Multi-disciplinary/scale modeling of the Scheldt Estuary and tidal river network (a collection of articles from 2009 to today)

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From 2007 to today, Anouk de Brauwere has been the driving force behind several innovating modelling developments with applications to the Scheldt Watershed. Functioning as a bridge between hydrodynamical modellers at UCL and two teams of environmental experimentalists at VUB (metals) and ULB (fecal bacteria), she coordinated the implementation of a multi-disciplinary, and multi-scale reactive transport model to study environmental questions in the Scheldt Basin. The key concept of this study was 'integration': integration of the necessary multi-displinary knowledge (hydrodynamics, computational fluid mechanics, microbiology, (geo)chemistry), but also the spatial integration of morphologically and dynamically distinct regions, resulting in a single model representing the whole tidal continuum from Ghent to the North Sea. Thanks to this integrative nature, the model has a unique potential to study processes and concentrations at the basin-scale, i.e. explicitly including all forcings. This offers possibilities not only to better understand the processes and their effects, but also to assess the impact of hypothetical future (management or accidental) scenarios for the whole Scheldt Watershed and the North Sea.

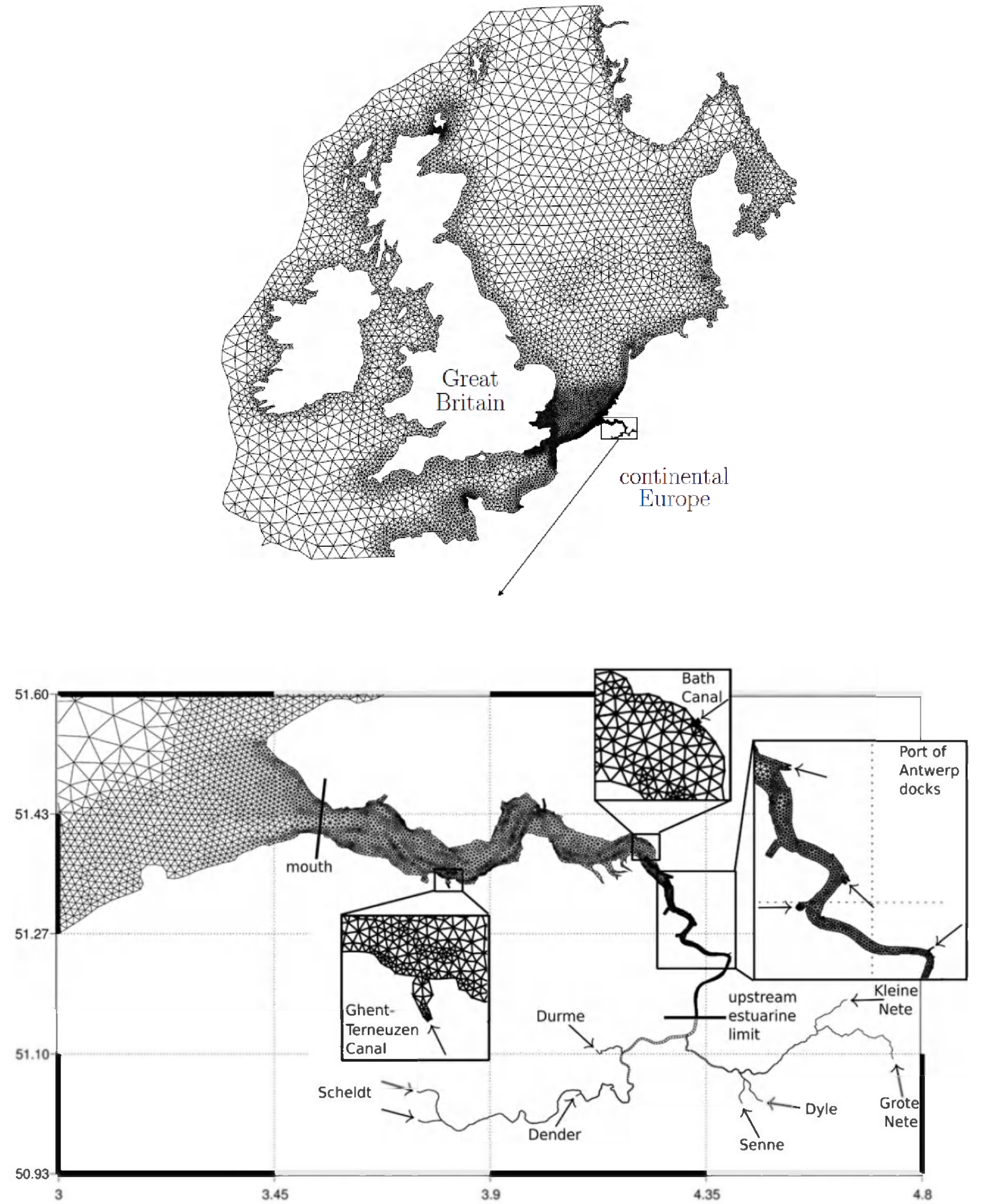
Three main study subjects were studied so far:

