Residence time, exposure time and connectivity in the Scheldt Estuary

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Abstract

Residence times and exposure times are computed for 13 boxes in the Scheldt Estuary, using the high resolution tracer transport model SLIM. The concepts are clearly defined and related to how they should be computed. First, the timescale values are compared with results published previously that were obtained with a simple box model, and an unexpected difference is revealed. This may suggest that a high resolution model is necessary, even for the computation of such integrated quantities as residence or exposure times. Secondly, the newly computed residence times are compared to the exposures times to illustrate their intrinsic differences. From this difference, it is possible to propose a *return coefficient*, expressing the fraction of the exposure time that is due to “returning water”, i.e. water which has already left the estuary at least once. Finally, the estuarine exposure times are decomposed into the different box exposure times, resulting in a *connectivity matrix*. This matrix expresses how much time is spent in each of the estuarine subdomains during the water parcels’ journey through the estuary.

Keywords: Residence time, exposure time, connectivity, return coefficient, Scheldt Estuary, water renewal.

1. Introduction

The fate of chemical and biological species in aquatic systems is determined by the combination of (passive) transport and species-specific transformations. The observed behaviour can vary significantly with small changes in these processes. A first order approach to assess the relative importance of different processes is to compare their characteristic timescales (see Monsen et al., 2002) and references therein for examples). However, this creates a new difficulty: which are the relevant timescales and how should they be computed?

In this study, we focus on two timescales for the transport processes: the *residence time* and the *exposure time*. Both express the time spent by a water parcel in some predefined area. They differ only slightly: while the residence time “recording” stops as soon as the water parcel hits one of the boundaries for the first time (Bolin and Rodhe, 1973; Delhez and Deleersnijder, 2006; Takeoka, 1984), the exposure time considers all subsequent re-entries in the domain (Delhez et al., 2004; Monsen et al., 2002). This seemingly minor distinction in definition may result in significantly different values when applied to tidal systems where the water leaves and returns several times.

The definition of these timescales suggests a Lagrangian formalism (Luther and Haitjema, 1998; Meyers and Luther, 2008; Monsen et al., 2002; Tartinville et al., 1997), in which water parcels are symbolised by discrete particles. In these methods the diffusive processes acting on these particles are represented by random walks (Allen, 1982; Nauman, 1981). However, the stochastic nature of the Lagrangian approach requires large numbers of particles to be released for the results to be relevant (Heemink, 1990; Spivakovskaya et al., 2007), which results in heavy computations if a reasonable spatial (and temporal) resolution is wanted. In this study, we use the alternaltive, forward Eulerian approach (Arega et al., 2008; Gourgue et al., 2007; Soetaert and Herman, 1995; Wang et al., 2004). The timescale properties are well-established for this formalism (Holzer and Hall, 2000; Delhez et al., 2004; Delhez, 2006). The disadvantage is that a different tracer simulation is required for each location and time for which the timescales are sought. Therefore, many simulations are necessary to estimate the timescales with a fine spatio-temporal resolution, often leading to unacceptable computation times. However, as in this study we focus on a limited number of estuarine compartments, the computation remains feasible. A very recent development consists of using an adjoint method to obtain the residence or exposure time at any time and location in the whole domain (Delhez et al., 2004; Delhez, 2006; Blaise et al., 2010). This approach significantly reduces the computational cost, but requires the model to be integrated backward in time, which is not standard in most models.

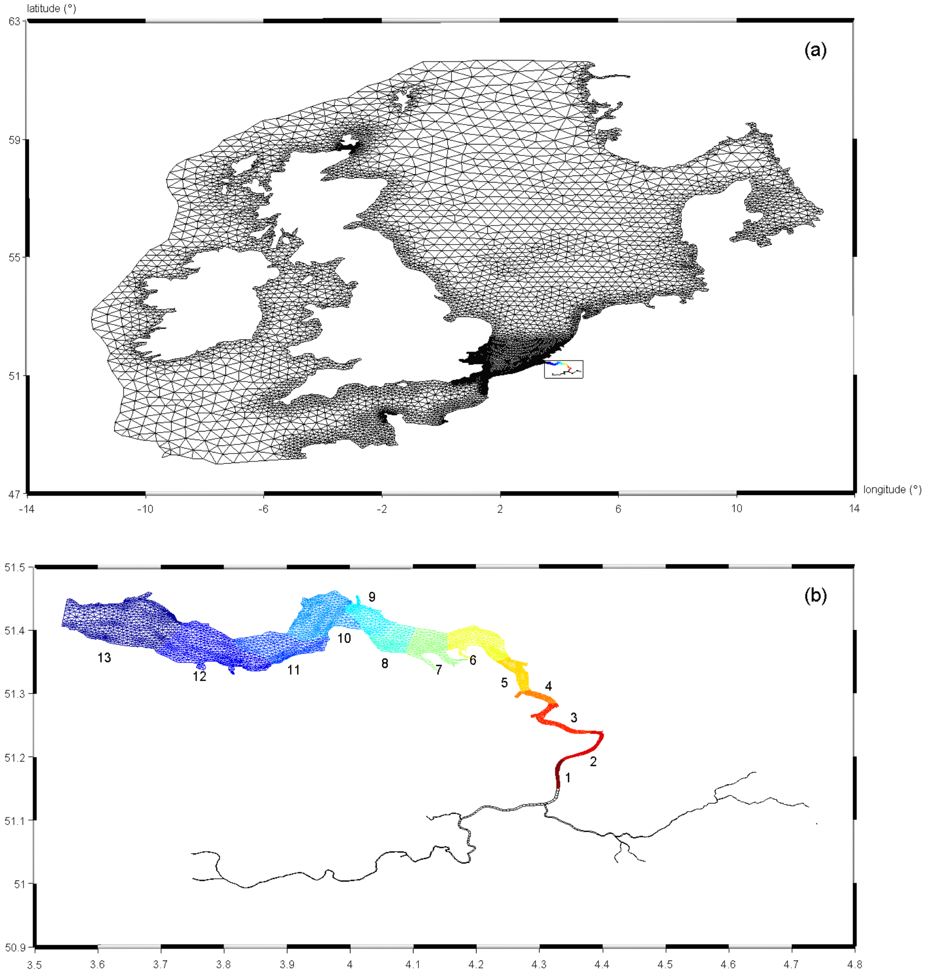

Figure 1: Computational domain and unstructured mesh used. Axes refer to latitude and longitude in degrees. (a) Whole computational domain (21000 triangles), showing the refined mesh along coasts and in the area of interest, the Scheldt Estuary (coloured part inside inset box). This domain is used for the hydrodynamics and the exposure time simulations. (b) Zoom of the computational domain, showing the Scheldt Estuary (2D) and the 1D-river network (inset box in panel a). The numbers and different colours indicate the different estuarine boxes, based on the compartimentalisation used by Soetaert and Herman (1995). For the residence time simulations, the tracers are only simulated in the coloured part.

