Conference Paper, Published Version

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Zur Verfügung gestellt in Kooperation mit/Provided in Cooperation with:
TELEMAC-MASCARET Core Group

Verfügbar unter/Available at: https://hdl.handle.net/20.500.11970/104323

Vorgeschlagene Zitierweise/Suggested citation:
Smolders, Sven; Maximova, Tatiana; Vanlede, Joris (2015): Salinity in the 3D TELEMAC model Scaldis (the Scheldt Estuary): tracer diffusion, dispersion and numerical diffusion. In: Moulinec, Charles; Emerson, David (Hg.): Proceedings of the XXII TELEMAC-MASCARET Technical User Conference October 15-16, 2021. Warrington: STFC Daresbury Laboratory. S. 133-140.

Salinity in the 3D TELEMAC model Scaldis (the Scheldt Estuary): tracer diffusion, dispersion and numerical diffusion

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***Abstract*— This paper describes how salinity was introduced as an active tracer in the 3D TELEMAC model of the Scheldt estuary. Boundary conditions are discussed and model results are compared with measured data. The role of the parameters: velocity diffusivity, tracer diffusion coefficient and numerical diffusion and their effect on the salinity field are shown. Next to the salinity data, tracer data from the model will be used to determine dispersion coefficients for a 1D ecological box model of our project partner, the University of Antwerp.**

I. Introduction

The Scheldt estuary is located in the south-western part of the Netherlands and in Belgium. In the framework of the projects "Integral Plan for the Upper Sea Scheldt" and "Agenda for the Future", it was necessary to develop an integrated model for the Scheldt estuary. Existing models lack a high resolution in the Upper Sea Scheldt, Durme, Rupel and Nete. For this reason, the SCALDIS model, a new unstructured high resolution model of the tidal Scheldt is developed in TELEMAC 3D for the entire estuary, but with special attention to the upstream parts. The calibrated model will be used to analyse the effects of several scenarios (different morphology of the Scheldt with different ranges of boundary conditions). Because this model will also be used for other projects in the future, including projects in the coastal zone, the model domain was extended to the coastal zone of Belgium.

The model domain (figure 1) covers the entire Scheldt estuary, including the mouth area, the Belgian coastal zone and the Eastern Scheldt. Upstream, the model extends to the limits of the tidal intrusion. The use of an unstructured grid allows to combine a large model extent with a high resolution upstream. The grid resolution varies from 500 m at the offshore boundaries to 7-9 m in the Upper Sea Scheldt.

Calibration parameters are bed roughness and velocity diffusivity. The model is calibrated for one spring-neap tidal cycle in 2013 against field data: water levels, velocities (in deep and shallow zones) and discharges. The calibration process is described in further detail in [1] and with extra focus on the velocities in [2]. For a complete overview of the model and calibration process we refer to [3]. This paper will go into detail on how salinity was implemented as an active tracer in the Scaldis model.

One of the project partners, the university of Antwerp, will need tracer calculations from different regions of the estuary to calibrate the dispersion coefficients for their 1D ecosystem box model [4]. Salinity is included in the 1D model as passive tracer (only transport). Every box in their 1D model corresponds to a part of the Scaldis model. For every box a dispersion coefficient is calibrated based on the dispersion coefficients of passive tracer simulations from the 3D Scaldis model of Flanders Hydraulics.

The coupling of both models by means of the dispersion coefficient, stresses the importance of the tracer calculations in the Scaldis model.

II. The Numerical Model

A. Model grid

The TELEMAC model developed in the framework of this project covers a part of the North Sea, the entire Scheldt estuary (until the tidal border) and the Eastern Scheldt. The flood control areas (FCA's) with or without a controlled reduced tide (CRT) are included in the model grid as they are important for the storm scenarios [3].

Figure 1. Scaldis model domain in red.

The model grid consists of 459,692 nodes in 2D mesh and 873,419 elements. In the 3D model we use five sigma layers, totalling 2,298,460 of nodes with the following distribution: 0D, 0.12D, 0.30D, 0.60D, 1D.

B. Bathymetry

The most recent available bathymetry is used in the model. Several datasets from different sources were pasted together.

The bathymetry for the Belgian continental shelf and the Belgian coastal zone comes from MDK-aKust (year 2007 - 2010). The bathymetry of the Dutch coast (2007-2012) was measured by Rijkswaterstaat and downloaded from Open Earth. For the ports of Zeebrugge, Blankenberge, Oostende and Nieuwpoort data from 2014 – 2015 are used. The bathymetry of the Western Scheldt (2013) and the Eastern Scheldt (2010) is available from Rijkswaterstaat. For the Lower Sea Scheldt, bathymetric data of 2011 were provided by Maritime Access division. The topographic data for the channel banks (2007) are taken from the Mercator databank.

The bathymetric data for the Upper Sea Scheldt and Rupel basin are available from Maritime Access division for the years 2013 - 2014. For the Durme bathymetry from 2012 - 2013 is defined. The data for the tributaries of Rupel are available for 2007 - 2013 (Dijle and Nete) and 2001 (Zenne and upstream part of Nete) from W&Z, Sea Scheldt division. For the Flood Control Areas along the river, the topographic data are derived from the Mercator Database.

