that play a role in the biochemical cycle of an aquatic ecosystem. In Table III the modules used in the present study are presented, along with the simulated variables of each module.

Table III AED2 modules and the simulated parameters used in the present model to study water quality in North sea

Module	Simulated variable
sedflux	oxygen sediment flux
Oxygen	Dissolved oxygen
Carbon	Inorganic carbon
Silica	Silica
Nitrogen	Ammonium
	Nitrate
Phosphorus	Phosphate
Organic matter	Particulate organic carbon (POC)
	Particulate organic nitrogen (PON)
	Particulate organic phosphorus (POP)
	Dissolve organic carbon (DOC)
	Dissolve organic nitrogen (DON)
	Dissolve organic phosphorus (DOP)
Phytoplankton	Diatoms
	Phaeocystis
Zooplankton	Copepods

In the North Sea, two phytoplankton groups are dominant and used in the present model: diatoms and phaeocystis. Diatoms are typically related with lower optimum water temperatures, whereas phaeocystis colonies are linked to higher ones [1]. Moreover, Copepods grazing only on diatoms are included in some of the sensitivity runs performed in the framework of the present study.

For the initialization of the model, representative values of oxygen, nutrient and chlorophyll-a concentration were used, based on measurement data collected from Belgian Marine Data Center (BMDC, https://www.bmdc.be/NODC/search_data.xhtml;jsessionid=k7Wb3MSNEd58EOEg-D4zbZJnaJKbOGnKOzVQMRu.teuthida) for the year 2015 at different locations in front of the Belgian coast zone. The exact locations of the BMDC measurement points are shown in Figure 6

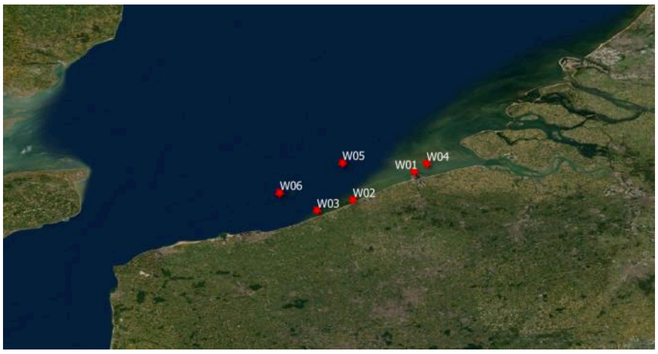

Figure 5. Figure V-1: Measurement stations of nutrients and chlorophyll-a concentration.

The main challenge for the calibration of the water quality model, is the large number of calibration parameters (more than 100). However, in the present study the calibration is focused on the most sensitive ones as identified from a previous sensitivity analysis. In addition, some parameters for the oxygen and nutrient were also manipulate (eg oxygen sediment flux, reaction rate of nitrification and reaction rate of denitrification). However, their influence on the results was less evident. The range of the calibration parameters is selected based on literature [1, 7].

As mentioned above the calibration of the water quality model is quite challenging and the available measurements limited. In this paper, calibration is mainly focused on the time evolution of chl-a concentration at the North Sea. In Figure 6 to Figure 11 the preliminary results in terms of surface chl-a concentration over an entire year, obtained from four different sensitivity runs are shown. The presented time series are extracted at the measurements points shown in Figure 6. An overview of the sensitivity runs performed in this study is presented in Table IV. The first three runs indicate the influence of silica uptake and Copepods grazing on the chl-a concentration. More specifically, in run01 silica uptake is not taken into account and the zooplankton module is not active. In run02, the silica uptake for diatoms is activated. Run03 is similar to run01 but Copepods grazing is considered only on diatoms. It can be noticed that silica uptake and the presence of zooplankton lead to a decrease of chlorophyll-a. Therefore, in run04, where both silica uptake and zooplankton are activated, the basic calibration parameters for the phytoplankton groups have been adjust to better reproduce the phytoplankton bloom.

Table IV Overview of the sensitivity runs performed

Runs	Activated modules	
run01	Sedflux oxygen carbon Organic matter	Nitrogen Phosphorus Phytoplankton
run02	Sedflux oxygen carbon Organic matter	Nitrogen Phosphorus Silica Phytoplankton
run03	Sedflux oxygen carbon Organic matter	Nitrogen Phosphorus Phytoplankton Zooplankton
run04	Sedflux oxygen carbon Organic matter	Nitrogen Phosphorus Silica Phytoplankton Zooplankton

For the validation of the numerical model, the obtained results are compared with both BMDC measurements and satellite data provided by Copernicus (https://marine.copernicus.eu/). It is worth noting that for year 2015 the available BMDC measurements are limited. Furthermore, an inconsistency can be observed between the two data sets. Based on BMDC data, the phytoplankton bloom occurs at the end of March whereas the satellite data suggest that the bloom occurs in the second half of April. Since satellite data is less scarce, they are here considered as more relevant for the validation of the model.

