

Pointwise and box-averaged water residence time in a 2D model of the Scheldt Estuary

- Let $\theta(t, x, y)$ denote the residence time of water particles present in the estuary at time t in an elemental control volume located at (x, y) . This timescale was computed by de Brye et al. (JMS, 2012) by means of the mathematically intricate (but computationally efficient) adjoint model developed by Delhez et al. (ECSS, 2004).
- The (space) average over box Ω_i (with $\Omega_i \subset \Omega$, where Ω is the domain of interest) of the above-mentioned timescale is

$$\theta_i(t) = \frac{1}{V_i(t)} \int_{\Omega_i} H(t, x, y) \theta(t, x, y) dx dy \quad (1)$$

where $V_i(t) = \int_{\Omega_i} H(t, x, y) dx dy$ is the volume of water contained in Ω_i

at time t

• If there is a relatively small number of boxes and if one can be satisfied with box-averaged residence times, then the forward approach of de Brauwere et al. (JMS, 2011) is likely to be computationally more efficient than that based on the adjoint model. First, one has to calculate for $t' \in [t, \infty[$ the concentration $C_i(t', x, y)$ of the water that is located in Ω_i at time t . The starting conditions are $C_i(t, x, y) = 1$ if $(x, y) \in \Omega_i$ and $C_i(t, x, y) = 0$ if $(x, y) \notin \Omega_i$. Then, the box-averaged residence time is

$$\theta_i(t) = \frac{1}{V_i(t)} \int_t^{\infty} \int_{\Omega} H(t', x, y) C_i(t', x, y) dx dy dt' \quad (2)$$

Timescales (1) and (2) are theoretically equivalent, but, in practice, their numerically-approximated values are likely to be slightly different from each other due to the different approaches they ensue from.

A one-dimensional, steady-state illustration

- The domain of interest is $x \in [0, L]$, and the velocity and diffusivity are positive constants U and K . From here on, only dimensionless variables will be used. They are obtained by having recourse to advective timescale L/U and length scale L , allowing for the introduction of Peclet number $Pe = UL/K$.

- For the sake of simplicity, it is assumed that there are only two boxes of equal lengths, i.e., $\Omega_1 = \{x | 0 \leq x < 1/2\}$ and $\Omega_2 = \{x | 1/2 < x \leq 1\}$. Water concentrations $C_1(t, x)$ and $C_2(t, x)$ obey (dimensionless) advection-diffusion equations

$$\frac{\partial C_i}{\partial t} = -\frac{\partial C_i}{\partial x} + \frac{1}{Pe} \frac{\partial^2 C_i}{\partial x^2} \quad (i = 1, 2) \quad (3)$$

which are to be solved under boundary conditions

$$[C_i(t, x)]_{x=0} = 0 = [C_i(t, x)]_{x=1} \quad (i = 1, 2) \quad (4)$$

and initial conditions

$$[C_1(t, x)]_{t=0} = \begin{cases} 1, & 0 \leq x < 1/2 \\ 0, & 1/2 < x \leq 1 \end{cases} \quad (5)$$

$$[C_2(t, x)]_{t=0} = \begin{cases} 0, & 0 \leq x < 1/2 \\ 1, & 1/2 < x \leq 1 \end{cases} \quad (6)$$

Then, following (2), the box-averaged residence times are

$$\theta_i = \frac{1}{(1/2)} \int_0^\infty \int_0^1 C_i(t, x) dx dt = 2 \int_0^\infty \int_0^1 C_i(t, x) dx dt \quad (i = 1, 2) \quad (7)$$

and the domain-averaged residence time simply is

$$\langle \theta \rangle = \frac{\theta_1 + \theta_2}{2} \quad (8)$$

- So far, I have not been capable of dealing analytically with (3)-(8). Nonetheless, there exists a workaround (e.g., Deleersnijder et al., EFM, 2006), which I start exploring for the present problem in the Appendix.
- A fully numerical approach should be feasible. The ensuing residence times should be compared with the exact values. They can be obtained rather easily from the adjoint approach of Delhez et al. (ECSS, 2004), which was applied to the Scheldt estuary by de Brye et al. (JMS, 2012) and the Mahakam delta by Pham Van et al. (Water, 2020).
- The (steady-state, dimensionless) pointwise residence time can be obtained from the adjoint model, which, in this case, reduces to an ordinary differential problem (e.g., Andutta et al., PiO, 2014), i.e.,

$$\frac{1}{Pe} \frac{d^2\theta}{dx^2} + \frac{d\theta}{dx} = -1, \quad [\theta(x)]_{x=0} = 0 = [\theta(x)]_{x=1} \quad (9)$$

leading to

$$\theta(x) = 1 - x - \frac{e^{-Pe x} - e^{-Pe}}{1 - e^{-Pe}} \quad (10)$$

Then, the (steady-state, dimensionless) box-averaged residence times are readily seen to be