The area of interest in this study is the Scheldt Estuary, located in Belgium and the Netherlands (Figure 1). The Scheldt River and its tributaries cross densely populated areas, which results in a highly polluted inflow in the estuary. In order to assess the impact this pollution can have, an estimate of the residence and exposure times of the estuarine water may be helpful. Previous studies in the Scheldt Estuary have already compared transport time estimates to bacterial growth rates (Goosen et al., 1995) pesticide fluxes (Steen et al., 2002), and phytoplankton growth rates (Carbonnel et al., 2009; Muylaert et al., 2005), but these studies use very rough estimates for the transport timescale. To the best of our knowledge, only one rigorous calculation of residence times in the Scheldt Estuary has been accomplished so far (Soetaert and Herman, 1995; from now on abbreviated as SH95). They developped a box model (or actually a 1D model with low spatial resolution) to simulate long-term reactive transport in the Scheldt Estuary and used this to compute the residence time for each of their 13 boxes.

The current study has three objectives:

1. Compute residence times in 13 boxes in the Scheldt Estuary with a high-resolution model and compare the results with the values found by SH95; this comparison serves to assess the added value (or not) of a high-resolution model for an integrated quantity such as box-averaged residence times.
2. Compute the exposure times in the 13 estuarine compartments with the same high-resolution model and compare them with the residence times. By comparing the two timescales, a measure may be derived of the proportion of the exposure time that is due to *returning water*.
3. Attempt to decompose the estuarine timescales into compartmental (sub-domain) timescales. By comparing these, a measure is proposed for the *connectivity* between subdomains, and is applied to the Scheldt Estuary.

Although this study focuses on the Scheldt Estuary, we attempted to make the description of the methods as general as possible, such that it may be of interest to a wider audience. Indeed, some effort was devoted to providing comprehensive definitions and descriptions of the concepts, including practical information on the computation of the different timescales.

2. Methods

2.1. Numerical model

The model used for the simulations in this study is the Second-generation Louvain-la-Neuve Ice-ocean Model (SLIM, www.climate.be/SLIM). SLIM is a finite-element model that solves the shallow-water and the tracer-transport equations. The model is able to solve such equations in an 1D framework (vertically for a water column or horizontally for a cross-section averaged river network), a 2D depth-integrated framework or in a full 3D framework (still under development). The spatial operators can be discretised by various finite-element schemes but the one used in this study is the Discontinuous Galerkin one with linear shape functions. This element proved to be especially efficient for flows highly dominated by advection processes (e.g. Kubatko et al., 2006; Bernard et al., 2007). The temporal derivative operator is discretized in this study with an implicit second order Runge-Kutta method. The corresponding non-linear system is solved by a Newton-Raphson method. Complete details about the numerical method are given in Comblen et al., 2010). The hydrodynamical part of the Scheldt model is fully described and validated in de Brye et al. (2010).

In this study we use a computational domain (see Figure 1) which is quasi-identical to that of de Brye et al. (2010) : although the focus is on the Scheldt Estuary (coloured in Figure 1), 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. This riverine part of the model is 1D in the longitudinal direction of the rivers, while the estuary and the downstream extension covering the whole North-Western European continental shelf are modelled by 2D, depth-averaged equations. The reasons why the computational domain was extended so drastically are threefold: (1) more accurate data are available for tidal forcing at the shelf break and at the upstream limits of the tidal influence; (2) inclusion of the shelf allows the simulation of meteorologic features such as storms; (3)

locating the open water boundary at a location that is distant from the area of interest allows for a better local setup of currents and, if the model is properly validated, removes any concerns on local fluxes into and out of the estuary of concern (e.g. Luettich and Westerink, 1995).

The colours and numbers in Figure 1b indicate the different subdomains that will be considered in this study. More details about the compartimentalisation is given in section 2.3.

Figure 1 also shows the unstructured mesh used, constructed by Gmsh (Geuzaine and Remacle, 2009; Lambrechts et al., 2008), which is made up of approximately 21000 triangles (in the 2D part) and 400 line segments (in the 1D part). This kind of mesh offers the advantage of its flexibility. Indeed, coastlines can be represented more accurately than with structured grids and, most importantly, the resolution can be adapted in space and time. In the current study a static mesh was used, but 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). The local mesh size was determined by the following rules (cf. de Brye et al., 2010):

- The resolution scales as $\sqrt{(gh)}$, in such a way that the grid size is proportional to the tidal wave velocity.
- The resolution is also increased near coasts.
- The mesh size is reduced in the area of interest, i.e. the Scheldt estuary and the Southern Bight of the North Sea (important for the hydrodynamics).
- The resolution is increased in function of the bathymetry gradient in the estuary.

The resulting local mesh refinement is the reason why it was feasible to extend the computational domain to the shelf break without increasing the number of triangles too much (7000 of the 21000 triangles are in the estuary, while the estuary comprises only 0.3% of the whole computational domain area), and thus keeping the computational cost reasonable. A comparable domain extension has been performed by a few previous studies (Arndt et al., 2007; Vanderborght et al., 2007). However both studies used a finite difference approach, and therefore they had to resort to nested grids for extending their domain in a computationally feasible way.

Full reference of the data sources used for the forcings (wind) and boundary conditions (water elevation at the shelf break and water discharges at the upstream ends and of the major rivers flowing in the North Sea: Seine, Rhine-Meuse and Thames) can be found in de Brye et al. (2010). However, note that in this study data for different years were used, namely the years 1983-1985, in order to be as comparable as possible to SH95, who computed their residence times for a winter and a summer situation in 1984. For 1984, we applied 10-days averaged water discharge values at the upstream boundaries, while de Brye et al. (2010) could use more recent daily values (all data from Hydrological Information Center, Flemish Government). In SH95 "[f]reshwater flows were allowed to change seasonally". In addition, in our simulations water enters the estuary by two canals at Terneuzen and Bath, and through the Antwerp Harbour locks. The discharge of these lateral inputs vary monthly, representing the average monthly values over the period 1990-2008 (period for which direct data are available, kindly provided by the Rijkswaterstaat Zeeland).

For the computation of the different renewal timescales, SLIM simulations of a passive tracer are used (section 2.2). The model's ability to simulate a passive tracer is validated by comparison to a number of salinity time series. The validation results are presented in detail in de Brye et al. (2010), but a summary thereof is also given in section 3.1.

2.2. Timescales for water transport

This study focuses on the concepts of residence time, exposure time and connectivity. In this section these concepts will be formally defined and it is explained how they were numerically computed. This is done is general terms, complemented by specific information about the Scheldt Estuary application.

2.2.1. Residence time

The *residence time* of a particle or water parcel is defined as the time it needs to leave the region of interest (for the first time). Therefore, for an unambiguous definition one needs to specify:

(a) the region of interest (Ω), i.e. the domain escaped by the water parcel. The residence time is the time until the water touches one of the (open) boundaries of this region *for the first time*. This implies that water which has left but later re-enters the region of interest is not considered. In the present study, the region of interest is the Scheldt Estuary. It has two open boundaries through which water can leave: one upstream (connection with the tidal river) and one downstream (mouth). Eventually all the estuarine water will leave through the mouth, but due to the tidal movements, some water is pushed through the upstream boundary during every tidal cycle.

(b) the initial time (t_o), when we “start to measure”. Only if the system is stationary, the residence time is constant in time, and does not depend on when we “start measuring” it. In this study we used the same initial times as SH95, namely 1 January 1984 (winter situation) and 1 June 1984 (summer situation). As the high-resolution model resolves the tide (taking time steps of 20 minutes), the initial time has to be defined in more detail than merely the date. In order to investigate the effect of the tide on the residence time, two initial times are considered for each season: one at high tide and one at low tide (approximate times for the whole estuary).

