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Automatic calibration of a tidal estuary model of the Scheldt using data assimilation algorithm

Automatic calibration of a tidal estuary model of the Scheldt using data assimilation algorithm

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Abstract – **A tidal estuary model of the Scheldt is developed in TELEMAC-3D. The model is calibrated on bottom roughness using an automatic procedure. The Python module TELAPY, is online coupled with the Python ADAO library from the SALOME platform. The 3D-Variational data assimilation algorithm is adopted to improve water level predictions along the estuary. The automatic calibration routine steers iterative runs, after each of which the bottom roughness is updated based on the minimization of a cost function. After automatic calibration, the model reproduces the hydrodynamics in the Scheldt Estuary accurately. For instance, the averaged root-mean-square-error (RMSE) of the water level is reduced to 12 cm and the M2 tidal amplitude is accurately reproduced. The Scheldt model is also validated for stormy period and validated against ADCP transect data. Therefore, the Scheldt model is considered as a reliable and efficient tool for various applications in the estuary.**

Keywords: Automatic calibration, tidal estuary, TELEMAC-3D, Scheldt, ADAO, TELAPY.

I. INTRODUCTION

The Scheldt is a tidal estuary situated in the Netherlands and Belgium, with a tidal reach up to 160 km upstream from the mouth near Vlissingen (The Netherlands). The Scheldt estuary has important environmental and commercial values. An accurate prediction of the tidal propagation along the estuary has numerous applications. Process-based numerical models, which include the most important processes and parameters for tidal predictions, have widely been adopted for this purpose.

Model calibration is often referred to as finding the optimal set of model parameters, which provide an accurate description of the system behaviour. It is normally achieved by confronting model predictions with measurements representing the system. Model calibration is an essential modelling step, but manual calibration often requires significant time and effort without guarantee of finding the optimal solution. Recently, automatic calibration of numerical models has shown its capacity in obtaining the optimal parameter settings in a fraction of the time needed for manual calibration. In the TELEMAC community, several studies [1,3,4,5] have shown successful calibration of TELEMAC models in both tidal rivers and the North Sea. All these studies have shown the potential of automatic model calibration in oceanic, estuarine and coastal waters.

In this study, a TELEMAC-3D hydrodynamic model is set up for the Scheldt Estuary. Tidal propagation is typically calibrated by adjusting the bottom roughness, which is performed in an automated manner in the present study. The Python module TELAPY, is coupled online with a Python library called ADAO (A module for Data Assimilation and Optimization) [2] from the SALOME platform [3]. The 3D-Variational data assimilation algorithm [6] is adopted to perform automatic model calibration. This algorithm compares time-series of water levels predicted by the Scheldt model to measurement data at 22 stations throughout the estuary, leading to a cost function which is subject to minimization. Twelve roughness polygons are selected for the Scheldt model domain, which is a compromise between model accuracy and computational efforts. The automatic calibration routine steers iterative runs, after each of which, the bottom roughness is updated based on the minimization of the cost function. After 75 iterations, an optimal bottom roughness field is found, which provides the lowest cost function.

After automatic calibration, the model is further validated for a stormy period and validated against ADCP transect data, showing that the model reproduces the hydrodynamics in the Scheldt Estuary accurately.

The Scheldt model is a very computationally efficient model. With a time step of 30 seconds, a simulation of 28 days period takes only 6.25 hours of computation time using 48 computational cores. Therefore, it is a reliable and efficient tool for various applications in the estuary, such as operational forecasting, sediment transport calculations [7] and transportation of macroplastics [8] etc.

II. ABBREVIATIONS AND CONVENTIONS

The used abbreviations are summarized in Table I. The following conventions are followed in this paper:

- Times are represented in UTC.
- The coordinate reference system, used by the model and for presentation of the model output is RD (Rijksdriehoekscoördinaten), expressed in meters.
- The vertical reference level used in the model is TAW which is 2.35m below NAP.
- Current directions refer to the direction to which the flow is directed: e.g. a current direction of 90°N means that the currents are directed towards the East.

