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An assessment of transport timescales and return coefficient in adjacent tropical estuariesFERNANDO P. ANDUTTA^{a,b*}, FERNANDA HELFER^a, LUIZ BRUNER DE MIRANDA^b, ERICDELEERSNIJDER^{c,d}, CHRISTOPHER THOMAS^e, CHARLES LEMCKERT^a^a Griffith School of Engineering, Griffith University, Gold Coast, QLD 4222, Australia.^b Oceanographic Institute, University of São Paulo, São Paulo SP, Brazil, CEP 05508-900, Brazil.^c Université catholique de Louvain (UCL), Institute of Mechanics, Materials and Civil Engineering (IMMC) & Earth and Life Institute (ELI), 4 Avenue Georges Lemaître, Bte L4.05.02, B-1348 Louvain-la-Neuve, Belgium^d Delft University of Technology, Delft Institute of Applied Mathematics (DIAM), Mekelweg 4, 2628CD Delft, The Netherlands^e Université catholique de Louvain (UCL), Institute of Mechanics, Materials and Civil Engineering (IMMC), 4 Avenue Georges Lemaître, Bte L4.05.02, B-1348 Louvain-la-Neuve, Belgium.**Abstract –**

Transport timescales (TTS), namely residence time and exposure time, were computed for adjacent shallow meso-tidal tropical estuarines system using the Lagrangian model D-Waq Part coupled with the hydrodynamic model Delft3D-Flow, and the Constituent-oriented Age and Residence time Theory, CART. The main results are threefold: **(a)** The TTS differs more between releases at high or low tide than between those at spring and neap tides. The exposure time was also calculated and found to be larger than the residence time by a few days. **(b)** The exposure and residence times were used to evaluate the return coefficient (r) for different scenarios. As with residence and exposure times, the return coefficient was found to differ more between releases at high or low tide than between those at spring and neap tides. **(c)** For the Caravelas Estuary, where the river inflow was low ($\sim 4 \text{ m}^3 \text{ s}^{-1}$), the residence time was found to be much larger than for the Peruípe Estuary, where the river discharge was greater and nearly constant during the sampling period ($\sim 20 \text{ m}^3 \text{ s}^{-1}$). These results shows the importance of advection in decreasing TTS in the Peruípe Estuary compared to the Caravelas Estuary. The influence of the advection and dispersion agrees with previous simple estimates obtained using the newly modified Land Ocean Interaction Coastal Zone (LOICZ) model by Andutta et al. (2014).

Keywords: tropical estuary; residence time; exposure time; return coefficient; numerical model; hydrodynamics.

1. Introduction

Since the dynamics of most estuarine systems is relatively complex, studies of transport timescales (TTS) provide valuable insight into estuarine behaviour. Transport timescales represent a more holistic way of interpreting the flow in complex systems (e.g. Monsen et al. 2002), and allow us to understand how advective and dispersive mechanisms transport water.

Transport timescales are driven by the water currents, which in turn are influenced by sea level oscillation, bathymetry and the temperature and salinity fields. It is therefore necessary to have an accurate representation of these quantities in order to satisfactorily estimate transport timescales.

This article has the following tasks:

(1) to demonstrate, using a 3D hydrodynamic model combined with particle simulations, how release times (e.g. slack waters of high and low tides, neap and spring tides) affect the exposure time and residence time in a shallow meso-tidal tropical estuary.

(2) to compare TTS results from numerical modelling with estimates using the simple newly modified Land Ocean Interaction Coastal Zone (LOICZ) model by Andutta et al. (2014).

(3) to calculate and evaluate the return coefficient (r) numerically and analytically using CART. This is a measure of the propensity of a water parcel to return into the domain of interest after leaving it.

a. Overview of Transport Timescales

Since the pioneering work by Ketchum (1951) and Bolin and Rodhe (1973), the theory of TTS has evolved (e.g. CART, www.climate.be/cart), and other TTS definitions have been introduced in order to fill scientific gaps. Therefore, there are many different transport timescale definitions, e.g. flushing time (Ketchum, 1951; Fischer et al., 1979; Monsen et al., 2002), residence

time (Bolin and Rodhe, 1973; Monsen et al., 2002; Delhez et al. 2004; Deleersnijder et al., 2006), exposure time (Monsen et al., 2002), transit time (Holzer and Hall 2000), influence time (Delhez et al., 2014), age (Bolin and Rodhe, 1973; Monsen et al., 2002), e-folding flushing time (Monsen et al., 2002), turnover time (Sheldon and Alber, 2006) and renewal time (Andutta et al., 2014) – all of which have their own interpretation.

Two timescales, residence time and exposure time, are used to provide an indication of increase or decrease of non-reactive and reactive substances in estuaries, bays, lagoons, and atolls (Andutta et al., 2014). The residence time (Θ) is the time needed for a particle constituent to reach for the first time an open boundary of the domain of interest (e.g. Delhez et al., 2004). The exposure time (φ) is the time the particle will stay in the domain (e.g. Monsen et al., 2002) (Figure 2). Therefore, at a given time and location, the exposure time is always larger than or equal to the residence time. The larger the difference between the two timescales, the more often the particles tend to re-enter the domain of interest after leaving it for the first time. To evaluate the exposure time, the computational domain must be larger than the domain of interest (de Brauwere et al., 2011, de Brye et al., 2012). Estimates of these timescales may be obtained in an Eulerian or a Lagrangian framework. The latter often requires sufficiently large number of numerical particles in order to provide a result that statistically approaches the real condition.

A dimensionless return coefficient, r , represents the propensity of particles to return into the estuary after reaching an open boundary for the first time, as illustrated in Figure 1A (de Brauwere et al., 2011). It is defined as the relative difference between φ and Θ , i.e.

$$r = \frac{(\Theta - \varphi)}{\Theta} . \quad (1)$$

Clearly, this coefficient lies in the interval [0,1].

The larger the r the more likely it is that particles will re-enter the estuary after crossing one of its open boundaries for the first time. Accordingly, particles that never return into the estuary have $r = 0$, while particles returning often or for long periods of time have r close to unity.

Preferred position for figure 1

b. Chosen estuary and coastal area

The domain of interest is the estuarine System of the Caravelas and Peruípe Rivers (ESCP), in southern Bahia state, Brazil (see Figure 2); more details may be found in Appendix 1. It is located at the approximate latitude of $17^{\circ}50'S$, nearly 60 km from the National Maritime Park of Abrolhos, which is one of the largest reef structures of the Atlantic ocean, providing habitat for innumerable marine species. The ESCP has two main mouths: the Caravelas Estuary in the north ($17^{\circ}45'S$), with two small channels named Barra Velha (~ 1 km wide) and Tomba's Mouth (~ 600 m wide), and the Peruípe Estuary in the south ($17^{\circ}54'S$) with a funnel shape ranging in width from ~ 3500 m to ~ 700 m in the first few hundred meters. These two mouths are separated by a distance of ~ 25 km alongshore, and are internally connected by shallow and narrow channels around Cassurubá or Cassumba Island. Our simulations consider the domain shown in Figure 1C, for which results were computed according to the number of particles in the control domain with boundaries ω_1 and ω_2 .

Preferred position for figure 2

2. Methods

a. Numerical model

The ESCP comprises a number of channels varying significantly in width, from 60 m upstream to 1000 m near the mouth, and thus a high resolution mesh is necessary to resolve the many small channels in the domain. The numerical model used is the curvilinear-mesh, three-dimensional Delft3D-Flow from Deltares (www.deltares.nl). This model is hydrostatic, and its

111 equations are solved by the method of finite differences (Delft Hydraulics, 2008). A curvilinear
 112 mesh is appropriate for the domain, although there are some disadvantages in the horizontal
 113 resolution distribution compared to unstructured meshes. Delft3D's curvilinear mesh is efficient in
 114 minimizing noise due to the steps in the horizontal plane, and allows the mesh cells to follow the
 115 channels more easily compared to non-curvilinear quadrangular meshes. The degree of non-
 116 orthogonality between mesh elements is always smaller than 0.02 thus satisfying the criteria ($\cos \theta$
 117 < 0.02), which helps to preserve numerical stability of the simulations (Delft Hydraulics, 2008).
 118 The diagonal horizontal resolution ranges from ~ 20 m to ~ 300 m. The number of quadrangular
 119 mesh cells on the horizontal plane is 22,928. A lower resolution is applied in the coastal region
 120 $\sim [130-300]$ m, but this is increased toward the coast and the estuary $\sim [20-100]$ m (Figure 1B). The
 121 refined mesh within the estuary combined with high water speeds requires the time-step to be
 122 relatively small (around 1 second), to satisfy the Courant–Friedrichs–Lewy condition. The mesh
 123 used in the simulations of the ESCP (Figure 1B) is relatively complex, covering a small part of the
 124 Peruípe River, near the city of Nova Viçosa. This river is the main channel connecting the northern
 125 and southern mouths. The main tributaries of the Caravelas River, namely the Cupído and Jaburuna
 126 Rivers, are covered by the mesh. With 10 equally spaced sigma vertical layers, this mesh also
 127 covers a few kilometers of the adjacent coastal region.

128 The bathymetry in the estuarine channels was obtained using an Echo sounder and Global
 129 Position System. Two tide gauges were installed in Caravelas and Nova Viçosa (see locations A and
 130 C in Figure 2), meant to remove the tides from the Echo sounder data. For the Peruípe River
 131 estuary, the bathymetry was measured only in the first 6 km, near anchor station D. Thus an
 132 extrapolation was applied, considering the depth to be 4 meters for the next 14 km along the Peruípe
 133 River. The bathymetry was combined from these sources, and the triangular interpolation
 134 application in Delft3D-Flow was used. The bottom topography has depths ranging from ~ 0.2 m to a
 135 maximum of ~ 18 m (Tomba's Mouth), whilst in the coastal region do not exceed ~ 10 m.

A more detailed description of the field work carried out to obtain measurements of thermohaline properties and other parameters is provided in Appendix 2.

b. Model Boundary conditions, initial conditions and physical parameters

Rainfall and river discharge measurements in the Peruípe River are shown in Figure 3B. The river discharge data, obtained from the National Agency of Waters ANA (<http://www.ana.gov.br/>), was measured at a gauge station upstream of the river, at station Helvécia nº 55510000 (code 1739006). This station covers a large part of the drainage basin of the river. During rainy conditions the total drainage basin of the river may be used to estimate the total river flow to be applied at the upstream inflow boundary of the river. The factor to account for the missing drainage basin area is $\alpha = \frac{A_1 + A_2}{A_1} = 1.6$, in which station Helvécia $A_1 \sim 2,840 \text{ km}^2$, and the downstream area not covered by this gauge station is $A_2 \approx 1,760 \text{ km}^2$. The area values were obtained from the ANA (<http://hidroweb.ana.gov.br/>).

Data from the gauge station were also used to estimate the river discharge range for the Cupído and Jaburuna rivers. This was done by comparing their watershed areas with the watershed of the Peruípe river, and assuming homogeneous rainfall and evapotranspiration distributions over these areas (Andutta, 2011; Pereira et al., 2010). The total river flow into Caravelas Estuary was then roughly estimated using $Q = Q_P \beta$, where $\beta = 600/4600$ is the ratio between the catchment areas of the Caravelas (600 km^2) and the Peruípe ($A_1 + A_2 = 4600 \text{ km}^2$) rivers, and Q_P is the average discharge for the Peruípe). This estimation was adjusted by comparing observed flow velocities at locations A and B with model predictions.

The monthly estimate of fresh water inflow for the Peruípe River reveals small inflow for the dry season, often between June and September (see Figure 3C). The combined freshwater input from the Jaburuna and Cupído rivers estimated using the factor β is less than 10% of the river discharge into the Peruípe River. Because the field work was conducted during a relatively dry wet

161 season, when rainfall was negligible prior to and during measurements obtained in January 2008
 162 (Figure 3A), it is logical not to consider the application of the factor α at the Helvécia gauge
 163 station. Although this approach of river flow estimation is not required, the technique described
 164 above would be required under homogeneous rainfall conditions over the drainage basin of the
 165 Peruípe, Jaburuna and Cupído rivers.

166 The best fit between observations and model results was obtained using the mean river
 167 discharge shown in Table 1 for the Cupído and Jaburuna rivers, and the daily measurements shown
 168 in Figure 3B for the Peruípe River. In other words, the value measured at Helvécia gauge station
 169 was used in the simulation with additional tuning to extrapolate results for the other two smaller
 170 rivers.

171 .

172 **Preferred position for figure 3**

173

174

175

176 **Preferred position for Table 1**

177

178 The measurements from this tide gauge were compared with the simulation results during
 179 neap and spring tides using the “Skill” method described below. In addition, a qualitative
 180 comparison was carried out between the axial salinity distribution found in the simulations, and the
 181 observed distribution presented in Schettini and Miranda (2010).

182 We used the initial condition of a homogeneous thermohaline distribution for the salinity (30
 183 practical salinity unit - psu) and temperature (27 °C). The spin up simulation was made for about
 184 two months to obtain a dynamic equilibrium condition. Since the temperature has previously been
 185 found to be nearly homogeneous in this estuary (Andutta, 2011), its mean value was used for all
 186 simulations. The first flow field and salinity distribution, obtained from the equilibrium condition,

187 was used to provide a varied initial field for simulations starting at slack waters in both spring and
 188 neap tidal conditions.

189 Computational modellers often assume that vertical eddy diffusion and viscosity coefficients
 190 vary in time, by using turbulent closure models, e.g. algebraic, *k-L*, *k-Epsilon* schemes. On the other
 191 hand, the horizontal eddy diffusivity, K_h , and horizontal viscosity coefficients, K_v , are often
 192 estimated according to the mesh element size (Okubo, 1971). Therefore, modellers need to choose a
 193 parameterisation scheme that provides the right amount of mixing in the estuary. We have
 194 considered the parameterisation of horizontal eddy viscosity by Uittenbogaard et al. (1992), which
 195 is available in Delft3D-Flow and reproduces well the turbulent fluxes of momentum.

196 The best fit between results and simulations was obtained assuming the horizontal eddy
 197 diffusivity, K_h , to be in the range of $\sim[2-30] \text{ m}^2 \text{ s}^{-1}$ with small and large values applied respectively
 198 to small and large mesh cells. The sensitivity analysis for K_h , was conducted following Okubo
 199 (1971). Because Okubo's formula applies for open-water, it was observed that it was not properly
 200 simulating the true dispersion in the estuary, thus a factor f was used to increase and decrease
 201 mixing at the sub-grid scale (See Equation 2). Varying f allowed us to achieve the best fit between
 202 measurements and model results.

$$203 \quad K_h = f [2.05 \times 10^{-4} \times d^{1.15}] \quad (2)$$

204
 205 where d is the mesh cell size (from ~ 20 to ~ 300 metres), and f is the factor set to different values
 206 but only shown for 2, 100, 150, 200, 250, 400 and 2000 in the sensitivity analyses (see Table 3).

207 The *k-Epsilon* turbulent closure scheme was used to compute values for the vertical viscosity
 208 and diffusivity. We assumed the typical Manning roughness coefficient of $(0.02 \text{ m}^{-1/3} \text{ s})$, which
 209 characterises the higher percentage of local sediment (Souza et al., 2013). This resulted in a Chézy
 210 coefficient of $\sim 40 \text{ m}^{-1/2}/\text{s}$. Wind speed and directions, assumed to be **constant** over this small region,
 211 were obtained at the Caravelas station from the Instituto Nacional de Meteorologia INMET (code
 212 INMET 86764), at (source: <http://www.inmet.gov.br/portal/>), see Figure 4.

Preferred position for figure 4

The wind was assumed to only **affect** mesh cells in coastal areas. In other words, the wind stress did not affect mesh cells inside the estuarine channels. Moreover, Andutta et al. (2013) applied Hansen and Rattray's analytical equation of the velocity and salinity components, and demonstrated that the wind effect in January 2008 was negligible at station C (near Nova Viçosa estuarine mouth), which is the closest to the coast. Hansen and Rattray's analytical solution required an adjustment of no more than 0.02 Pascal for the wind stress, which correspond to wind speeds of $\sim 3 \text{ m s}^{-1}$ (Andutta et al., 2013). South-southwestward alongshore currents occur between October and January, while north-northeastward alongshore currents are observed during the fall and winter months Lessa and Cirano (2006).

Sea level data from TOPEX were used to force tides at the open boundary nodes. A time series of water surface elevation from May to July 2007 was recorded at Terminal Aracruz (TA in Figure 2), which is a few kilometers away from the coastal open boundary. At TA a total of 16,264 tidal measurements were recorded at five minute intervals, and were processed using the tidal component **extraction** program PACMARÉ (Franco, 2000). These tidal measurements were used to obtain the amplitude and phase of the main tidal components, shown in Table 2. Additionally, sea-level data were recorded at stations A and C from 14th to 19th of January 2008, and these data were used to validate modelled sea-level oscillation (comparison shown in Results and Discussion section). Sea surface elevation observations from sites A and C showed the same phase, strongly suggesting that tides propagate across the shelf, because tides propagating along the coast would results in a phase shift between sea level observations at sites A and C (see Figure 2). The measurements of tidal heights of $\sim 1 \text{ m}$ and $\sim 3 \text{ m}$ during neap and spring tides, respectively. This ranks as meso-tidal, according to the criteria of Davies (1964) for tidal classification. From the tidal heights shown in Table 3, the tidal form-number is $[N_f = (K_1 + O_1) / (M_2 + S_2) = 0.19]$, indicating a semidiurnal tidal estuary (Defant, 1960). The tidal components from Table 2 represent over 97% of sea level variations for the estuarine system (Andutta, 2011).

