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Modelling *Escherichia coli* concentrations in the tidal Scheldt river and estuary

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ABSTRACT

Recent observations in the tidal Scheldt River and Estuary revealed a poor microbiological water quality and substantial variability of this quality which can hardly be assigned to a single factor. To assess the importance of tides, river discharge, point sources, upstream concentrations, mortality and settling a new model (SLIM-EC) was built. This model was first validated by comparison with the available field measurements of *Escherichia coli* (*E. coli*, a common fecal bacterial indicator) concentrations. The model simulations agreed well with the observations, and in particular were able to reproduce the observed long-term median concentrations and variability. Next, the model was used to perform sensitivity runs in which one process/forcing was removed at a time. These simulations revealed that the tide, upstream concentrations and the mortality process are the primary factors controlling the long-term median *E. coli* concentrations and the observed variability. The tide is crucial to explain the increased concentrations upstream of important inputs, as well as a generally increased variability. Remarkably, the wastewater treatment plants discharging in the study domain do not seem to have a significant impact. This is due to a dilution effect, and to the fact that the concentrations coming from upstream (where large cities are located) are high. Overall, the settling process as it is presently described in the model does not significantly affect the simulated *E. coli* concentrations.

1. Introduction

With its population density of more than 500 inhabitants per km^2, its active industrial development and its intensive agriculture and animal farming, the Scheldt watershed (20,000 km^2 from the North of France to the Belgian–Dutch border, see Fig. 1) represents an extreme case of surface water and groundwater pollution (EEA, 2004). Improvement of water

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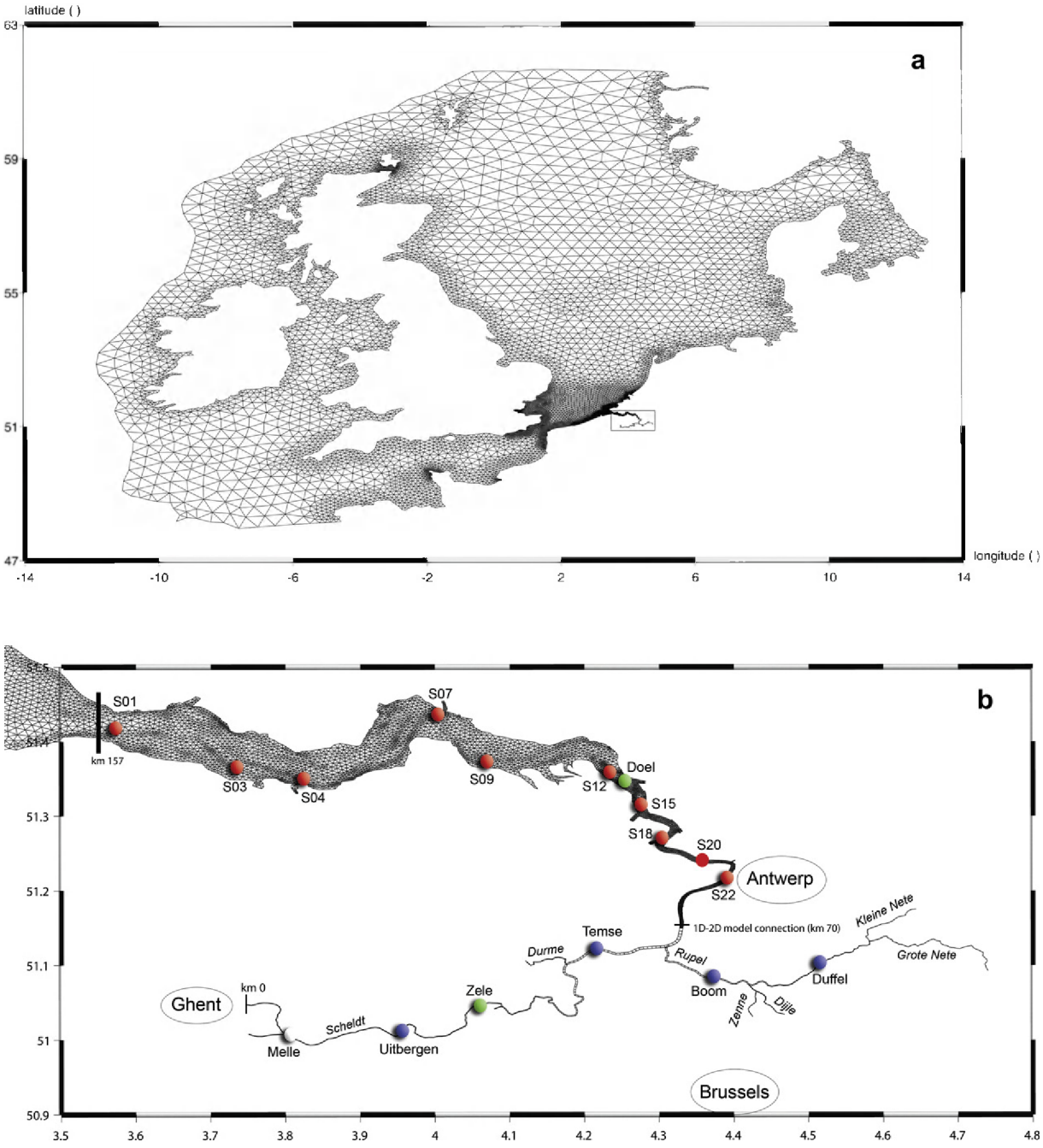

Fig. 1 – Model domain and grid, showing the area of interest (Scheldt River and Estuary) covering only a small fraction, but containing a significant number of grid cells. (a) Complete mesh; (b) zoom on estuary and tidal rivers, also showing the connection between the 1D and 2D models, the different tributaries modelled as well as a few important locations. Important cities are encircled, sampling locations are indicated by coloured circles (blue: our monitorings, green: VMM stations, red: estuarine stations sampled during cruises). The same colours are used throughout the figures. Km indications refer to the longitudinal axis along the Scheldt used for visualising the simulations. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

quality is however expected for 2015, owing to the ongoing implementation of the EU water framework directive (EU, 2000). Identification of pollutant sources, description of their fate along the Scheldt land-sea continuum and prediction of the evolution of water quality in response to future implemented environmental policies and climate change – these are the objectives of the Interuniversity Attraction Pole (IAP) TIMOTHY (www.climate.be/timothy). This must be achieved through the integration of different existing and new mathematical models for describing the water flows and biogeochemical and microbial transformations for all aquatic compartments of the Scheldt land-sea continuum. The current study is to be situated in this broad framework, and more particularly focuses on the understanding of the microbiological water quality in the part of the

Scheldt influenced by the tide. Recent field measurements (Ouattara et al., 2011) have demonstrated a rather poor microbial water quality in the Scheldt watershed concentrations above the minimal water quality standards of the new EU Directive for bathing water (EU, 2006). In addition, a large variability in the measured concentrations was observed. Understanding these observations is the primary motivation for the current study.

The monitoring of microbiological water quality is based on the concept of fecal bacterial indicators, whose abundance is related to the risk of pathogens being present (Havelaar et al., 2001). Today, *Escherichia coli* (*E. coli*) is the more commonly used fecal bacterial indicator, as there was evidence from epidemiological studies (Kay et al., 2004) that its abundance is a good indicator to predict the sanitary risks associated with waters (Edberg et al., 2000).

E. coli concentrations measured in river waters often exhibit a variability which is so high that the concentrations are classically visualised on a log-scale. This variability is especially important in systems under tidal influence, as the part of the Scheldt studied here. Table 1 summarises the factors generally thought to affect *E. coli* concentrations and variability in natural waters. However, it is often not clear which factors are the *main* drivers explaining the mean concentrations and the concentration variability.

Hydrological factors include the tide, river discharge and lateral runoff, which all influence the local transport, and hence the local residence time, of the bacteria. These factors vary at different scales (and interact with each other); but it is clear that short term variations at the scale of the hour cannot be neglected.