- Wind directions refer to the direction the wind is coming from: e.g. a wind direction of 90°N means that the wind is coming from the East.
- SI units are used.

Table I Used abbreviations

ADAO	A module for Data Assimilation and Optimization
ADCP	Acoustic Doppler Current Profiler
API	Application Program Interface
HIC	Hydrological Information Centre
HMCZ	Hydro Meteo Centrum Zeeland
iCSM	IMDC Continental shelf Model of the North Sea
NAP	Normaal Amsterdams Peil (Dutch vertical reference level)
RD	Rijksdriehoekscoördinaten (Dutch horizontal system)
RMAE	Relative Mean Absolute Error
RMSE	Root Mean Square Error
RWS	Rijkswaterstaat
TAW	Tweede Algemene Waterpassing (Belgian vertical reference level)
UTC	Universal Time Coordinate

III. Model Setup

A. Mesh and Bathymetry

The mesh of the Scheldt model covers the estuary mouth and the entire Scheldt River (Figure 1). The mesh resolution gradually decreases from ~450 m near the offshore boundary to ~3.5 m in the upper river tributaries. The total number of computational nodes is 143,872, with 260,595 triangular elements in a horizontal plane. To better represent the flow patterns, the Scheldt model runs in 3-D mode with 5 vertical nodes using sigma coordinates at (0, 0.12, 0.3, 0.6 and 1.0 from bottom to top).

The mesh is made such that it is aligned with the flow lines of the water movement inside the estuary, e.g. using soft-lines along the channel to guide the generation of the mesh. In the upstream parts, channel meshes are used to structure the triangles of the mesh in such a way that they better follow the channel geometry and the flow direction.

The bathymetric data of 2019 are used, which are identical to the data described in [9]. The data is formatted as combigrids (combination between LIDAR and Bathy data into one consistent dataset). The dataset has a spatial resolution of 5 m.

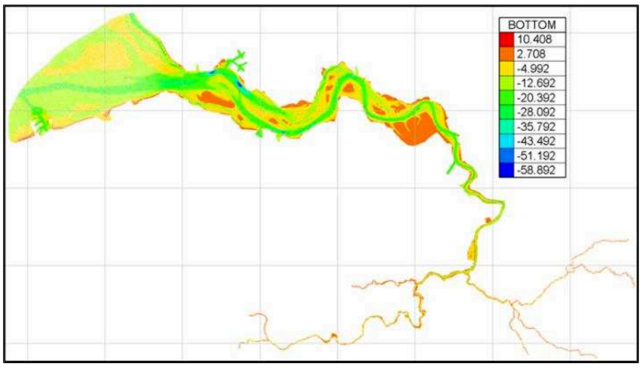

Figure 1. Mesh and bathymetry (m TAW) of the Scheldt model.

B. Boundary and Initial Condition

The model contains one open boundary at the mouth of the Western Scheldt and eight upstream boundary sections. At the downstream boundary, time series of water levels and depth-averaged velocities are imposed from the in-house iCSM model [10]. Recently, the iCSM was automatically calibrated [5] on bottom friction on the platform of SALOME-Hydro with three-dimensional variational assimilation (3D-Var). The iCSM model accurately reproduce the hydrodynamics in the North Sea. For instance, the root mean square error (RMSE) of the water levels along the Belgian coastal zone is 10 cm. The RMSE of the velocity magnitude in the Belgian Coastal Zone (determined form stationary velocity measurements) is of the order 0.1 m/s, which is considered as top-of-range numerical model accuracy.

The water levels and velocities computed by iCSM are interpolated on the open sea boundary nodes of the Scheldt model via an in-house boundary nesting tool. For the eight upstream boundaries, measured time series of river discharge (provided by HIC and RWS) and salinity (set to zero) are imposed.

The initial condition from the models comes from a two-day spin-up simulation for the water levels and velocities. The initial condition for the salinity was obtained from spatial interpolation of measurements data from point measurements along the Scheldt estuary.