(c) the initial position or region where the water parcel is present at t_o. Obviously the residence time will vary in space, generally being smaller closer to the open boundaries of the region of interest. Sometimes only an integrated value is needed and the residence is calculated for the whole region of interest, i.e. the initial region equals the region of interest. In this study, 13 initial regions Ω_i ($i = 1, \ldots, 13$) are considered, dividing the Scheldt Estuary in approximately longitudinal boxes. These boxes are again similar to those used by SH95; more details on this topic are given in section 2.3.

The residence time can be computed using a numerical model which is able to simulate the transport of a passive tracer in the region of interest. The water present at t_o in subdomain Ω_i is then represented by a virtual passive tracer whose concentration C_i is initially 1 in Ω_i and 0 elsewhere (Gourgue et al., 2007). For a 2D depth-averaged model this results in:

$$\begin{cases} \dfrac{\partial}{\partial t}\left(HC_i\right)+\nabla\cdot\left(H\mathbf{u}C_i\right)=\nabla\cdot\left(H\kappa\nabla C_i\right) \\ C_i(t_0,\mathbf{x}\in\Omega_i)=1 \\ C_i(t_0,\mathbf{x}\in\Omega\setminus\Omega_i)=0 \end{cases}, \tag{1}$$

with H standing for water height, $\mathbf{u}$ the depth-averaged velocity vector and κ the diffusivity coefficient. The water entering the region of interest after t_o must be prescribed to contain no tracer, and once the tracer leaves through one of the open boundaries it is lost forever.

The residence time of water initially (at t_o) present in Ω_i equals (again assuming the use of a 2D depth-averaged model)

$$\Theta_i(t_0)=\frac{\int_{t_0}^{\infty}\int_{\Omega}H(t,\mathbf{x})C_i(t,\mathbf{x})d\mathbf{x}dt}{\int_{\Omega}H(t_0,\mathbf{x})C_i(t_0,\mathbf{x})d\mathbf{x}}, \tag{2}$$

with $\mathbf{x}$ referring to horizontal coordinates (x, y).

In practice, the residence time for water present in region Ω_i at t_o can be computed by simulating $C_i(t, \mathbf{x})$ (equation 1) and $H(t, \mathbf{x})$ for a “very long” time, i.e. until most tracer has left the region of interest Ω and hence the residence time estimate has converged. Afterwards, the integrals in (2) can be computed to find the residence time.

If, as in our case, the residence time should be computed for several (say n) initial subdomains Ω_i ($i = 1, \ldots, n$), n tracers should be simulated, each of which is initially only present in one of the subdomains (cf. (1) for $i = 1, \ldots, n$). Clearly, the more (initial) subdomains are considered, the more tracers must be simulated and the heavier the computation will become. If the spatial variability of the residence time is of real interest, this procedure is not efficient. To compute the residence time for any initial time and any initial location, one should resort to the adjoint method (Delhez et al., 2004, Blaise et al., 2010). An alternative to achieve a higher spatial coverage is to use a Lagrangian approach (e.g. Monsen et al., 2002) where particles are released at the initial time thoughout the domain and they are tracked until they leave the domain of interest. However, in order to be accurate, this kind of simulations should be performed with a number of particles which is high enough (Heemink, 1990; Spivakovskaya et al., 2007), making the task quite extensive again if one wants to achieve high spatial resolution with acceptable accuracy.

For the current study, the hydrodynamics (i.e. the depth-averaged horizontal velocities and water height) were simulated in advance on the whole domain including the shelf and rivers (see Figure 1a). Subsequently, for each initial time, a tracer simulation was run only in the Scheldt Estuary with 13 tracers, each of which has an initial concentration equal to one only in one of the subdomains.

2.2.2. Exposure time and return coefficient

An important conceptual drawback of the residence time as a timescale to measure water renewal is its incapacity to consider water parcels which re-enter the region of interest. This results in particularly unrealistic timescales in tidal systems where water parcels close to the boundaries will leave and re-enter the domain many times before escaping definitively. Therefore, computing the residence time will significantly underestimate the *total* time spent in the region of interest. The latter timescale is called *exposure time* (Monsen et al., 2002).

Exposure time and residence time are very similar concepts. Both require the definition of (a) a region of interest, (b) an initial time and (c) an initial region (see section 2.2.1). The numerical computation of exposure times is also very similar to the procedure outlined above for residence times. For each initial region for which exposure times should be computed, a different tracer is introduced, whose initial conditions are defined in (1). However, the numerical model should simulate the spatiotemporal evolution of the tracers in a region *larger* than the region of interest, at least covering the regions where the processes occur that make water parcels re-enter the estuary. Otherwise it is impossible to explicitly take into account returning water parcels. This means equation (2) still describes the exposure time, but the simulation is performed in domain larger than the region of interest. For the computation of the exposure times in the Scheldt Estuary, the computational domain is extended both upstream and downstream (Figure 1a), resulting in the same computational domain as used for the hydrodynamics.

Whether residence times or exposure times are the more relevant timescales to express how long a water parcel stays in a certain region can be debated. Delhez et al. (2004) discussed the two concepts in detail, including their applicability. In short, it appears that the strict residence time is more relevant if the domain of interest is clearly distinct from the exterior, i.e. if the open boundaries correspond to a steep physical/chemical/biological gradient. If, on the other hand, the boundaries are rather artificial or arbitrary, the exposure time approach can be preferable. Which timescale to use also depends on the application under study. If the studied species undergo significant changes when leaving the domain of interest (e.g. related to the changing conditions), the strict residence time is appropriate. The exposure time should be used if the aim is to assess the time during which a pollutant can affect the domain of interest, because in this case the full extent of the pollution event includes subsequent returns.

In any case, computing both residence and exposure times for a given setup, offers the possibility to compare both measures. From the difference between exposure time and residence time, some information can be gained about the contribution of returning water to the exposure time. Indeed, the residence time being equal to the exposure time implies that any water parcel leaving the domain of interest never returns to it.

We will compute the following *return coefficient* representing the relative difference between exposure time (E) and residence time (R):

$$r = \frac{E - R}{E}\,. \tag{3}$$

With this definition, r is comprised between 0 and 1. If no water returns, $E = R$, implying that $r = 0$. The other limit ($r = 1$) is reached when $R << E$, i.e. when water quickly leaves the domain of interest but stays for a very long time in the domain after re-entering (or re-entering many times). The intermediate situation when $E = 2R$ gives $r = 0.5$, meaning that half of the exposure time is due to "returning water", which has already left the domain of interest at least once.

This return coefficient is similar to the definition proposed by Arega et al. (2008) in their study of East Scott Creek Estuary (USA). In their derivation they nicely show the relation with the "return flow factor" used to refine simple tidal prism models, and defined as "the fraction of water leaving during ebb that returns during flood" (Sanford et al., 1992; Luketina, 1998). This factor can only be estimated accurately by taking into account the flow outside the basin of interest (cf. the exposure time). Sanford et al. (1992) proposed a physically based method; alternatively, empirical regression relations with lateral diffusion outside the embayment have been proposed (Abdelrhman, 2007). MacDonald, 2006) defined a complementary "exchange ratio" as the "volumetric ratio which represents the fraction of incoming flood water that is replaced for ambient estuarine water prior to exiting on the ebb". All these factors express the relative importance of returning waters, and do this in terms of volumes, while our return coefficient is defined in terms of times. However, both viewpoints can easily be shown to be equivalent at least in the case of a well mixed domain (e.g. see derivation by Arega et al. (2008)).