C. Boundary conditions

The downstream model boundary is located in the North sea. The upstream boundary is located at the tidal border. The model domain includes all the tidal tributaries of the Scheldt estuary. The TELEMAC model is nested in the overall ZUNO model (figure 2) (a correction of the harmonic components is done: M2 phase +4°; M4 phase -6°; S2 phase +7° and Z_0 -0.21 m) [5]. The 10 minute time series of the water level calculated in ZUNO are defined at the downstream boundary of TELEMAC. The subroutine bord3d.f was changed to allocate a water level and a salinity value for each boundary node separately (469 nodes).

There are 8 upstream boundaries with prescribed discharge and free tracer. The measured daily average discharges are defined as upstream boundary conditions at Merelbeke (Upper Sea Scheldt), Dender, Zenne, Dijle, Kleine Nete, Grote Nete, channel Ghent – Terneuzen and channel Bath.

Wind is applied on the coastal zone through the subroutine meteo.f. To include the culvert function in TELEMAC 3D the function t3d.debsce was changed [1].

The salinity boundary conditions are generated by nesting the SCALDIS in the CSM-ZUNO model train. Model results for salinity are highly influenced by values imposed at the boundaries. Therefore, it is very important to have accurate salinity boundary conditions. Salinity boundary values in the SCALDIS model are corrected based on the comparison of the calculated and measured salinity time series at Vlakte van de Raan (located in the North sea; red dot in figure 4 in the larger mouth area of the Scheldt Estuary).

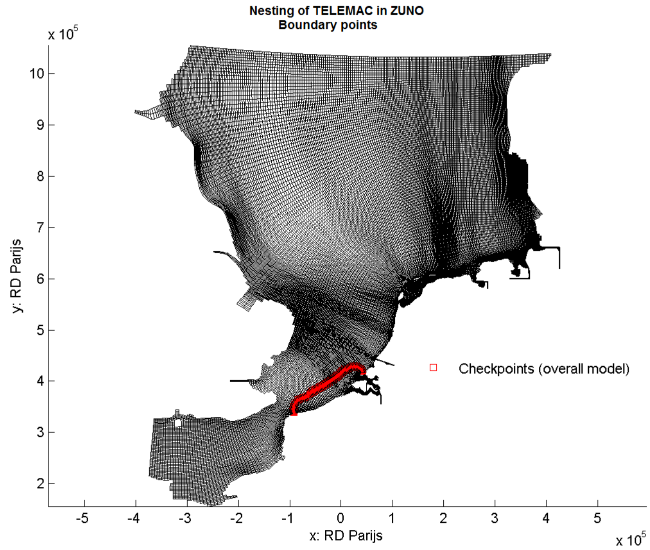

Figure 2. Nesting of Scaldis model in ZUNO. Scaldis boundary nodes given in red.

The modeled and measured salinity at Vlakte van de Raan are compared in figure 3. Thicker lines show the daily average curves. The missing values in the daily average measured salinity were filled by a linear interpolation. The ZUNO model underestimates the salinity values in the area of interest a lot. Therefore, a salinity correction at the boundaries was necessary.

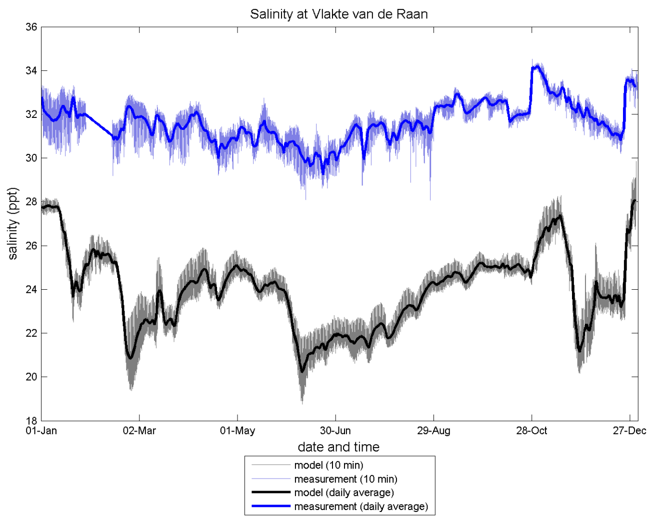

Figure 3. Comparison of modelled salinity in ZUNO and measured salinity for Vlakte van de Raan station.

The correction, the difference between the daily averaged measured and modelled values were added to the boundaries point values of the Scaldis model; the values of which were extracted from the ZUNO model. Salinity is the only active tracer in the Scaldis model.

D. Simulation period and initial condition

Salinity simulations are done with a three month simulation. The model starts from a previous computation file (a short simulation to start up the tidal motion in the model). The model runs from 17/09/2013 00:00 to 20/12/2013 00:00.