C. Wind

Wind measurement data is available at Hansweert with time interval of 10 minutes (data source: HMCZ, https://waterberichtgeving.rws.nl/water-en-weer/dataleveringen/ophalen-opgetreden-data). The time series of wind measurement at Hansweert of 2019 are used to force the Scheldt model. Figure 2 shows the wind rose plot for the entire year of 2019. The dominant wind comes from the south-west direction with a typical wind speed between 6 - 12 m/s.

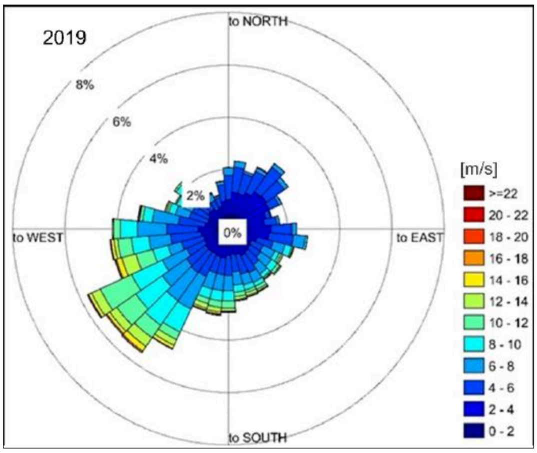

Figure 2. Wind rose for the entire year of 2019 at Hansweert.

D. *Parameter Settings*

The parameter settings of the Scheldt model are summarized in Table II.

Table II Model parameters of the Scheldt model.

Parameter	**Description**
Time Step	30 s
Initial condition	two-day spin-up
Number of vertical nodes	5
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
Vertical turbulence model	6: GOTM (using K-epsilon model with second order closure for the buoyancy flux) [11].
Horizontal turbulence model	4: Smagorinsky
Scheme for advection of velocities	1: characteristic method
Scheme for advection of tracers	13: Leo Postma for tidal flats
Solver	7: GMRES
Scheme for diffusion of tracers	0: No diffusion horizontally. Vertical diffusion is calculated using the set_dif.f subroutine [12].

IV. Model Calibration

A. *Modelling Period*

The model calibration period is 29 days from 22/03/2019 to 20/04/2019, which is a relatively calm period with an average wind speed of 4.3 m/s (Figure 3).

Thanks to the use of improved drying-flooding methods [13], the Scheldt model could run with a time step of 30 seconds which significantly increases the computational efficiency. For instance, it takes 6.25 hours for 29 days simulation on 48 cores.

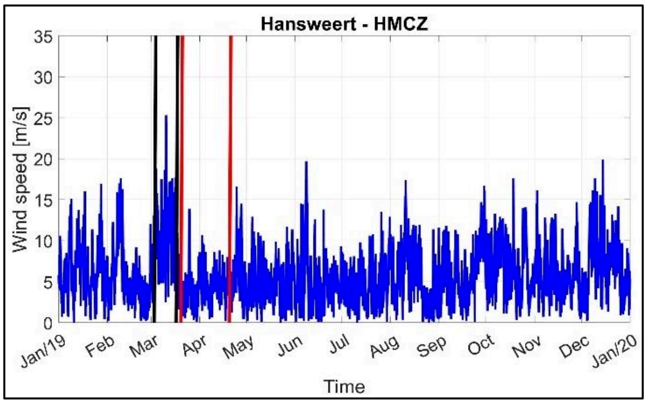

Figure 3. Time series of the wind speed at Hansweert. The calibration period (22/03 – 20/04/2019) is indicated by red lines.. The stormy period used for the validation (03/03 - 17/03/2019) is indicatedby black lines.

B. *Automatic calibration*

The objective of the automatic calibration is to improve water levels along the estuary predicted by the Scheldt model. The Python module TELAPY is coupled online to the Python ADAO library from the Salome-Hydro platform. The 3D-Variational data assimilation algorithm is adopted to execute the automatic model calibration. This algorithm compares time-series of water levels predicted by the Scheldt model to measurement data at 22 measurement stations along the river Scheldt (Figure 7 and Table III), leading to a cost function which is subject to minimization. The automatic calibration routine steers iterative runs, after each of which, the bottom roughness is updated based on the minimization of cost function.