1. Hydrodynamical modelling and timescales for water transport

This new model was built using the general architecture of the Second-generation Louvain-la-Neuve Ice-ocean Model (SLIM, www.climate.be/slim). The specificity of this model is that it uses the finite element method to solve the governing equations, which allows for the use of unstructured meshes for the spatial discretisation of the domain. An unstructured mesh has a resolution that can greatly vary over the domain, i.e. in sub-regions of interest or subject to more complex dynamics the resolution (and thus the computational effort) can be increased compared to other areas. This implies a great flexibility that has unique advantages for multi-scale/physics problems. In the case of the Scheldt, this flexibility has enabled the integration of the upstream tidal river network, the Scheldt Estuary as well as the North-western European Continental Shelf in one single model. The large marine part facilitates a more accurate simulation of the tides or storm surges as they enter the Scheldt Estuary. Yet, as the mesh is less resolved in this large part of the domain (grid size ~ 50 km compared to a resolution down to 60 m in the estuary), the computational cost is only doubled compared to a situation where only the Scheldt Estuary and the tidal rivers would be included.

After having validated the hydrodynamical model (de Brye *et al.*, 2010), the model was not yet practical for environmental applications. In this form, the information is still very complex (fields varying spatially and temporally at a high resolution) and hence difficult to use for diagnostic purposes. Therefore, it is useful to derive diagnostic variables which summarize some of the main transport features present in the complex raw hydrodynamical outputs. This is the general motivation behind the use of timescales like water residence time and water age, which are often used in biological/chemical/geological studies to express the time spent by water in a given domain – which can then be conveniently compared to other timescales of more biological/chemical/geological relevance. We computed these timescales for the Scheldt Estuary, combining rigorous theoretical formulas with the complex hydrodynamical model, such that we can be confident that they integrate all relevant physical processes (time-varying residual current, tides, turbulent diffusion).

The definition of the residence time is the time that will be spent by a given water parcel in the estuary until it leaves it for the first time. According to this definition, it is clear that the residence time is both variable in space (as it depends on where the water parcel is at the moment the time measurement is started) and time (since it will depend on the actual hydrodynamical conditions at the initial or release time). Therefore, in a first study we computed the residence time for 13 boxes in the estuary (spatial variability) and for different initial times (temporal variability) (de Brauwere *et al.*, 2011a).



The spatial variation was approximately as expected, i.e. monotonically decreasing towards the mouth – except that for the most upstream box the residence time was close to zero. At first, this may seem counter-intuitive but in fact it is in line with the definition: close to the upstream boundary of the estuary the water will also quickly 'leave the estuary for the first time', due to the tides periodically pushing the water upstream. Obviously, this is not consistent with the empirical meaning generally attributed to the residence time: it is supposed to express the total exposure of a water body in a domain. In order to account for this generalisation an alternative timescale has been defined: the exposure time. When computed for the 13 boxes in the Scheldt Estuary, the exposure time in the most upstream box is indeed the highest, and in any box it is higher than the respective residence time.
To investigate the temporal variability of the residence and exposure time, we compared the timescales computed for initial times in winter and summer, and for each season at high and low tide. As expected, the timescales are longer in summer, due to the lower upstream river discharge.

Equally expected was the fact that at low tide the timescales were longer than when starting at high tide – because at low tide the water will first be pushed up the estuary. However, it was totally unexpected to find that the difference between the high and low tide timescales were so large: up to almost 20 days. In other words, at the most downstream box, the exposure time of water parcels 'released' at a 6 hour interval varies between 9 (start at high tide) and 28 days (start at low tide)!