Inputs of *E. coli* bacteria into the domain are also major factors controlling the *E. coli* concentrations in the system. Indeed, it is generally assumed that fecal bacteria cannot grow in natural water, and hence must be brought into the system through external sources. Regarding the tidal Scheldt River and Estuary, bacteria can enter through the upstream boundaries and tributaries. Obviously these inputs are highly variable. In addition, *E. coli* are brought into the domain by point sources of domestic waste water. Domestic wastewater is released into the aquatic system after treatment in waste water treatment plants (WWTPs); the type of treatment greatly affects the concentration of fecal bacteria in the released effluents (George et al., 2002; Servais et al., 2007b). Wastewater discharges are expected to vary greatly on short time scales, especially during rain events. Finally, fecal pollution can also be brought to surface waters through diffuse sources (surface runoff and soil leaching). In a recent study, (Ouattara et al., (2011) compared the respective contribution of point and non-point sources of fecal contamination at the scale of the whole Scheldt watershed. They concluded that point sources were largely predominant when compared to non-point sources (around 30 times more for *E. coli* at the scale of the Scheldt watershed). Predominance of point sources was also demonstrated for the Seine watershed which is just south of the Scheldt one and is also highly urbanised (Garcia-Armisen and Servais, 2007; Servais et al., 2007b). However, these results are based on catchment-scale calculations and diffuse sources can still have a significant local impact on the *E. coli* concentrations, especially in small rivers in rural areas.

After their release in rivers, fecal bacteria abundance decreases more or less rapidly. The disappearance of fecal bacteria in aquatic environments results from the combined actions of various biological (grazing by protozoa, virus-induced cell lysis and autolysis) and physico-chemical conditions (stress due to osmotic shock when released in seawater, nutrient depletion, exposition to sunlight and temperature decrease) and also to possible settling to the sediments (Barcina et al., 1997; Rozen and Belkin, 2001). Unfortunately, it is difficult to identify the respective contribution of each of these factors to the decay rate at a given moment but it can be expected that their rate of disappearance varies on timescales from hours to years. In models, the decay of fecal bacteria is usually described by a first order kinetics (Servais et al., 2007b).

From the above overview it is clear that many factors act on the local *E. coli* concentrations, and most of them vary on short time scales. The goal of this study is to bring some insight into the (relative) importance of these different factors in causing the observed *E. coli* concentrations in the tidal Scheldt River and Estuary. The focus will be on understanding both the long-term median concentrations (varying in space) and the local variability in concentration. For this purpose, the SLIM-EC model is set up which includes as many of these factors as possible (Table 1). This is the first *E. coli* model developed for the Scheldt tidal River, tributaries and Estuary, and the current paper presents the first realistic simulation results.

As a number of factors can be included only approximately (due to a lack of information), it is not expected that concentrations can be predicted for a specific point and time. Furthermore, although the model is capable of simulating the intra-tidal *E. coli* concentrations, the necessary high-resolution observations and boundary conditions are not available to evaluate the model performance at this scale. Rather, the

Table 1 – Summary of factors affecting *E. coli* concentration in natural surface waters and the way these factors are represented in the model used in this study (SLIM-EC) for the Scheldt simulations.

Factor affecting *E. coli* concentration	Representation in SLIM-EC
Hydrological factors	
Tide	15 min resolution
Upstream discharges	Daily resolution
Lateral runoff	Parameterised (only in river part), at daily resolution
E. coli inputs	
Upstream concentrations (boundaries)	Constant concentration
Concentration entering by tributaries	Main tributaries explicitly in model
WWTP point sources	Constant discharge
Diffuse sources	No
E. coli processes	
Mortality	First order kinetic process, with time-dependent coefficient (seasonal variation linked to temperature)
Sedimentation	First order process, coefficient v_{sed}/H (with constant v_{sed})

objective is to reconstruct the right median *E. coli* concentrations (taken over time periods of the order of one day to a year) and concentration variability, both in time and in space. The ability of the model to achieve this goal is assessed by comparison with the available data.

2. Model description

The model used in this study is a version of the Second generation Louvain-la-Neuve Ice-ocean Model (SLIM: www.climate.be/slim). As its name indicates, this model originally focuses on the physical processes in the aquatic environment, and does so by solving the governing equations using the finite element method on unstructured meshes ("second generation"). Unstructured grids offer the possibility of a more accurate representation of coastlines and grid sizes varying in space (and time) – without having to increase the total number of discrete unknowns. A validated SLIM version for the hydrodynamics in the Scheldt (de Brye et al., 2010) is combined with a simple reactive tracer module for the simulation of *E. coli* concentrations, forming SLIM-EC. Table 1 summarises the main processes and inputs and at which temporal resolution they are represented by the model.

2.1. Model domain and mesh

The computational domain (see Fig. 1) is identical to that used by de Brye et al. (2010): although the focus is on the Scheldt Estuary (indicated by the rectangle in Fig. 1a and shown in the zoom of Fig. 1b), the domain is extended both upstream and downstream. Upstream the domain reaches as far as the tidal influence is significant, covering a riverine network of the Scheldt and its tributaries. So, although the Scheldt is the main focus of this study, all main (tidally influenced) tributaries are also modelled explicitly. This riverine part of the model is 1D (averaged over the cross section), while the estuary and the downstream extension covering the whole North-Western European continental shelf are modelled by 2D, depth-averaged equations.

Fig. 1 also shows the unstructured mesh used, constructed by Gmsh (Geuzaine and Remacle, 2009; Lambrechts et al., 2008), which is made up of approximately 21,000 triangles (in the 2D part) and 400 line segments (in the 1D part). In the current study a mesh was used with triangle sizes covering several orders of magnitude (the ratio of the size of the largest triangle to the smallest exceeds 1000, the smallest with a characteristic length of ~60 m are in the Scheldt Estuary). For a more detailed discussion of the computational domain and construction of the mesh, please refer to de Brye et al. (2010).

2.2. Hydrodynamics

A detailed presentation and validation of the hydrodynamical model SLIM can be found in de Brye et al. (2010). We only repeat here the aspects determining its temporal resolution. The model has a time step of 15 min. It is forced

- at the shelf break: by elevation and velocity harmonics of the global ocean tidal model TPXO7.1;
- by wind fields at 10 m above the sea level. These fields are 4 times daily NCEP Reanalysis data provided by the NOAA/OAR/ESRL PSD;
- at the upstream river boundaries, the mouths of the Seine, Thames, Rhine/Meuse, the Bath Canal, Ghent-Terneuzen Canal and the Antwerp Harbour locks: by discharges interpolated from daily measurements.

2.3. E. coli module

SLIM-EC combines the hydrodynamic SLIM with a module describing the dynamics of *E. coli* in the aquatic system. In this module the bacteria are modelled as a single type of reactive tracer, i.e. once they enter the model domain (through external sources), they are transported by the hydrodynamics and their concentration is affected by *E. coli*-specific processes.

In the 2D part of the model domain, the depth-averaged concentration C of *E. coli* is described by the following advection-diffusion-reaction equation:

$$\frac{\partial}{\partial t}(HC) + \nabla \bullet (H\mathbf{u}C) = \nabla \bullet (KH\nabla C) + HR \tag{1}$$

where t is the time, ∇ the horizontal del operator, H the water depth, $\mathbf{u}$ the depth-averaged velocity vector, K the diffusivity coefficient and R the reaction term (which will be described in more detail below). As the mesh size varies greatly over the computational domain, it is essential to that the horizontal diffusivity varies with the mesh size. In this study the diffusivity coefficient K depends on the mesh size Δ according to a relation inspired by Okubo (1971): $K = \alpha\ \Delta^{1.15}$, with $\alpha = 0.03\ \mathrm{m}^{0.85}\mathrm{s}^{-1}$.

In the 1D part of the model the following advection-diffusion-reaction equation is solved for the section-averaged concentration C of *E. coli*:

$$\frac{\partial}{\partial t}(SC) + \frac{\partial}{\partial x}(SuC) = \frac{\partial}{\partial x}\left(KS\frac{\partial}{\partial x}\right) + SR \tag{2}$$

where S is the section of the river and u the section-averaged velocity. The variable x represents the along-river distance.

The processes affecting *E. coli* concentration in the water column that are considered in the SLIM-EC model are mortality and sedimentation. The approach used to model these processes is similar to that of Servais et al. (2007a, b) to model the dynamics of fecal coliforms in the rivers of the Seine drainage network. Both mortality and settling are modelled by first order (type) reaction terms:

$$R = -k_{mort}C - \frac{v_{sed}}{H}C \tag{3}$$

The sedimentation velocity v_{sed} is assumed to be constant and equal to $5.56 \times 10^{-6}\ \mathrm{ms}^{-1}$. This value is based on experiments conducted to study the fecal bacteria settling rate in rivers from the Scheldt and Seine watersheds (Garcia-Armisen and Servais, 2008). Note that this representation of the disappearance rate by sedimentation is a parameterisation for depth-averaged models, implying that the water column is well-mixed. In practice, this assumption may not be entirely valid, but it has been shown that the error made remains relatively small (de Brauwere and Deleersnijder, 2010).