The automatic model calibration is executed using the SALOME platform (https://www.salome-platform.org/), which is an open-source tool developed at EDF, which provides pre- and post-processing of model simulations, supports cascading and coupling of different software tools, modules and codes [14]. SALOME is based on an open and flexible architecture with reusable components, which can be used to construct a computation scheme assembling internal module or external codes through specific communication protocols [1]. In this study, the Scheldt model developed in TELEMAC-3D is coupled using the TelApy and dynamically linked to ADAO within SALOME (Figure 4).

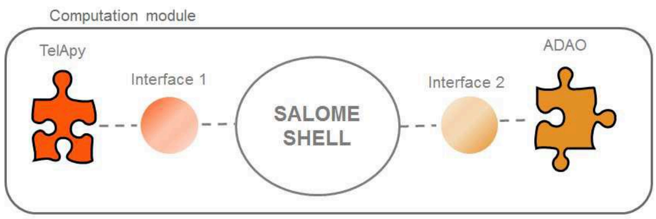

Figure 4. The SALOME composition linking TELAPY to ADAO, adopted after [1].

The TELAPY is an internally built-in component in the open-source TELEMAC system [15]. It is essentially a python module which wraps and controls TELEMAC simulations through a Fortran API (Application Program Interface). The API is used to steer a simulation while running a model. The TelApy component has the capability to be extended to new types of TELEMAC simulations including high performance computing for the computation of uncertainties, other optimization methods and coupling [3].

ADAO is a Python library (https://pypi.org/project/adao/) providing standard and advanced data assimilation and optimization algorithms on the SALOME platform [1]. ADAO can be easily coupled with other modules or external simulation codes, for instance TELEMAC-2D and TELEMAC-3D.

The automatic calibration is based on a 3D-Variational data assimilation scheme [6]. This method minimizes a cost function J(x) which describes the deviation between a model state and an observation as expressed in Eq. (1). The cost function is essentially a sum of squared differences between the observations and the corresponding model values:

$$J(x) = (x - x^b)^T B^{-1}(x - x^b) + (y^0 - H(x))^T R^{-1}(y^0 - H(x)) \quad (1)$$

where the vector x represents the parameters to be calibrated (bottom roughness in this study), x^b represents the prior knowledge of x (the background state, e.g. the initial guess); y^0 is the observation vector (time series of measured water levels in this study), H is an observation operator enabling the passage of the parameter space to the observation space (the TELEMAC-3D Scheldt model in this study) such that y = H(x). B, R are the so-called background and observation error covariance matrices respectively.

The first term in the right hand side of Eq. (1) is often referred to the 'penalty term' introduced by [16], meaning that additional cost is added to the cost function when the calibrated parameter x drifts away from the background state x^b. This is useful for fine-tune the calibration, when the modeler has high confidence in his initial guess x^b. In this study, the background error covariance B is set to a very large value (10^8) such that the 'penalty term' of the cost function is ignored.

The minimization of the cost function is based on the so-called constrained Broyden Fletcher Goldfarb Shanno Quasi-Newton method (c-BFGS-QN). Using this constrained optimization method makes it possible to impose boundaries during the search process of the model parameters, guaranteeing that only physically meaningful values are used. A detailed description of the BFGS is given by [1]. Thus, it will not be further discussed here.

As a preparation step for the auto-calibration, twelve roughness polygons are selected for the Scheldt model domain as shown in Figure 7. The number of polygons in use is a compromise between model accuracy and computational efforts. The selection of polygons is based on knowledge gained from manual calibration experience from the past. For instance if modelled water level behaves differently at two neighbouring stations with the same roughness values, those two stations shall be assigned to two different polygons. The bottom roughness in the model is calculated using the Nikuradse equation:

$$C_d = \left(\frac{\kappa}{\log\left(\frac{30h}{ek_s}\right)}\right)^2 \quad (2)$$

where C_d is the bed drag coefficient [-], h is the water depth [m]; κ is the Von Kármán constant of 0.41 [-]; e is Euler's constant of 2.71828, and k_s is the Nikuradse roughness value [m].