These results illustrate that the seemingly simple concept of residence time hides several subtleties that are often not considered in applications, but may be of significant importance. These observations motivated us to further refine this study. A first refinement consisted of computing the 'partial exposure times' of the 13 estuarine boxes, i.e. the total time spent in each box, instead of in the whole estuary. Doing this for water initially in each box at a time, we obtained a 'connectivity matrix', relating the initial position of water with the time it spends in each box. This information is nothing but a sophisticated summary of the complex underlying hydrodynamics, but now it is much more useful for applications, e.g. to quickly assess the impact of an accidental pollution event somewhere in the estuary on the different sub-regions of the estuary, or to evaluate how long water stays in subregions known to be favourable for the growth of a certain species.

In a subsequent refinement effort, we increased the resolution of the computed residence and exposure time, such that their value is now known for every model grid cell and model time step (de Brye *et al.*, 2012). This is appealing because it provides actual 'movies' of the timescales varying in time and space. However, the results are again too complex to be easily usable for diagnostic applications. The tidally-averaged pictures reveal that the residence and exposure times exhibit surprisingly little lateral variation, i.e. the longitudinal trend observed with the 13 boxes is relatively accurate. In contrast, there is great spatial heterogeneity in the temporal variability associated with the timescales, resulting from a complex interplay of bathymetry and water discharge.

Besides this detailed study of the residence and exposure times, the water age was also investigated. As opposed to the first timescales, the age is defined as the time since a given water parcel has entered the estuary. Again, the age varies in space and time, but it is also dependent on the 'entrance' through which the water entered. In other words, for each different water source, a different age can be defined. In the case of the Scheldt Estuary, a distinction was made between water coming from upstream (freshwater), from downstream (sea water) and from lateral inputs like canals and harbour locks.

With the above timescale studies in the Scheldt Estuary, it has become a benchmark application. For instance, one recent study illustrated the meaning of another timescale for water renewal, the so-called 'influence time', again on the Scheldt Estuary (Delhez *et al.*, in review). New ongoing work consists of computing yet another new timescale, the 'partial age' (a generalisation of the age concept), in the Scheldt Estuary.

2. Modelling *Escherichia coli* concentrations as an indicator of fecal pollution

Due to its intensive agriculture, high concentration of industry and large population density, the Scheldt Watershed is subject to significant pollution pressure. Discharge of wastewaters or run-off loaded with animal or human fecal material degrades the microbiological water quality, i.e. increases the risk of having microbial pathogens present in the natural surface water. Because these pathogens are too diverse, and often present only at very low concentrations, it is not feasible to systematically monitor all their concentrations. Instead, it has been decided to measure the concentration of a small number of so-called 'fecal indicator bacteria', of which *Escherichia coli* (*E. coli*) is one of the most important. Its concentration in the Scheldt Watershed has been monitored in 2007-8 by colleagues at the ULB, but the results were so variable in time that they were difficult to interpret. It is well known that *E. coli* concentrations can vary over orders of magnitude in natural systems, but the possible causes in the case of the Scheldt were too numerous (water discharge, upstream inputs, wastewater treatment plant inputs, interaction with sediment, tides, temperature effect) to disentangle them empirically. If we could only simulate all these effects in a single model, we might be able to quantify their relative importance… So, an *E. coli* module was added to SLIM.

A first model considered only the tidal part of the Scheldt Basin, and represented the bacteria as a single pool (de Brauwere *et al.*, 2011b). Yet, the results were already quite interesting. Indeed, it appeared that the inputs due to the wastewater treatment plants, as well as the temperature effect were negligible to explain the observed variability. In contrast, the water entering the tidal domain from upstream was already highly polluted, such that it to a great extent determined the levels observed in the tidal river. This was especially the case for the water coming from Brussels and entering the tidal Scheldt via the Zenne, Dijle and Rupel. In combination with the tidal mixing action, these highly concentrated upstream (and side) inputs caused greatly varying concentrations in the Scheldt. Downstream of the main tributaries, the gradual decay of the bacteria and continuous dilution results in a steep decrease of the *E. coli* concentrations downstream of Antwerp. Close to the estuary mouth, the bacteria have almost disappeared, and the estuary has thus effectively operated as a cleaning filter.