The mortality rate varies with temperature following a sigmoid relation (Servais et al., 2007a, 2007b):

$$k_{mort}(T) = k_{20}\frac{\exp\left(-\frac{(T-25)^2}{400}\right)}{\exp\left(-\frac{25}{400}\right)} \quad (4)$$

with T representing temperature in °C and k_{20}=1.25 × 10^{-5} s^{-1}.

We do not have high-frequency high-resolution temperature measurements in the Scheldt. But using the temperature measurements made at the monthly intervals during 2007–2008 at several locations, we fitted a sine through these points in order to get the average seasonal temperature in the whole domain as a function of time (Fig. 2). Using this relation, we can now approximate the temperature at any time during the simulations. Substituting this in equation (4), we effectively get a mortality rate varying seasonally. The value of the mortality rate was similar to the one used by Servais et al. (2007a, b) for modelling the dynamics of fecal bacteria in the Seine watershed. We verified in batch experiments (data not shown) that the mortality rates in the large rivers of the Scheldt watershed were not significantly different from those estimated for the large rivers of the Seine watershed. In this model, to the "base mortality" no additional mortality term was added related to solar effects, as is done in some other studies (Liu et al., 2006; Thupaki et al., 2010). The main reason for this is that in the modelled domain water is quite turbid (from 20 mg/l of suspended matter to more than 1 g/l in the maximum turbidity zone of the estuary), resulting in a low light penetration and thus a limited impact of solar irradiation on fecal bacteria.

2.4. *Input of* E. coli *into the system*

2.4.1. *Input by WWTPs*

As Ouattara et al., (2011) showed that *E. coli* enter the Scheldt mostly through point sources (cf. Introduction), WWTP outlets are the only sources included in the model (see also Table 1). WWTP data are compiled from information provided by the Vlaamse Milieumaatschappij (Flemish Environmental Agency, VMM), Rijkswaterstaat Zeeland and Waterschap Zeeuwse Eilanden for the whole (tidal) basin. Data processing steps involved the localisation of the WWTP outlet, the actual discharge point in the model domain, and the distance between these two points. The number of *E. coli* discharged by a WWTP per second was approximated to be proportional to the average volume treated in the WWTP (which depends on the number of inhabitants-equivalents connected to the WWTP) multiplied by an *E. coli* concentration depending on the treatment type applied in the WWTP (George et al., 2002; Servais et al., 2007b). The *E. coli* concentrations considered in the treated effluents was 2.8 × 10^5 E. coli (100 ml)$^{-1}$ when a the primary treatment followed by an activated sludge process was applied, 1.7 × 10^5 E. coli (100 ml)$^{-1}$ when the N removal treatment (nitrification + denitrification) was added to an activated sludge process and 1.1 × 10^5 *E. coli* (100 ml)$^{-1}$ when the treatment included activated sludge followed by N and P removal; these values result from measurements performed in treated effluents of various WWTPs located in the Scheldt watershed. After this procedure, the *E. coli* discharges in the model domain by the WWTPs ranged from 8 × $10^6$$s^{-1}$ to 8 × $10^8$$s^{-1}$.

2.4.2. *Open boundary concentrations*

The concentration of *E. coli* entering the domain through the open boundaries must also be assigned (see Fig. 1 for location and Table 2 for values). The concentration at the shelf break was assumed to be zero, as well as the concentrations entering the estuary laterally (the Bath and Terneuzen Canals, and water coming from the Antwerp harbour locks). The assumption for the shelf break seems undisputable, due to its large distance from land. The concentrations in the canals were not measured but estuarine observations indicate that their effect is very limited (see below). The effect of the harbour was neglected based on specific measurements made inside and outside the locks, which were quasi-identical (*unpublished data*). Furthermore the harbour authorities estimated the average residence time in the harbour to be of the order of several months, suggesting that bacteria entering the harbour are probably long dead before they could reach the locks.

The only boundaries through which a significant amount of bacteria enters the domain are the upstream river boundaries. These boundary concentrations are based on field measurements taken at the boundary locations (*unpublished data*). If only one measurement is available, this value was considered, otherwise the median value of all measurements available at that point was used. The data did not allow to impose boundary concentrations varying in time – although we did investigate whether the measured concentrations correlated with discharge, but no significant relation was revealed (Ouattara et al., 2011).

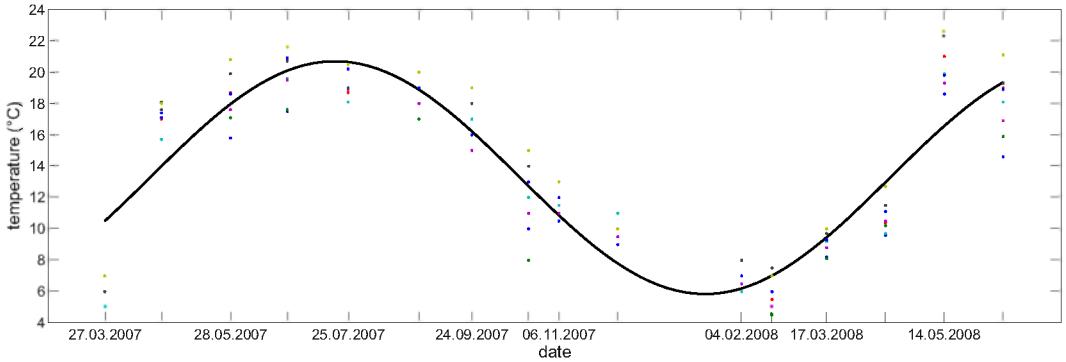

Fig. 2 – Fitted sine (black line) through temperature measurements made at several locations in the Scheldt and its tributaries (dots).

Table 2 – *E. coli* concentrations imposed at the model boundaries in SLIM-EC.

Boundary concentrations in *E. coli* (100 ml)$^{-1}$	
Durme	2600
Scheldt upper branch	10000
Scheldt lower branch	15000
Kleine Nete	1900
Grote Nete	1500
Dender	700
Dijle	3400
Zenne	400000
Shelf break, rivers discharging in North Sea and canals discharging in estuary	0

3. Validation measurements

The *E. coli* concentrations calculated by the model were compared to field measurements made in the study domain in order to validate the model. The modelling period was chosen such that it covers the measurements made in the scope of the IAP TIMOTHY project, i.e. February 2007–June 2008. Two types of sampling campaigns were conducted during this period:

- From 26 March 2007 to 13 June 2008, monthly samples were taken at several monitoring stations in the Scheldt watershed. This gives monthly timeseries at several locations, but also enables to assess the long-term variability.
- In February 2007 and 2008, two one day cruises along the saline estuary were conducted. This resulted in two longitudinal estuarine profiles.

The results of the latter monitoring survey are fully described in Ouattara et al., (2011). *E. coli* concentrations were estimated by a plate count method using Chromocult Coliform agar medium. By performing replicates, the coefficient of variation (CV) of the plate counts on specific media used in this study was estimated to be 25%. This value of CV is usual for this type of bacterial enumeration (Prats et al., 2008).

In addition, a second set of data was used: measurements of fecal coliforms made by the VMM at one station in the Scheldt River (Zele) and three locations in the estuary very close to each other (around Doel). The fecal coliform concentrations were converted into *E. coli* concentrations by multiplying the fecal coliform data by 0.77; this value is the average ratio between *E. coli* and fecal coliforms numbers measured in river water samples (Garcia-Armisen et al., 2007). The VMM measurements span different periods, ranging from 2000 to 2008, and hence do not exactly correspond to the modelled period. Therefore, these measurements should be regarded with some caution.

4. Results and discussion

4.1. *Reference simulation*

The simulations are compared to the available observations in three different ways, enabling model validation from different perspectives:

(1) Simulated median and range (over the period of the our monthly monitoring) of *E. coli* concentrations along the Scheldt axis (Fig. 3) and along the Rupel-Nete-Grote Nete axis (Fig. 4) are compared to the median and range of measured values. This enables an assessment of the simulated median and variability, and its variation in space.
(2) Simulated and measured timeseries at a given point in space (two locations in the Scheldt River, Fig. 6). This comparison more clearly visualises the simulated and measured long-term variability in time.
(3) Simulated and measured concentrations on two specific days, at a number of specific estuarine stations (sampled during two cruises, Fig. 5). This comparison focuses on the estuarine part; it visualises the short term model variability, but only point-wise comparisons with the observations are possible.