The above-mentioned return flow factor and exchange ratio were introduced to improve simple models used to estimate residence times. Our return coefficient could also be used to transform the residence time into an exposure time. However, from the above references it is clear that an independent estimation of the amount of returning water is not straightforward, and for our return coefficient probably the same information is needed than for an exposure time calculation. Therefore, we view the return coefficient more as an alternative way to present the information available if both residence and exposure time are computed. As it summarises the importance inside the estuary of water which has already left the estuary at least once, it could be used to roughly assess the impact of a waterborne contaminant or biological species which is altered when it leaves the estuary. This information cannot be obtained by individual inspection of the residence time or exposure time.

2.2.3. Connectivity

So far, the discussed timescales (residence and exposure time) express how much time a water parcel spends in a single region of interest. These timescales can be computed for different initial regions, the usual and natural procedure being to subdivide the region of interest in a number of initial subdomains. In this case, an additional time diagnostic is a measure of how long a water parcel initially present in subdomain i spends in each of the subdomains $j \in \{1, ..., n\}$. This measure would then allow to identify special "connections" between subdomains: without having to look into the complex circulation and transport patterns, one can have a rough picture of where the water parcels released at different places spend most of the time on their journey out of the domain of interest.

In analogy with the definition of the residence time for the whole domain of interest (1)-(2), a "subdomain exposure time" $\Theta_{i,j}(t_0)$ can be defined as

$$\Theta_{i,j}(t_0) = \frac{\int_{t_0}^{\infty}\int_{\Omega_j} H(t,\mathbf{x}) C_i(t,\mathbf{x}) d\mathbf{x} dt}{\int_{\Omega_i} H(t_0,\mathbf{x}) d\mathbf{x}}, \tag{4}$$

or the time spent in subdomain *j* by water initially in subdomain *i*. As the water is allowed to leave and re-enter the subdomains, we are indeed dealing with exposure times. However, to be fully consistent with the exposure time definition, it is also necessary to perform the tracer simulations on a computational domain larger than the domain of interest (in practice the simulation performed for the estuarine exposure time can provide all needed values). This implies that $\Theta_{i,j}(t_0)$ actually represents a "subdomain *exposure time*", i.e. including all stays in the subdomain. For the special case *i=j*, $\Theta_{i,i}(t_0)$ is the exposure time of box *i*, i.e. the total time spent in the initial box *i*.

The following dimensionless quantity can be proposed

$$d_{i,j} = \frac{\Theta_{i,j}(t_0)}{\Theta_i(t_0)} = \frac{\Theta_{i,j}(t_0)}{\sum_{j=1}^{n} \Theta_{i,j}(t_0)} \tag{5}$$

to express the ratio between the time spent in subdomain Ω_j and the total time spent in the domain of interest Ω by particles initially present in subdomain Ω_i. It is easily seen that $\sum_{j=1}^{n} d_{i,j} = 1$ and , such that a $d_{i,j}$ value close to 1 means that the relative time that particles from Ω_i spend in Ω_j is long, i.e. of the total time these particles spend in the domain of interest, they are mostly in Ω_j. The $d_{i,j}$'s form a matrix which we call *connectivity matrix*. Indeed, this matrix visualises how different subregions of the domain of interest are connected to eachother. For instance, row *i* can be used to identify which areas of the domain will be mostly affected by a pollution source in subdomain *i*. Knowledge of special connections between "original subdomains" and "exposed subdomains" may be useful for management purposes. For instance, it is inefficient to protect or clean an area which is clearly connected to an original subdomain whose problems are not solved.

This connectivity matrix concept is loosely inspired by the *dependency matrix* proposed by Braunschweig et al., 2003, which expresses the integrated influence from one box to another during a predefined period, e.g. 30 days. The term and concept of *connectivity* is rarely used in physical studies (Condie and Andrewartha, 2008), but it is common in ecological studies, where it refers to the very similar issue of spatial connections between habitats (e.g. Fahrig and Merriam, 1985; Condie and Andrewartha, 2008; Munday et al., 2009; Wolanski et al., 1997).

2.3. Compartimentalisation

To facilitate comparison, it was decided to use the same 13 estuarine compartments as SH95 to compute the residence times. The boxes were defined such that they could be "supposed to be more or less homogeneous with respect to the modelled processes. One of the restrictions on the number of compartments is that they should be sufficiently large such as to allow a reasonably large time step, however without the risk of an untolerably large numerical dispersion" (p.9 in Soetaert et al., 1992). The compartimentalisation had been defined for an earlier model (SAWES, 1991), and has been used several times since then (e.g. Goosen et al., 1995; Van Damme et al., 1999).

As the model in SH95 was developed for ecological modelling, the timescales of interest are seasons or even years. Therefore, SH95 were not interested in variations within a tidal cycle and transposed “the transport equation to a new reference frame, which oscillates with the tide” (Soetaert et al., 1992) to allow the use of a simplified transport equation in which the tidal effect is filtered out. This procedure implies that the compartments are not fixed in space but also “oscillate with the tide”. As a consequence, it is not straightforward to use *exactly* the same compartments in this study; instead we used fixed compartments corresponding to the SH95 compartments at mid-tide. Furthermore, the first, most upstream compartment in our setup is smaller than in SH95, because the upstream boundary of our 2D estuary model lies slightly more downstream.

3. Results and discussion

3.1. Salinity validation

Timescales like residence and exposure time are difficult (if possible at all) to measure *in situ*, because this would require a tracer release (e.g. dye) experiment which is monitored at numerous locations across the estuary for weeks to months (in the Scheldt Estuary). Therefore, timescales estimated from computer simulations are very difficult to validate directly (Deleersnijder and Delhez, 2007). This does not mean that the model results are completely unvalidated. The general practice is to validate the model by comparing with observed tracers (usually salinity), and assume that this also validates computed timescales, as these are simulated by an identical transport (Deleersnijder and Delhez, 2007). As mentioned in section 2.1, the hydrodynamics and salinity fields simulated by SLIM are validated against available measurements – and so did SH95 for their model. We will briefly summarize the salinity validation results for SLIM in this section, because these results are a primary confirmation of the quality of the timescales shown below.

More precisely, the salinity simulation allowed us to calibrate the tracer diffusivity. As the mesh size varies greatly over the computational domain, it is essential to have a horizontal diffusivity varying with the mesh size. This is an issue for any multi-scale model. In this study the diffusivity coefficient κ depends on the mesh size Δ according to a relation inspired by Okubo, 1971): $\kappa = \beta \, \Delta^{1.15}$. The proportionality factor β is calibrated in order to best fit the 2008 salinity observations in the Scheldt Estuary (Figure 3). Its value was set to 0.022606.

The salinity simulation is performed for the year 2008, because a best coverage of measurements was available for this year. Freshwater (i.e. salinity = 0) enters the model domain at the upstream boundaries of the fresh tidal river network. The Ghent-Terneuzen and the Bath canals also bring freshwater in the estuary as well as the Antwerp Harbour locks (see Figure 2). In the North West European Continental Shelf, freshwater is introduced by the Seine, the Thames, the Meuse and the Rhine Rivers. Precipitation and evaporation are not taken into account but the salinity outside of the Southern Bight is relaxed towards monthly climatological data (Berx and Hughes, 2009).