To get the salinity distribution in the estuary immediately good, the model starts from an initial salinity field: a map like the BOTTOM or BOTTOM FRICTION is made based on a combination of salinity measurements and model results from ZUNO. Figure 4 shows the outline of the model. The dots in the North Sea and Eastern Scheldt are extracted from the ZUNO model for the start date situation. All these point values are first corrected in the same way as the boundary conditions. The red dots in figure 4 give the location of stations where salinity is measured. The measured values at 17/09/2013 00:00 were interpolated using inverse distance method together with the corrected model values from ZUNO to give an initial salinity map (figure 5) that is read by a modified subroutine fonstr.f. The values of the 2D map are copied to the other four layers in the model.

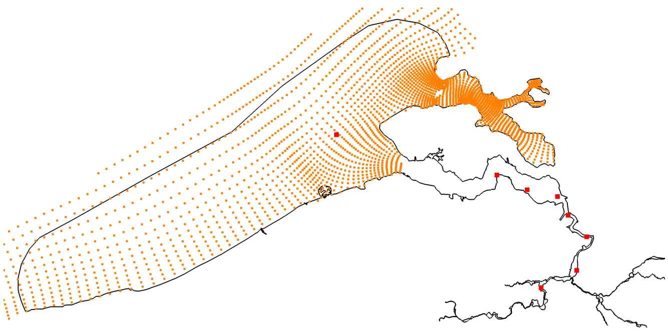

Figure 4 – Salinity values at 17/09/2013 00:00 extracted from ZUNO (orange dots) and location of the stations that measure salinity in the Scheldt Estuary (red dots). These stations are named (from downstream to upstream) Vlakte van de Raan, Overloop van Hansweert, Baalhoek, Prosperpolder, Liefkenshoek, Boei 84, Hemiksem and Driegoten.

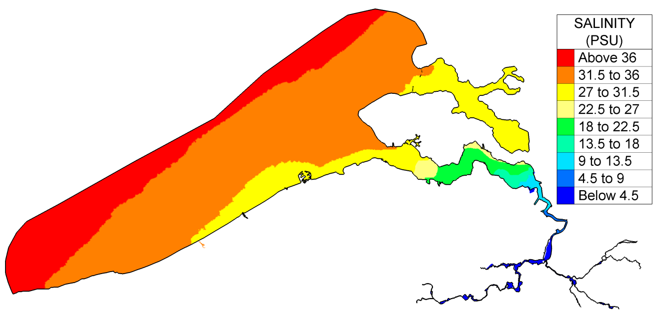

Figure 5 – Initial salinity field for start simulation at "17/09/2013 00:00"

E. Initialising tracer calculation

Salinity is the first tracer in the Scaldis model. But the salinity does not reach all the way upstream the estuary. So it is not sufficient to calculate dispersion coefficients for the 1D box model. The Scaldis model was divided into 89 parts by means of polygons. The focus lies on the Scheldt estuary itself and not on the tributaries. Figure 6 shows an example of how the model partitioning by the polygons was done. In the downstream part of the estuary, the polygons have a length of 5 km. In the upstream part the distance along the estuary axis is 1,5 km with a gradually transition. All flooding areas with controlled reduced tide [3] are also given a separate polygon.

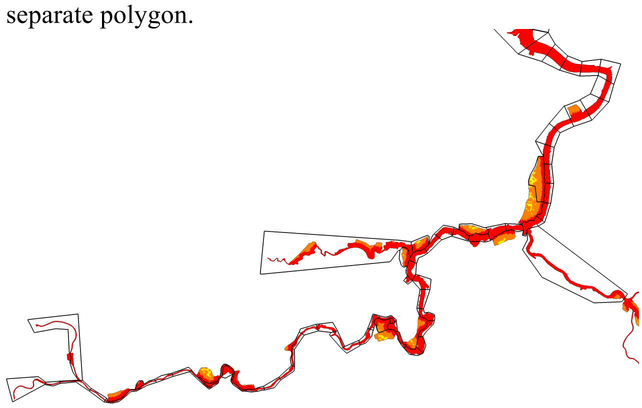

Figure 6. example of model domain divided by polygons

A concentration of 1000 kg/m³ for 19 passive tracers will be initialized in different parts of the Scheldt estuary. The simulation will start the same way as the salinity simulation, but will only simulate three days. For every tracer the concentration inside every polygon will be calculated for every graphical output time step (= 1 hour). From this data, the university of Antwerp can extract the necessary dispersion coefficients for their 1D box model.

III. MODEL VS MEASUREMENTS

The advection scheme for tracers is scheme 13 (Leo Postma for tidal flats; necessary for combination with sinks and sources). The coefficient for vertical and horizontal diffusion of tracers was kept at the default value of 1.E-6 m²/s. The coefficient for horizontal and vertical diffusion of velocities was calibrated and found optimal at 2.E-2 m²/s [3]. When after a simulation period of three months the model results are compared with the measurements (figures 7-11), the results show that for Vlakte van de Raan (figure 7) (for location of the stations see figure 4) the comparison is not good. The model is not able to reproduce the measurements. The results of Baalhoek (figure 8), however, are much better. Despite the discrepancy between model and measurement in the Coastal area, inside the estuary results look good. The results improve going further upstream for Liefkenshoek (figure 9) and Boei 84 (results not shown). For Hemiksem (figure 10) and Driegoten (figure 11) the model seems to follow the tendencies of the measured salinity, but the average salinity level in the model is too low.