However the Nikuradse value k_s has a highly nonlinear relation with the drag coefficient C_d (see Eq. 2), meaning that the change in the water level as function of the roughness behaves differently for high Nikuradse values than for low Nikuradse values, and that the physically admissible range of Nikuradse values is rather large (it can vary from 0.1 cm to 10 cm). This will slow down the automatic calibration process. Therefore instead of directly calibrating k_s, we calibrated $\log_{10}(k_s)$, see relation in Figure 5. An initial guess of 0.03 m of Nikuradse value ($\log_{10}(k_s) = -1.52$) is assumed for the automatic calibration. Note that although $\log_{10}(k_s)$ is calibrated, the model is still forced with k_s during the simulation.

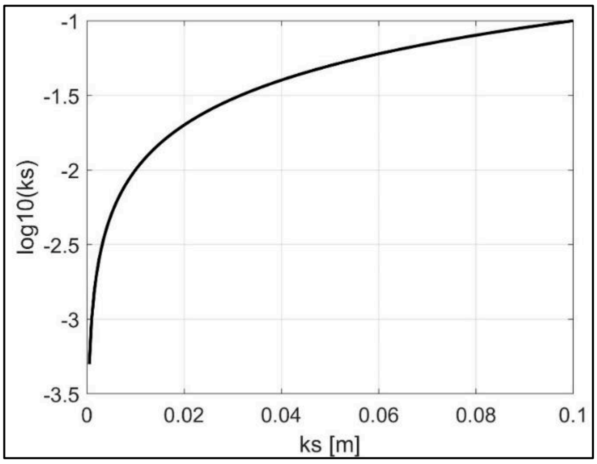

Figure 5. Relation between Nikuradse value (ks) and its transformation of log10(ks).

V. CALIBRATION RESULTS

Figure 6 illustrates the evolution of the cost function. After 75 iterations, an optimal bottom roughness field is found (Figure 7), leading to the lowest cost function.

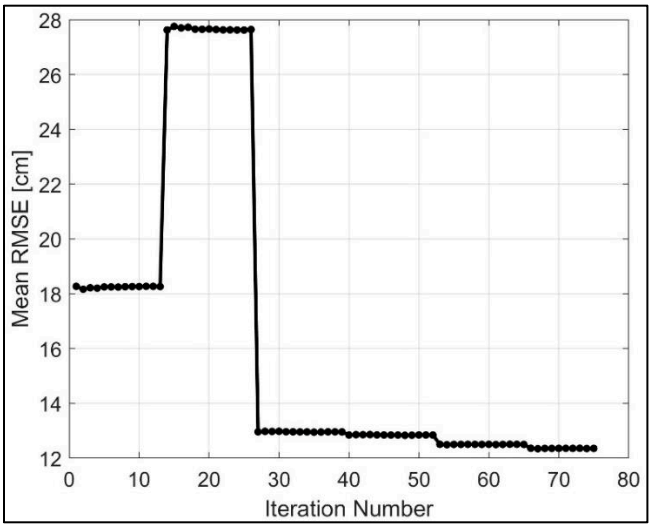

Figure 6. Evolution of mean RMSE during the automatic calibration.

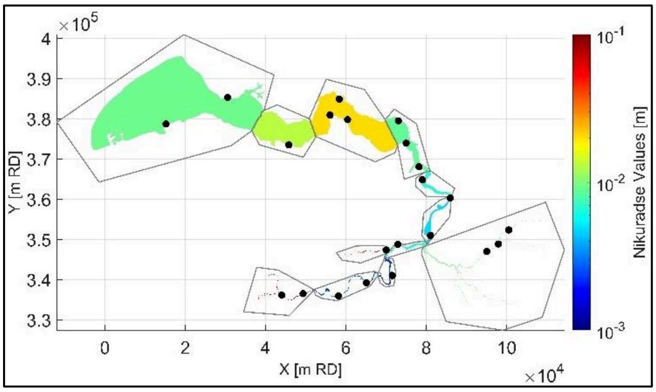

Figure 7. Roughness map showing the Nikurase values after automatic calibration. The 12 polygons in grey define different roughness zones. The black dots represent water level measurement stations as indicated in Table III.