Preferred position for Table 2

d. Model validation criteria

In order to quantify the agreement between the simulated velocity and salinity profiles the method suggested by Wilmott (1981), based on the Skill parameter was used. Accordingly, the skill is measured as follows

$$Skill = 1 - \frac{\sum |X_{\text{mod}} - X_{\text{obs}}|^2}{\sum \left(|X_{\text{mod}} - \bar{X}_{\text{obs}}| + |X_{\text{obs}} - \bar{X}_{\text{obs}}| \right)^2}, \quad (3)$$

where X_{obs} and X_{model} denote the observational and simulated properties, respectively, $\bar{X}_{\text{obs}}$ being the mean observational values. The Skill parameter varies from 1 to zero, with 1 indicating the best fit, and zero indicating a complete disagreement between observation and model results.

e. Modelling approach to calculate the Transport Timescales

To quantify the residence time and exposure time 35 thousand numerical particles were released in the estuary by coupling D-Waq PART with results from the Delft3D-FLOW (i.e. within the subdomain denoted ω). Numerical particles were deployed near the bottom and top layers. The particle concentration using conservative tracer module was normalized to value 1 within the volume of ω . Therefore, the number of particles decreases when particles exit ω , and increases when particles re-enter ω . The minimal initial number of particles, i.e. 25 thousand, was computed considering a minimum thickness of 2 m and a grid cell of ~ 20 by 10 meters.

A total of four simulation scenarios were made: (S_1) particle released at high water in neap tide, (S_2) particle released at low water in neap tide, (S_3) particle released at high water in spring tide, and (S_4) particle released at low water in spring tide.

In order to be consistent with CART timescales, for the computation of the residence time, particles are discarded once they have reached an open boundary, e.g. estuarine head or an open

boundary in coastal waters (de Brauwere et al., 2011; de Brye et al., 2012). The arithmetic mean of the individual residence times, φ , was computed as the time necessary for particles to exit the domain (ω) for the first time. As for the exposure time, the particles are assumed to immediately bounce back into the domain only at estuarine heads. This simplifying hypothesis is unlikely to entail any major error, since a particle crossing the upstream estuarine boundary in the upstream direction (because of diffusive processes) will most likely return into the estuary after a relatively small time under the influence of the river flow, e.g., the St. Johans River in Florida, which experiences backflows over significant durations (Hendrickson et al., 2003).

Results from residence and exposure times were used to estimate the return coefficient distribution. The residence and exposure times may vary according to the time of release, such as during neap/spring tides or high/low tides, and this would also affect the return coefficient. This notwithstanding, results of exposure and residence times must be calculated for the same conditions when computing the return coefficient, i.e. $r = (\Theta - \varphi) / \Theta$.

277

278 *f. The modified LOICZ analytical model*

The modified LOICZ model of Andutta et al. (2014) applies the salinity balance proposed by Fischer et al. (1979) into the original formulation of the LOICZ. This water renewal timescale model has been shown to be sensitive to changes to some of its free parameters (e.g. river flow and salinity grandient). We expect that the estimates of the timescales from our numerical results would fit within the ranges derived from the LOICZ model. Details of its derivation are provided in Andutta et al. (2014); however we provide the simplified relation for water renewal timescale.

285

$$286 \quad \frac{1}{T_p} = \frac{1}{T_1} + \frac{1}{T_2}, \quad (4)$$

287

where $T_1 = L/U$ and $T_2 = L^2/K$ are the advective and dispersive timescales, respectively. L , U , K and T_p are respectively the selected estuarine segment length, the flow speed, the characteristic value of the longitudinal diffusivity and the water renewal timescale. This expression may be re-

290

written in terms of the dimensionless Péclet number $Pe = ULK^{-1}$, the ratio $P_e = T_2/T_1$ of the dispersive to the advective timescale. Similarly, this number provides a comparison of contributions from advective and dispersive processes to transport timescales, yielding

$$T_P = \frac{VP_e}{Q_R(1 + P_e)}. \quad (5)$$

Where V and Q_R denote the estuarine volume and river discharge, respectively. The contribution of advection to the total water renewal timescale T_P , θ ($0 \leq \theta \leq 1$), is given by

$$\theta = T_P/T_1 = Q_R/(Q_R + Q_D), \quad (6)$$

where Q_D is the discharge. Equations (4) and (6) were used to generate the advective-dispersive diagram (shown later), whose results will be compared to the numerical results.

g. The CART analytical model

As previously mentioned, in the framework of CART, the TTS that may be used to calculate water renewal rates can be obtained at any time and position as the solution of partial differential equations (Deleersnijder et al., 2006; de Brye et al., 2012; Andutta et al., 2014). For instance, residence time and exposure time were estimated using calibrated/validated numerical simulations for the Scheldt Estuary (de Brauwere et al. 2011, de Brye et al. 2012). As an easy acceptable method, analytical solutions may provide results that are representative of real situations (e.g. CART and LOICZ). The idealised CART timescales were used to obtain the exact analytical solution of the so called return coefficient for the ESCP. Different values of the Péclet number were considered, in order to assess the axial variation of return coefficient values. The advective timescale, $T_1 = V/Q_R$, and a dispersive timescale, $T_2 = P_e V/Q_R$, are defined taking into consideration the estuarine volume V . Andutta et al. (2014) provides a detailed description depicting an idealized channel for the time scales.

318 Consider an estuarine channel ($-\infty < x < \infty$) with a constant cross-sectional area A , and a
 319 flow under steady-state. The volumetric flow rate is denoted as Q_R . The downstream and upstream
 320 boundaries of our idealised estuary are located at $x = L_0$ and $x = L_1$, respectively. The estuarine
 321 length is $L = L_0 - L_1$, and thus the volume is $V = AL$. The water velocity is then
 322 $U = Q_R / A = LQ_R / V$. For the abovementioned conditions, the residence time satisfies the adjoint
 323 of the classical passive tracer transport equation (Delhez et al. 2004, Andutta et al. 2014), i.e.

324

$$325 \quad \frac{d}{dx} \left(AK \frac{d\varphi}{dx} + Q_R \varphi \right) = -A \quad (7)$$

326

327 where, x , denotes the particle position. The solution for the equation needs to satisfy the upstream
 328 and downstream boundary conditions,

329

$$330 \quad \varphi(L_1) = 0 = \varphi(L_0). \quad (8)$$

331

332 It represents the average time required by particles initially located in the interval $[x, x + \delta x]$
 333 (with $\delta x \rightarrow 0$) to reach one of the open boundaries. The solution is then easily derived:

334

$$335 \quad \varphi(x) = \frac{V}{Q_R} \left(1 - \frac{\xi}{L} \right) + \frac{V}{Q_R} \left(\frac{e^{-Pe} - e^{-Pe \xi/L}}{1 - e^{-Pe}} \right) \quad (9)$$

336 where $\xi = x - L_1$.

337 The exposure time was also derived (Andutta et al., 2014), and is defined in the domain of interest
 338 and its surrounding environment.

$$339 \quad -\infty \leq x \leq L_1 \quad : \quad \Theta(x) = \frac{V}{Q_R} \quad (10a)$$

$$340 \quad L_1 \leq x \leq L_0 \quad : \quad \Theta(x) = \frac{V}{Q_R} \left(1 - \frac{\xi}{L} \right) + \frac{V}{Q_R} \left(\frac{1 - e^{-Pe \xi/L}}{Pe} \right) \quad (10b)$$

$$341 \quad L_0 \leq x < \infty \quad : \quad \Theta(x) = \frac{V}{Q_R} \left(\frac{e^{-Pe} - 1}{Pe} e^{-Pe \xi/L} \right) \quad (10c)$$

From Equations (9) and (10), which are valid within the upstream and downstream open boundaries, the return coefficient is:

$$r = \frac{\Theta(x) - \varphi(x)}{\Theta(x)} = \frac{\left(\frac{1 - e^{-Pe \zeta/L}}{Pe} \right) - \left(\frac{e^{-Pe} - e^{-Pe \zeta/L}}{1 - e^{-Pe}} \right)}{\left(1 - \frac{\zeta}{L} \right) + \left(\frac{1 - e^{-Pe \zeta/L}}{Pe} \right)} \quad (11)$$

Note that r is bounded by $[0,1]$, as mentioned before.

In principle, the residence time and the exposure time can be obtained by solving classical passive transport equations. However, to do so, time- and position-dependent concentrations must first be **obtained and**, then, time and space integral must be performed to derive the relevant timescales. This is not straightforward, even for highly idealised flows. This is why it is preferable to have recourse to the adjoint method established by Delhez et al. (2004), which requires the solution of simpler differential problems to be determined: in the present case, only ordinary differential equations are to be dealt with rather than partial differential ones. The disadvantage of this approach is that the theoretical underpinning of an adjoint model sometimes appears elusive, which is probably the reason why Errico (1997) wrote a general, enlightening paper on this matter, explaining the nature and purpose of adjoint models.

3. Results and Discussion

a. Model calibration of salinity, velocity and tides

We carried out a sensitivity analysis considering different values for the horizontal diffusion coefficient k_h using Equation 2. These adjustments of factor f for the horizontal diffusivity based on the grid size allowed us to obtain a proper representation of the salinity field and its time variability.

Preferred position for Table 3

The mean Skill parameters for the simulation are shown in Table 3 for different values of factor f , which was described with Equation 2. The comparison of sea-level oscillation over a tidal modulation period, from the 14th to the 29th of January 2008, showed good skill values for locations A (Figure 5) and C (not shown), and the Skill parameter for tides was calculated to be over 0.97 for both locations, i.e. A and C. The comparison of tides, velocity, and salinity showed good skill values during spring tides (not shown), and reasonable values during neap tides (Figure 6).

Preferred position for figure 5
Preferred position for figure 6

The Skill parameter for the water column height variation in time was calculated to be over 0.98 for all the sites under neap and spring tides (Table 4), and the tidal ranges were ~1.0 m and ~2.5 m for neap and spring tides, respectively. Observations have shown that the tidal phase between sites A (Caravelas mouth) and C (Peruípe mouth) is almost the same. The similarity of their phases indicates that tides propagate mainly perpendicular to the coast line in this region, a result which is in close agreement with observations previously reported by Lessa and Cyrano (2006).

For the modeled velocity validation, good results (Skill from 0.77 to 0.93) were obtained in spring tides in the estuaries of Caravelas (sites A and B) and Nova Viçosa (sites C and D). For neap tides due to small differences on tidal asymmetry, the Skill was lower, at ~ 0.6.

The model agreed well with observations of maximum ebb and flood currents at site A. The model also properly simulated the velocity profiles for sites B, C, and D. Therefore, the description of maximum ebb and flood currents from in-situ data also apply to the model simulations. At site B there were maximum speeds of ~0.5 m s⁻¹ and 1.0 m s⁻¹ (ebb events), and ~-0.3 m s⁻¹ and ~-0.6 m s⁻¹ (flood events), during neap and spring tides, respectively. For site A the vertical shear of the velocity was negligible in flood and ebb conditions, while for site B there was a small vertical shear of the horizontal velocity during ebb events. During flood events, the water velocity was homogenous over the water column. In addition, a residual velocity of ~0.05 m s⁻¹ was calculated at

394 site B, indicating a residual circulation from Nova Viçosa towards the Caravelas River. Site A had a
 395 residual current of $\sim 0.06 \text{ m s}^{-1}$, indicating a small discharge from the Cupído and Jaburuna Rivers.
 396 At sites C and D, located in the Peruípe River, the downstream velocities showed more intensity
 397 than observed in the Caravelas Channel. For site C the downstream velocities varied from $\sim -0.9 \text{ m}$
 398 s^{-1} to $\sim -1.5 \text{ m s}^{-1}$, for neap and spring tides, respectively. During flood events, the velocities were $\sim$
 399 0.3 m s^{-1} and $\sim -0.7 \text{ m s}^{-1}$, for neap and spring tides, respectively. At site D the maximum
 400 downstream velocities were only $\sim 0.7 \text{ m s}^{-1}$ and $\sim 1.0 \text{ m s}^{-1}$ at neap and spring tides, and upstream
 401 velocities were $\sim -0.3 \text{ m s}^{-1}$ and $\sim -0.4 \text{ m s}^{-1}$. The residual velocities at sites C and D, which have
 402 values of $\sim 0.10 \text{ m s}^{-1}$ to $\sim 0.15 \text{ m s}^{-1}$, indicate a higher advective contribution from the Peruípe River
 403 compared with the Caravelas estuary.

404 In addition to the tides and the velocity field, the model simulated the temporal variation of
 405 the salinity well for all sites (A, B, C, and D). During spring tides the calculated Skill values were
 406 over 0.83, while for neap tides they were over 0.73 (Table 4). At the Caravelas estuarine channel,
 407 $\sim 3 \text{ km}$ near the mouth (site A), during low tide, salinity was observed in intervals of $\sim 34.5 \text{ psu}$ to
 408 $\sim 35.0 \text{ psu}$ and $\sim 34.0 \text{ psu}$ to $\sim 34.5 \text{ psu}$ for the observational and theoretical results,
 409 respectively. About 6 km away from the mouth we obtained a good agreement for the salinity, with
 410 $\sim 32.0 \text{ psu}$ and $\sim 32.5 \text{ psu}$ for observation and simulation, respectively. In the vicinity of the
 411 interconnection with Cupído and Jaburuna Rivers (site B), which is about 12 km upstream from the
 412 mouth, the salinity decreased to $\sim 30.0 \text{ psu}$ and $\sim 28.5 \text{ psu}$ for the observational and calculated
 413 results, respectively. At high tide, near the mouth (site A) and at a distance of 6 km from the mouth,
 414 the salinity was $\sim 36.5 \text{ psu}$ and $\sim 36.0 \text{ psu}$, respectively, for both simulation and field measurements.
 415 In the upper reaches of the estuary, near the junction of the rivers, Cupído and Jaburuna ($\sim 12 \text{ km}$
 416 from the mouth), a close agreement between simulated and observed salinity values ($\sim 33.0 \text{ psu}$) was
 417 obtained at high tide. Along the Peruípe River estuary at neap tides, the surface salinities vary in the
 418 range of 20.0 psu to 34.0 psu at the surface, and 32.5 psu to 36.0 psu near the bottom. The region of
 419 Nova Viçosa has more vertical stratification of the salinity than at sites A and B in the Caravelas

420 River. This is due to Peruípe River's larger freshwater discharge. The observed value of ~36.0 psu
 421 near the bottom is characteristic of the Tropical Water Mass, which was already reported to enter
 422 this estuarine system (Schettini et al., 2010). During spring tides the vertical mixing causes the
 423 erosion of the halocline, and thus decreases vertical stratification. This results in a smaller vertical
 424 variation of 31.0 psu to 36.0 psu from the surface to the bottom.

425 **Preferred position for Table 4**

426 A comparison of the axial distribution of salinity was made for the Caravelas River (Figure
 427 7A,B). For the first 12 km along the estuarine channel, results from simulations were compared to
 428 observations made by Schettini and Miranda (2010). The measurements were obtained on the 10th
 429 of April, 2001 during spring tides. Although the field data are likely to be from different conditions
 430 of river flow, the simulation showed a good correlation of the axial distribution of the salinity in the
 431 Caravelas River (See Figures 7C and 7D), with values of $R^2 \sim 0.97$ and $R^2 \sim 0.99$ for low and high
 432 tides respectively. This indicates that the model has well represented the mixing processes in the
 433 Caravelas Estuary. During low tide (Figure 7A,C), a good agreement is found near the mouth, with
 434 salinity values of ~35.2 psu and ~34.5 psu, for the model results and observations, respectively. At
 435 nearly 6 km upstream, there is still a good agreement ($R^2 \sim 0.99$) with the salinity values of ~33
 436 psu (model), and ~32 psu (observation). Further upstream and near the inter-connection between the
 437 Cupído and Jaburuna rivers (i.e. ~12 km upstream), the agreement is slightly poorer with the
 438 salinity values of ~30 psu (model) and ~29 psu (observation). At high tide (Figure 7B, D), the
 439 model predicted the longitudinal salinity variations well along the Caravelas Channel. The salinity
 440 values near the mouth were ~36.4 psu (model and observation), and reduced to ~36 psu 6 km
 441 further upstream. Moreover, during high tides the agreement was also good near the channel
 442 between the Cupído and Jaburuna rivers with salinity of ~33 psu.

443 **Preferred position for figure 7**

444
 445 *b. Results of the residence time, the exposure time and the return coefficient*

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447 The transport timescales, namely residence time (φ), exposure time (Θ), and the return
 448 coefficient (r), were estimated for the Caravelas and Peruípe estuarine channels with simulation
 449 under different scenarios, i.e. S_1 to S_4 (Figures 8, and 9).