Fig. 3a shows that the model is able to reproduce the measured median concentrations and concentration range in the tidal Scheldt River (1D model). The median values correspond very well to the observed medians (Table 3). The difference certainly falls within the measurement precision of approximately 25% (cf. section 3). On the other hand, it appears that the model finds a larger range of concentrations than those measured (when expressed as interquartile range, cf. Table 3). This is probably due to the fact that the model covers a much wider range of hydrological regimes than the monthly measurements. Indeed, the modelled range is primarily a reflection of extreme events occurring during the simulation period. It is not surprising that these brief extreme conditions are not captured by a monthly point sample. Furthermore, it was attempted to carry out the monitoring samplings approximately at low water, but due to logistic constraints this is not exactly the case for all stations. This could be an additional factor lowering the observed range.

According to Fig. 3 the WWTPs have little effect on the concentrations, while the tributaries and the water from upstream have a more significant influence. This is especially true for the water coming from the Rupel, as this river also carries water coming from the Zenne crossing the city of Brussels (cf. Fig. 1). Fig. 4 shows the simulation results for the Rupel, including the measurements made during the monthly monitoring, clearly illustrating the huge concentrations entering through the Dyle/Zenne. Ouattara et al., (2011) reported on the Zenne water quality in more detail, noting that the section downstream of Brussels is heavily contaminated with *E. coli* abundances comparable to those usually measured in treated waste waters.

The effect of the tide is also clearly visible in Figs. 3 and 4, as high concentrations are also transported upstream of the input point (e.g. when the Dyle/Zenne join the Rupel in Fig. 4, or when the Rupel joins the Scheldt in Fig. 5). Indeed, the tides periodically push water up the rivers, thus counteracting the "normal", downstream directed, river flow. Without tides, the high concentrations would primarily be transported downstream. This important feature could only be captured by a model resolving tides, and suggests that the tidal process may indeed be an important factor explaining the observed concentrations and/or variability. In particular, it seems that the concentrations measured at Temse (Fig. 3a) are highly

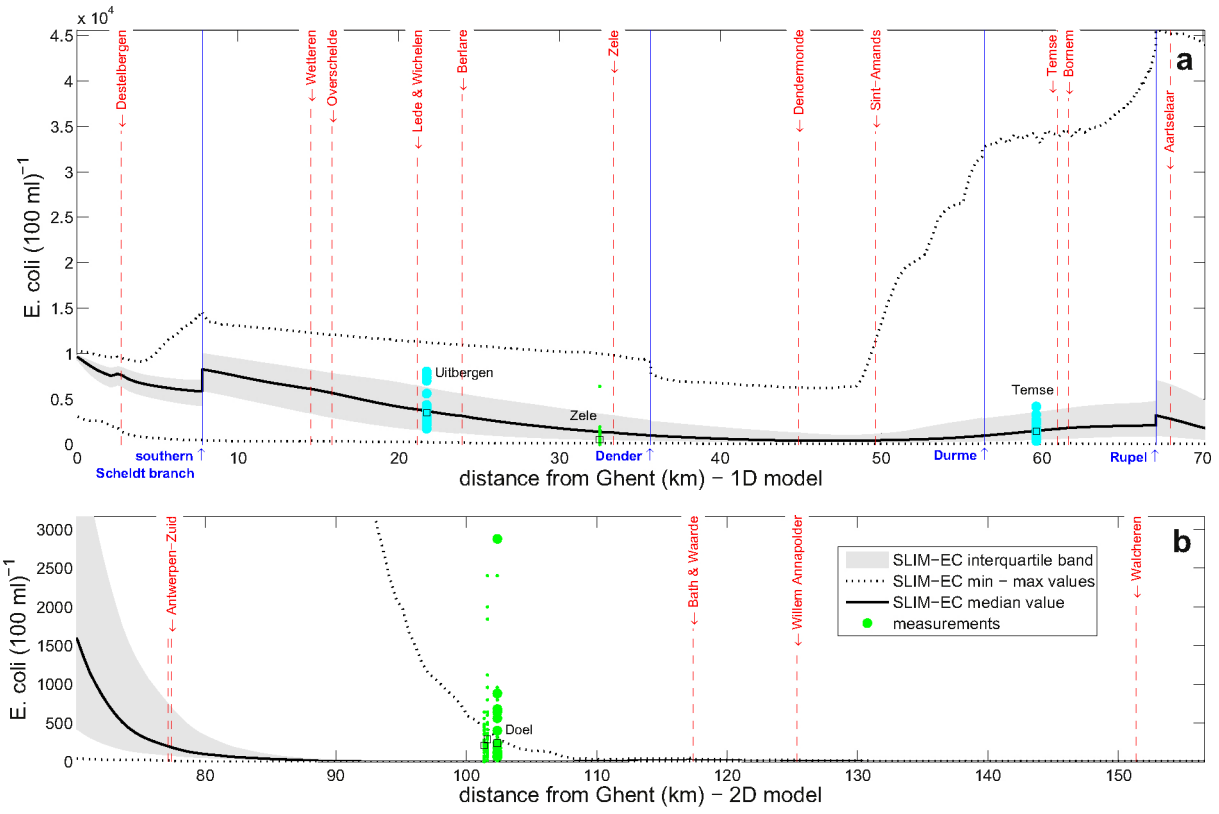

Fig. 3 – *E. coli* concentration profile along the Scheldt, from Ghent (km 0, cf. Fig. 1) to the mouth. (a) Results from 1D model. (b) Results from the 2D model. Red vertical lines indicate the location of the WWTPs, blue vertical lines the location of tributaries joining the Scheldt. Only the simulation results covering the our monthly monitoring period are considered. The simulations are summarised as their median value at every position (black line), the interquartile range (grey band) and the min-max range (dotted lines). The available measurements are shown as dots: cyan dots referring to our monthly monitoring, and green dots referring to VMM measurements (only the bigger dots represent samples taken during the simulation period), squares indicate the median value of the measurements at each location. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

influenced by the Rupel although Temse is situated upstream of the Rupel connection. The importance of the tide will be further discussed in section 4.2.

In the estuary, the major feature is a steep decrease in simulated concentrations (Fig. 3b). This decrease is coincident with the maximum turbidity zone (MTZ) in the Scheldt, which is reported approximately between km 60 and 100, or between salinity values 2 and 10 (Baeyens et al., 1998; Chen et al., 2005; Muylaert and Sabbe, 1999). Measured timeseries in the estuary are scarce. The only timeseries in the estuary available to us are those performed by VMM. As discussed in section 3, these measurements are to be interpreted with care, but it appears that the model underestimates the concentrations in this part of the estuary, or at least cannot reproduce some of the higher values measured. The model performance in the estuary is further assessed in Fig. 5, comparing measurements made during two estuarine cruises with model outputs from the same days. These results suggest that the model predicts the correct concentrations in the beginning and at the mouth of the estuary, but simulates too fast a decrease between these two extremes. Again, the concentration decrease occurs in the MTZ. Therefore, the poor model performance in this part of the Scheldt is probably related to the fact that the *E. coli* dynamics are modelled as independent of suspended matter. For instance, explicitly modelling resuspension and longer survival times for *E. coli* bacteria attached to sediment particles (Craig et al., 2004; Davies and Bavor, 2000; Davies et al., 1995) may indeed increase the modelled concentrations in the MTZ. A second possible explanation for the model underestimation is missing sources. WWTPs are included in the model, but not the possible pollution effect of canals, or of diffuse sources (most of the estuary lies in a rural area).