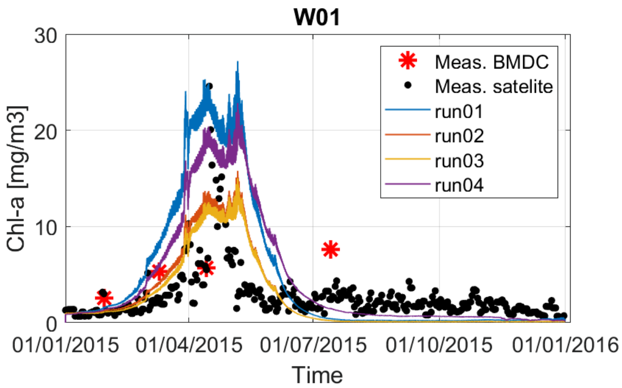

Figure 6. Figure V-2 Comparison of model output and measured data (both BMDC and satellite data) in terms of chl-a concentration for 2015, at the measurements point W01.

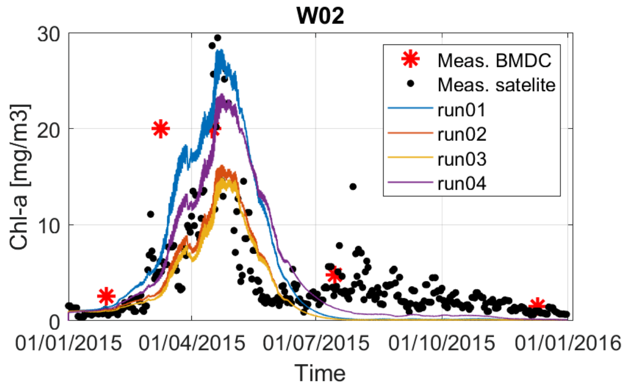

Figure 7. Figure V-3 Comparison of model output and measured data (both BMDC and satellite data) in terms of chl-a concentration for 2015, at the measurements point W02.

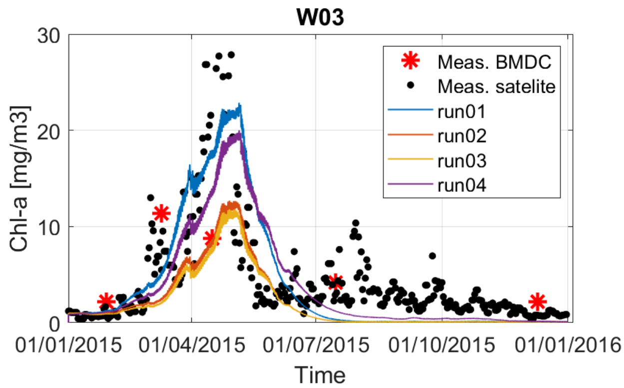

Figure 8. Figure V-4 Comparison of model output and measured data (both BMDC and satellite data) in terms of chl-a concentration for 2015, at the measurements point W03.

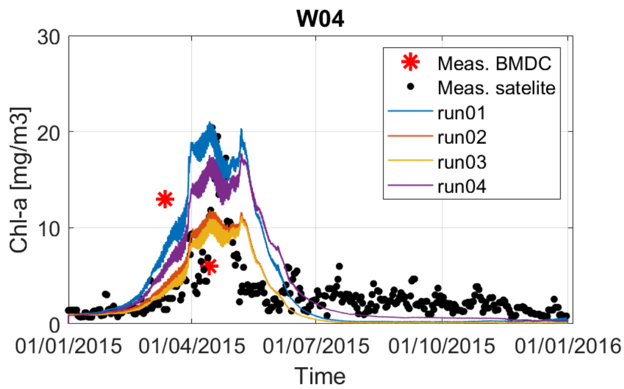

Figure 9. Figure V-5 Comparison of model output and measured data (both BMDC and satellite data) in terms of chl-a concentration for 2015, at the measurements point W04.