The output of the model, i.e the depth-averaged salinty, is compared with salinity timeseries measured at two different depths (if both sensors were operational) and three different stations across the estuary (Hoofdplaat, Overloop van Hansweert and Baalhoek, cf. Figure 2). Data were provided by the Hydrologish Meteorologisch Centrum Zeeland (www.hmcz.nl).

There is a good agreement between the model and the observations: the rms errors between modelled and measured salinity in 2008 range between 0.8 and 1.6, while the relative errors lie between 3.8% and 10.7% (cf. Figure 3 for a zoom on September 2008). It is on these observations (i.e. at the three estuarine stations) that the diffusivity is calibrated, which is also used for the timescale simulations below. The remaining differences are attributed to salinity boundary condition imperfections (e.g. constant discharge of Canal Ghent-Terneuzen, imperfect salinity simulation outside the estuary), i.e. problems specific to the salinity simulation and which should not reduce the confidence in the diffusivity calibration (or in the timescale computations).

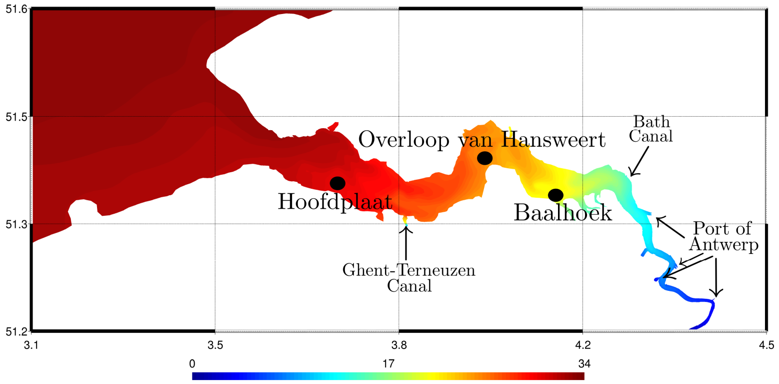

Figure 2: Location of the salinity observation time-series (dots). The points where freshwater enters the estuary are indicated by arrows. The colours represent a snapshot of the salinity field computed by SLIM (2008/09/01 00:00).

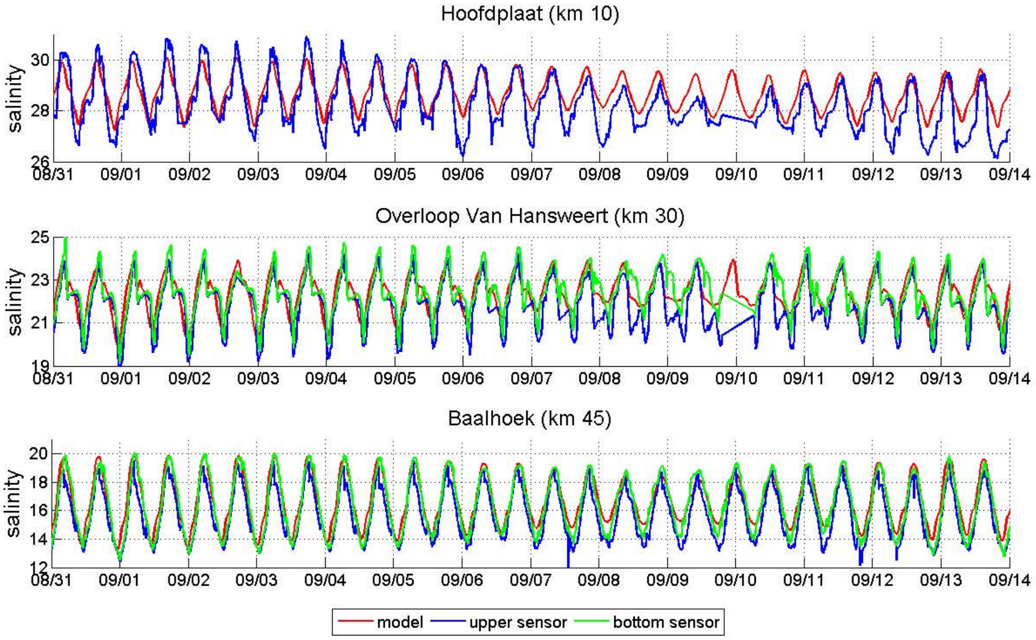

Figure 3: Modelled salinity compared to measured timeseries at the three stations (location shown in Figure 2) for approximately two weeks in September 2008 (the whole year was simulated). Measurements are generally made by two sensors, one being approximately 1 m below the water surface and one at 1 m above the bottom. At Hoofdplaat the bottom sensor is not working and some occasional errors may occur in the other recordings.

3.2. Residence time

The first objective was to compute the residence time with a high-resolution 2D transport model and compare the results to those reported in SH95. To facilitate the comparison, the "high-resolution" residence times were computed for the same boxes as used by SH95 (section 2.3), and for the same initial dates: 1 January 1984 and 1 June 1984.

Figure 4 shows the residence times (in blue) found in this study and those from SH95 (in red). Both series were computed by simulating 13 tracers each initialised in one of the 13 boxes, as explained in section 2.2.1. In our case, the simulations were run for at least 10 months to ensure that most of the tracers left the estuary; in practice less than 0.5% of the initial tracer is still in the domain at the end of the simulation.