In Fig. 6 the model results are visualised as timeseries at two monitoring stations in the Scheldt. These figures visualise more explicitly the temporal variability in the observations and simulations. It can be seen that the model is not able to reproduce the observations exactly, i.e. the model is not accurate for predictions of the exact concentration at a given time and location. However, the median value and range are satisfactorily modelled, especially when comparing with the generally reported performances of microbial quality models described in the literature, where one is generally satisfied with model simulations falling within half a log unit of the observations (Collins and Rutherford, 2004; Garcia-Armisen et al., 2006; Sanders et al., 2005). The modelled variability has a different nature at the two locations: in Temse (Fig. 6a) a large portion of the variability is due to the tide (compare raw outputs with

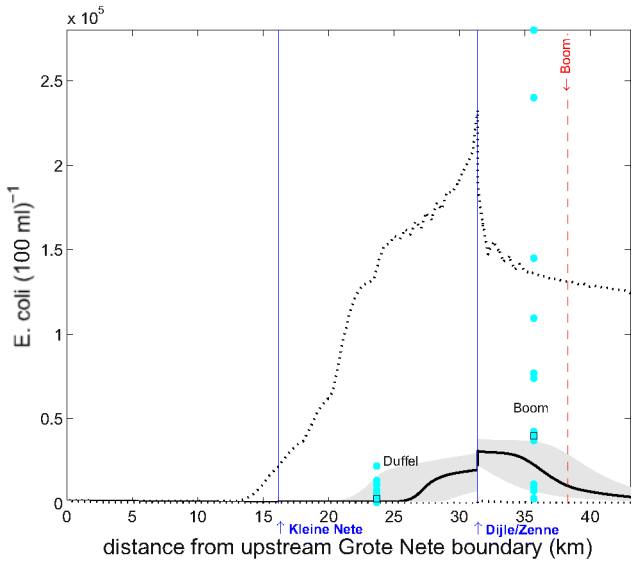

Fig. 4 – *E. coli* concentration profile along the Rupel-Nete-Grote Nete axis (cf. Fig. 1). Km 0 refers to the upstream boundary of the model in the Grote Nete. For legend refer to Fig. 3.

tidally averaged concentrations), while in Uitbergen (Fig. 6b) most of the variability seems to occur at longer timescales and is probably more related to the hydrological regime. This agrees with what we could expect as Uitbergen is located more upstream than Temse. It is also in agreement with Ouattara et al., (2011), who identified a positive correlation between *E. coli* concentrations and discharge at Uitbergen, while there was no significant correlation at Temse. The tidal influence in Temse was already suggested when inspecting Fig. 3a, and is related to the Rupel joining the Scheldt downstream of Temse. The high *E. coli* concentrations carried by the Rupel are pushed upstream (to Temse) at a tidal frequency, explaining the important tidal fingerprint in the timeseries at this location. Conversely, at Uitbergen, there is no important source in the vicinity which could cause a similar tidal influence.

In this section, the model results of the reference simulation were assessed and generally a good agreement is found for the median concentration and its variability. This validation is not trivial as the model parameters (for mortality and settling) and inputs (WWTPs and boundary concentrations) were not tuned, but directly taken from field measurements or external studies. The (potential) influence of tide, river discharge, WWTP inputs and upstream concentrations have been briefly discussed. The importance of these factors will be further investigated in the next section.

4.2. *Impact of different processes on* E. coli *concentrations*

One of the objectives of this study is to better understand the importance of the different factors affecting the long-term median *E. coli* concentration and its variability in the Scheldt River and Estuary. Starting from the reference simulation

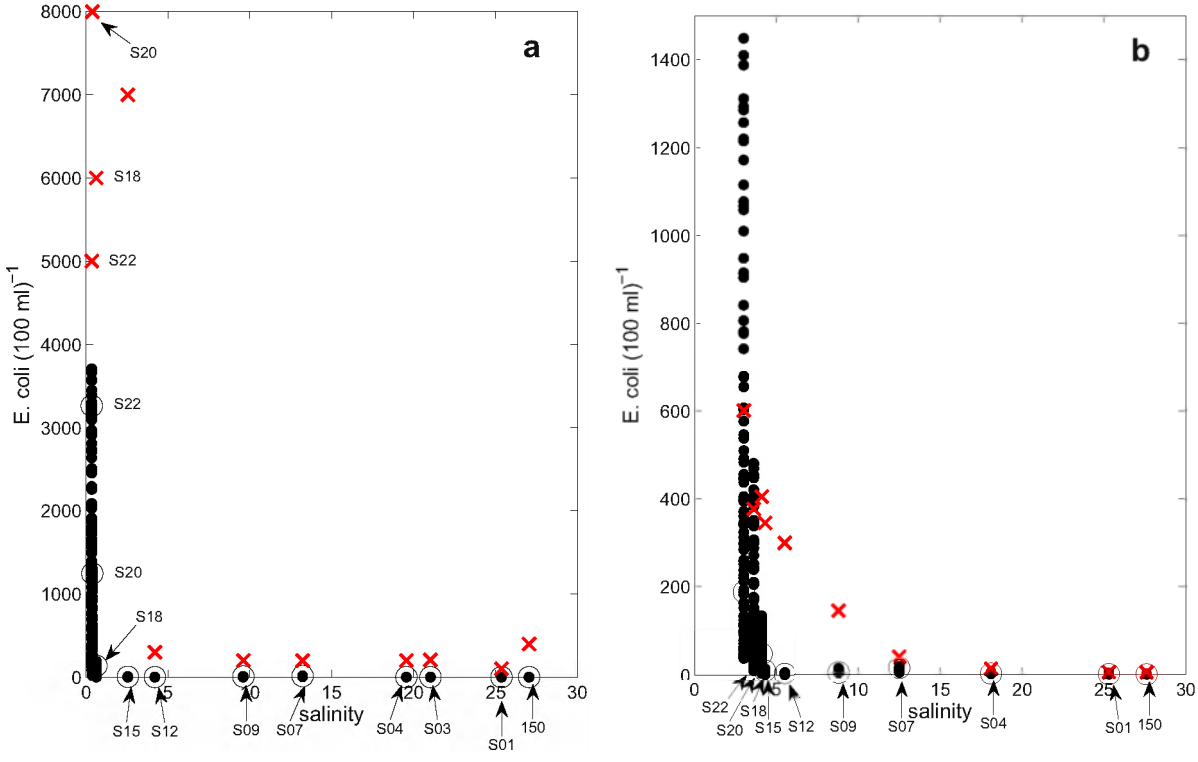

Fig. 5 – Estuarine profiles of *E. coli* concentrations on two specific days of longitudinal cruises in the estuary: (a) 14 February 2007, (b) 12 February 2008. Black dots represent the simulated *E. coli* concentrations at the same location as the cruise stations during the whole cruise day. The larger black circle shows the simulated value approximately at the time of sampling. The crosses represent the measurements. Station names are also added to facilitate localisation of the stations (see Fig. 1, station 150 is a sea station outside the mouth of the Scheldt).

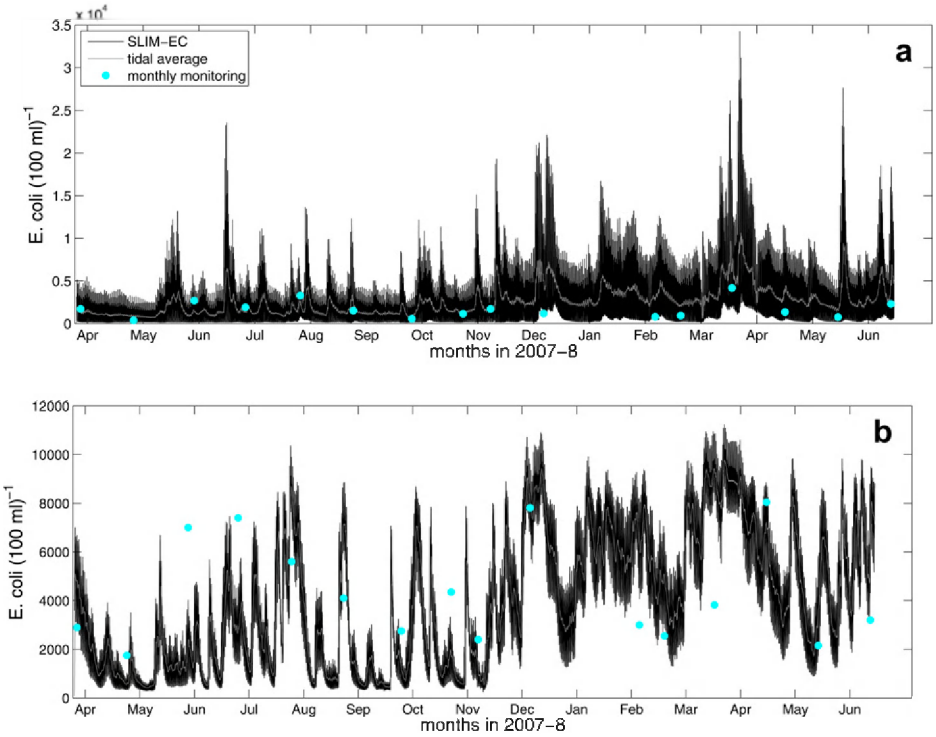

Fig. 6 – *E. coli* concentration timeseries at two locations in the Scheldt River (see Figs. 1 and 3 for location): (a) Temse, (b) Uitbergen. Simulation period covers our monthly monitoring. Black line shows the model output, grey line the tidal moving average of these outputs. Dots represent field measurements made during this monitoring.

presented in the previous section, we removed, one by one, the major processes (cf. Table 1). Table 3 summarises the results of these different simulations.