Overall the results are satisfying. Certainly knowing that the model was not "calibrated" for this tracer. No calibration was done, because the only parameter to change was the horizontal diffusivity of tracer para meter and at this moment we don't know exactly what it does. From the comparsion of measurments and model an overestimation of the measurement by the model in the downstream part can be seen (figures 8 and 9) and a small underestimation is noticed in the downstream part (figures 10 and 11). This might be due to changes in mesh resolution going from coarse downstream to fine upstream.

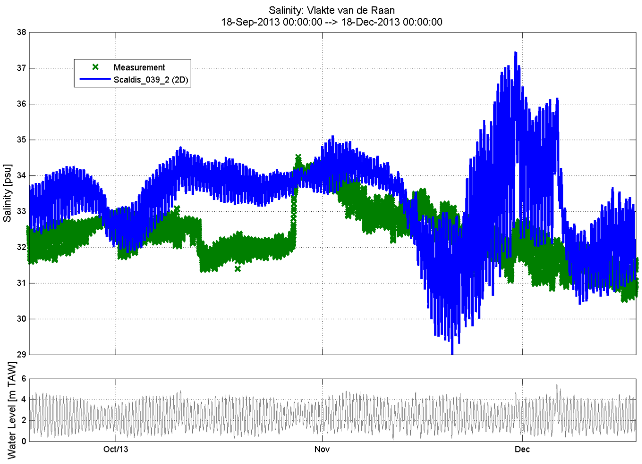

Figure 7. Salinity: model vs. measurement. Vlakte van de Raan.

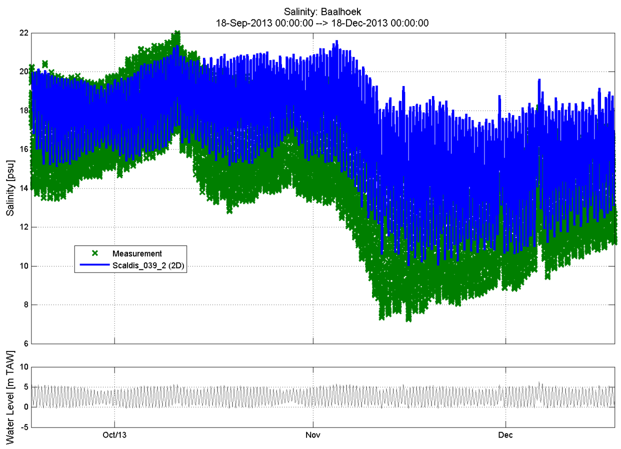

Figure 8. Salinity: model vs. measurement. Baalhoek.

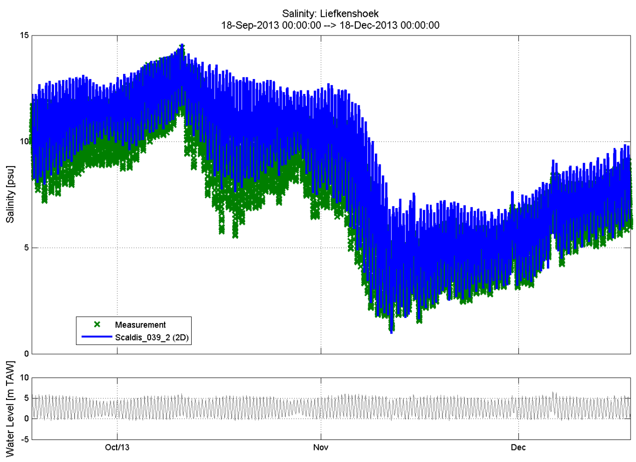

Figure 9. Salinity: model vs. measurement. Liefkenshoek.

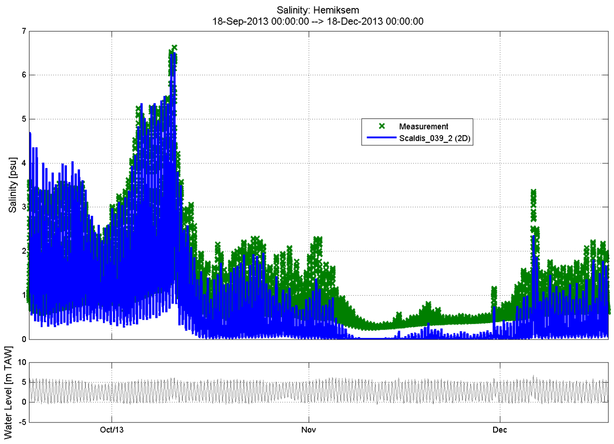

Figure 10. Salinity: model vs. measurement. Hemiksem.