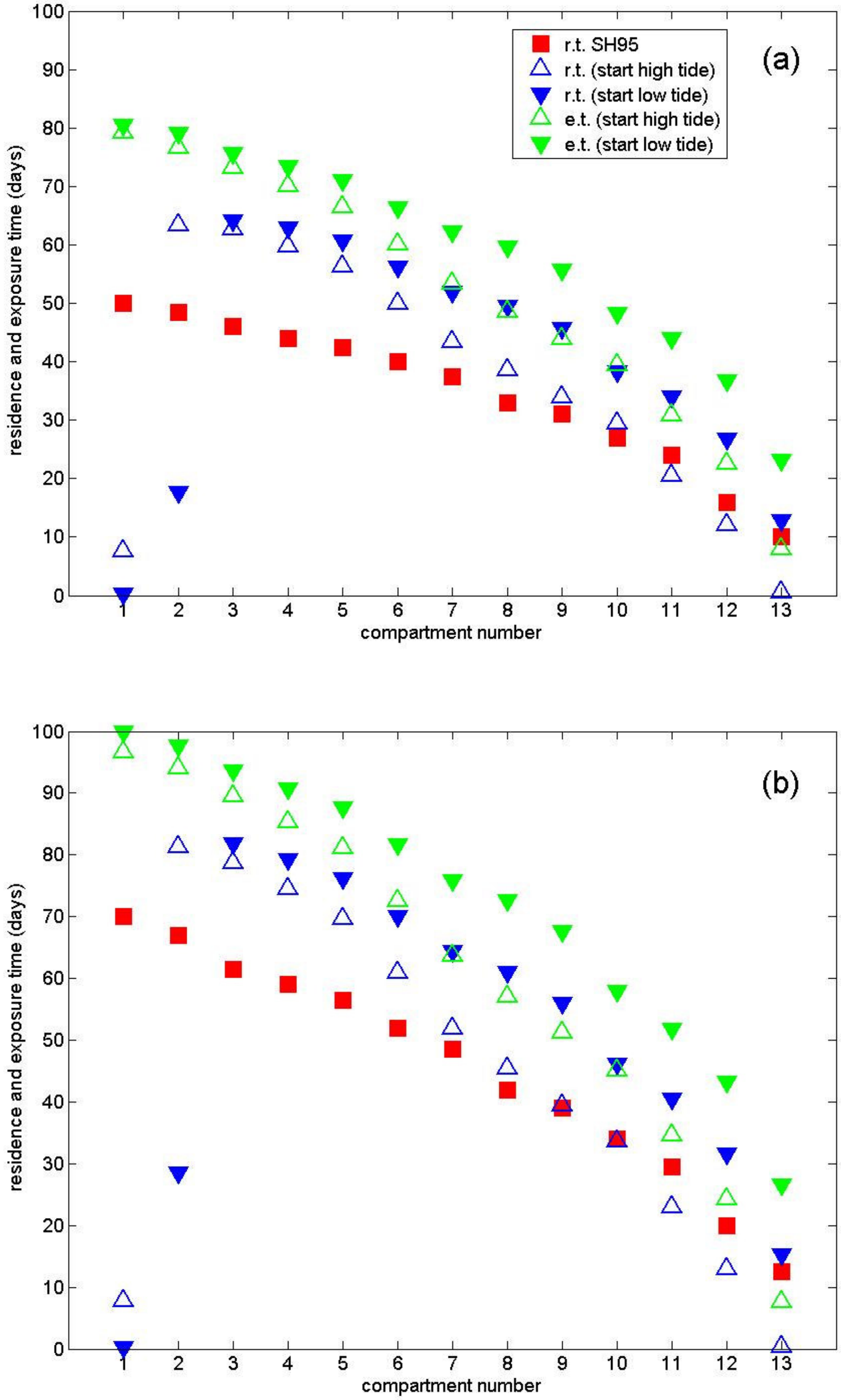

Figure 4: Comparison of different timescales. r.t. stands for "residence time", while e.t. refers to "exposure time". (a) Winter situation (starting 1 January 1984); (b) summer situation (starting 1 June 1984).

First, let us note that the winter (Figure 4a) and summer (Figure 4b) situations display very similar patterns. The residence times computed by SH95 exhibit the expected pattern, i.e.

monotonically decreasing towards the mouth. The residence times found in our study reveal a similar trend, but decreasing towards *both* open boundaries of the domain, i.e. the mouth *and* the upstream end of the estuary. This behaviour directly follows from the definition of the residence time which only considers water parcels present in the area of interest until they leave for the first time. As the model used in our study considers the tidal motion, water parcels close to either of the boundaries will quickly leave the domain, although they would actually re-enter at the next tidal cycle, but this is not taken into account by the strict application of the residence time definition (Delhez and Deleersnijder, 2006). The reason why SH95 did not find residence times decreasing towards the upstream end, is that their box model only considers the residual motion, and therefore tracer cannot leave through the upstream boundary. Also at the downstream end, their value should be more representative because the tracer will only leave the estuary at the rate of the residual current, instead of being "flushed out" at each low tide. In this respect, the SH95 residence time is related to our exposure time.

If we now neglect the boundary boxes, the second striking observation in Figure 4 is that the new residence times are significantly higher than the SH95 estimates, both for the winter and summer situations. The difference appears to increase with the distance to the mouth. The presence of such a significant discrepancy is unexpected, because the simulation setups and residence time computations of both studies are so similar (same initial time, same domain of interest, same initial boxes, same residence time definition). In addition, both models are calibrated in order to reproduce salinity well, which is usually regarded as a sufficient validation for tracer simulations. It cannot completely be ruled out that some differences still exist between the forcings used (cf. section 3.4). However, the major remaining difference lies in the very different model complexities and associated resolution. However, the box-averaged residence times consider timescales of several days to months; therefore, one tends to expect that resolving finer-scale processes both in space (2D model vs. box model) and time (tidal dynamics vs. multiple-day timesteps) is unnecessary. Unfortunately, no independent estimates for the box-averaged residence times in the Scheldt Estuary exist, as a result it is not possible to validate either of the model results directly.

Explaining to the full extent this difference goes beyond the scope of this study, but we will attempt a preliminary justification. First of all, we are inclined to put more confidence in the complex model, because it considers more processes and scales, one of which may be important for the residence time calculation. This important process must be significant for the residence time estimation, while it must have a negligible impact on the simulated (average) salinity distribution, as both model can represent this accurately. Both tracer simulations consider passive tracers, but they differ in that (average) salinity is in quasi-steady-state while the residence time is estimated using a transient tracer simulation. We thus hypothesize that although a tidally-averaged box model can represent steady-state quantities accurately, this may not be the case for transient tracers, even if their overall timescales are much larger than the model timestep. Regnier et al., 1998) already showed that low-frequency tidal compounds (spring-neap cycle and its monthly modulation) "result in nonnegligible fluctuations in the residual flow field". For instance, "[i]f a low river flow coincides with a spring tide, the residual flow is directed toward the land (…) within a significant proportion of the estuary. This situation may last for several days and results in a longer flushing time". These effects are neglected in a tidally-averaged box model. England and Maier-Reimer, 2001) also noted that (for global circulation models) transient tracer experiments provide substantially more information about water circulation en ventilation than temperature-salinity. In addition, one may imagine that the lateral water motions may have the effect to increase the residence times, because some areas will be associated with significantly lower flow rates effectively "trapping" the tracer. Although this explanation must certainly be substantiated by additional tests, these results could thus suggest that for the simulation of residence times (even box-averaged), a high-resolution model makes sense, because these quantities are estimated using transient simulations. For quantities that can be assumed to be stationary, such as salinity and average fate of nutrients, 1D or box models would still be relevant.

Final observation from Figure 4 the residence time is clearly time-dependent. As already noted by SH95 and Steen et al., 2002) (studying flushing times in the Scheldt), there is a strong dependence on the upstream discharge. This is primarily reflected by the long-term (seasonal and interannual) variations in residence time. Summer residence times are generally longer than in winter (compare Figure 4a and b), because the upstream discharges decrease during the summer months. Residence times also differ between years: e.g. 2001 was a particularly wet year with extreme river discharges and this results in significantly shorter residence times (Blaise et al., 2010). A second, less obvious, factor influencing the residence time in time is the tide. Indeed, Figure 4 illustrates that at low tide the residence time close to the mouth is longer than at high tide. This can be explained because in the first case the water will be pushed further in the estuary during the coming rising water, this way increasing the residence time. One would expect the difference between residence times starting at high and low tide to be of the order of the tidal period, which would be rather insignificant, but the difference is much larger. The residence time starting at low tide may be more than 10 days higher than the residence time at the same location but starting at high tide. According to Figure 4, this effect of the initial time on the residence time generally decreases with the distance to the mouth, but becoming significant again for the boxes close to the upstream end. However, an in-depth understanding of the exact relation between the residence time and the tide is asking too much from the box averages computed here. An adjoint approach providing the residence time at any point in space at any moment in time is more relevant for such an investigation, some first results on the Scheldt Estuary are reported in Blaise et al. (2010).