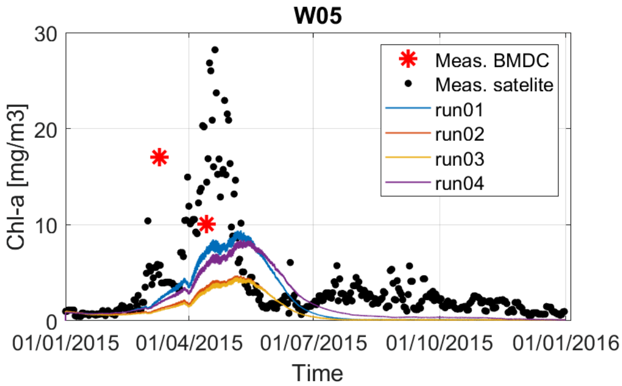

Figure 10. Figure V-6 Comparison of model output and measured data (both BMDC and satellite data) in terms of chl-a concentration for 2015, at the measurements point W05.

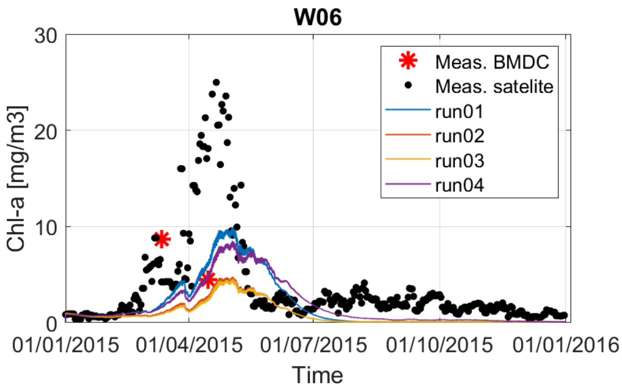

Figure 11. Figure V-7 Comparison of model output and measured data (both BMDC and satellite data) in terms of chl-a concentration for 2015, at the measurements point W05.

It can be observed that the model results are in good agreement with the satellite data, for the stations located closer to the coast. The chl-a peak during the second half of April is well represented as well as the limited availability of phytoplankton biomass the rest of the year. However, an noticeable underestimation of chl-a is observed at the stations W05 and W06 located more offshore. This may be related to the fresh water plumes generated in the mouth of Scheldt and Rhine river. Fresh water is one of the main carries of nutrients into the North Sea which are necessary for phytoplankton growth. It seems that in the model the fresh water zone is too small, which may be related to the treatment of the lateral boundary conditions. Further work is planned in the future to improve this issue.

The nitrate and phosphate concentration at stations W02 and W03 are also shown in Figure 12 to Figure 15. The nutrients dynamics reproduced by the numerical model are consistent with the patterns of the phytoplankton biomass. The phytoplankton growth observed in the second half of April consumes the stock of nutrients in the water column (particularly of nitrate). However, it can be observed that nitrate concentration do not recover after the decay of the phytoplankton. Thus, nitrate concentration is very low at the end of the simulated year. This issue may be related to the offshore BC conditions, for which it is difficult to prescribe correct values due to the lack of available data. One of the possible solutions to overcome this issue is to apply zero-gradient boundary conditions for tracers, which allow the nutrients at the boundary to adapt to the nutrient concentrations inside the domain. A more detailed validation of the nutrient dynamics is planned in the future.

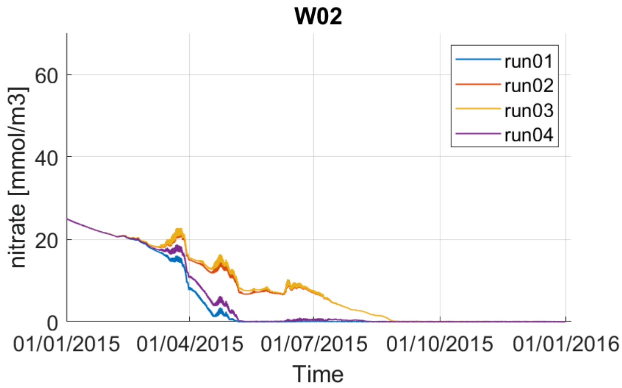

Figure 12. Figure V-8 Model results of nitrate concentration for the four sensitivity runs, at station W01.