Figure 8 shows that the RMSE of the water levels in general reduces after the automatic calibration, especially in the upstream part of the Scheldt estuary. Figure 9 shows that the M2 amplitude is very well reproduced. The full statistics of the water levels after the automatic calibration are referred to Table III. The average RMSE of the water level in the Scheldt estuary is reduced from 18 cm to 12 cm after automatic calibration.

Table III Statistics of water level after automatic calibration along the estuary (from downstream to upstream).

Stations	**Bias of the water level [cm]**	**RMSE of the water level [cm]**	**Bias of the M2 Amplitude [cm]**	**Bias of the M2 Phase [deg]**
Cadzand	0.5	9.9	-2.1	1.6
Vlissingen	-0.2	8.9	0.2	1.2
Terneuzen	-0.6	8.8	3.0	-1.4
Overloop Hansweert	-0.7	7.9	2.3	0.3
Hansweert	-1.7	8.2	2.5	-0.4
Walsoorden	-2.9	9.1	1.5	-0.1
Bath	2.0	10.0	1.1	0.3
Prosperpolder	4.8	10.7	1.8	-0.4
Liefkenshoek	-1.6	10.3	2.5	-0.7
Kallosluis	4.2	11.2	1.3	-0.4
Antwerpen	-1.3	10.9	2.0	-0.5
Hemiksem	-1.4	12.7	6.0	-1.6
Temse	-2.7	15.8	8.9	-2.8
Tielrode	-1.5	14.9	8.6	-1.7
Sint-Amands	-1.6	14.0	6.3	-2.1
Dendermonde	0.6	11.1	-3.5	1.6
Schoonaarde	-3.0	11.9	-3.3	3.5
Wetteren	-6.8	12.7	-1.6	2.2
Melle	-8.7	14.8	-1.5	2.1
Duffel	-2.5	12.5	-6.8	1.3
Lier Molbrug	-3.0	15.0	-7.9	6.1
Emblem	-22.9	30.4	1.3	-2.8
|Average|	**3.4**	**12.4**	**3.5**	**1.6**

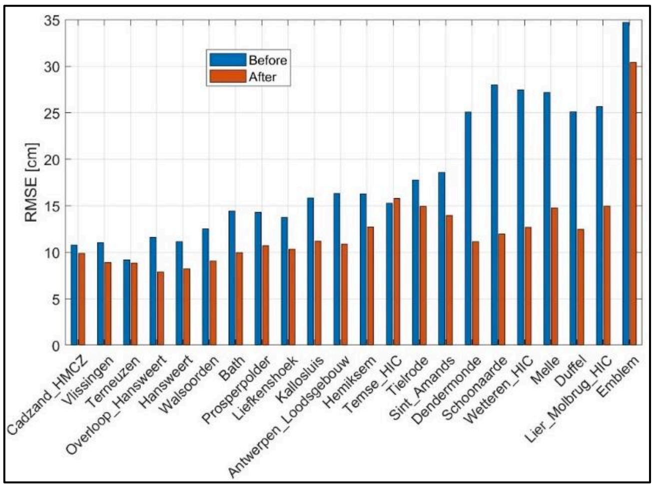

Figure 8. RMSE of the water level along the Scheldt before and after automatic calibration.