3.3. Exposure time and return coefficient

In a tidal system, the exposure time may be a more informative measure of the time spent in a domain, because it allows water parcels (or tracer) to leave and return to the domain of interest. Therefore, the second objective of this study was to compute the exposure time, compare it to the residence time, and from this comparison derive some measure quantifying the amount of returning water – these points will be discussed in this section.

In Figure 4 (in green) the estimated exposure times are shown for the 13 Scheldt boxes. These values are different from the residence times in two respects. First, the exposure times at the open boundaries are more in line with the "common sense": the values are not artificially small anymore, because the water leaving is allowed to re-enter at the next tidal cycle. This also results in a more realistic monotonic pattern (as SH95), with the highest exposure times for the upstream boxes.

Second (expected) difference is that the exposure time is always larger than the residence time – as it should from the definitions. The difference between the two timescales is approximately constant (10 days, except for the most upstream boxes), expressing that the difference is mainly due to the incorporation of the subsequent re-entries once the water has arrived close to the mouth.

The exposure times are also computed at high and low tide, and the differences observed between these two initial times are in line with the observations made for the residence times: the difference decreases with the distance to the mouth, and are significantly longer than the tidal period.

From the difference between the residence and exposure times a measure can be computed expressing the proportion of "returning water" (equation 3). In Figure 5 the return coefficients, associated to the results in Figure 4a, are shown. It is seen that the fraction of returning water is highest close to the open boundaries, as expected. In box 1, at the upstream end, the proportion of returned water is approximately 1, as expected, because all water present in this box leaves at least once through the upstream end but always returns. At the downstream end, the return coefficient varies between 45% and 93% (winter situation, but summer situation gives virtually identical results (not shown)), with the highest values found at high tide. At that moment, indeed, the water will be pushed out of the estuary soon, resulting in a lower residence time (Figure 4) and consequently a higher return coefficient.

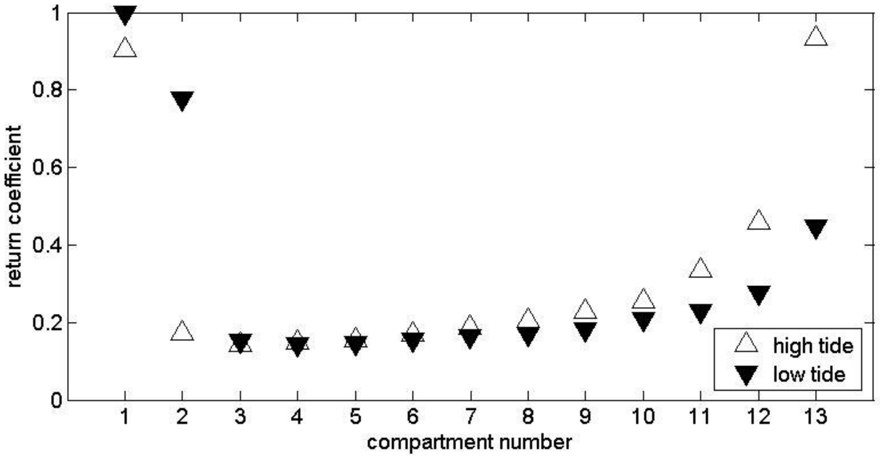

Figure 5: Return coefficients for the winter situation (starting 1 January 1984); results for the summer situation are very similar.

3.4. Effect of lateral inflow in the estuary

As underlined above, we tried to perform the timescale simulations as comparable as possible to SH95. In SH95 it is not mentioned whether they consider lateral inflow of water in the estuary, by for instance the canals entering the estuary at Terneuzen and Bath, and through the harbour locks (see Figure 2). In fact, it seems that their formulation uses a constant discharge through the whole estuary, which would be incompatible with lateral inflows. As our simulations do take these inflows into account, we performed an additional simulation without them to assess their potential impact on the timescale estimates. The sum of the discharges of these lateral inputs is on average 40% of the freshwater flowing in the estuary through the upstream end near Antwerp, which suggests that the impact may be significant.

Figure 6 shows the results of this comparison. Surprisingly, the effect of adding or removing these lateral inputs is minor (maximum 3 days). Although this result may seem counter-intuitive, it has already been observed previously that adding lateral inflow can even *increase* the overall residence time (Tartinville et al., 1997; Deleersnijder, 2003). Finally, and most importantly, the fact that SH95 (probably) did not include these lateral inputs into the Scheldt Estuary cannot explain the discrepancy observed in Figure 4.

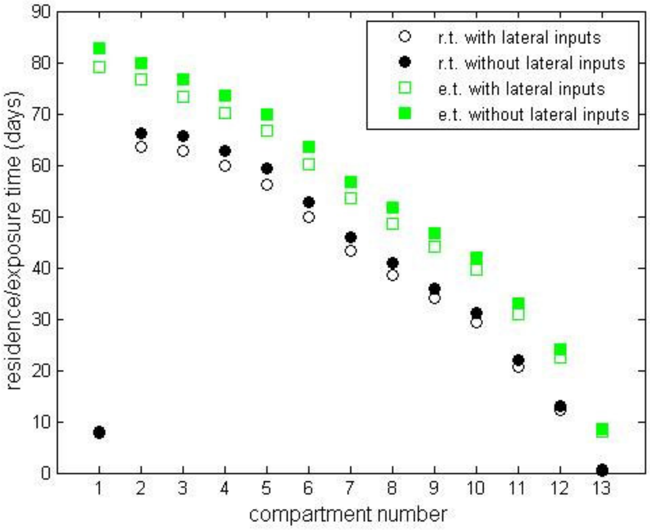

Figure 6: Comparison of timescales computed with and without lateral inputs of water in the estuary. Simulations start 1 January 1984 at high tide.