450 For scenarios S_1 and S_3 (Figure 8), the residence time along the Caravelas Channel, from the
 451 mouth to 12 km upstream, was found to vary from 0 to ~ 15.0 days. The inflow boundaries of the
 452 Cupído and Jaburuna rivers were found to have residence times of ~ 27 and ~ 22 days, respectively.
 453 For the Peruípe Channel the residence times ranged from 0 to ~ 7.4 days, from the mouth to 5 km
 454 upstream, with a maximum value of ~ 18 days at the inflow boundary of the Peruípe Estuary.

455 The residence time estimated at ~ 6 km further upstream in the Caravelas Estuary ($\varphi = 11.7$
 456 days) is almost three times larger than the residence time calculated for the same distance along the
 457 Peruípe Estuary ($\varphi < 4.4$ days). The difference between results in the Caravelas and the Peruípe
 458 estuaries is due to the larger velocity contribution in the Peruípe Estuary.

459 Comparing scenarios S_1 and S_3 , the residence time was found to be slightly lower for S_3 (c.a.
 460 a few hours) and this difference is due to increased diffusive contribution during stronger spring
 461 tidal conditions. In contrast to scenarios S_1 and S_3 , the simulations considering scenarios S_2 and S_4
 462 yielded an increased residence time. This increase was maximum near the estuarine mouths (~ 5
 463 days), and observed to reduce in the upstream direction (few hours). The increase in residence time
 464 for particles released in slack water of low tide is caused by tidal excursion from reversing currents
 465 (i.e. flood currents). These results reflect and add value to recent simulations by de Brye et al.
 466 (2012) for the Scheldt Estuary (in Belgium and the Netherlands), whose results showed larger
 467 residence time values for particles released at slack water of low tides than for high tides (difference
 468 of a few days).

469 The virtual Lagrangian particles showed that a negligible number of particles crossed the
 470 connecting channel between the Caravelas (ω_1) and Peruípe Estuaries (ω_2), which indicates that this
 471 relatively narrow and shallow interconnection channel allows little exchange of water properties
 472 between these estuaries. Moreover, the residence time is observed to be larger within the

473 enlargement of the interconnecting channel between these two estuaries. Schettini and Miranda
 474 (2010) and Schettini et al. (2013) have addressed the importance of the interconnection channel
 475 between Caravelas and Peruípe, and found that sediment deposited near the Caravelas mouth was
 476 both inner shelf **local resuspension** and upstream transport, or sourced from the Peruípe River via
 477 the interconnection channel.

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Preferred position for figure 8

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Exposure time results showed that particles re-entered the system for up to two days (Figure
 9). Note that the difference between the exposure time and the residence time ($\Theta - \varphi$) showed little
 spatial variation for scenarios S_1 and S_3 .

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Preferred position for figure 9

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The spatially averaged difference between exposure and residence times ($\Theta - \varphi$) are
 calculated in days, and its respective RMSE to be $\sim 1.98 \pm 0.06$ for S_1 , $\sim 1.87 \pm 0.12$ for S_2 , ~ 1.92
 ± 0.07 for S_3 , $\sim 2.19 \pm 0.08$ for S_4 . These results strongly suggest that ($\Theta - \varphi \sim \text{const.}$) for the
 ESCP under the four different scenarios considered. The results also suggest that $t_3 - t_2$ varies little
 away from the open boundaries, so particles deployed at different times and locations in the estuary
 re-enter for similar lengths of time, assuming the circulation in coastal waters does not considerably
 change over time due to additional forcings, e.g. sudden alongshore wind driven currents.

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Equation (5) was used to estimate the range of water renewal timescales for the Caravelas
 and Peruípe estuaries using the parameters given in the appendices of Andutta et al. (2014), see
 Figure 10. The straight line labelled θ (lowercase) indicate the relative advective contribution to
 water renewal, where $0 \leq \theta \leq 1$. The line at $\theta = 0.5$ separates the areas where transport is
 dominated by advection (diagram upper zone, $\theta > 0.5$) and dispersion (diagram lower zone, $\theta <$
 0.5).

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The Caravelas and Peruípe estuaries have mean depths of ~ 6.5 and ~ 7.5 meters,
 respectively, and the maximum and minimum tidal ranges in these estuaries are ~ 2.5 and ~ 0.5

501 meters. According to Andutta et al. (2013), these tidal ranges combined with the relatively the small
 502 depths result in a high rate of change of the potential energy ($\sim 6.1 \text{ J m}^{-3} \text{ s}^{-1}$), which contributes
 503 towards large dispersion. It is valid to compare these results to the Sheldt Estuary, where tidal
 504 oscillation is typically 4-5 meters along the first $\sim 100 \text{ km}$, and where the mean water depth is ~ 10
 505 meters. Tidal range in the Sheldt can reach $\sim 7 \text{ m}$, which is about 45% of the mean water depth
 506 value for the first $\sim 25 \text{ km}$ near the estuarine mouth (Soertaert and Herman, 1995; de Brye et al.
 507 2012), and this system is classified as well-mixed due to dispersion prevailing over advection. The
 508 numerical results for the ESCP fit within the timescale ranges estimated using the simple LOICZ
 509 method.

510
 511 **Preferred position for figure 10**
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513 The return coefficient cannot be calculated using the modified LOICZ model. However, it
 514 was computed numerically and compared to the non-dimensional solution obtained using CART.
 515 The return coefficient converges to one at the estuarine mouths and near estuarine heads (Figure 11,
 516 for all scenarios S_1 to S_4 and Figure 12B). However, this is only a direct consequence of the
 517 definition of the residence time, which converges to zero at the entrance, and thus the return
 518 coefficient will always increase towards unity. r was observed to be smaller upstream, because the
 519 ratio $(\Theta - \varphi)/\Theta$ is likely to decrease. It can be noticed that the axial variation of the return
 520 coefficient is similar for both CART solution and numerical approach (Figures 11 and 12C). The
 521 return coefficient calculated from CART and from numerical simulations is observed to increase
 522 towards the upstream boundary. This increase towards the estuarine head is due to the boundary
 523 condition assumed in the analytical and numerical solutions, where particles do not re-enter the
 524 domain after crossing the estuarine head, although in a real estuary water particles would re-enter
 525 through the estuarine head due to river flow conditions.

526 Figure 12A shows results of the residence and exposure time and return coefficient for a
 527 range of values of the Péclet number. High values of the Péclet number yield a boundary layer in
 528 the vicinity of the upstream location.

529 The greater the relative importance of advection, the less likely it is that dispersion will
 530 cause a water particle to hit the upstream boundary of the domain ($x = L_0$). In accordance with their
 531 definitions, the exposure time is larger than the residence time for any location in the domain ($L_1 \leq$
 532 $\xi/L \leq L_0$). These idealised results of the return coefficient were used to access results obtained
 533 from our numerical simulations.

534

Preferred position for figure 11

Preferred position for figure 12

In the illustration shown in Figure 11A, the ratio is simply the difference between times t_3 and t_2 . Evidently this is a simple case where the particle is assumed to have re-entered the domain only once.

Particles are expected to first cross the estuarine mouth during ebb currents, which would be alternating with flood currents and dispersive processes. Therefore, we could presume that Lagrangian particles would have a time window of ~ 6.5 hours to cross the entrance (for semi-diurnal tidal estuaries), and this time window would then close for ~ 6.5 hours (the period of flood currents).

Our simulations were for relatively calm weather conditions, which were predominant over the region, c.a. wind speeds in the range $1\text{--}4\text{ m s}^{-1}$ (wind from NE). Andutta et al. (2013) showed that wind conditions did not affect the water circulation in this estuarine system in January 2008. However, for stronger wind conditions the results would not be the same. Evidently alongshore wind-driven currents would reduce the difference between the exposure time and the residence time, and the return coefficient would thus decrease towards zero. This is because alongshore currents inhibit the propensity of particles to re-enter the estuarine system. The alongshore shelf currents are observed to be driven by the N-S migration of the South Atlantic High between summer and winter. South-southwestward alongshore currents occur between October and January, while stronger north-northeastward alongshore currents are observed during the fall and winter months (Lessa and Cirano, 2006).

4. Conclusions

Overall goal

This study provides the first estimates of the residence time, exposure time and the return coefficient for the Caravelas and Peruípe estuaries and might be a reference for future studies related to the control of pollutants and sediment transport. These transport timescales were estimated using a Lagrangian model only as a tool, and this model has been properly calibrated and validated using field data.

Specific conclusions

- *Achievements regarding goals (1 and 2)*

The residence time for particles released far upstream in the Caravelas Estuary was found to be nearly 3 weeks for particles, regardless of whether they are released at high or low tide, and is driven by tidal dispersion combined with the discharge from the Cupído and Jaburuna Rivers (typical range of 4 to 9 m³ s⁻¹). These results are consistent with previous estimates derived from simple analytical solutions (Andutta et al., 2014), see Figure 10. For the Peruípe Estuary, our estimates of the residence time were for less than one week, due to the tidal dispersion combined with the larger river input from the Peruípe River (typical range of 20 to 70 m³ s⁻¹).

The transport timescales (exposure and residence times) were found to be quite similar for particles released in high tide under spring and neap tidal conditions, thus confirming previous estimations made for the Scheldt Estuary (de Brye et al., 2012). In contrast, the transport timescales were shown to be more sensitive to tidal-phase release time (i.e. high or low tides) in this estuarine system. Similar observations were made for the Scheldt Estuary (de Brauwere et al., 2011), in which there was a difference of days for results of residence time using particles released at high and low tides. This suggests that tidal-phase release time for a meso-tidal shallow estuary forced by low-moderate river discharge conditions is important for quantification of TTS, especially for water particles near mouths where larger tidal excursions are expected compared to locations further upstream, and since their initial movement would be upstream/downstream if released during low/high tide, respectively.

588 The Lagrangian simulation also showed that the narrow and shallow inter-connecting
 589 channel between the Peruípe and Caravelas estuaries allows **little** water exchange between the two
 590 estuaries, and only a few particles were capable of crossing the inter-connection passage with
 591 prevailing direction from the Peruípe to the Caravelas, in agreement with Schettini et al. (2013).
 592 Therefore, both exposure time and residence time were large at that location, and the exchange of
 593 water properties is likely to happen through alongshore currents at inner coastal areas.

594 • *Achievements regarding goal (3)*

595 Similarly to the exposure and residence times, the return coefficient was shown to be more
 596 sensitive to tidal phase (high and low tide), than to neap and spring tidal conditions. It may be
 597 summarized as follows: (1) the return coefficient is larger for particles released at high tide than at
 598 low tide; (2) the return coefficient is larger for particles released during spring tides than during
 599 neap tides.

600 For these two estuaries the exposure time was higher than the residence time in all
 601 simulations, thus showing that water may return to the system after having first crossed the mouth.
 602 The propensity of this water to return to the estuary was quantified using the return coefficient,
 603 which depends on the difference between the exposure and residence times, and thus also on the
 604 residual circulation due to river discharge, as well as the circulation in coastal waters. For instance,
 605 swift longshore currents decrease the difference between the exposure and residence times, and
 606 therefore reduce the return coefficient. The wind conditions over our measurement period were
 607 characteristic of calm weather, c.a. a few m s^{-1} (see Figure 4), and different scenarios may produce
 608 different results for the transport timescales, for **instance** under stronger north-northeastward
 609 alongshore currents which are often observed during the fall and winter months Lessa and Cirano
 610 (2006). Due to its definition, the return coefficient is predicted to be larger at the estuarine mouths,
 611 because the residence time tends to zero (see Equation 1). Our results have additionally shown that
 612 for our scenarios the difference between exposure and residence times ($\Theta - \varphi$) is nearly constant
 613 within our domain. This can also be observed from our analytical solution (Figure 12C).

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An assessment of transport timescales and return coefficient in adjacent tropical estuaries

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Abstract –

Transport timescales (TTS), namely residence time and exposure time, were computed for adjacent shallow meso-tidal tropical estuarines system using the Lagrangian model D-Waq Part coupled with the hydrodynamic model Delft3D-Flow, and the Constituent-oriented Age and Residence time Theory, CART. The main results are threefold: **(a)** The TTS differs more between releases at high or low tide than between those at spring and neap tides. The exposure time was also calculated and found to be larger than the residence time by a few days. **(b)** The exposure and residence times were used to evaluate the return coefficient (r) for different scenarios. As with residence and exposure times, the return coefficient was found to differ more between releases at high or low tide than between those at spring and neap tides. **(c)** For the Caravelas Estuary, where the river inflow was low ($\sim 4 \text{ m}^3 \text{ s}^{-1}$), the residence time was found to be much larger than for the Perúpe Estuary, where the river discharge was greater and nearly constant during the sampling period ($\sim 20 \text{ m}^3 \text{ s}^{-1}$). These results shows the importance of advection in decreasing TTS in the Perúpe Estuary compared to the Caravelas Estuary. The influence of the advection and dispersion agrees with previous simple estimates obtained using the newly modified Land Ocean Interaction Coastal Zone (LOICZ) model by Andutta et al. (2014).

Keywords: tropical estuary; residence time; exposure time; return coefficient; numerical model; hydrodynamics.

1. Introduction

Since the dynamics of most estuarine systems is relatively complex, studies of transport timescales (TTS) provide valuable insight into estuarine behaviour. Transport timescales represent a more holistic way of interpreting the flow in complex systems (e.g. Monsen et al. 2002), and allow us to understand how advective and dispersive mechanisms transport water.

Transport timescales are driven by the water currents, which in turn are influenced by sea level oscillation, bathymetry and the temperature and salinity fields. It is therefore necessary to have an accurate representation of these quantities in order to satisfactorily estimate transport timescales.

This article has the following tasks:

(1) to demonstrate, using a 3D hydrodynamic model combined with particle simulations, how release times (e.g. slack waters of high and low tides, neap and spring tides) affect the exposure time and residence time in a shallow meso-tidal tropical estuary.

(2) to compare TTS results from numerical modelling with estimates using the simple newly modified Land Ocean Interaction Coastal Zone (LOICZ) model by Andutta et al. (2014).

(3) to calculate and evaluate the return coefficient (r) numerically and analytically using CART. This is a measure of the propensity of a water parcel to return into the domain of interest after leaving it.

a. Overview of Transport Timescales

Since the pioneering work by Ketchum (1951) and Bolin and Rodhe (1973), the theory of TTS has evolved (e.g. CART, www.climate.be/cart), and other TTS definitions have been introduced in order to fill scientific gaps. Therefore, there are many different transport timescale definitions, e.g. flushing time (Ketchum, 1951; Fischer et al., 1979; Monsen et al., 2002), residence

time (Bolin and Rodhe, 1973; Monsen et al., 2002; Delhez et al. 2004; Deleersnijder et al., 2006), exposure time (Monsen et al., 2002), transit time (Holzer and Hall 2000), influence time (Delhez et al., 2014), age (Bolin and Rodhe, 1973; Monsen et al., 2002), e-folding flushing time (Monsen et al., 2002), turnover time (Sheldon and Alber, 2006) and renewal time (Andutta et al., 2014) – all of which have their own interpretation.

Two timescales, residence time and exposure time, are used to provide an indication of increase or decrease of non-reactive and reactive substances in estuaries, bays, lagoons, and atolls (Andutta et al., 2014). The residence time (Θ) is the time needed for a particle constituent to reach for the first time an open boundary of the domain of interest (e.g. Delhez et al., 2004). The exposure time (φ) is the time the particle will stay in the domain (e.g. Monsen et al., 2002) (Figure 2). Therefore, at a given time and location, the exposure time is always larger than or equal to the residence time. The larger the difference between the two timescales, the more often the particles tend to re-enter the domain of interest after leaving it for the first time. To evaluate the exposure time, the computational domain must be larger than the domain of interest (de Brauwere et al., 2011, de Brye et al., 2012). Estimates of these timescales may be obtained in an Eulerian or a Lagrangian framework. The latter often requires sufficiently large number of numerical particles in order to provide a result that statistically approaches the real condition.

A dimensionless return coefficient, r , represents the propensity of particles to return into the estuary after reaching an open boundary for the first time, as illustrated in Figure 1A (de Brauwere et al., 2011). It is defined as the relative difference between φ and Θ , i.e.

$$r = \frac{(\Theta - \varphi)}{\Theta} . \quad (1)$$

Clearly, this coefficient lies in the interval [0,1].

The larger the r the more likely it is that particles will re-enter the estuary after crossing one of its open boundaries for the first time. Accordingly, particles that never return into the estuary have $r = 0$, while particles returning often or for long periods of time have r close to unity.