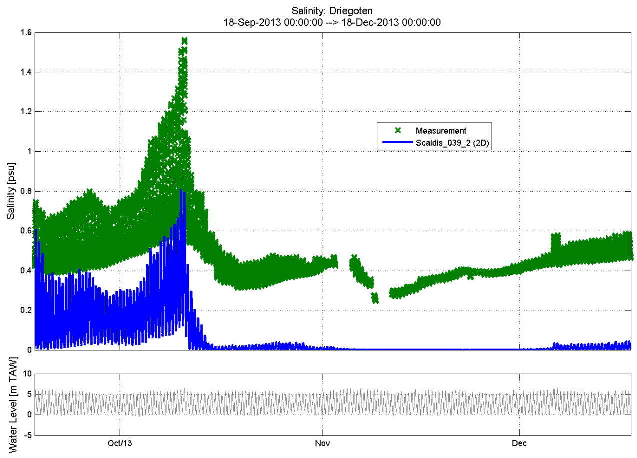

Figure 11. Salinity: model vs. measurement. Driegoten.

IV. TRACER DIFFUSION

A. Diffusion, advection and dispersion

Tracer diffusion is the mass transfer that happens because of the random thermal motion of molecules (so called Brownian motion). The salinity will move from a region of high concentration to a region of low concentration over the concentration gradient. Under the assumption of steady state this is also known as Fick's first law and is written for one dimension as follows:

$$J = -D\frac{\partial c}{\partial x} \quad (1)$$

with J the mass flux, c the concentration of tracer, x the distance and D the diffusion coefficient or diffusivity. Dispersion is known as the mass transfer due to diffusion in non-ideal flow or turbulent flow. Diffusion helps molecules to move from one streamline to the next, and thereby transported over different distances due to the difference in velocities. The dispersive mass flux can be written with the same equation as Fick's first law (equation 1), but instead of D a dispersion coefficient E is used. The amount of dispersion reduces with increasing diffusion coefficient, because molecules will just be moving from one streamline to another constantly. They will not spent enough time on one streamline to be transported far away from each other. In the tracer transport equation:

$$\frac{\partial T}{\partial t}+U\frac{\partial T}{\partial x}+V\frac{\partial T}{\partial y}+W\frac{\partial T}{\partial z}=\frac{\partial}{\partial x}\left(\nu_T\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\nu_T\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\nu_T\frac{\partial T}{\partial z}\right)+Q \quad (2)$$

with T, the tracer; t, the time; x,y,z, the space components; Q, the sink or source of tracer and ν_T, the tracer diffusion coefficient or diffusivity, both advective transport (left hand side of equation 2) and diffusive transport (right hand side of equation 2) are present.

In numerical models the total tracer dispersion is affected by the inherent numerical diffusion. This is an “uncontrolled” diffusion that is automatically introduced in the calculation. Numerical solver schemes can be diffusive. In the model we can choose for one or another scheme but all schemes are in some way diffusive. Another factor that affects numerical diffusion is the mesh resolution. For a 1D case the numerical diffusion can be estimated by U*dX/2. For 2D and 3D cases this formula just gives you an order of magnitude. This formula shows that the coarser your mesh, the larger the numerical diffusion will be.

The problem in the Scaldis model is that it has a very large model domain with a mesh resolution of 200-500 m in the coastal zone up to 5 m resolution at the upstream boundaries (figure 12). So the numerical diffusion will be different at different locations of the model domain. The total tracer diffusion will be a result of the tracer molecular diffusion parameter (tracer diffusivity) and the numerical diffusion. If we want to get the salinity distribution in the model as accurate as possible, we need to get an idea of the order of magnitude of the effect of the mesh resolution on the tracer transport. A second question is how to choose our tracer diffusivity parameter in order to have an effect on the total tracer transport. To test the effects of several parameters a small test case was made.

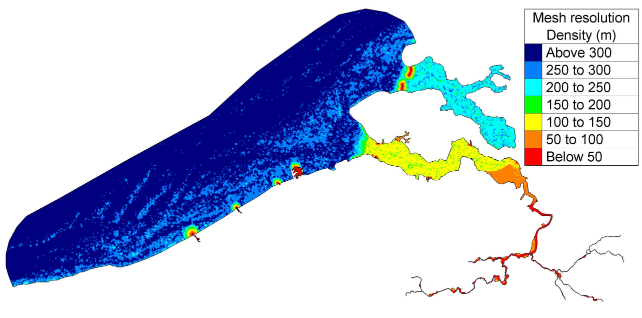

Figure 12. Scaldis 3D model mesh resolution

V. Small Test Cases

We want to test two things:

1. What is the effect of the mesh resolution on the tracer movement?
2. What order of magnitude is the numerical diffusion or from which value does the parameter, horizontal diffusivity of tracer, start to play a role in the tracer movement?

A. *test case 1: the effect of mesh resolution*

1) *test model description*

A part of the estuary channel is modelled by taking a rectangular channel of 10 km long and 500 m wide. The depth is set at -10 m TAW (= the Belgian reference level, close to low water sea level). As we are only interested in the horizontal diffusion of the tracer, the model was only run in 2D. Three different mesh resolutions were applied: 5 m, 20 m and 100 m. On one side a schematic tidal water level (WL) boundary was set according to: WL = A*sin(ω*t) where A is the tidal amplitude (=2 m), t is the time and ω is the frequency (= 0,000141 for a semi diurnal tide). The simulation period was up to 90 days. On the other side a fixed discharge of 1 m³/s was set as boundary condition. The time step was 4 s and all other parameters were kept at the default values. The mesh resolution is the only parameter that changed. At the tidal boundary a fixed tracer concentration was set at 30 PSU.