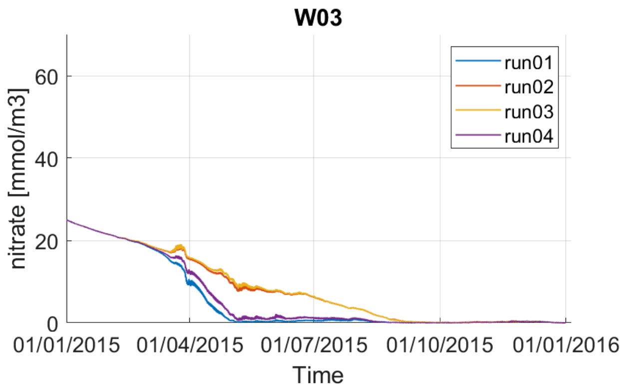

Figure 13. Figure V-9 Model results of nitrate concentration for the four sensitivity runs, at station W02.

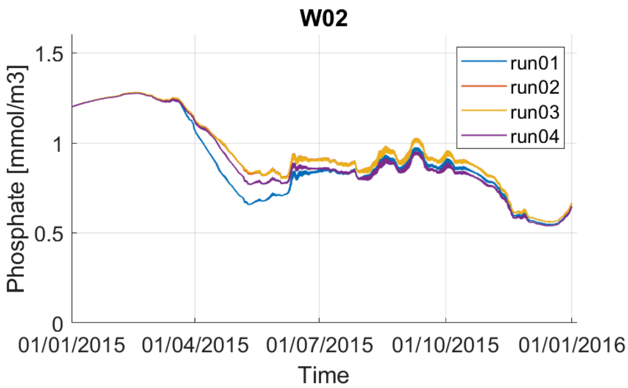

Figure 14. Figure V-10 Model results of phosphate concentration for the four sensitivity runs, at station W01.

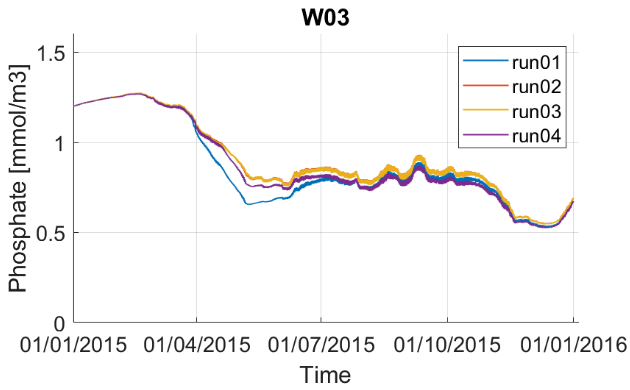

Figure 15. Figure V-11 Model results of phosphate concentration for the four sensitivity runs, at station W02.

VI. Summary and Conclusions

In this work, TELEMAC-3D coupled to the AED2 library were used in the KaZNo model to simulate the thermal dynamics and biochemical cycle in the North Sea for the year 2015. However, in order to perform this study a couple of modification were required in TELEMAC-3D. A brief description of the implemented changes are given in the paper.

Due to the high importance of the water temperature in the biochemical cycle of an aquatic ecosystem this work is initially focused on temperature calibration. Two different atmospheric exchange models were used. A linearized model, which uses the water temperature at the surface and the air temperature at an elevation of 2m above the sea and a more complex model, in which the complete energy balance is taken into account. Both models showed a very good performance based on measurement data of sea water temperature from the Meetnet Vlaamse Banken, collected at a number of stations at the Belgian Coastal. The averaged RMSE was around 0.8^{o}C, for both atmospheric models.

In terms of chlorophyll-a concentration the model results show a correct simulation of the phytoplankton growth compared to the available satellite data. Phytoplankton biomass starts growing in March and reaches its peak at the second half of April. The rest of the year chl-a concentration remains low. It is also indicated that for 2015 the simulated nutrient cycle is consistent with the patterns of the phytoplankton biomass.

A future goal of the present work is to further calibrate the nutrient cycle and zooplankton grazing. However, a necessary condition for the further calibration of the model is the availability of monitoring data. In addition, in order to improve the distribution of the chl-a concentration offshore further work is required for the better representation of the fresh water plume in the mouth of Scheldt and Rhine river. To do so a new zero-gradient boundary conditions for tracers will be applied. Finally, the use of a large number of racers (around 25) leads to substantial calculation times. In order to speed up the model, faster advection schemes for tracers are needed. Therefore, alternative advection schemes, based on the characteristic method, but with correction to ensure mass conservations are currently being implemented in TELEMAC-3D.

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