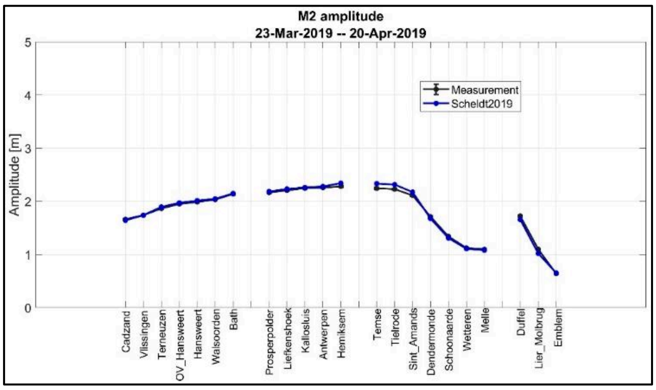

Figure 9. M2 amplitude of the Scheldt model after auto-calibration.

VI. Model Validation

A. *Validation for a stormy period*

The Scheldt model was run for a stormy period from 03/03/2019 to 17/03/2019. This period contains a maximum wind speed of 25 m/s and mean wind speed of 11 m/s (Figure 3).

Figure 10 presents the RMSE of the water level along the Scheldt Estuary during this stormy period, compared to the RMSE determined from the calibration period. In general, the model performance from the estuary mouth to Sint-Amands is comparable to the performance for calibration period (with a RMSE that is 2-3 cm larger). It is noticeable that the model performs slightly worse in the upstream part for this stormy period (e.g. the RMSE is more than 30 cm at Melle), which requires further investigation. It might be due to the uncertainties in the river discharge data at Melle, and/or the use of stationary wind data at Hansweert, which is quite far away from the upstream branches, for the entire model domain. It also worthwhile to mention that such a deviation is usually a classical diagnostic in data assimilation which can be considered as a positive systematic side-effect of using data assimilation framework.

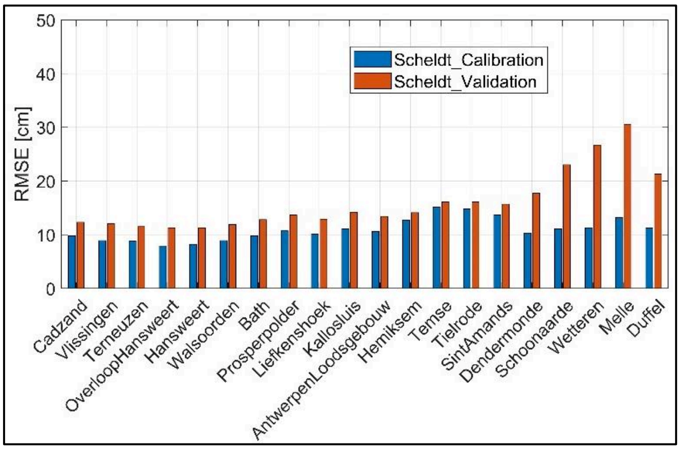

Figure 10. Comparison of the RMSE of the water levels along the Scheldt between the calibration period and the validation period.

B. *Validation on ADCP transect data*

The model is also validated against eleven ADCP transect data in the Western Scheldt as described in [7]. The measured tide during the through tide measurement campaigns are used to determine the modelling period using the comparable tide analysis [17]. This is a method that allows the comparison of model results to measurements, which are outside of the simulation period. In this method, the water levels that occurred during the through tide measurement (ADCP) are compared to the water level measurements during the simulation period. Those tidal cycles that match best with the tidal cycles during the through tide measurement are selected and used for the model validation.

By using a model qualification based on the RMAE (Relative-Mean-Absolute Error), which includes the accuracy of both the velocity magnitude and direction, the comparison can be quantified (Table IV). Table V shows the RMSE and RMAE statistics of the simulated velocities during the eleven ADCP campaigns. All the eleven different transects show a RMAE with the qualification ‘Good’ or ‘Excellent’. The average RMSE of the flow magnitude is 16.8 cm/s, which can be considered a good performance given that the average tidal peak velocity is 1.5 m/s. In general the flow pattern is adequately reproduced by the Scheldt model. Figure 11 shows the modelled and measured velocity field at Waarde during maximum ebb tide. Both flow magnitude and direction are well reproduced by the model.