Preferred position for figure 1

b. Chosen estuary and coastal area

The domain of interest is the estuarine System of the Caravelas and Peruípe Rivers (ESCP), in southern Bahia state, Brazil (see Figure 2); more details may be found in Appendix 1. It is located at the approximate latitude of $17^{\circ}50'S$, nearly 60 km from the National Maritime Park of Abrolhos, which is one of the largest reef structures of the Atlantic ocean, providing habitat for innumerable marine species. The ESCP has two main mouths: the Caravelas Estuary in the north ($17^{\circ}45'S$), with two small channels named Barra Velha (~1 km wide) and Tomba's Mouth (~600 m wide), and the Peruípe Estuary in the south ($17^{\circ}54'S$) with a funnel shape ranging in width from ~3500 m to ~700 m in the first few hundred meters. These two mouths are separated by a distance of ~25 km alongshore, and are internally connected by shallow and narrow channels around Cassurubá or Cassumba Island. Our simulations consider the domain shown in Figure 1C, for which results were computed according to the number of particles in the control domain with boundaries ω_1 and ω_2 .

Preferred position for figure 2

2. Methods

a. Numerical model

The ESCP comprises a number of channels varying significantly in width, from 60 m upstream to 1000 m near the mouth, and thus a high resolution mesh is necessary to resolve the many small channels in the domain. The numerical model used is the curvilinear-mesh, three-dimensional Delft3D-Flow from Deltares (www.deltares.nl). This model is hydrostatic, and its

111 equations are solved by the method of finite differences (Delft Hydraulics, 2008). A curvilinear
 112 mesh is appropriate for the domain, although there are some disadvantages in the horizontal
 113 resolution distribution compared to unstructured meshes. Delft3D's curvilinear mesh is efficient in
 114 minimizing noise due to the steps in the horizontal plane, and allows the mesh cells to follow the
 115 channels more easily compared to non-curvilinear quadrangular meshes. The degree of non-
 116 orthogonality between mesh elements is always smaller than 0.02 thus satisfying the criteria ($\cos \theta$
 117 < 0.02), which helps to preserve numerical stability of the simulations (Delft Hydraulics, 2008).
 118 The diagonal horizontal resolution ranges from ~ 20 m to ~ 300 m. The number of quadrangular
 119 mesh cells on the horizontal plane is 22,928. A lower resolution is applied in the coastal region
 120 $\sim [130-300]$ m, but this is increased toward the coast and the estuary $\sim [20-100]$ m (Figure 1B). The
 121 refined mesh within the estuary combined with high water speeds requires the time-step to be
 122 relatively small (around 1 second), to satisfy the Courant–Friedrichs–Lewy condition. The mesh
 123 used in the simulations of the ESCP (Figure 1B) is relatively complex, covering a small part of the
 124 Peruípe River, near the city of Nova Viçosa. This river is the main channel connecting the northern
 125 and southern mouths. The main tributaries of the Caravelas River, namely the Cupído and Jaburuna
 126 Rivers, are covered by the mesh. With 10 equally spaced sigma vertical layers, this mesh also
 127 covers a few kilometers of the adjacent coastal region.

128 The bathymetry in the estuarine channels was obtained using an Echo sounder and Global
 129 Position System. Two tide gauges were installed in Caravelas and Nova Viçosa (see locations A and
 130 C in Figure 2), meant to remove the tides from the Echo sounder data. For the Peruípe River
 131 estuary, the bathymetry was measured only in the first 6 km, near anchor station D. Thus an
 132 extrapolation was applied, considering the depth to be 4 meters for the next 14 km along the Peruípe
 133 River. The bathymetry was combined from these sources, and the triangular interpolation
 134 application in Delft3D-Flow was used. The bottom topography has depths ranging from ~ 0.2 m to a
 135 maximum of ~ 18 m (Tomba's Mouth), whilst in the coastal region do not exceed ~ 10 m.

A more detailed description of the field work carried out to obtain measurements of thermohaline properties and other parameters is provided in Appendix 2.

b. Model Boundary conditions, initial conditions and physical parameters

Rainfall and river discharge measurements in the Peruípe River are shown in Figure 3B. The river discharge data, obtained from the National Agency of Waters ANA (<http://www.ana.gov.br/>), was measured at a gauge station upstream of the river, at station Helvécia nº 55510000 (code 1739006). This station covers a large part of the drainage basin of the river. During rainy conditions the total drainage basin of the river may be used to estimate the total river flow to be applied at the upstream inflow boundary of the river. The factor to account for the missing drainage basin area is $\alpha = \frac{A_1 + A_2}{A_1} = 1.6$, in which station Helvécia $A_1 \sim 2,840 \text{ km}^2$, and the downstream area not covered by this gauge station is $A_2 \approx 1,760 \text{ km}^2$. The area values were obtained from the ANA (<http://hidroweb.ana.gov.br/>).

Data from the gauge station were also used to estimate the river discharge range for the Cupído and Jaburuna rivers. This was done by comparing their watershed areas with the watershed of the Peruípe river, and assuming homogeneous rainfall and evapotranspiration distributions over these areas (Andutta, 2011; Pereira et al., 2010). The total river flow into Caravelas Estuary was then roughly estimated using $Q = Q_P \beta$, where $\beta = 600/4600$ is the ratio between the catchment areas of the Caravelas (600 km^2) and the Peruípe ($A_1 + A_2 = 4600 \text{ km}^2$) rivers, and Q_P is the average discharge for the Peruípe). This estimation was adjusted by comparing observed flow velocities at locations A and B with model predictions.

The monthly estimate of fresh water inflow for the Peruípe River reveals small inflow for the dry season, often between June and September (see Figure 3C). The combined freshwater input from the Jaburuna and Cupído rivers estimated using the factor β is less than 10% of the river discharge into the Peruípe River. Because the field work was conducted during a relatively dry wet

161 season, when rainfall was negligible prior to and during measurements obtained in January 2008
 162 (Figure 3A), it is logical not to consider the application of the factor α at the Helvécia gauge
 163 station. Although this approach of river flow estimation is not required, the technique described
 164 above would be required under homogeneous rainfall conditions over the drainage basin of the
 165 Peruípe, Jaburuna and Cupído rivers.

166 The best fit between observations and model results was obtained using the mean river
 167 discharge shown in Table 1 for the Cupído and Jaburuna rivers, and the daily measurements shown
 168 in Figure 3B for the Peruípe River. In other words, the value measured at Helvécia gauge station
 169 was used in the simulation with additional tuning to extrapolate results for the other two smaller
 170 rivers.

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172 **Preferred position for figure 3**

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176 **Preferred position for Table 1**

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178 The measurements from this tide gauge were compared with the simulation results during
 179 neap and spring tides using the “Skill” method described below. In addition, a qualitative
 180 comparison was carried out between the axial salinity distribution found in the simulations, and the
 181 observed distribution presented in Schettini and Miranda (2010).

182 We used the initial condition of a homogeneous thermohaline distribution for the salinity (30
 183 practical salinity unit - psu) and temperature (27 °C). The spin up simulation was made for about
 184 two months to obtain a dynamic equilibrium condition. Since the temperature has previously been
 185 found to be nearly homogeneous in this estuary (Andutta, 2011), its mean value was used for all
 186 simulations. The first flow field and salinity distribution, obtained from the equilibrium condition,

187 was used to provide a varied initial field for simulations starting at slack waters in both spring and
 188 neap tidal conditions.

189 Computational modellers often assume that vertical eddy diffusion and viscosity coefficients
 190 vary in time, by using turbulent closure models, e.g. algebraic, *k-L*, *k-Epsilon* schemes. On the other
 191 hand, the horizontal eddy diffusivity, K_h , and horizontal viscosity coefficients, K_v , are often
 192 estimated according to the mesh element size (Okubo, 1971). Therefore, modellers need to choose a
 193 parameterisation scheme that provides the right amount of mixing in the estuary. We have
 194 considered the parameterisation of horizontal eddy viscosity by Uittenbogaard et al. (1992), which
 195 is available in Delft3D-Flow and reproduces well the turbulent fluxes of momentum.

196 The best fit between results and simulations was obtained assuming the horizontal eddy
 197 diffusivity, K_h , to be in the range of $\sim[2-30] \text{ m}^2 \text{ s}^{-1}$ with small and large values applied respectively
 198 to small and large mesh cells. The sensitivity analysis for K_h , was conducted following Okubo
 199 (1971). Because Okubo's formula applies for open-water, it was observed that it was not properly
 200 simulating the true dispersion in the estuary, thus a factor f was used to increase and decrease
 201 mixing at the sub-grid scale (See Equation 2). Varying f allowed us to achieve the best fit between
 202 measurements and model results.

$$203 \quad K_h = f [2.05 \times 10^{-4} \times d^{1.15}] \quad (2)$$

204
 205 where d is the mesh cell size (from ~ 20 to ~ 300 metres), and f is the factor set to different values
 206 but only shown for 2, 100, 150, 200, 250, 400 and 2000 in the sensitivity analyses (see Table 3).

207 The *k-Epsilon* turbulent closure scheme was used to compute values for the vertical viscosity
 208 and diffusivity. We assumed the typical Manning roughness coefficient of $(0.02 \text{ m}^{-1/3} \text{ s})$, which
 209 characterises the higher percentage of local sediment (Souza et al., 2013). This resulted in a Chézy
 210 coefficient of $\sim 40 \text{ m}^{-1/2}/\text{s}$. Wind speed and directions, assumed to be constant over this small region,
 211 were obtained at the Caravelas station from the Instituto Nacional de Meteorologia INMET (code
 212 INMET 86764), at (source: <http://www.inmet.gov.br/portal/>), see Figure 4.

Preferred position for figure 4

The wind was assumed to only affect mesh cells in coastal areas. In other words, the wind stress did not affect mesh cells inside the estuarine channels. Moreover, Andutta et al. (2013) applied Hansen and Rattray's analytical equation of the velocity and salinity components, and demonstrated that the wind effect in January 2008 was negligible at station C (near Nova Viçosa estuarine mouth), which is the closest to the coast. Hansen and Rattray's analytical solution required an adjustment of no more than 0.02 Pascal for the wind stress, which correspond to wind speeds of $\sim 3 \text{ m s}^{-1}$ (Andutta et al., 2013). South-southwestward alongshore currents occur between October and January, while north-northeastward alongshore currents are observed during the fall and winter months Lessa and Cirano (2006).

Sea level data from TOPEX were used to force tides at the open boundary nodes. A time series of water surface elevation from May to July 2007 was recorded at Terminal Aracruz (TA in Figure 2), which is a few kilometers away from the coastal open boundary. At TA a total of 16,264 tidal measurements were recorded at five minute intervals, and were processed using the tidal component extraction program PACMARÉ (Franco, 2000). These tidal measurements were used to obtain the amplitude and phase of the main tidal components, shown in Table 2. Additionally, sea-level data were recorded at stations A and C from 14th to 19th of January 2008, and these data were used to validate modelled sea-level oscillation (comparison shown in Results and Discussion section). Sea surface elevation observations from sites A and C showed the same phase, strongly suggesting that tides propagate across the shelf, because tides propagating along the coast would results in a phase shift between sea level observations at sites A and C (see Figure 2). The measurements of tidal heights of $\sim 1 \text{ m}$ and $\sim 3 \text{ m}$ during neap and spring tides, respectively. This ranks as meso-tidal, according to the criteria of Davies (1964) for tidal classification. From the tidal heights shown in Table 3, the tidal form-number is $[N_f = (K_1 + O_1) / (M_2 + S_2) = 0.19]$, indicating a semidiurnal tidal estuary (Defant, 1960). The tidal components from Table 2 represent over 97% of sea level variations for the estuarine system (Andutta, 2011).

Preferred position for Table 2

d. Model validation criteria

In order to quantify the agreement between the simulated velocity and salinity profiles the method suggested by Wilmott (1981), based on the Skill parameter was used. Accordingly, the skill is measured as follows

$$Skill = 1 - \frac{\sum |X_{\text{mod}} - X_{\text{obs}}|^2}{\sum \left(|X_{\text{mod}} - \bar{X}_{\text{obs}}| + |X_{\text{obs}} - \bar{X}_{\text{obs}}| \right)^2}, \quad (3)$$

where X_{obs} and X_{model} denote the observational and simulated properties, respectively, $\bar{X}_{\text{obs}}$ being the mean observational values. The Skill parameter varies from 1 to zero, with 1 indicating the best fit, and zero indicating a complete disagreement between observation and model results.

e. Modelling approach to calculate the Transport Timescales

To quantify the residence time and exposure time 35 thousand numerical particles were released in the estuary by coupling D-Waq PART with results from the Delft3D-FLOW (i.e. within the subdomain denoted ω). Numerical particles were deployed near the bottom and top layers. The particle concentration using conservative tracer module was normalized to value 1 within the volume of ω . Therefore, the number of particles decreases when particles exit ω , and increases when particles re-enter ω . The minimal initial number of particles, i.e. 25 thousand, was computed considering a minimum thickness of 2 m and a grid cell of ~ 20 by 10 meters.

A total of four simulation scenarios were made: (S_1) particle released at high water in neap tide, (S_2) particle released at low water in neap tide, (S_3) particle released at high water in spring tide, and (S_4) particle released at low water in spring tide.

In order to be consistent with CART timescales, for the computation of the residence time, particles are discarded once they have reached an open boundary, e.g. estuarine head or an open

boundary in coastal waters (de Brauwere et al., 2011; de Brye et al., 2012). The arithmetic mean of the individual residence times, φ , was computed as the time necessary for particles to exit the domain (ω) for the first time. As for the exposure time, the particles are assumed to immediately bounce back into the domain only at estuarine heads. This simplifying hypothesis is unlikely to entail any major error, since a particle crossing the upstream estuarine boundary in the upstream direction (because of diffusive processes) will most likely return into the estuary after a relatively small time under the influence of the river flow, e.g., the St. Johans River in Florida, which experiences backflows over significant durations (Hendrickson et al., 2003).

Results from residence and exposure times were used to estimate the return coefficient distribution. The residence and exposure times may vary according to the time of release, such as during neap/spring tides or high/low tides, and this would also affect the return coefficient. This notwithstanding, results of exposure and residence times must be calculated for the same conditions when computing the return coefficient, i.e. $r = (\Theta - \varphi) / \Theta$.

277

278 *f. The modified LOICZ analytical model*

The modified LOICZ model of Andutta et al. (2014) applies the salinity balance proposed by Fischer et al. (1979) into the original formulation of the LOICZ. This water renewal timescale model has been shown to be sensitive to changes to some of its free parameters (e.g. river flow and salinity gradient). We expect that the estimates of the timescales from our numerical results would fit within the ranges derived from the LOICZ model. Details of its derivation are provided in Andutta et al. (2014); however we provide the simplified relation for water renewal timescale.

285

$$286 \quad \frac{1}{T_p} = \frac{1}{T_1} + \frac{1}{T_2}, \quad (4)$$

287

where $T_1 = L/U$ and $T_2 = L^2/K$ are the advective and dispersive timescales, respectively. L , U , K and T_p are respectively the selected estuarine segment length, the flow speed, the characteristic value of the longitudinal diffusivity and the water renewal timescale. This expression may be re-

290

291 written in terms of the dimensionless Péclet number $Pe = ULK^{-1}$, the ratio $P_e = T_2/T_1$ of the
 292 dispersive to the advective timescale. Similarly, this number provides a comparison of contributions
 293 from advective and dispersive processes to transport timescales, yielding

294

$$295 \quad T_P = \frac{VP_e}{Q_R(1 + P_e)}. \quad (5)$$

296 Where V and Q_R denote the estuarine volume and river discharge, respectively. The contribution of
 297 advection to the total water renewal timescale T_P , θ ($0 \leq \theta \leq 1$), is given by

$$298 \quad \theta = T_P/T_1 = Q_R/(Q_R + Q_D), \quad (6)$$

299

300

301 where Q_D is the discharge. Equations (4) and (6) were used to generate the advective-dispersive
 302 diagram (shown later), whose results will be compared to the numerical results.

303

304 *g. The CART analytical model*

305 As previously mentioned, in the framework of CART, the TTS that may be used to calculate
 306 water renewal rates can be obtained at any time and position as the solution of partial differential
 307 equations (Deleersnijder et al., 2006; de Brye et al., 2012; Andutta et al., 2014). For instance,
 308 residence time and exposure time were estimated using calibrated/validated numerical simulations
 309 for the Scheldt Estuary (de Brauwere et al. 2011, de Brye et al. 2012). As an easy acceptable
 310 method, analytical solutions may provide results that are representative of real situations (e.g.
 311 CART and LOICZ). The idealised CART timescales were used to obtain the exact analytical
 312 solution of the so called return coefficient for the ESCP. Different values of the Péclet number were
 313 considered, in order to assess the axial variation of return coefficient values. The advective
 314 timescale, $T_1 = V/Q_R$, and a dispersive timescale, $T_2 = P_e V/Q_R$, are defined taking into consideration
 315 the estuarine volume V . Andutta et al. (2014) provides a detailed description depicting an idealized
 316 channel for the time scales.

318 Consider an estuarine channel ($-\infty < x < \infty$) with a constant cross-sectional area A , and a
 319 flow under steady-state. The volumetric flow rate is denoted as Q_R . The downstream and upstream
 320 boundaries of our idealised estuary are located at $x = L_0$ and $x = L_1$, respectively. The estuarine
 321 length is $L = L_0 - L_1$, and thus the volume is $V = AL$. The water velocity is then
 322 $U = Q_R / A = LQ_R / V$. For the abovementioned conditions, the residence time satisfies the adjoint
 323 of the classical passive tracer transport equation (Delhez et al. 2004, Andutta et al. 2014), i.e.