2) *Results*

At 5000 m from the tidal boundary a tracer value time series was extracted for the three different mesh resolutions. The results are plotted in figure 13. It is clear that a coarse mesh has a larger effect on the tracer transport.

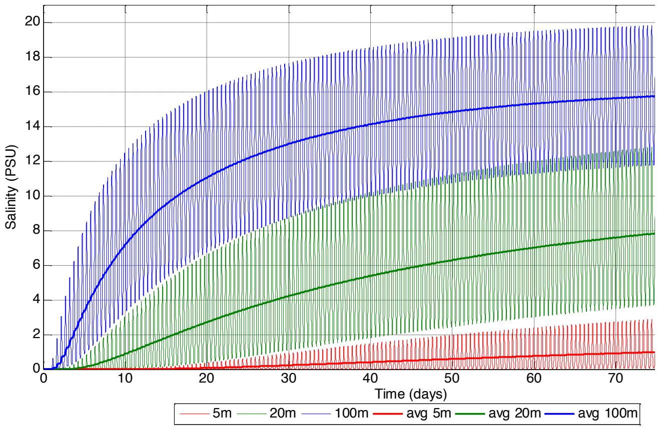

Figure 13. effect of mesh resolution on tracer diffusion

The results suggest that salt will diffuse further upstream when the mesh is coarse. In this channel test case a channel mesh of 100 m resolution in the length and 20 m in width gave the same results as the overall 100 m resolution mesh as expected since the main velocity vectors are directed along the channel axis.

B. test case 2: effect of the tracer diffusivity parameter

For a certain mesh resolution there is an amount of numerical diffusion present. We would like to know what order of magnitude this numerical diffusion has or at which parameter value of the tracer diffusivity we start to influence the tracer diffusion in the test model.

1) test model description

We used the same default parameter values and boundary conditions as the previous test case. For the 20, 50 m and 100 m mesh resolution we even used the same model domain, but for the 5 and 10 m mesh resolution we used a smaller model domain of 2000 m in length and 50 m wide. The depth was kept the at -10 m TAW. The time step was always 4 s. The tracer diffusivity was varied between 1.E-6 and 1.E3 m²/s.

2) Results

At 1000 m from the tidal and tracer boundary a tracer value time series was extracted. This was done for the small model domain with mesh resolution of 5 and 10 m.

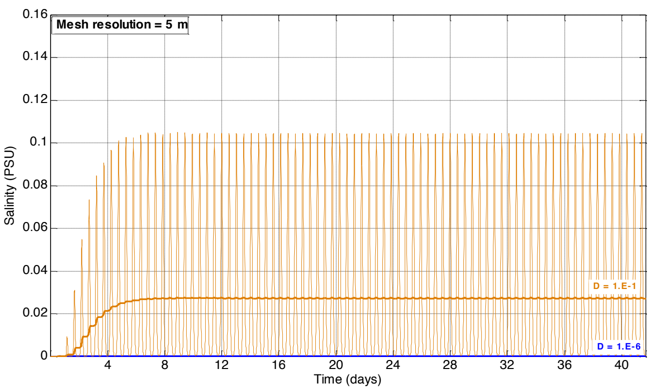

Figure 14. Mesh resolution 5 m: tracer diffusion results for D=1.E-1m²/s (orange line) and D=1.E-6 m²/s (blue line = zero)

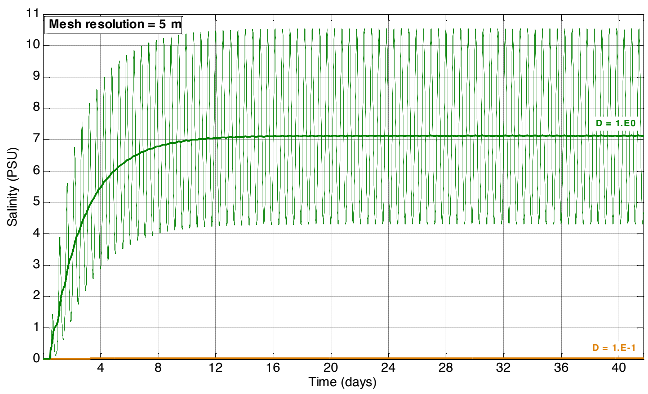

Figure 15. Mesh resolution 5 m: tracer diffusion results for D=1.E0 m²/s (green line) and D=1.E-1 m²/s (orange line = almost zero)

For the 5 m mesh a parameter value for the tracer diffusivity D of 1.E-6 m²/s gave no tracer concentration after 90 days at 1000 m from the boundary (figure 14). In the small model domain the upstream boundary discharge condition of 1m³/s has a larger effect than in the bigger model domain, because in figure 13 we see for the same diffusivity value a small tracer diffusion. If the tracer diffusivity is increased from 1.E-6 to 1.E-1 m²/s an increase of tracer diffusion to 0,025 PSU (daily averaged value) can be seen in figure 14. If the diffusivity is further increased to 1.E0 m²/s a much larger increase in tracer diffusion can be seen in figure 15.