4.2.1. *Tide and upstream discharge*

To assess the role of the tides, a simulation was run with the tides removed from the hydrodynamics, while all other forcings and processes are kept identical.

Table 3 – Comparison of observed and simulated median and interquartile concentrations all expressed as *E. coli* (100 ml)$^{-1}$. The comparison is done at two monitoring locations, where samples were taken at approximately monthly intervals from 26 March 2007 to 13 June 2008. The simulations cover the same period, but all model outputs (at 15 min intervals) are used to compute the statistics.

	Temse		Uitbergen	
	Median	Interquartile range	Median	Interquartile range
Observations	1400	1200	3500	3700
Simulations				
Reference	1500	3000	3600	4700
No tide	80	280	5500	4700
No upstream conc.	110	51	300	120
No WWTPs	1400	3000	3300	4900
$k_{mort} = 0$	16000	20000	10000	2900
$v_{sed} = 0$	1900	3800	4700	5100

First inspecting what happens at the two monitoring stations Temse and Uitbergen (Table 3), it is seen that the change is largest at Temse. Indeed, both median concentration and variability (interquartile range) are significantly reduced. Surprisingly, the median concentration at Uitbergen increases, while the variability remains equal. This confirms the hypothesis formulated when discussing Fig. 6 that Temse is much more influenced by the tide, because it is the tide that allows water mass to flow from downstream to upstream and thus brings the high Rupel concentrations upstream. When the tide is switched off, the Rupel concentration cannot reach as far upstream anymore (Fig. 7). Fig. 8a shows the simulated timeseries at Temse, showing the reduced concentrations and variability. The remaining variability is related to the upstream discharge (average daily discharges are prescribed). Fig. 8c shows the daily water discharge at Melle (see Fig. 1 for location) and there is indeed a clear similarity with the concentration timeseries at Temse. High concentrations at Temse generally coincide with high discharge periods.

The concentrations at Uitbergen are overall less influenced by the tide. Therefore, it is no surprise that the simulated concentration timeseries at Uitbergen (without tide, Fig. 8b) also exhibits a clear similarity with the discharge timeseries, although the concentrations seem to be less "sensitive" to high discharges than was the case at Temse. This suggests that the two counteracting effects of high discharge – reduced transit time (increasing *E. coli* concentrations downstream) and increased dilution (decreasing concentrations) – are balanced differently at these two locations. But the overall result at both locations is an increase of the *E. coli* concentrations with discharge.

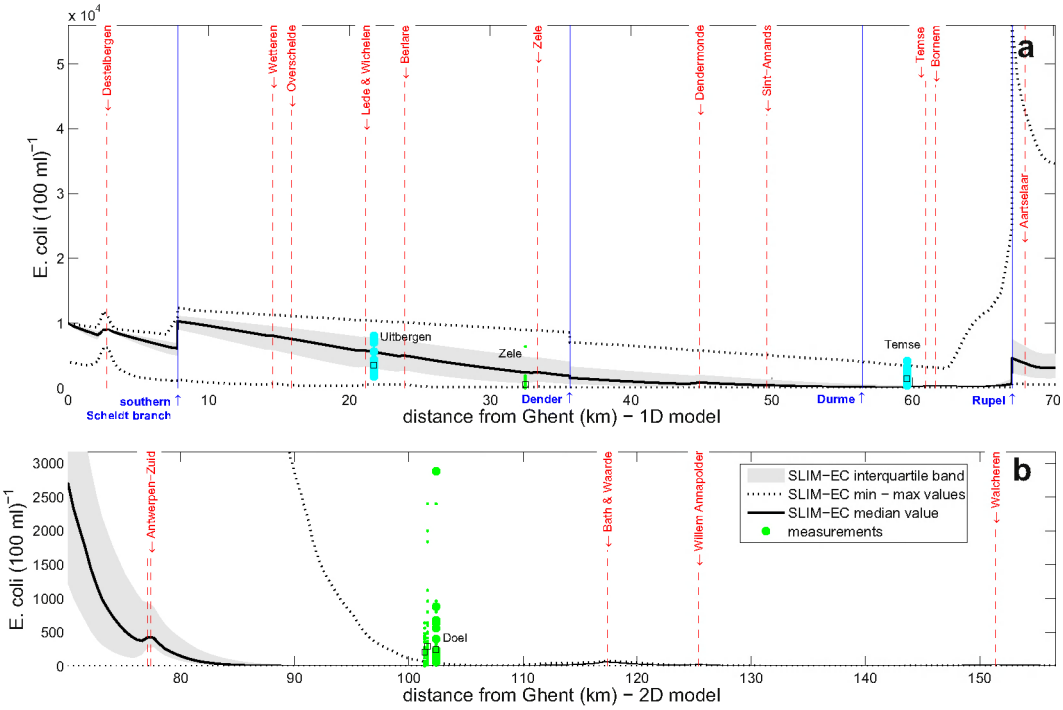

Fig. 7 – *E. coli* concentration profile along the Scheldt (cf. Fig. 3 for legend). Model results refer to simulation without tide.

Further inspecting the simulations at Uitbergen without tides, it is remarkable that the median simulated concentration is increased, while the interquartile range remains unchanged. When comparing Fig. 8b with Fig. 6b, it appears that switching off the tide induces two main changes:

(i) the short term variability due to the tidal effect vanishes, as expected. Because this variability has a smaller amplitude than the long-term variations, this barely influences the overall interquartile range.
(ii) the minimal concentrations are higher (although the maximal concentrations remain quasi-identical). Indeed, in the simulation with tides, the concentrations drop to lower, almost-zero values. As for Uitbergen no major sources lie downstream, during rising tide, waters with lower *E. coli* concentrations are brought upstream to Uitbergen, effectively reducing the concentration at Uitbergen. It is remarkable that the concentrations remain at these low levels for significantly longer periods than a tidal cycle. Therefore, these low values cannot (only) result from the periodic tidal current upstream. Rather, it seems that the tidal oscillation has a mixing effect acting on longer timescales, especially during periods of low discharge, when there is less counteraction from the river flow.

These results clearly demonstrate that the concentrations at both monitoring locations are influenced by the tides, but in a different manner. In order to get a more detailed picture of the spatially varying effect of the tides on median concentration and variability, we visualised the differences between Fig. 3 (with tides) and Fig. 7 (without tides) in Fig. 9. This figure reveals a complex role of the tides: they can locally either increase or decrease the median concentration and, surprisingly, the same holds for the variability. Indeed, in the central part (between km 22 and 50) the tides effectively reduce the observed variability in *E. coli* concentrations. Further downstream (from km 50 to the Rupel) the tides hugely increase both the variability and the median concentrations, until almost 100% of their value is due to the tides. This is the upstream Rupel influence zone, as discussed for the sampling station Temse. Upstream of km 50 the median concentrations are lowered by the tides (cf. discussion for Uitbergen), and this reduction is higher than 50% for a significant section of the river.

In order to better understand why the tides reduce median and interquartile range in the central part of the river, we performed an additional model test. A narrow patch of tracer was initialised at Uitbergen on 1/2/2007 at 0:00 and followed during 10 days – once transported by the "full" hydrodynamics (tides + river flow), and once with only the river flow. For simplicity, all other sources and decay reactions were removed (passive tracer). Fig. 10 shows the results of these two simulations. It is seen that, in addition to moving the patch up and down the river, the tides increase the width of the patch and accordingly reduce the maximal concentration. This suggests that the tides indeed have an increased "mixing" effect, smoothing the patch more efficiently than without tidal action, which is compatible with the observed lower median concentrations and variability in this section of the river.