324

$$325 \quad \frac{d}{dx} \left(AK \frac{d\varphi}{dx} + Q_R \varphi \right) = -A \quad (7)$$

326

327 where, x , denotes the particle position. The solution for the equation needs to satisfy the upstream
 328 and downstream boundary conditions,

329

$$330 \quad \varphi(L_1) = 0 = \varphi(L_0). \quad (8)$$

331

332 It represents the average time required by particles initially located in the interval $[x, x + \delta x]$
 333 (with $\delta x \rightarrow 0$) to reach one of the open boundaries. The solution is then easily derived:

334

$$335 \quad \varphi(x) = \frac{V}{Q_R} \left(1 - \frac{\xi}{L} \right) + \frac{V}{Q_R} \left(\frac{e^{-Pe} - e^{-Pe \xi/L}}{1 - e^{-Pe}} \right) \quad (9)$$

336 where $\xi = x - L_1$.

337 The exposure time was also derived (Andutta et al., 2014), and is defined in the domain of interest
 338 and its surrounding environment.

$$339 \quad -\infty \leq x \leq L_1 \quad : \quad \Theta(x) = \frac{V}{Q_R} \quad (10a)$$

$$340 \quad L_1 \leq x \leq L_0 \quad : \quad \Theta(x) = \frac{V}{Q_R} \left(1 - \frac{\xi}{L} \right) + \frac{V}{Q_R} \left(\frac{1 - e^{-Pe \xi/L}}{Pe} \right) \quad (10b)$$

$$341 \quad L_0 \leq x < \infty \quad : \quad \Theta(x) = \frac{V}{Q_R} \left(\frac{e^{-Pe} - 1}{Pe} e^{-Pe \xi/L} \right) \quad (10c)$$

From Equations (9) and (10), which are valid within the upstream and downstream open boundaries, the return coefficient is:

$$r = \frac{\Theta(x) - \varphi(x)}{\Theta(x)} = \frac{\left(\frac{1 - e^{-Pe \zeta/L}}{Pe} \right) - \left(\frac{e^{-Pe} - e^{-Pe \zeta/L}}{1 - e^{-Pe}} \right)}{\left(1 - \frac{\zeta}{L} \right) + \left(\frac{1 - e^{-Pe \zeta/L}}{Pe} \right)} \quad (11)$$

Note that r is bounded by $[0,1]$, as mentioned before.

In principle, the residence time and the exposure time can be obtained by solving classical passive transport equations. However, to do so, time- and position-dependent concentrations must first be obtained and, then, time and space integral must be performed to derive the relevant timescales. This is not straightforward, even for highly idealised flows. This is why it is preferable to have recourse to the adjoint method established by Delhez et al. (2004), which requires the solution of simpler differential problems to be determined: in the present case, only ordinary differential equations are to be dealt with rather than partial differential ones. The disadvantage of this approach is that the theoretical underpinning of an adjoint model sometimes appears elusive, which is probably the reason why Errico (1997) wrote a general, enlightening paper on this matter, explaining the nature and purpose of adjoint models.

3. Results and Discussion

a. Model calibration of salinity, velocity and tides

We carried out a sensitivity analysis considering different values for the horizontal diffusion coefficient k_h using Equation 2. These adjustments of factor f for the horizontal diffusivity based on the grid size allowed us to obtain a proper representation of the salinity field and its time variability.

Preferred position for Table 3

The mean Skill parameters for the simulation are shown in Table 3 for different values of factor f , which was described with Equation 2. The comparison of sea-level oscillation over a tidal modulation period, from the 14th to the 29th of January 2008, showed good skill values for locations A (Figure 5) and C (not shown), and the Skill parameter for tides was calculated to be over 0.97 for both locations, i.e. A and C. The comparison of tides, velocity, and salinity showed good skill values during spring tides (not shown), and reasonable values during neap tides (Figure 6).

Preferred position for figure 5
Preferred position for figure 6

The Skill parameter for the water column height variation in time was calculated to be over 0.98 for all the sites under neap and spring tides (Table 4), and the tidal ranges were ~1.0 m and ~2.5 m for neap and spring tides, respectively. Observations have shown that the tidal phase between sites A (Caravelas mouth) and C (Peruípe mouth) is almost the same. The similarity of their phases indicates that tides propagate mainly perpendicular to the coast line in this region, a result which is in close agreement with observations previously reported by Lessa and Cyrano (2006).

For the modeled velocity validation, good results (Skill from 0.77 to 0.93) were obtained in spring tides in the estuaries of Caravelas (sites A and B) and Nova Viçosa (sites C and D). For neap tides due to small differences on tidal asymmetry, the Skill was lower, at ~ 0.6.

The model agreed well with observations of maximum ebb and flood currents at site A. The model also properly simulated the velocity profiles for sites B, C, and D. Therefore, the description of maximum ebb and flood currents from in-situ data also apply to the model simulations. At site B there were maximum speeds of ~0.5 m s⁻¹ and 1.0 m s⁻¹ (ebb events), and ~-0.3 m s⁻¹ and ~-0.6 m s⁻¹ (flood events), during neap and spring tides, respectively. For site A the vertical shear of the velocity was negligible in flood and ebb conditions, while for site B there was a small vertical shear of the horizontal velocity during ebb events. During flood events, the water velocity was homogenous over the water column. In addition, a residual velocity of ~0.05 m s⁻¹ was calculated at

394 site B, indicating a residual circulation from Nova Viçosa towards the Caravelas River. Site A had a
 395 residual current of $\sim 0.06 \text{ m s}^{-1}$, indicating a small discharge from the Cupído and Jaburuna Rivers.
 396 At sites C and D, located in the Peruípe River, the downstream velocities showed more intensity
 397 than observed in the Caravelas Channel. For site C the downstream velocities varied from $\sim -0.9 \text{ m}$
 398 s^{-1} to $\sim -1.5 \text{ m s}^{-1}$, for neap and spring tides, respectively. During flood events, the velocities were $\sim$
 399 0.3 m s^{-1} and $\sim -0.7 \text{ m s}^{-1}$, for neap and spring tides, respectively. At site D the maximum
 400 downstream velocities were only $\sim 0.7 \text{ m s}^{-1}$ and $\sim 1.0 \text{ m s}^{-1}$ at neap and spring tides, and upstream
 401 velocities were $\sim -0.3 \text{ m s}^{-1}$ and $\sim -0.4 \text{ m s}^{-1}$. The residual velocities at sites C and D, which have
 402 values of $\sim 0.10 \text{ m s}^{-1}$ to $\sim 0.15 \text{ m s}^{-1}$, indicate a higher advective contribution from the Peruípe River
 403 compared with the Caravelas estuary.

404 In addition to the tides and the velocity field, the model simulated the temporal variation of
 405 the salinity well for all sites (A, B, C, and D). During spring tides the calculated Skill values were
 406 over 0.83, while for neap tides they were over 0.73 (Table 4). At the Caravelas estuarine channel,
 407 $\sim 3 \text{ km}$ near the mouth (site A), during low tide, salinity was observed in intervals of $\sim 34.5 \text{ psu}$ to
 408 $\sim 35.0 \text{ psu}$ and $\sim 34.0 \text{ psu}$ to $\sim 34.5 \text{ psu}$ for the observational and theoretical results,
 409 respectively. About 6 km away from the mouth we obtained a good agreement for the salinity, with
 410 $\sim 32.0 \text{ psu}$ and $\sim 32.5 \text{ psu}$ for observation and simulation, respectively. In the vicinity of the
 411 interconnection with Cupído and Jaburuna Rivers (site B), which is about 12 km upstream from the
 412 mouth, the salinity decreased to $\sim 30.0 \text{ psu}$ and $\sim 28.5 \text{ psu}$ for the observational and calculated
 413 results, respectively. At high tide, near the mouth (site A) and at a distance of 6 km from the mouth,
 414 the salinity was $\sim 36.5 \text{ psu}$ and $\sim 36.0 \text{ psu}$, respectively, for both simulation and field measurements.
 415 In the upper reaches of the estuary, near the junction of the rivers, Cupído and Jaburuna ($\sim 12 \text{ km}$
 416 from the mouth), a close agreement between simulated and observed salinity values ($\sim 33.0 \text{ psu}$) was
 417 obtained at high tide. Along the Peruípe River estuary at neap tides, the surface salinities vary in the
 418 range of 20.0 psu to 34.0 psu at the surface, and 32.5 psu to 36.0 psu near the bottom. The region of
 419 Nova Viçosa has more vertical stratification of the salinity than at sites A and B in the Caravelas

420 River. This is due to Peruípe River's larger freshwater discharge. The observed value of ~36.0 psu
 421 near the bottom is characteristic of the Tropical Water Mass, which was already reported to enter
 422 this estuarine system (Schettini et al., 2010). During spring tides the vertical mixing causes the
 423 erosion of the halocline, and thus decreases vertical stratification. This results in a smaller vertical
 424 variation of 31.0 psu to 36.0 psu from the surface to the bottom.

425 **Preferred position for Table 4**

426 A comparison of the axial distribution of salinity was made for the Caravelas River (Figure
 427 7A,B). For the first 12 km along the estuarine channel, results from simulations were compared to
 428 observations made by Schettini and Miranda (2010). The measurements were obtained on the 10th
 429 of April, 2001 during spring tides. Although the field data are likely to be from different conditions
 430 of river flow, the simulation showed a good correlation of the axial distribution of the salinity in the
 431 Caravelas River (See Figures 7C and 7D), with values of $R^2 \sim 0.97$ and $R^2 \sim 0.99$ for low and high
 432 tides respectively. This indicates that the model has well represented the mixing processes in the
 433 Caravelas Estuary. During low tide (Figure 7A,C), a good agreement is found near the mouth, with
 434 salinity values of ~35.2 psu and ~34.5 psu, for the model results and observations, respectively. At
 435 nearly 6 km upstream, there is still a good agreement ($R^2 \sim 0.99$) with the salinity values of ~33
 436 psu (model), and ~32 psu (observation). Further upstream and near the inter-connection between the
 437 Cupído and Jaburuna rivers (i.e. ~12 km upstream), the agreement is slightly poorer with the
 438 salinity values of ~30 psu (model) and ~29 psu (observation). At high tide (Figure 7B, D), the
 439 model predicted the longitudinal salinity variations well along the Caravelas Channel. The salinity
 440 values near the mouth were ~36.4 psu (model and observation), and reduced to ~36 psu 6 km
 441 further upstream. Moreover, during high tides the agreement was also good near the channel
 442 between the Cupído and Jaburuna rivers with salinity of ~33 psu.

443 **Preferred position for figure 7**

444
 445 *b. Results of the residence time, the exposure time and the return coefficient*

446

447 The transport timescales, namely residence time (φ), exposure time (Θ), and the return
 448 coefficient (r), were estimated for the Caravelas and Peruípe estuarine channels with simulation
 449 under different scenarios, i.e. S_1 to S_4 (Figures 8, and 9).

450 For scenarios S_1 and S_3 (Figure 8), the residence time along the Caravelas Channel, from the
 451 mouth to 12 km upstream, was found to vary from 0 to ~ 15.0 days. The inflow boundaries of the
 452 Cupído and Jaburuna rivers were found to have residence times of ~ 27 and ~ 22 days, respectively.
 453 For the Peruípe Channel the residence times ranged from 0 to ~ 7.4 days, from the mouth to 5 km
 454 upstream, with a maximum value of ~ 18 days at the inflow boundary of the Peruípe Estuary.

455 The residence time estimated at ~ 6 km further upstream in the Caravelas Estuary ($\varphi = 11.7$
 456 days) is almost three times larger than the residence time calculated for the same distance along the
 457 Peruípe Estuary ($\varphi < 4.4$ days). The difference between results in the Caravelas and the Peruípe
 458 estuaries is due to the larger velocity contribution in the Peruípe Estuary.

459 Comparing scenarios S_1 and S_3 , the residence time was found to be slightly lower for S_3 (c.a.
 460 a few hours) and this difference is due to increased diffusive contribution during stronger spring
 461 tidal conditions. In contrast to scenarios S_1 and S_3 , the simulations considering scenarios S_2 and S_4
 462 yielded an increased residence time. This increase was maximum near the estuarine mouths (~ 5
 463 days), and observed to reduce in the upstream direction (few hours). The increase in residence time
 464 for particles released in slack water of low tide is caused by tidal excursion from reversing currents
 465 (i.e. flood currents). These results reflect and add value to recent simulations by de Brye et al.
 466 (2012) for the Scheldt Estuary (in Belgium and the Netherlands), whose results showed larger
 467 residence time values for particles released at slack water of low tides than for high tides (difference
 468 of a few days).

469 The virtual Lagrangian particles showed that a negligible number of particles crossed the
 470 connecting channel between the Caravelas (ω_1) and Peruípe Estuaries (ω_2), which indicates that this
 471 relatively narrow and shallow interconnection channel allows little exchange of water properties
 472 between these estuaries. Moreover, the residence time is observed to be larger within the

enlargement of the interconnecting channel between these two estuaries. Schettini and Miranda (2010) and Schettini et al. (2013) have addressed the importance of the interconnection channel between Caravelas and Peruípe, and found that sediment deposited near the Caravelas mouth was both inner shelf local resuspension and upstream transport, or sourced from the Peruípe River via the interconnection channel.

Preferred position for figure 8

Exposure time results showed that particles re-entered the system for up to two days (Figure 9). Note that the difference between the exposure time and the residence time ($\Theta - \varphi$) showed little spatial variation for scenarios S_1 and S_3 .

Preferred position for figure 9

The spatially averaged difference between exposure and residence times ($\Theta - \varphi$) are calculated in days, and its respective RMSE to be $\sim 1.98 \pm 0.06$ for S_1 , $\sim 1.87 \pm 0.12$ for S_2 , $\sim 1.92 \pm 0.07$ for S_3 , $\sim 2.19 \pm 0.08$ for S_4 . These results strongly suggest that ($\Theta - \varphi \sim \text{const.}$) for the ESCP under the four different scenarios considered. The results also suggest that $t_3 - t_2$ varies little away from the open boundaries, so particles deployed at different times and locations in the estuary re-enter for similar lengths of time, assuming the circulation in coastal waters does not considerably change over time due to additional forcings, e.g. sudden alongshore wind driven currents.

Equation (5) was used to estimate the range of water renewal timescales for the Caravelas and Peruípe estuaries using the parameters given in the appendices of Andutta et al. (2014), see Figure 10. The straight line labelled θ (lowercase) indicate the relative advective contribution to water renewal, where $0 \leq \theta \leq 1$. The line at $\theta = 0.5$ separates the areas where transport is dominated by advection (diagram upper zone, $\theta > 0.5$) and dispersion (diagram lower zone, $\theta < 0.5$).

The Caravelas and Peruípe estuaries have mean depths of ~ 6.5 and ~ 7.5 meters, respectively, and the maximum and minimum tidal ranges in these estuaries are ~ 2.5 and ~ 0.5

501 meters. According to Andutta et al. (2013), these tidal ranges combined with the relatively the small
 502 depths result in a high rate of change of the potential energy ($\sim 6.1 \text{ J m}^{-3} \text{ s}^{-1}$), which contributes
 503 towards large dispersion. It is valid to compare these results to the Sheldt Estuary, where tidal
 504 oscillation is typically 4-5 meters along the first $\sim 100 \text{ km}$, and where the mean water depth is ~ 10
 505 meters. Tidal range in the Sheldt can reach $\sim 7 \text{ m}$, which is about 45% of the mean water depth
 506 value for the first $\sim 25 \text{ km}$ near the estuarine mouth (Soertaert and Herman, 1995; de Brye et al.
 507 2012), and this system is classified as well-mixed due to dispersion prevailing over advection. The
 508 numerical results for the ESCP fit within the timescale ranges estimated using the simple LOICZ
 509 method.

510
 511 **Preferred position for figure 10**
 512

513 The return coefficient cannot be calculated using the modified LOICZ model. However, it
 514 was computed numerically and compared to the non-dimensional solution obtained using CART.
 515 The return coefficient converges to one at the estuarine mouths and near estuarine heads (Figure 11,
 516 for all scenarios S_1 to S_4 and Figure 12B). However, this is only a direct consequence of the
 517 definition of the residence time, which converges to zero at the entrance, and thus the return
 518 coefficient will always increase towards unity. r was observed to be smaller upstream, because the
 519 ratio $(\Theta - \varphi)/\Theta$ is likely to decrease. It can be noticed that the axial variation of the return
 520 coefficient is similar for both CART solution and numerical approach (Figures 11 and 12C). The
 521 return coefficient calculated from CART and from numerical simulations is observed to increase
 522 towards the upstream boundary. This increase towards the estuarine head is due to the boundary
 523 condition assumed in the analytical and numerical solutions, where particles do not re-enter the
 524 domain after crossing the estuarine head, although in a real estuary water particles would re-enter
 525 through the estuarine head due to river flow conditions.