For the mesh with 10 m resolution the diffusion is very comparable as the mesh with the 5 m resolution for the same diffusivity values. The daily averaged values just lie a little bit higher : compare results in figure 15 with results in figure 16.

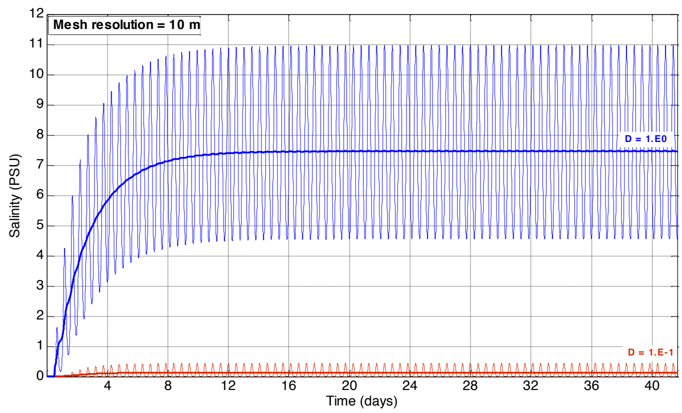

Figure 16. Mesh resolution 10 m: tracer diffusion results for D=1.E-1 m²/s (red line) and D=1.E0 m²/s (blue line)

For the mesh with 20 m resolution the diffusion of tracer increases again slightly for the same diffusivity values. A diffusivity D = 1.E1m²/s was also tested for the 20 m resolution mesh and gave a further increase in diffusion (figure 17) . It is noticed that the higher the diffusivity, the faster the tracer reacts to the concentration gradients, which is to be expected, and the faster a steady state is reached.

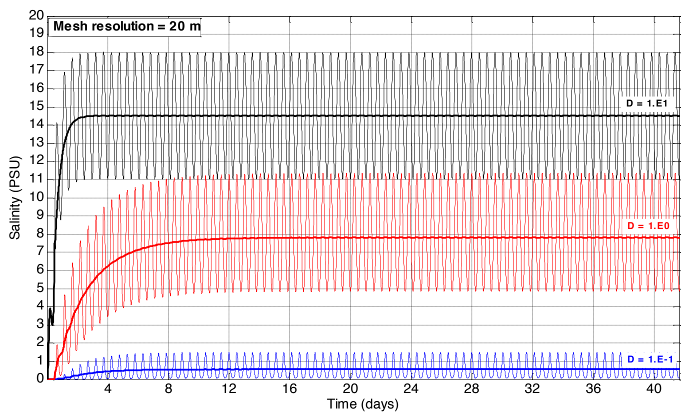

Figure 17. Mesh resolution 20 m: tracer diffusion results for D=1.E-1 m²/s (blue line), D=1.E0 m²/s (red line) and D=1.E1 m²/s (black line)

For the mesh with 50 m resolution the difference between the simulation with D=1.E-4 m²/s and D=1.E-1m²/s is small and less than 1 PSU. Increasing D with a factor ten (D=1.E0 m²/s) gives a big change in tracer transport (figure 18). Increasing the diffusivity again with a factor ten (D=1.E1 m²/s) results in the same order of magnitude increase as from D=1.E-1 m²/s to D=1.E0 m²/s (figure 19).

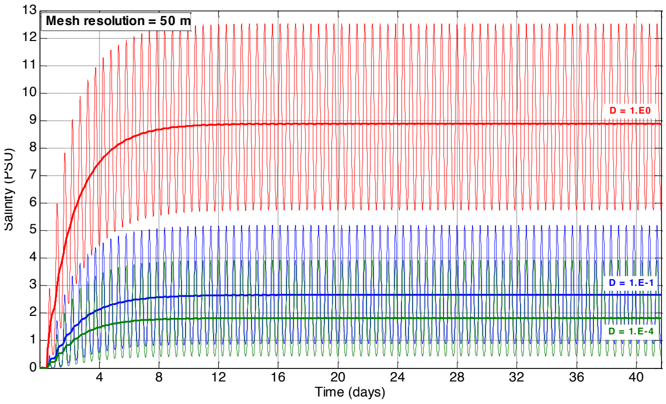

Figure 18. Mesh resolution 50 m: tracer diffusion results for D=1.E-4 m²/s (green line), D=1.E-1 m²/s (blue line) and D=1.E0 m²/s (red line)

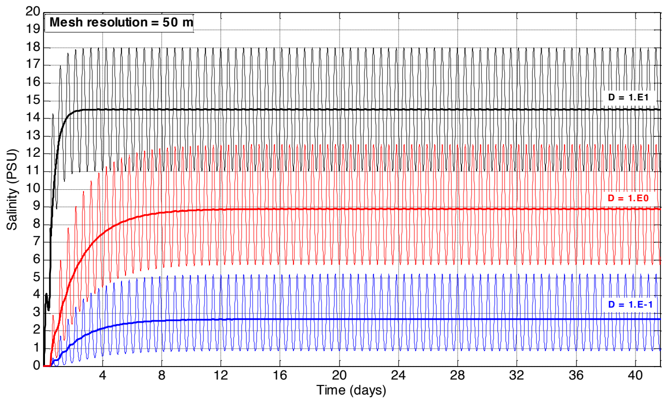

Figure 19. Mesh resolution 50 m: tracer diffusion results for D=1.E-1 m²/s (blue line), D=1.E0 m²/s (red line) and D=1.E1 m²/s (black line)