In the estuary, the picture does not change so much by removing the tidal effect (Fig. 7b). Without tides, the high Rupel concentrations propagate less far downstream. Only

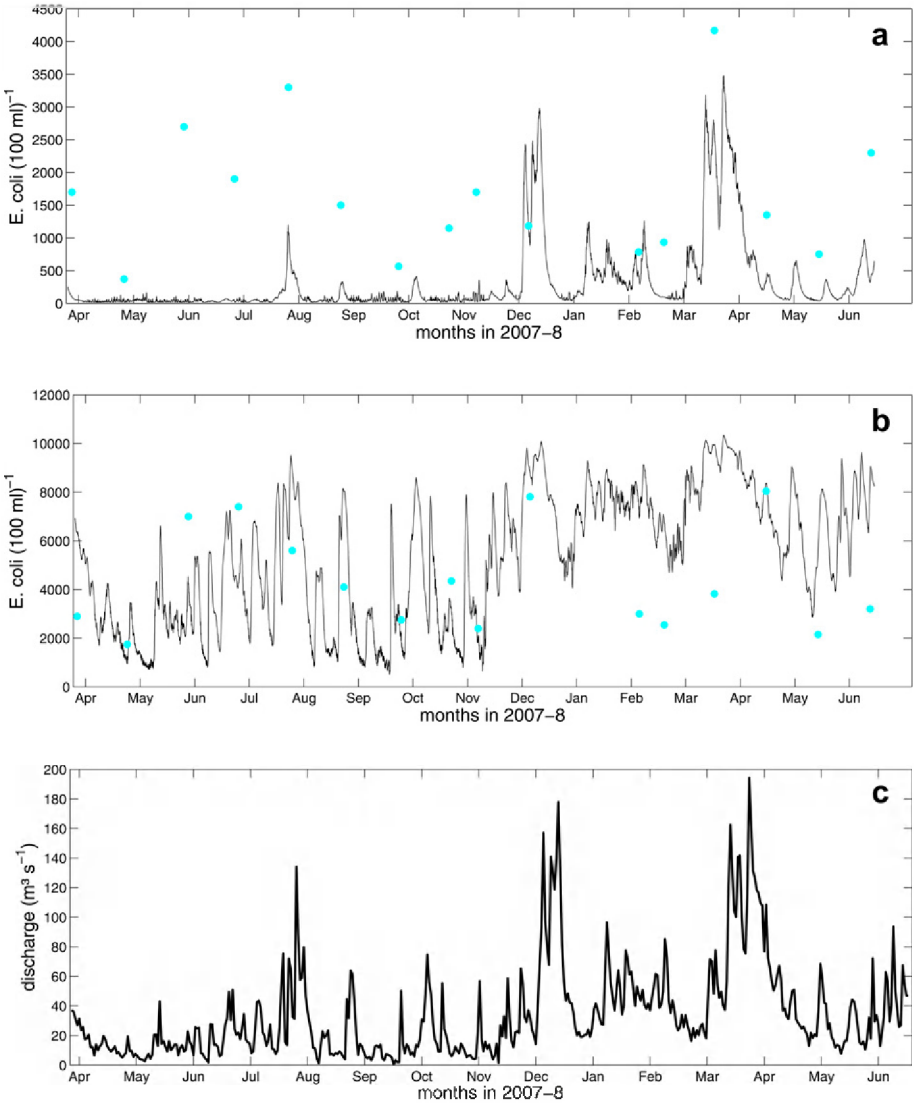

Fig. 8 – *E. coli* concentration timeseries at (a) Temse and (b) Uitbergen (cf. Fig. 1 for location). Model results refer to simulation without tide. (c) Measured daily discharge at Melle.

the residual current drives the concentrations downstream, resulting in slightly higher concentrations close to the Rupel and a faster decrease to quasi-zero values.

In conclusion, the tide appears to have a significant influence on the *E. coli* concentrations (median and range) – but the effect is different depending on the location. Overall, the tide has the effect to enlarge the influence radius of a source (or tributary) by pushing water upstream and further downstream than if there were no tides. In zones lying (not too far) upstream of important sources, the tides therefore cause an *increase* of the average concentrations, otherwise the average concentrations tend to *decrease*. In this particular case of the Scheldt, this means that the extent of the region influenced by the high Rupel concentrations is significantly enlarged by the presence of tides, mostly upstream but also downstream. Conversely, the most upstream section of the Scheldt is mainly influenced by what comes from further upstream, and only to a lesser extent by the tide. In this part, the tides rather have the effect to decrease the concentrations by bringing downstream water which contains lower concentrations of *E. coli*. Finally, by removing the tidal forcing it was also clearly seen that both at Temse and Uitbergen the modelled *E. coli* concentrations correlate positively with upstream discharge, although their response is different. Clearly, the impact of the tides on the *E. coli* concentrations is crucial but very complex, implying that "tidal corrections" in models which would not explicitly simulate the tides are unlikely to be reliable.

4.2.2. *Upstream concentrations and WWTPs*

Table 3 clearly shows that from the two inputs considered in this study (upstream concentrations and WWTPs), the main "source" of *E. coli* in the Scheldt is what comes through the upstream boundaries. This is probably due to the fact that

(i) a huge amount of bacteria enter the model domain through the Zenne boundary, caused by the large volumes of

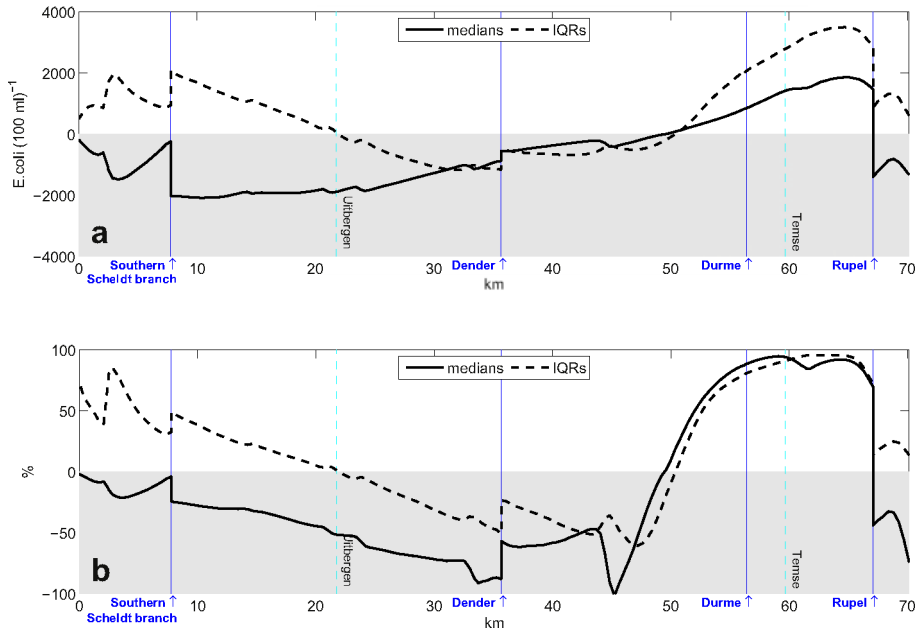

Fig. 9 – Difference between simulation with tides and simulation without tides. (a) Absolute difference and (b) relative difference between medians (full line) and interquartile ranges (IQRs, dashed line). Positive values mean that the simulation with tides is associated with higher median or IQR. The location of tributaries joining the Scheldt and the two monitoring stations Temse and Uitbergen are also indicated.

waste water discharged in the Brussels area (upstream of the model boundary) in the relatively small river Zenne. These massive concentrations propagate through the Rupel into the Scheldt, where they overwhelm the effect of local WWTPs.

(ii) the largest WWTPs in the Scheldt (the part under tidal influence) have a limited effect. Most of them are located in the Antwerp area, where they either discharge in canals or in the Antwerp harbour, avoiding a direct effect on the Scheldt. The few large WWTPs that discharge directly in the Scheldt (e.g. Antwerpen-Zuid and Aartselaar), do so in the downstream part of the river (downstream of the Rupel connection) where water discharges are much higher and therefore their impact is immediately reduced by dilution.

Although Table 3 only focuses on Temse and Uitbergen, the concentrations are reduced in the whole domain when the boundary concentrations are set to zero (not shown). The effect of the WWTPs is then more visible but remains only very local, suggesting an efficient mixing/dilution.