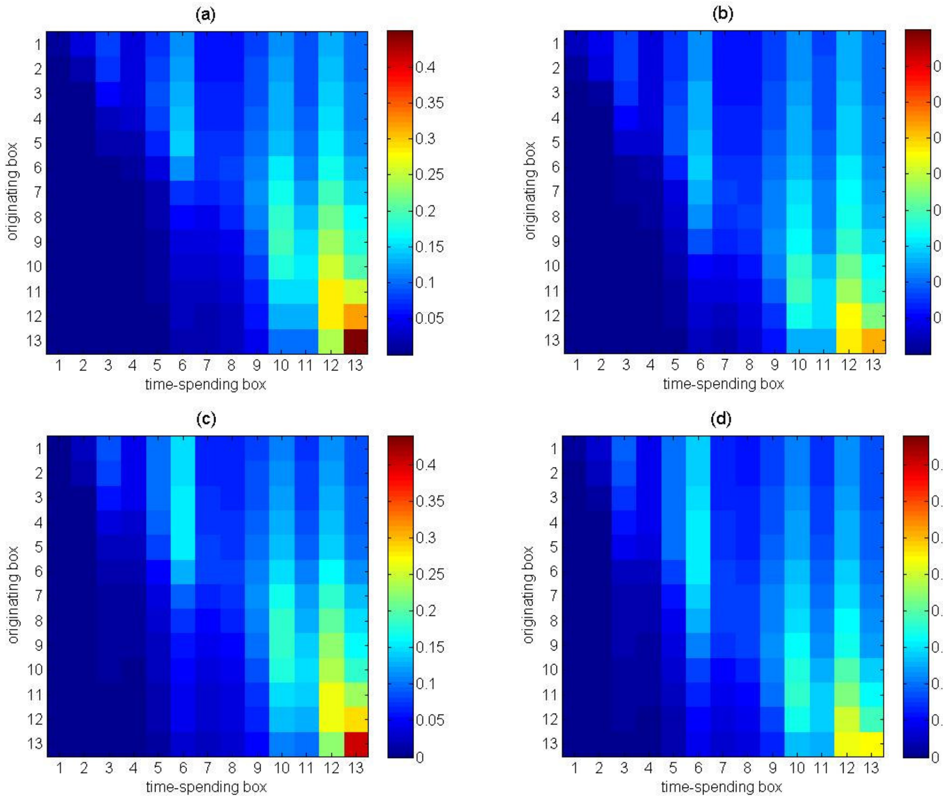

Figure 7: Connectivity matrices as defined in equations (4)-(5), representing the relative time spent in box 1, ..., 13 by water initially in box 1, ..., 13. Initial times: (a) 1 January 1984 at high tide; (b) 1 January 1984 at low tide; (c) 1 June 1984 at high tide; (d) 1 June 1984 at low tide.

3.5. Connectivity

The final results shown concern the "connectivity" matrix proposed in section 2.2.3. In Figure 7 the matrices are visualised for the four initial times considered in this study (1 January 1984 and 1 June 1984, at high and low tide).

First, there is clearly little difference between the different matrixes, so we will focus on the general, common patterns. Recalling that the connectivity matrix expresses the proportion of the estuarine exposure time spent in each of the subboxes, one can see that water spends relatively more time in some boxes than others during its journey out of the estuary. Water spends generally most of its time in compartments downstream of its original box (lower left part of matrix is close to zero), which is naturally expected. Water originally in boxes 1-7, spend relatively more time in boxes 6, 10 and 12. For the more downstream boxes only boxes 10 and 12 appear to be preferential. In summer the preference for box 6 is slightly more pronounced. The longer times spent in box 6 can be explained partly by the fact that this compartment is larger than the surrounding ones. Its volume is almost twice the volume of box 5 and 1.5 times the volume of box 7. The relatively long exposure time in box 12 is more remarkable, because for water initialised in boxes 1-7 it is even longer than the time spent in the last box. This would suggest that the repeated returns close to the mouth are not so important. The connectivity matrix (Figure 7) also shows that water initially in box 13 spends less than half of its total time in the estuary in this box, i.e. most of the time this water is in more upstream boxes (~25% of the time in box 12). This suggests that water in box 13 is more "connected" to upstream boxes than to the sea.

The above discussion illustrates how the connectivity matrix can be used to interpret spatial exposure time variations. Although a few preferential boxes appear in the Scheldt Estuary, they seem independent of the box of origin. In other words, no special connection was observed between individual boxes. It is difficult to infer this kind of information directly from flow patterns. We computed the Eulerian and Lagrangian residual transport (unpublished results and de Brye et al., 2010), but these diagnostics for long-term transport are very difficult to interpret (especially inside the estuary) and therefore do not provide much information to understand/predict local variations in exposure time. In fact, it is well known that velocities and associated quantities are difficult to interpret because of their “noisy” nature. This is exactly why tracers are used to trace the overall circulation patterns and timescales (e.g. England and Maier-Reimer, 2001).

4. Summary and conclusions

Timescales for water renewal are very useful tools for interpreting observations (Lucas et al., 2009; Monsen et al., 2002). However, it is not always clear which timescales should be used. The importance of clearly defining the transport timescales used has been emphasized in the past (e.g. Bolin and Rodhe, 1973; Monsen et al., 2002). Furthermore, numerous methods have been proposed and applied to estimate these different timescales, ranging from very simplistic formula to the application of numerical models delivering high-resolution timescales both in time and space (Guo and Lordi, 2000; Luketina, 1998; Sheldon and Alber, 2002, 2006; Blaise et al., 2010). In this study, we computed box-averaged residence times and exposure times using a high-resolution model, including the effect of the tide.

The main conclusions of the study are in accordance with the objectives:

(1a) When comparing our results for the residence times and the exposure times to the values reported by SH95, a significant difference was revealed. Indeed, our exposure time values exceed the ones of SH95 by 40 - 80%. This difference was rather unexpected because we performed the timescale computation for the same compartments, the same time period and with the same equations for the residence/exposure time. Moreover, both models were calibrated and validated against salinity measurements. The only difference resides in the different model complexities (and associated spatiotemporal resolution): a 13-box model versus a tidal model with ~21000 grid cells (of which 7000 are in the estuary of interest). However, it is generally accepted that coarse models (both in time and space) can be used for long-term, spatially averaged processes (e.g. Hofmann et al., 2008) defending the use of such simple models for the Scheldt), and hence should be applicable to compute the box-averaged timescales in the Scheldt Estuary. From the current results, this paradigm might have to be reconsidered. It appears that a clear distinction should be made between quasi-stationary quantities (e.g. salinity) and quantities with a transient nature (like a tracer released instantaneously). This being said, simple models certainly remain useful, e.g. due to the easier interpretation of their output they can help understand the essential features in the results produced by complex models (e.g. Deleersnijder et al., 1997; Mouchet and Deleersnijder, 2008).

(1b) It was also shown that the initial time for which the timescales are computed can have an unsuspected impact on the water renewal timescale. This was already noted for the seasonal influence by SH95 (higher residence times in summer due to lower river discharges). We have now shown that even a small difference of only 6 hours (high tide versus low tide) can result in significantly different residence/exposure times of up to 15 days (for the downstream boxes).

(2) The presented residence times and exposure times also illustrated the expected differences between them. First, the residence time decreases towards both the upstream and downstream boundaries, while the exposure times decrease monotonically only towards the mouth. Secondly, the exposure time is higher than the residence time. From this difference, a measure can be derived expressing the amount of returning water. This return coefficient was computed for the 13 boxes in the Scheldt Estuary, showing a sharp increase of the returning water for the

downstream boxes. Also, a large difference between high and low tide was clearly visible for the boxes closest to the boundaries.

(3) By relating "local" exposure times (within boxes) to the "global" estuarine exposure time for water originating from each box, a connectivity matrix can be constructed which expresses how much time is spent in each of the individual boxes. This metric can be used to identify preferential connections between parts of the domain. For the Scheldt Estuary, the boxes do not appear to have special individual connections. This is a consequence of their longitudinal positioning forcing the overall circulation to pass through all of the boxes. A more complex pattern might have arisen with a different compartimentalisation. Nevertheless, a few boxes appear to be associated with longer relative exposure times, independent of the origin of the water.

These results illustrate the information richness hidden in relatively simple timescales for water renewal. The concepts of residence time and exposure time are far from new, but the novelty of this study lies in their rigorous application to the Scheldt Estuary and the computation of related metrics like return coefficient and connectivity matrix. This revealed some interesting patterns which were interpreted in terms of the local hydrodynamics. The next step will be to use the computed values to interpret ecological and environmental observations – indeed we hope that these improved estimates will be useful for the numerous scientists studying the Scheldt.

A first attempt has been made to justify the difference with the SH95 model results, suggesting the added value of a high-resolution model even for the computation of long-term processes, if these have a transient nature. Yet, this issue certainly merits more attention and we hope it will be the subject of a future, more detailed, study.

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