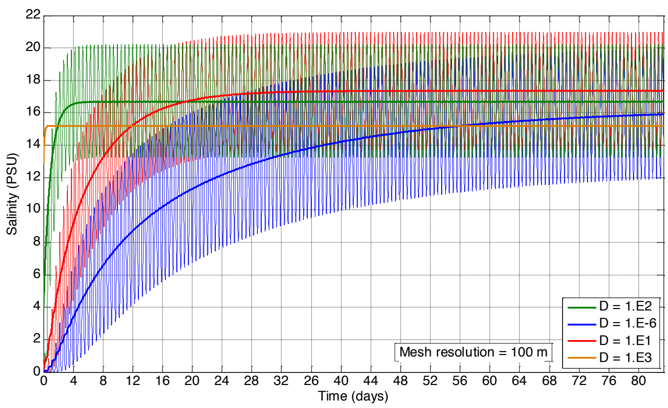

Figure 20. Mesh resolution 100 m: tracer diffusion results for D=1.E-6 m²/s (orange line), D=1.E1m²/s (red line), D=1.E2 m²/s (green line) and D=1.E3 m²/s (orange line)

For the mesh with 100 m resolution the results show that the size of the diffusivity parameter mostly influences the speed at which the steady state is reached (figure 20) and less the steady state salinity level. For D=1.E-6 m²/s (blue line in figure 20) the steady state salinity level lies even higher than for D=1.E3 m²/s, a very high diffusivity.

VI. Discussion

Even in simple test cases like the small test cases described in this paper it is very difficult to differentiate the effect on tracer transport caused by tracer advection, molecular tracer diffusion, numerical diffusion and dispersion. But the test cases show a clear and large influence of the mesh resolution on the tracer results. The test cases also show that the tracer diffusivity parameter D has a different effect at different mesh sizes. This makes it really difficult to calibrate or to improve the salinity as a tracer in our big model because of the different mesh resolutions at different locations. at least we need a place varying diffusivity parameter so we can influence tracer calculations in the model domain part where the mesh resolution is not too coarse; or in other words where the numerical diffusion is not so overwhelming that it dominates the tracer transport.

For our partner in the project, the University of Antwerp, we did some tracer calculations in the Scaldis model. Figure 21 shows the tracer concentrations of two identical tracers for seven tidal cycles. Tracer 11 (blue line) was released in the downstream part of the model (where the mesh is coarser; about 50-70 m) and tracer 17 was released in the upstream part of the model (where the mesh resolution was 7 m). Figure 21 shows that tracer 11 is more diffusive than tracer 17. But again it is difficult to differentiate and point only towards numerical diffusion. The cross sectional area downstream is much larger than upstream and so the fresh water discharge has less effect on tracer diffusion downstream than upstream. This can also be seen in the higher advective transport of the tracer upstream. This makes it very difficult to judge the models performance for tracers.

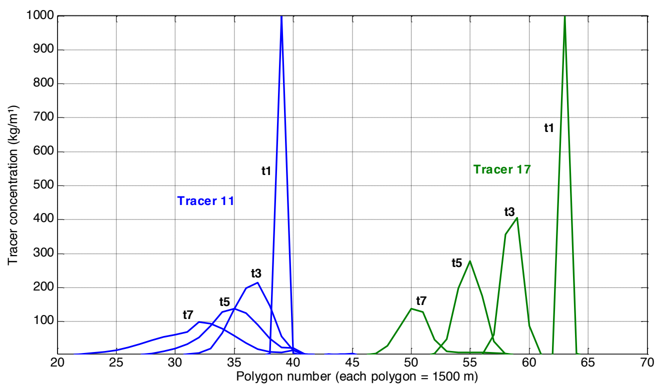

Figure 21. Tracer transport at two different locations (downstream=blue lines; and upstream= green lines) after one (t1), three (t3), five (t5) and seven (t7) tidal cycles in the Scaldis model

VII. CONCLUSIONS

For the Scaldis 3D model we do not succeed to get the salinity values right in the Coastal zone of the model. The salinity field corresponds better with the measurements inside the Scheldt Estuary. Due to the high dependency of the salinity as a tracer from the numerical diffusion (mainly due to mesh resolution) we get no grip on how to improve this salinity field in the coastal zone.

The small test cases clearly show the dependency of the tracer diffusion on the mesh resolution. If one keeps all parameters fixed, but changes only the grid resolution of his model, the whole salinity field will change, like already reported by [6].

For mesh resolution ranging from 5 to 100 m the tracer diffusivity parameter has no effect with values below 1.E-1 m^2/s. But due to the interference of tracer advection, molecular tracer diffusion, dispersion and numerical diffusion it is very difficult to estimate the real contribution of this parameter.

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