In a second model, we further extended both the geographical domain and the representation of the bacteria pools. By coupling SLIM (tidal rivers + estuary + sea) with an ecohydrological model of the upstream river catchment (Ouattara *et al.,* in press), we effectively integrated the complete Scheldt Watershed in a single simulation (de Brauwere *et al.*, 2014). Instead of using these two tools as competing models, each of them was used in the domain for which it was originally designed and clearly outperforms the other model. This resulted in a unique coverage of the whole Scheldt land-sea continuum from the source all the way to the North Sea. As the first model showed the importance of the upstream rivers (and especially the Brussels area), this integration allowed to include all *E. coli* sources explicitly. In addition to the geographical model integration, we further refined the model by dividing the bacteria pool in free-floating bacteria and those attached to particles. While the first are transported along with the water, the latter are also subject to settling and resuspension processes. To explicitly represent these processes, a new suspended sediment model has been developed within the SLIM architecture (Gourgue *et al.*, in press). The results of this second model study confirm the previous observation on the importance of the tides, and the weak effect of the wastewater treatment plants in the tidal part. Besides, they suggest that the sediment-related processes are actually not essential to reproduce the median *E. coli* concentrations along the Scheldt, nor the observed variability at a given location. Nevertheless, the explicit distinction between free and attached bacteria increases the insight in the system and offers more interpretation possibilities. As an illustration of the potential of this new modelling tool, we also performed two simulations considering extreme (worst case and best case) situations of Brussels wastewater management. The effect of both scenarios is clearly observable all the way to Antwerp.

Several side-studies were also performed related to the *E. coli* model in the Scheldt. These studies range from semi-theoretical considerations on the parameterisation of the settling flux (de Brauwere and Deleersnijder, 2010), establishing where and when new water quality samples should be taken in order to reduce the model uncertainty most (de Brauwere *et al.*, 2009), derivation and computation of the age associated to the bacteria (Matton, 2012), to the publication of an exhaustive literature review of the existing models for fecal indicator organisms in natural surface waters (de Brauwere *et al.*, in press).

3. First steps towards modelling metal speciation

Besides microbiological water quality, SLIM could also be extremely useful for the study of other pollutants. Especially its large domain, and its ability to provide highly resolved (both spatially and temporally) outputs makes it an interesting tool for risk assessments. Therefore, we started to build a new SLIM module to allow the simulation of dissolved and particulate metals (Elskens *et al.*, in review).

By merging the long-term data records collected by VUB, ULB and VMM, empirical functions were derived, relating the total metal concentration to environmental variables (salinity and suspended sediment concentration). This means that if SLIM simulates these environmental variables, we can reconstruct or predict the metal concentration at each location and each timestep of the simulation. A second empirical function was estiblished linking the metal partitioning coefficient (i.e. the ratio between particulate and dissolved metal concentration) to environmental variables. Applying this function to the SLIM outputs and the reconstructed metal concentrations then allowed producing high-resolution fields of dissolved and particulate metal concentration. This means that SLIM can be used to produce ‘movies’ of dissolved and particulate metal concentrations, allowing infinitely more detailed analyses than based on direct point measurements alone. This being said, the limitation of this approach lies in the empirical functions, which are only valid within their calibration domain. In other words, although this combined model is already a significant step forward, it cannot be trustfully used for scenario evaluations or even predictions for periods outside the one covered by the calibration dataset (1980-2010). Therefore, we now focus on the development of a fully mechanistic metal module.

Conclusion

The cited work has obviously been produced by a team of researchers. Nevertheless, it is the merit of Anouk de Brauwere to have facilitated their collaboration, crossing not only scientific boundaries, but also language and institutional ones. After 6 years, we are proud of the results, but are also well aware that the work is far from finished. There are clear scientific challenges waiting for us: closer collaboration with geochemists and environmental chemists to develop a mechanistic metal model, investigate the potential of modelling newly emerging pollutants like nanomaterials and endocrine disruptors, ecological modelling. Notwithstanding the significant effort put so far in the scientific integration, we want to further increase it in order to demonstrate the usefulness of our developed tools. Yet, if we really want to go to the next level, we should include players and interests beyond the science platform. The Scheldt Basin being densely populated, better understanding and predicting the complex dynamics of the river system and its response to the diverse pollution pressures has a clear importance for society. We see our application to the VLIZ North Sea Award as a first attempt to take this step.

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