4.2.3. *Disappearance processes*

Finally, we tested the impact of taking out either of the two considered disappearance processes: mortality and settling. Table 3 shows that sedimentation has a negligible effect, but mortality certainly not. In other words, it is the mortality process which is primarily responsible for the decrease in concentrations following the input by a WWTP or tributary (Fig. 3). The negligible importance of the settling process on the overall disappearance rate is probably due to the fact that the rivers considered in this study are relatively deep, implying that bacteria need to cross a significant water depth before they actually disappear by settling. The (local) relative importance of mortality versus sedimentation can be expressed as $q = k_{mort}H/v_{sed}$, with H the water height. In the freshwater (1D) part of the Scheldt and during the study period (26 March 2007–15 June 2008) this ratio ranges between 2 and 35, with a median value of 9. In other words, disappearance by mortality is always faster than by sedimentation. For the Seine watershed, it was already found that the relative importance of settling versus mortality in the total disappearance rate decreases with increasing hydrological order of the stream (Servais et al., 2009). For small streams, settling was the dominant cause of *E. coli* disappearance, while its importance became negligible in the largest rivers of the watershed. Nevertheless, we must keep in mind that the settling process was modelled by means of a very simple first order parameterisation, while a more accurate representation would include an explicit model of suspended matter (including resuspension). It was already discussed that such a representation is expected to improve the model performance in the estuarine MTZ. However, it is not obvious whether it will significantly influence the results in the riverine part. Based on the *E. coli* concentrations measured in the bottom sediments and the concentrations of suspended matter, Ouattara et al., (2011) estimated the potential contribution of sediment resuspension to the *E. coli* concentration in the water column. Sediment resuspension contributed significantly to the water contamination only at two sites in the Scheldt watershed. These results suggest that resuspension can have important but localised impacts in the rivers. Modelling these effect will be a challenge for the future.

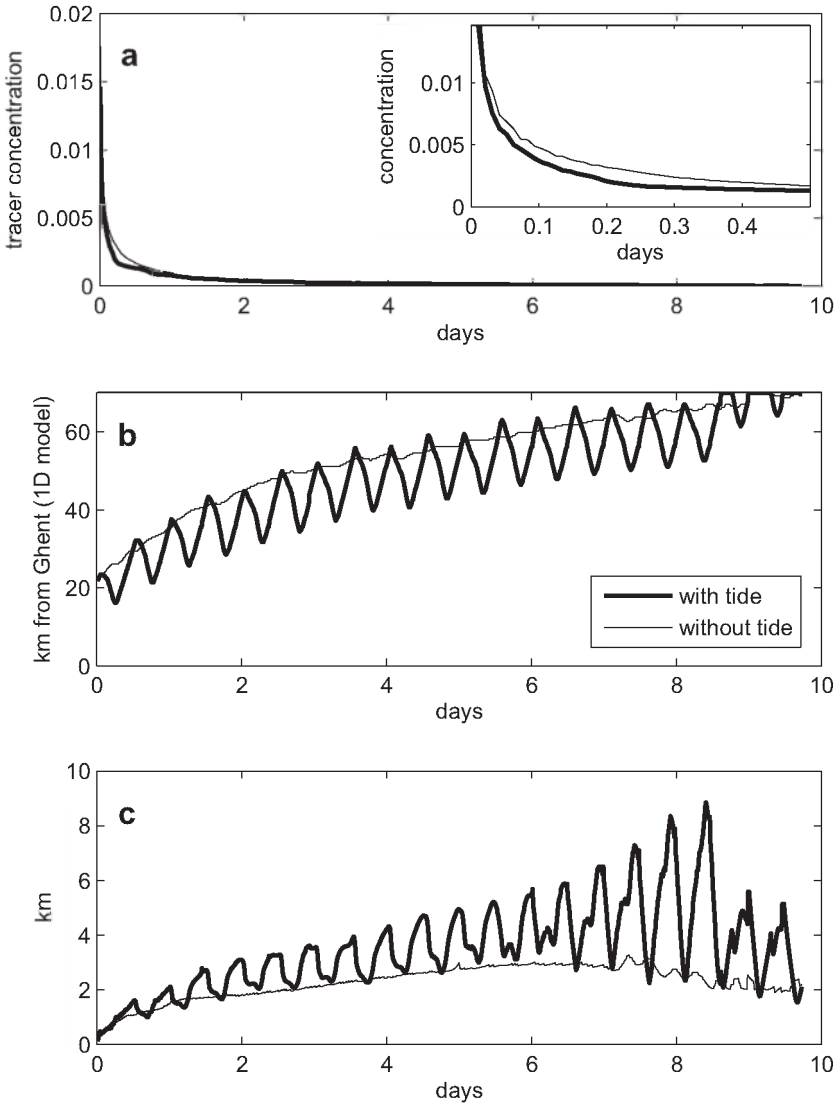

Fig. 10 – Results of simulation in which a patch of passive tracer was released at Uitbergen. No sources or decay processes were considered. In a first simulation, the tracer was transported by the "full" hydrodynamics (tides + river flow, thick lines) and in a second simulation only the river flow was considered (thin lines). Results shown: (a) evolution of maximal concentration (arbitrary units), with inset showing zoom on first hours; (b) position of maximum; (c) measure for the width of the patch.

5. Summary and conclusions

The current study aimed at providing some insight into the (observed) *E. coli* concentration in the tidal Scheldt River and Estuary. At a few locations along the tidal Scheldt long-term monitorings (>1 year) have been performed, and the resulting (monthly) measurements exhibited a remarkable variability, which could not readily be explained. Although measurements are available only at a monthly interval, we hypothesised that the short term physical processes (tide and upstream discharge) could be major drivers. To verify this hypothesis, the SLIM-EC model was built, in order to simulate the spatio-temporal distribution of *E. coli* concentrations, including these high-resolution physical forcings, in addition to specific *E. coli* sources (WWTPs, boundary concentrations) and processes (mortality and settling). The *E. coli* dynamics are kept relatively simple, motivated by analogous studies (e.g. disregard of diffuse sources) and by lack of data (constant WWTP discharge, boundary concentrations, single pool of bacteria). Nevertheless, the model simulations were capable of reproducing the long-term median and range of *E. coli* concentrations in the Scheldt. The main deficiency of the model is its inability to accurately simulate the decrease in concentration in the MTZ – which is most probably due to the lack of sediment-related dynamics for *E. coli*.

This is not the first *E. coli* model resolving the tide, but previous studies did not investigate the long-term effect of this forcing. Kashefipour et al. (2002) focus on single days, Garcia-Armisen et al. (2006) only study the concentration profile after a 28 days simulation with constant upstream discharge. On the other hand, we must admit that the current model is not fit for "point predictions" at a precise time and location. Still, the model has proven accurate in predicting

long-term median and range, making it a potentially interesting tool for long-term risk assessment studies. Indeed, for risk studies, understanding of the median behaviour is not sufficient; it is crucial to have some insight into the variability and the processes driving it.

Comparing the reference simulation to reduced model setups, a deeper understanding of the controlling processes was possible:

(1) The tide, the concentrations coming from upstream and the mortality process are the main factors causing the observed *E. coli* concentrations and variability.
(2) The tide is crucial to find correct median and range of concentrations. However, its effect is complex: it can either increase or decrease the local (median) concentrations (depending on the location of the closest sources) and increase or decrease the local variability.
(3) The impact of the WWTPs inside the model domain are minor, suggesting that investment in these WWTPs may not be the most efficient management action to improve the water quality in terms of fecal contamination. At the opposite, improving wastewater treatment in some WWTPs located upstream of the studied domain (especially in the Brussels area) would be important from a water quality point of view.

These results point towards a few directions for future developments:

(1) Model improvements:

a. A better model representation of the estuarine decrease in *E. coli* concentrations may be achieved by complexifying the *E. coli* module by including a direct link with sediment dynamics.

b. Include further variability in the forcings, especially the boundary concentrations. Including varying WWTP discharges does not seem relevant, due to the small impact of these sources. However, a more accurate representation of what enters from upstream could be achieved by extending the model to the more upstream (non-tidal) river sections, especially the Zenne section crossing Brussels, as this appears to be a major source of contamination.

(2) Additional data. Indeed, the above-mentioned model improvement are only possible if additional measurements are made/become available. But also for the validation of the model additional data are necessary. Visually it is clear that data (timeseries) are lacking in the estuary, but also in the riverine part additional monitoring stations would be useful. The model may be a useful guide to determine the optimal position and/or timing of future samples (e.g. de Brauwere et al., 2009).

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