Due to the lack of data, the Scheldt model is not validated for the Sea Scheldt and the Upper Sea Scheldt, which shall be further evaluated in the future.

Table IV Model qualification based on RMAE [18].

Model qualification	**RMAE [-]**
Excellent	<0.2
Good	0.2-0.4
Reasonable/fair	0.4-0.7
Poor	0.7-1.0
Bad	>1.0

Table V RMSE and RMAE of velocities along 11 ADCP transects. The campaign names indicate the location and date of the measurement.

Campaign	**RMSE [cm/s]**	**RMAE [-]**
R6_GatVanOssenisse_20120509	20.2	0.25
R6_Middelgat_20120508	21.5	0.35
Diepe_Put_Hansweert_20170720	21.5	0.22
Diepe Put Hansweert 20181214 Dwarsraai	18.6	0.28
Diepe Put Hansweert 20181214 Langsraaien	17.1	0.28
Diepe Put Hansweert 20181220 Dwarsraai	15.9	0.21

Diepe Put Hansweert 20181220 Langsraaien	13.3	0.18
Waarde_20060323_Neap	12.9	0.25
Waarde_20060928_Average	11.9	0.24
R5_SchaarVanWaarde_20130424	15.4	0.30
R5_Zuidergat_20130425	17.4	0.26
Average	**16.8**	**0.26**

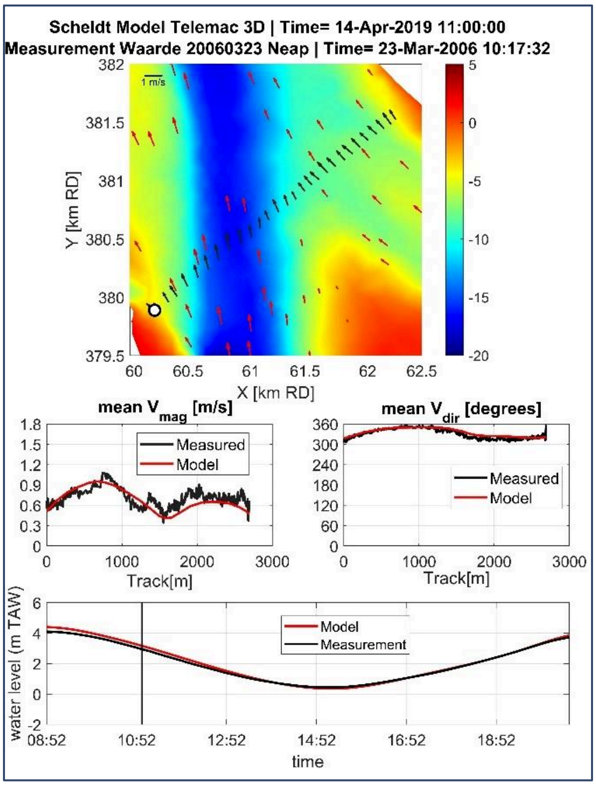

Figure 11. Modelled and measured velocity at Waarde during ebb.

VII. Conclusion

In the present study, a TELEMAC-3D hydrodynamic model is set up for the Scheldt Estuary. The bed roughness in the model is calibrated automatically using the 3D-Varational data assimilation algorithm, which compares time-series of the water levels from the Scheldt model and measurement data at 22 stations throughout the estuary, leading to a cost function which is subject to minimization. Twelve roughness polygons are selected for the Scheldt model domain. After 75 iterations, an optimal bed roughness field is found, leading to the lowest cost function. Using the bed roughness determined by the automatic calibration procedure, the model reproduces the hydrodynamics in the Scheldt Estuary accurately, with an average RMSE of the water levels of 12 cm.

The Scheldt model generally shows good predictive skills for a stormy period, that was selected for the validation, except at the upstream branches of the estuary. The reason for this needs further investigation in the future.

The model is also validated against measured velocity along ADCP transects, leading to an averaged RMSE of the flow magnitude of 0.16 m/s which is considered a good performance given that the average tidal peak velocity is 1.5 m/s.

Acknowledgement

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