526 Figure 12A shows results of the residence and exposure time and return coefficient for a
527 range of values of the Péclet number. High values of the Péclet number yield a boundary layer in
528 the vicinity of the upstream location.

529 The greater the relative importance of advection, the less likely it is that dispersion will
530 cause a water particle to hit the upstream boundary of the domain ($x = L_0$). In accordance with their
531 definitions, the exposure time is larger than the residence time for any location in the domain ($L_1 \leq$
532 $\xi/L \leq L_0$). These idealised results of the return coefficient were used to access results obtained
533 from our numerical simulations.

534

Preferred position for figure 11

Preferred position for figure 12

In the illustration shown in Figure 11A, the ratio is simply the difference between times t_3 and t_2 . Evidently this is a simple case where the particle is assumed to have re-entered the domain only once.

Particles are expected to first cross the estuarine mouth during ebb currents, which would be alternating with flood currents and dispersive processes. Therefore, we could presume that Lagrangian particles would have a time window of ~ 6.5 hours to cross the entrance (for semi-diurnal tidal estuaries), and this time window would then close for ~ 6.5 hours (the period of flood currents).

Our simulations were for relatively calm weather conditions, which were predominant over the region, c.a. wind speeds in the range $1\text{--}4\text{ m s}^{-1}$ (wind from NE). Andutta et al. (2013) showed that wind conditions did not affect the water circulation in this estuarine system in January 2008. However, for stronger wind conditions the results would not be the same. Evidently alongshore wind-driven currents would reduce the difference between the exposure time and the residence time, and the return coefficient would thus decrease towards zero. This is because alongshore currents inhibit the propensity of particles to re-enter the estuarine system. The alongshore shelf currents are observed to be driven by the N-S migration of the South Atlantic High between summer and winter. South-southwestward alongshore currents occur between October and January, while stronger north-northeastward alongshore currents are observed during the fall and winter months (Lessa and Cirano, 2006).

4. Conclusions

Overall goal

This study provides the first estimates of the residence time, exposure time and the return coefficient for the Caravelas and Peruípe estuaries and might be a reference for future studies related to the control of pollutants and sediment transport. These transport timescales were estimated using a Lagrangian model only as a tool, and this model has been properly calibrated and validated using field data.

Specific conclusions

- *Achievements regarding goals (1 and 2)*

The residence time for particles released far upstream in the Caravelas Estuary was found to be nearly 3 weeks for particles, regardless of whether they are released at high or low tide, and is driven by tidal dispersion combined with the discharge from the Cupído and Jaburuna Rivers (typical range of 4 to 9 m³ s⁻¹). These results are consistent with previous estimates derived from simple analytical solutions (Andutta et al., 2014), see Figure 10. For the Peruípe Estuary, our estimates of the residence time were for less than one week, due to the tidal dispersion combined with the larger river input from the Peruípe River (typical range of 20 to 70 m³ s⁻¹).

The transport timescales (exposure and residence times) were found to be quite similar for particles released in high tide under spring and neap tidal conditions, thus confirming previous estimations made for the Scheldt Estuary (de Brye et al., 2012). In contrast, the transport timescales were shown to be more sensitive to tidal-phase release time (i.e. high or low tides) in this estuarine system. Similar observations were made for the Scheldt Estuary (de Brauwere et al., 2011), in which there was a difference of days for results of residence time using particles released at high and low tides. This suggests that tidal-phase release time for a meso-tidal shallow estuary forced by low-moderate river discharge conditions is important for quantification of TTS, especially for water particles near mouths where larger tidal excursions are expected compared to locations further upstream, and since their initial movement would be upstream/downstream if released during low/high tide, respectively.

588 The Lagrangian simulation also showed that the narrow and shallow inter-connecting
 589 channel between the Peruípe and Caravelas estuaries allows little water exchange between the two
 590 estuaries, and only a few particles were capable of crossing the inter-connection passage with
 591 prevailing direction from the Peruípe to the Caravelas, in agreement with Schettini et al. (2013).
 592 Therefore, both exposure time and residence time were large at that location, and the exchange of
 593 water properties is likely to happen through alongshore currents at inner coastal areas.

594 • *Achievements regarding goal (3)*

595 Similarly to the exposure and residence times, the return coefficient was shown to be more
 596 sensitive to tidal phase (high and low tide), than to neap and spring tidal conditions. It may be
 597 summarized as follows: (1) the return coefficient is larger for particles released at high tide than at
 598 low tide; (2) the return coefficient is larger for particles released during spring tides than during
 599 neap tides.

600 For these two estuaries the exposure time was higher than the residence time in all
 601 simulations, thus showing that water may return to the system after having first crossed the mouth.
 602 The propensity of this water to return to the estuary was quantified using the return coefficient,
 603 which depends on the difference between the exposure and residence times, and thus also on the
 604 residual circulation due to river discharge, as well as the circulation in coastal waters. For instance,
 605 swift longshore currents decrease the difference between the exposure and residence times, and
 606 therefore reduce the return coefficient. The wind conditions over our measurement period were
 607 characteristic of calm weather, c.a. a few m s^{-1} (see Figure 4), and different scenarios may produce
 608 different results for the transport timescales, for instance under stronger north-northeastward
 609 alongshore currents which are often observed during the fall and winter months Lessa and Cirano
 610 (2006). Due to its definition, the return coefficient is predicted to be larger at the estuarine mouths,
 611 because the residence time tends to zero (see Equation 1). Our results have additionally shown that
 612 for our scenarios the difference between exposure and residence times ($\Theta - \varphi$) is nearly constant
 613 within our domain. This can also be observed from our analytical solution (Figure 12C).

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Figure 1

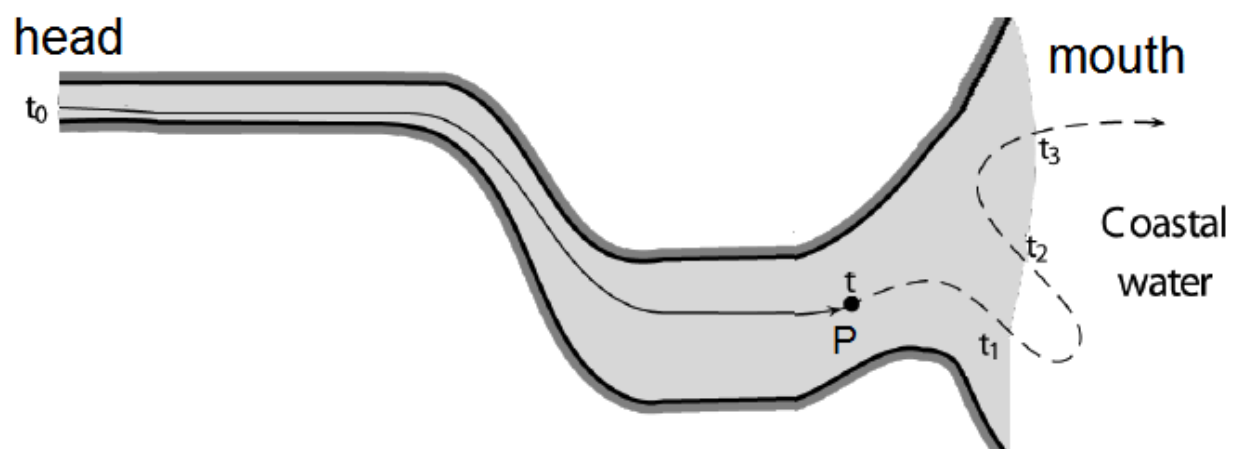


Figure 1 –Path of a particle in the estuary from the upstream boundary (head) to the downstream boundary (mouth). For a particle initially at position P at time t , the residence time is $t_1 - t$, the exposure time is $(t_3 - t_2) + (t_1 - t)$.

Figure 2

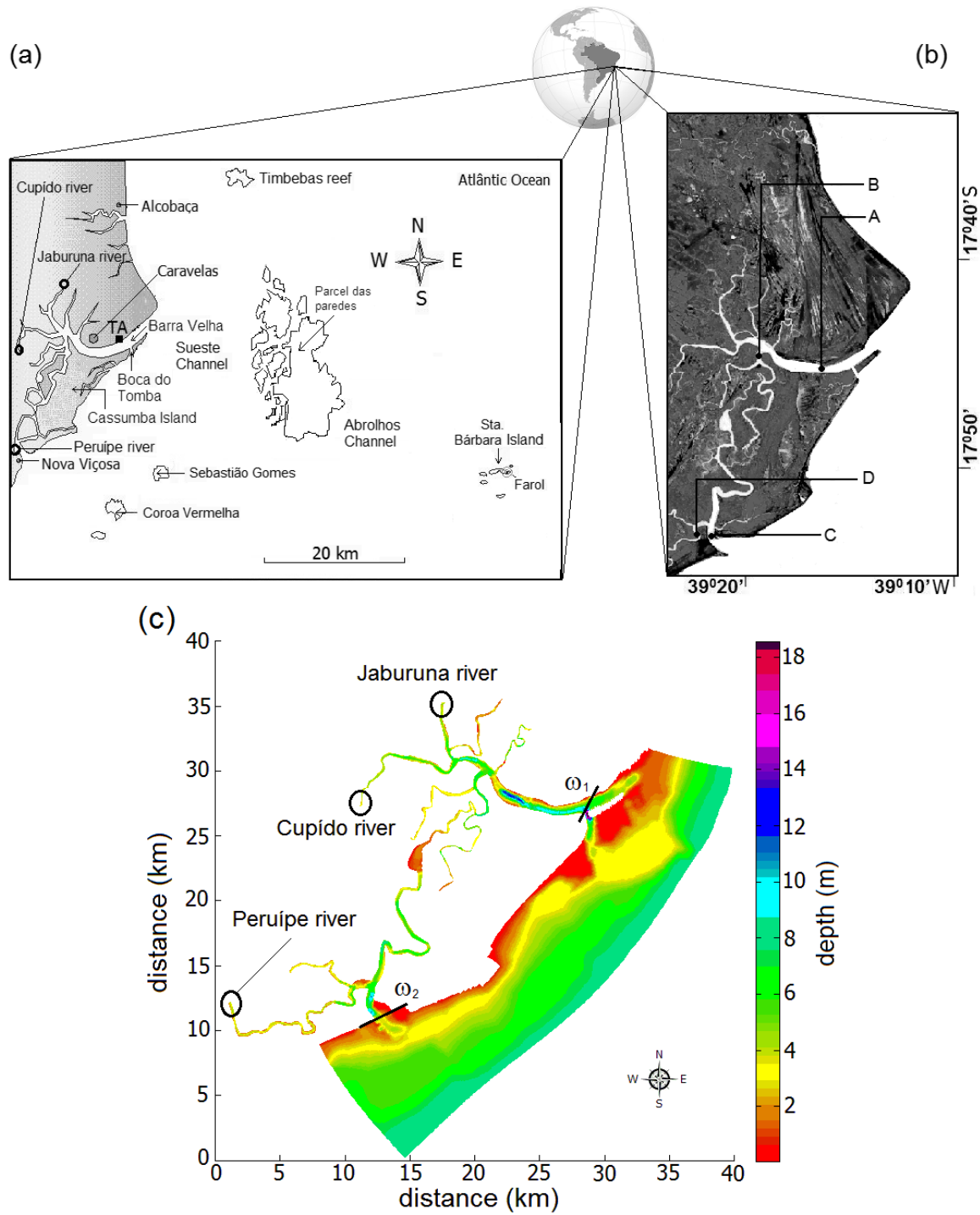


Figure 2 – (a) Geographic location of the estuarine system comprising the Caravelas and Peruípe rivers. Aracruz terminal harbour – TA, and the Sueste and Abrolhos channels, the Parcel das paredes and the National Marine Park of Abrolhos. (b) Detailed image of the estuarine system, and location of the oceanographic mooring sites A and B in Caravelas area, and C and D in Nova Viçosa area, where D is referred as site E at Andutta et al., 2013b. (c) numerical domain with ω_1 and ω_2 denoting the limit of the control domain ω to compute the transport timescales.

Figure 3

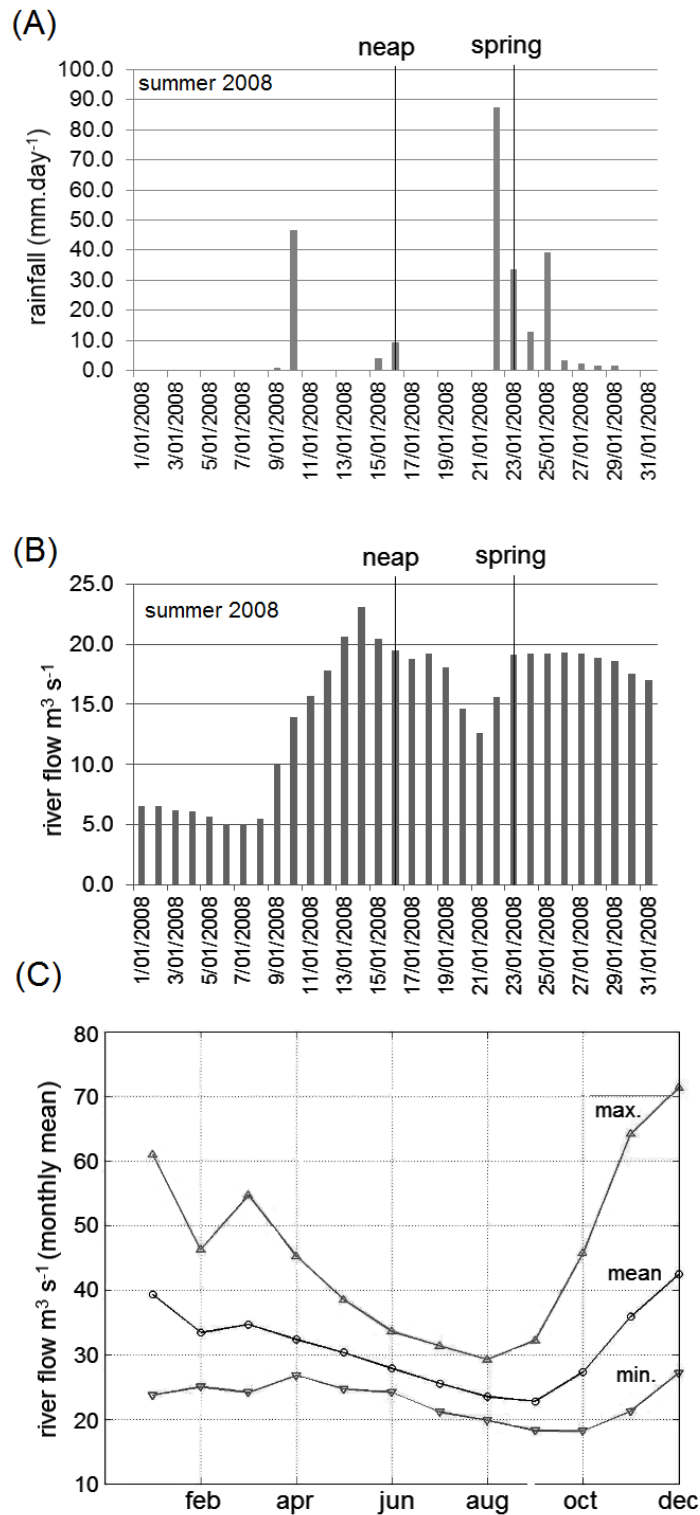


Figure 3 – Daily variation of the rainfall (A), and river discharge (B) during January (2008), observations were made at the gauge station Helvécia nº 55510000 (código 1739006) – National Agency of Waters. (C) Climatological estimate of the mean, minimum (min.) and maximum (max.) monthly river discharge using data from 1975 to 2008 (34 years of measured river flow) and corrected using the factor 1.6 to account for the entire drainage basin area of the Perú River.

Figure 4

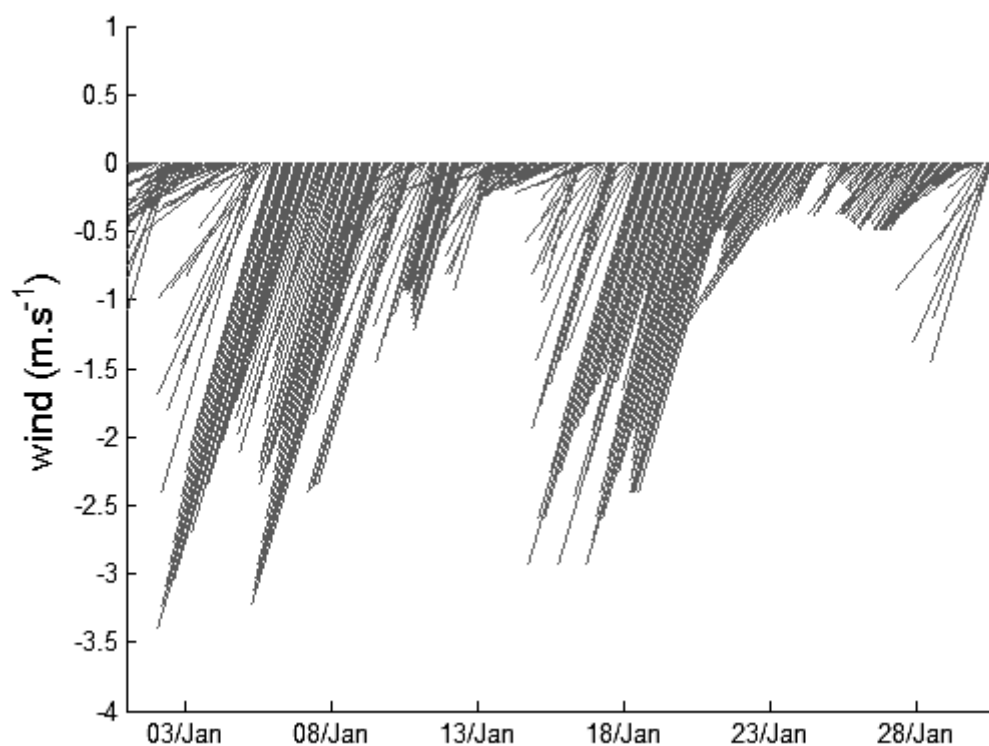


Figure 4 – Wind data obtained from the Instituto Nacional de Meteorologia INMET. Data during January 2008 at Caravelas station, code INMET A405, and coordinates (Lat. 17°43'48.0" S; Long. 39°15'00.0" W).

Figure 5

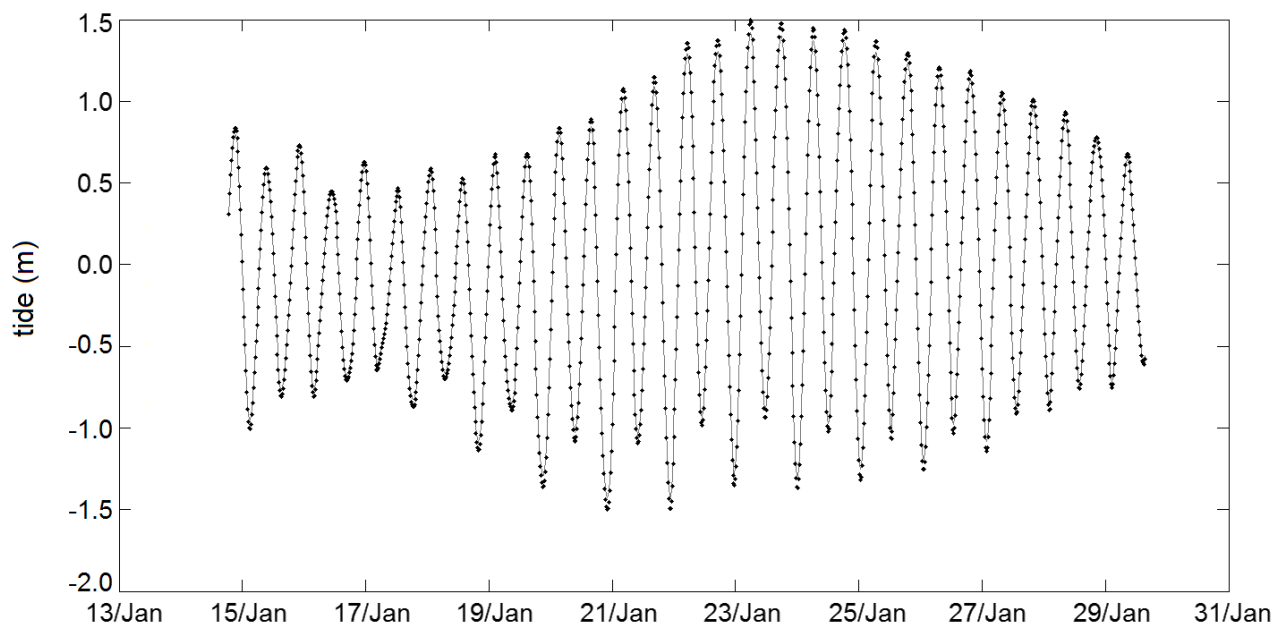


Figure 5 – Modelled water column (m) at station A compared to measured tides, from 14th to 29th of January 2008. Dots denote observations, and line denotes model result.

Figure 6

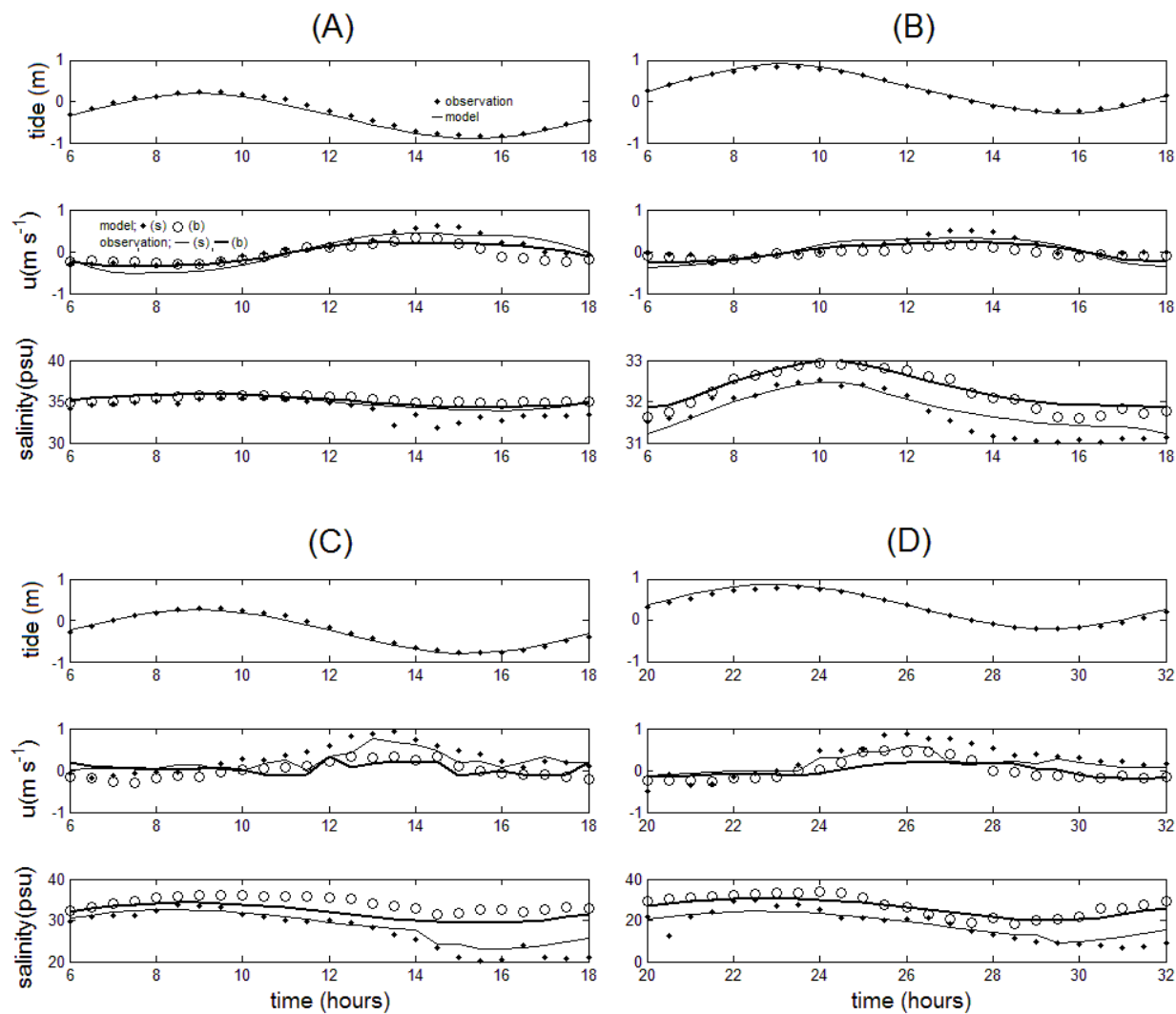


Figure 6 – Modelled tide (m), axial channel velocity u (m s^{-1}) and salinity (psu) compared to measured time series at stations A, B, C, and D, during neap tides. Measurements and simulation represented at the surface and bottom layers. Skill values are synthesised in Table 4.

Figure 7

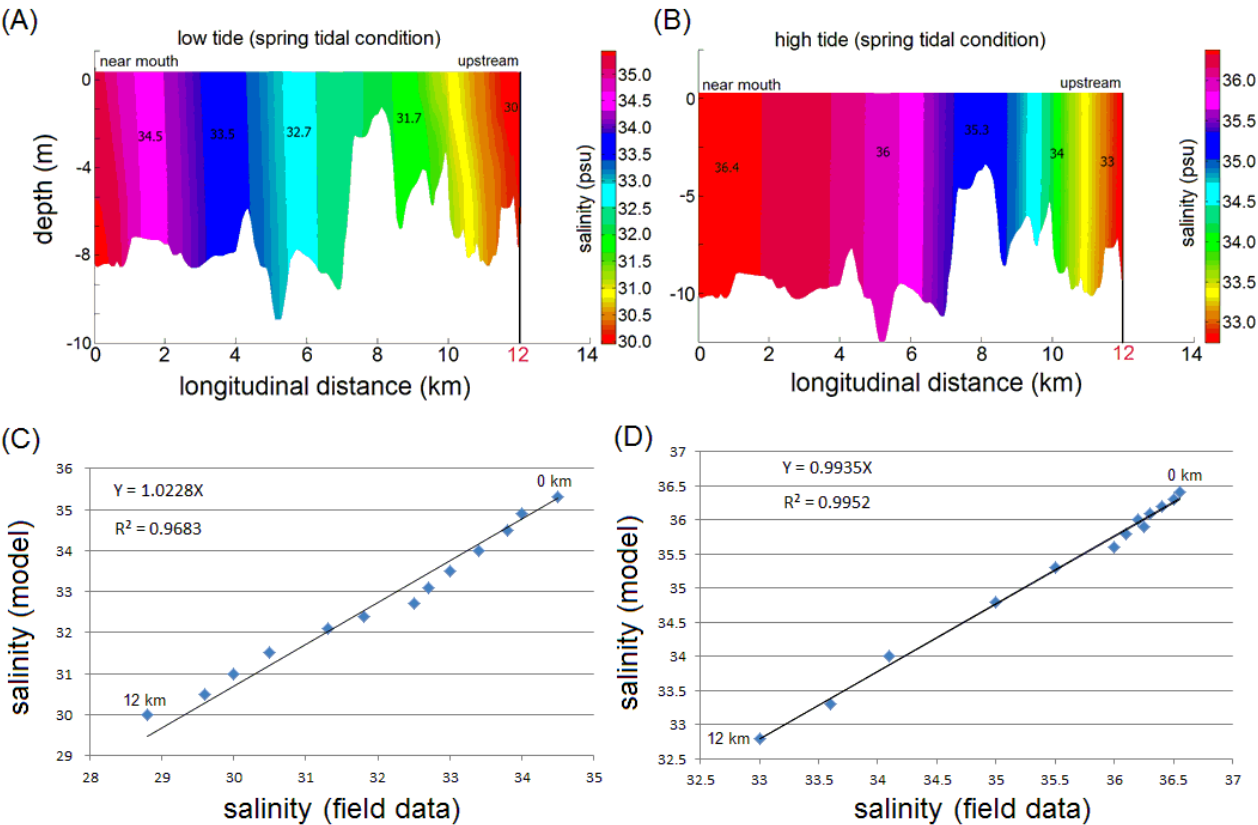


Figure 7 – Axial distribution of salinity () in the Caravelas Estuary in spring tidal conditions, at low (A) and high (B) tide. Correlation of axial distribution of the mean water column salinity between model and observation at low (C) and high (D) tide in spring tide, where Y and X denote model results and measurement, respectively. First dot on left denotes position at estuarine mouth (0 km), while lat dot denotes a position 12 km further upstream, the increment of 1 km is applied from first to last dot. Observations obtained from Schettini and Miranda (2010).

Figure 8

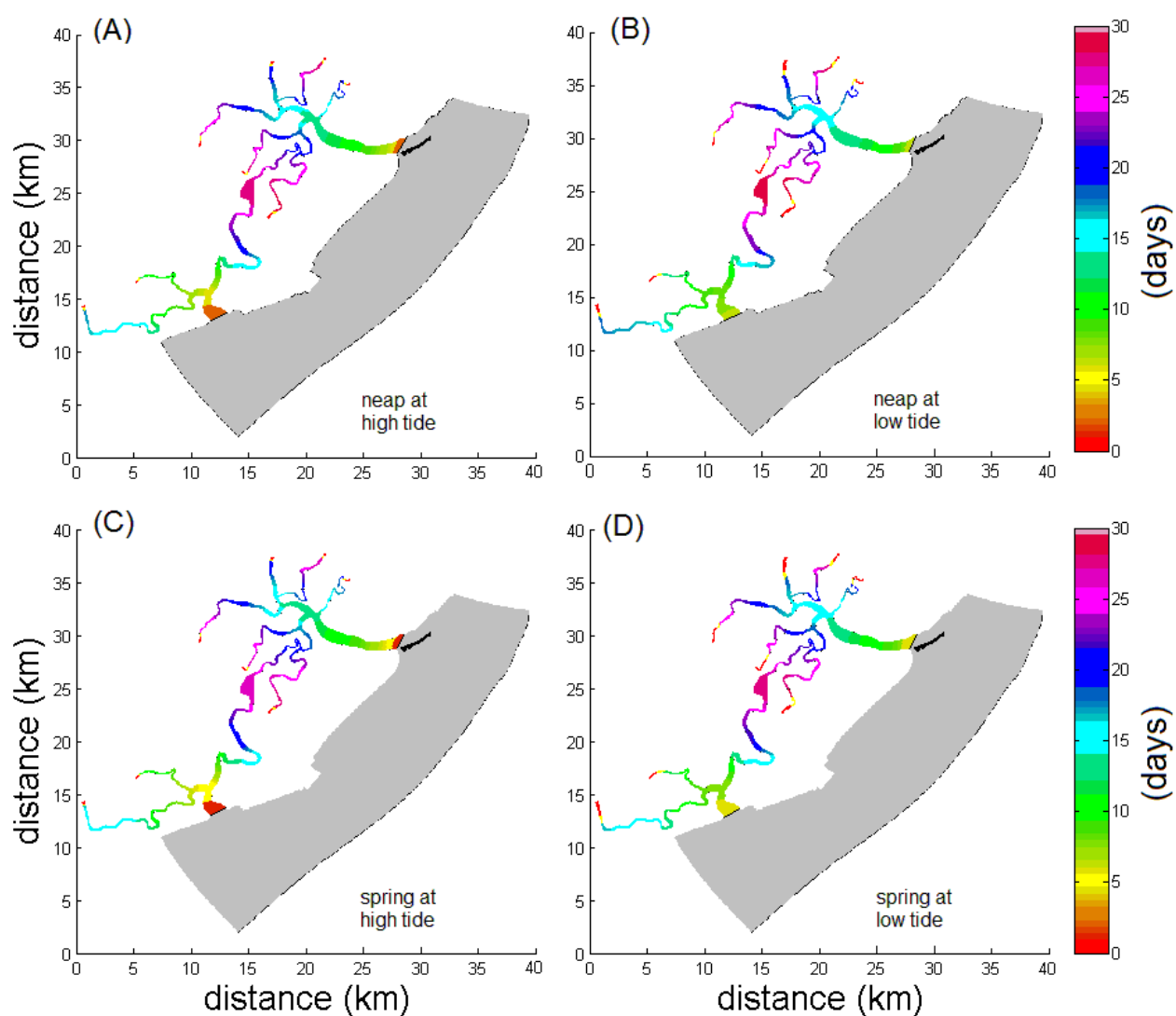


Figure 8 – Verically averaged residence time spatial distribution (ϕ), for scenarios S_1 (A), S_2 (B), S_3 (B) and S_4 (C). Colored bar indicates the timescales in days.

Figure 9

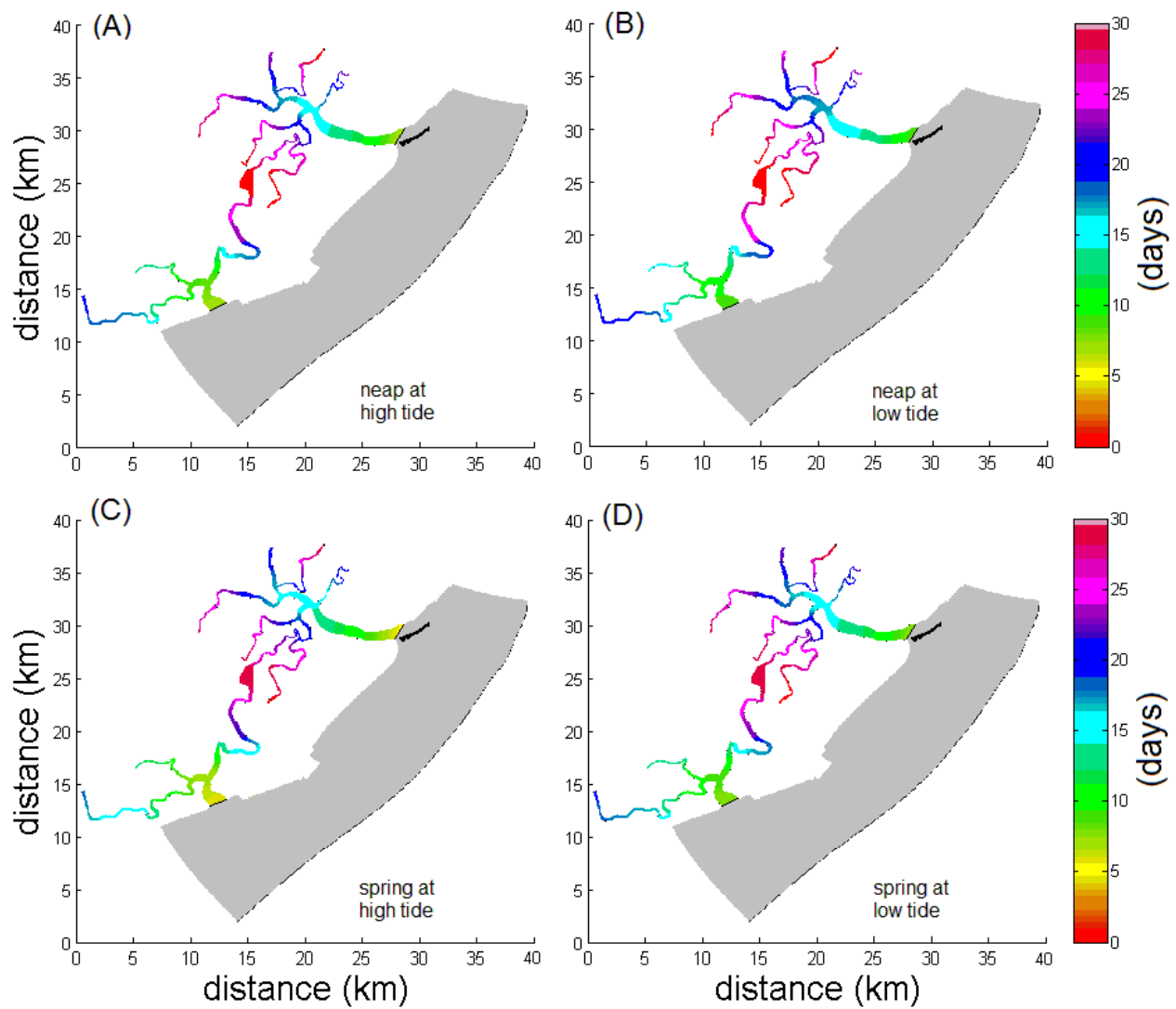


Figure 9 – Vertically averaged exposure time spatial distribution (θ), for scenarios S_1 (A), S_2 (B), S_3 (B) and S_4 (C). Colored bar indicates the timescales in days.

Figure 10

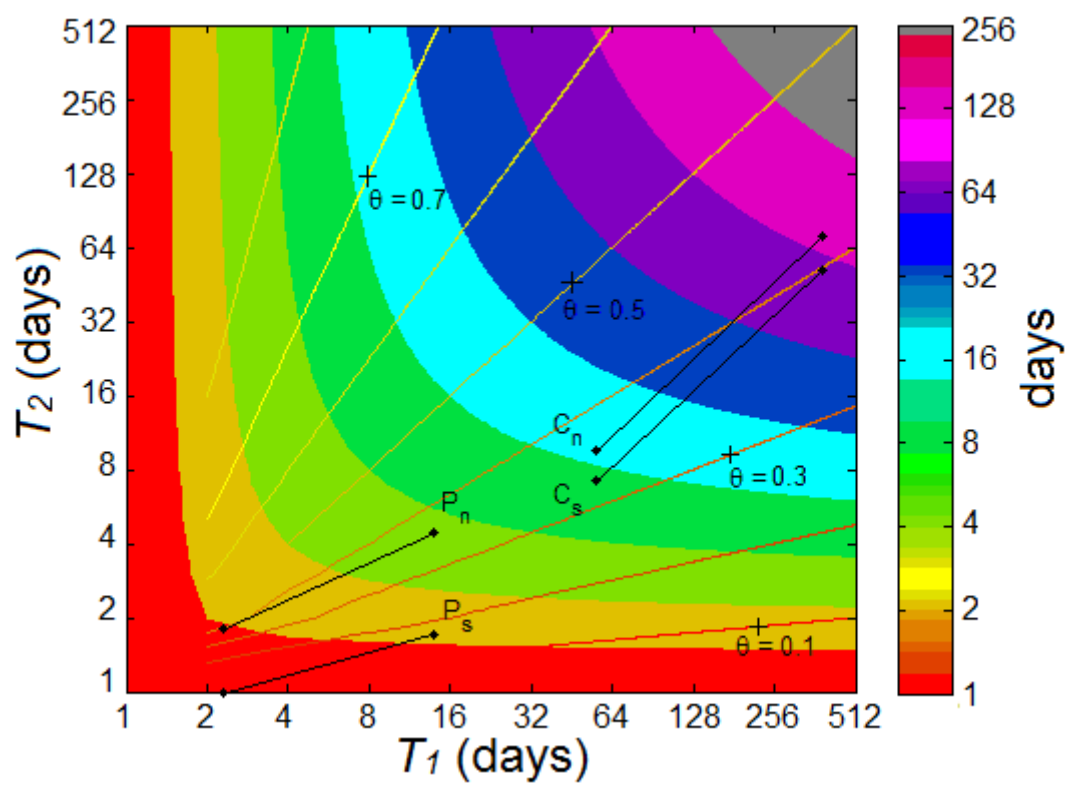


Figure 10 – The position of Caravelas (CA) and Peruípe (P) estuaries on the advection-diffusion diagram to indicate the relative contribution to the water renewal T_P by the advective (T_1) and dispersive (T_2) timescales using a logarithmic scale. Subscript (n) and (s) indicate neap and spring tide conditions.

Figure 11

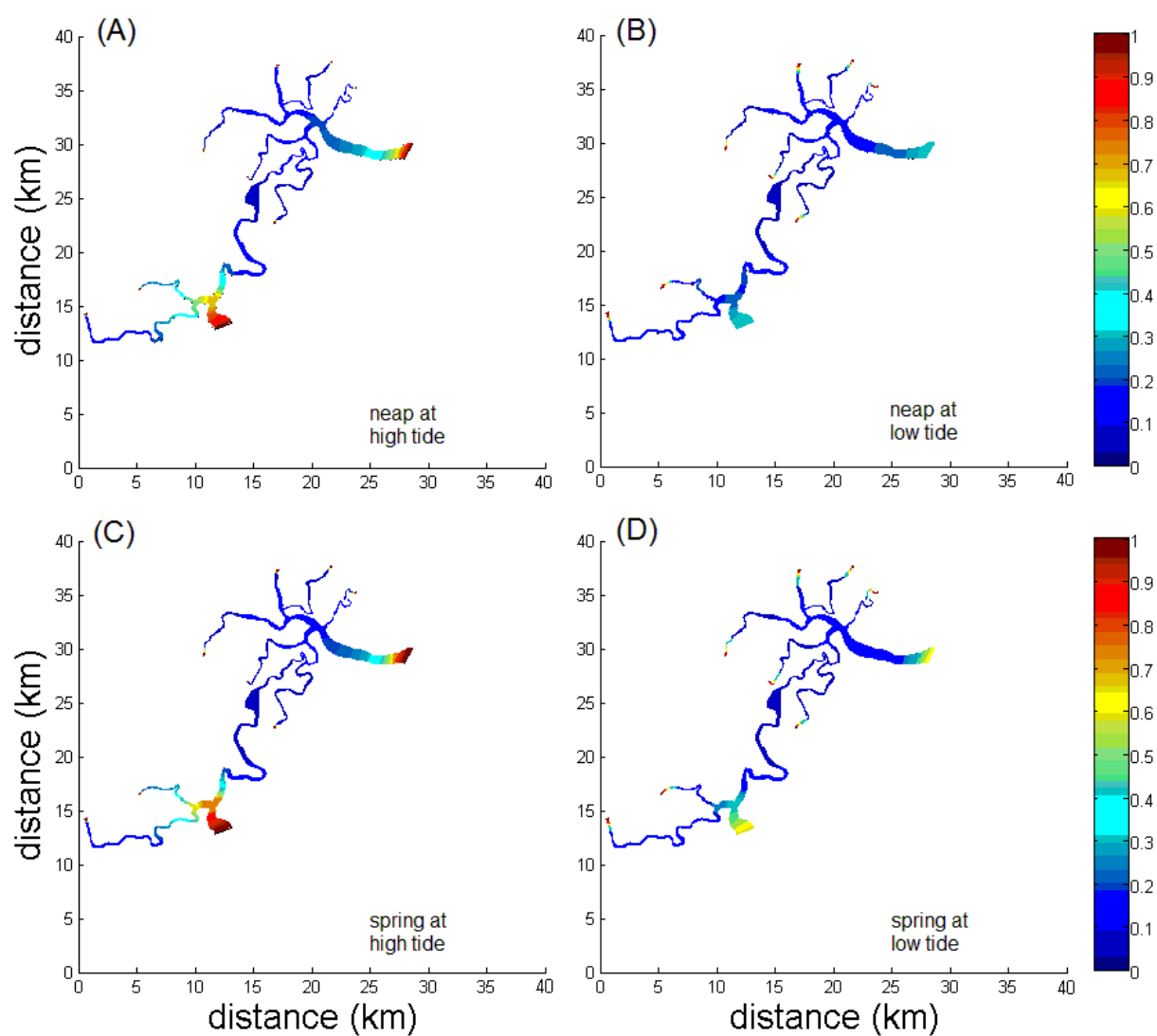


Figure 11 – Return coefficient spatial distribution (r), for scenarios S_1 (A), S_2 (B), S_3 (B) and S_4 (C). Colored bar indicates the timescales in days.

Figure 12

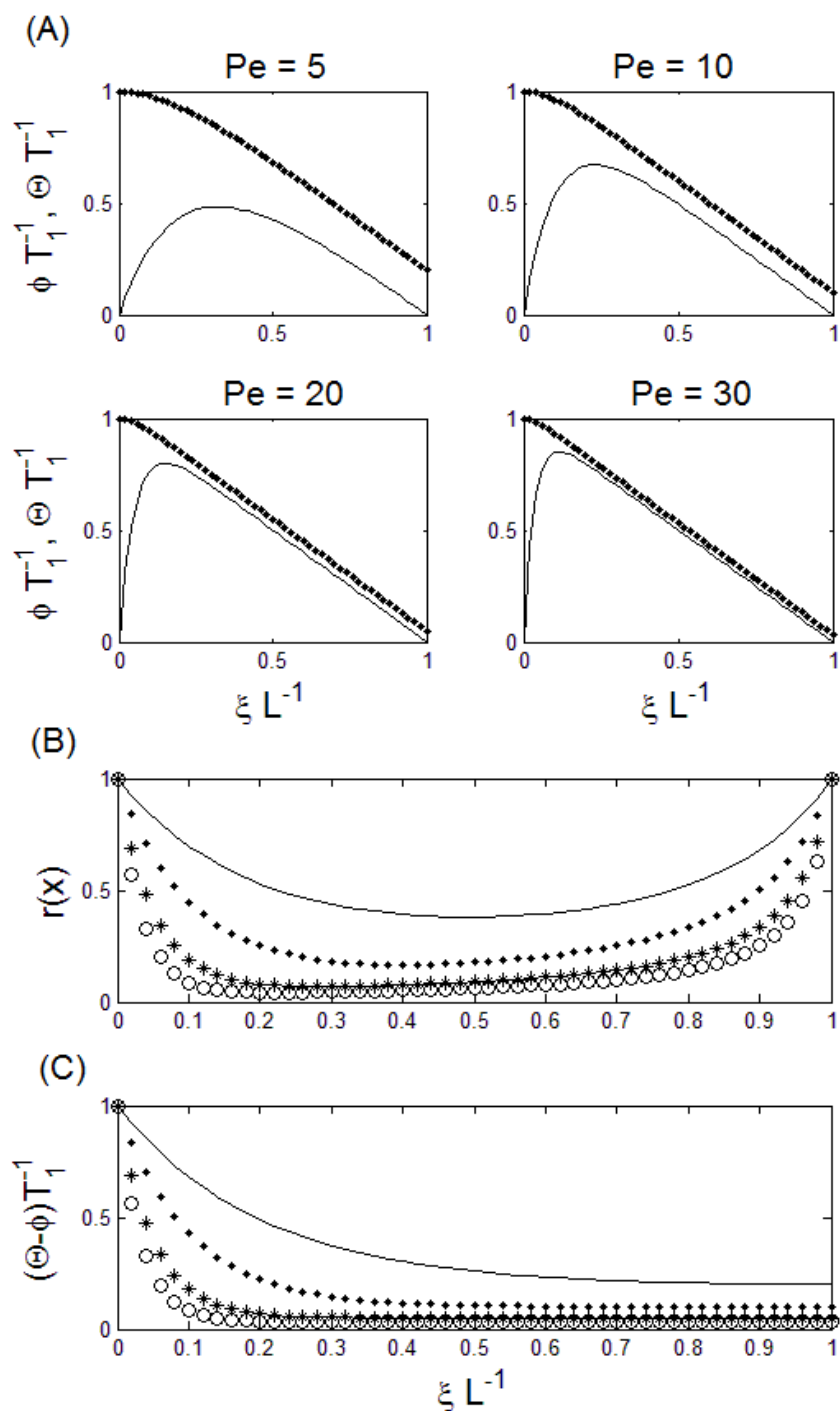


Figure 12 – (A) Representation of the exposure time Θ (dots) and residence time ϕ (line) as a function of the distance x from the upstream boundary of the domain. (B) Return coefficient and (C) and the difference between the exposure and residence time $(\Theta - \phi)$ calculated for different values of Peclet number, $Pe = 5$ (line), $Pe = 10$ (dot), $Pe = 20$ (star), and $Pe = 30$ (circle). The timescales are normalised by means of the advective timescale T_1 .

Table 1 – Summary of flow conditions in the simulations for the Peruípe, Cupído, and Jaburuna rivers. Data from ANA.

river	flow ($\text{m}^3 \text{s}^{-1}$)	typical range of flow ($\text{m}^3 \text{s}^{-1}$)	Salinity applied to
	January 2008	in wet season	boundary cells
Peruípe	~5-20	17 to 70	0
Cupído	2	2 to 9	6
Jaburuna	2		4

Table 2 – Amplitude and frequency of the main tidal components recorded at Terminal Aracruz - TA.

Component	Amplitude (cm)	Frequency (degree hr ⁻¹)
O ₁	8.89	13.94
K ₁	5.76	15.04
P ₁	1.91	14.96
Q ₁	1.62	13.40
M ₂	75.10	28.98
S ₂	33.48	30.00
L ₂	15.06	29.53
N ₂	13.45	28.44
K ₂	9.11	30.08

Table 3 – Sensitivity analysis of the salinity to the value of the horizontal diffusivity K_h using the Skill method from Wilmott (1981). Skill values are in the range 0 to 1. The factor f was used in the sensitivity analyses following formulae by Okubo (1971).

Parameter	Site A (Skill)	Site B (Skill)	Site C (Skill)	Site D (Skill)
$f = 2$				
Salinity (neap)	0.78	0.58	0.55	0.70
Salinity (spring)	0.85	0.62	0.60	0.75
$f = 100$				
Salinity (neap)	0.86	0.72	0.68	0.74
Salinity (spring)	0.90	0.76	0.75	0.82
$f = 150$				
Salinity (neap)	0.80	0.76	0.64	0.72
Salinity (spring)	0.95	0.80	0.80	0.88
$f = 200$				
Salinity (neap)	0.85	0.80	0.73	0.78
Salinity (spring)	0.97	0.85	0.83	0.93
$f = 250$				
Salinity (neap)	0.81	0.77	0.72	0.74
Salinity (spring)	0.94	0.81	0.78	0.89
$f = 400$				
Salinity (neap)	0.81	0.74	0.66	0.65
Salinity (spring)	0.85	0.78	0.70	0.79
$f = 2000$				
Salinity (neap)	0.64	0.56	0.50	0.60
Salinity (spring)	0.66	0.60	0.54	0.65

Table 4 – Results of the validation using the Skill method from Wilmott (1981).

Parameter	Site A (Skill)	Site B (Skill)	Site C (Skill)	Site D (Skill)
Tidal height (neap)	0.99	1	0.99	0.99
Tidal height (spring)	1	0.99	1	0.98
Velocity (neap)	0.68	0.65	0.62	0.65
Velocity (spring)	0.77	0.93	0.84	0.88
Salinity (neap)	0.85	0.80	0.73	0.78
Salinity (spring)	0.97	0.85	0.83	0.93
Parameter	Site A (Skill)	Site B (Skill)		
Velocity (14 th to 26 th Jan 2008)	0.72	0.78		

Appendix 2

[Click here to download Supplementary material for on-line publication only: Andutta-et.al-2015-Caravelas-Appendix 02.doc](#)