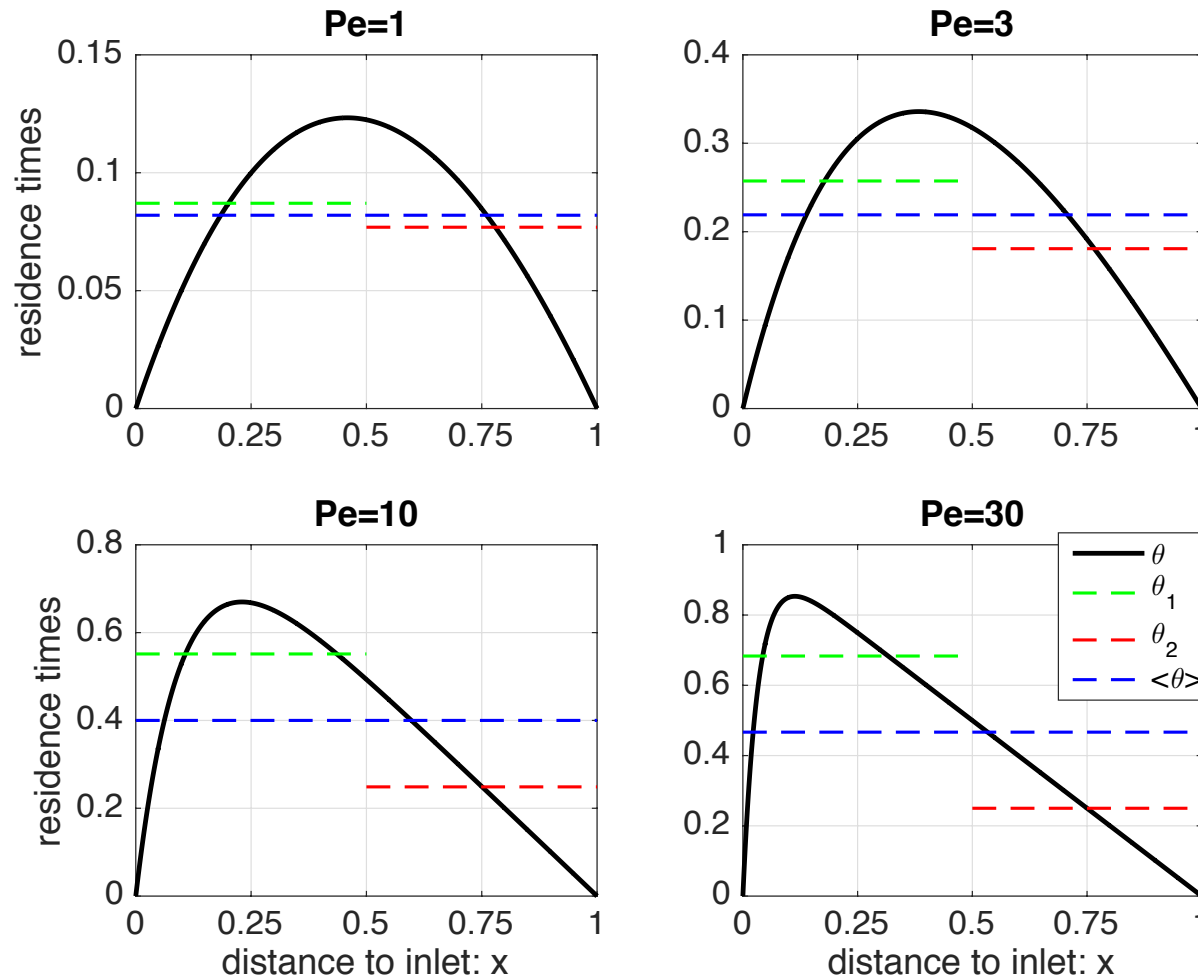
$$\theta_1 = \frac{1}{1/2} \int_0^{1/2} \theta(x) dx = \frac{3}{4} + \frac{1}{e^{Pe} - 1} - \frac{2}{Pe} \frac{1}{e^{-Pe/2} + 1} \quad (11)$$

$$\theta_2 = \frac{1}{1/2} \int_{1/2}^1 \theta(x) dx = \frac{1}{4} + \frac{1}{e^{Pe} - 1} - \frac{2}{Pe} \frac{1}{e^{Pe/2} + 1} \quad (12)$$

Finally, the (steady-state, dimensionless) domain-averaged residence time reads

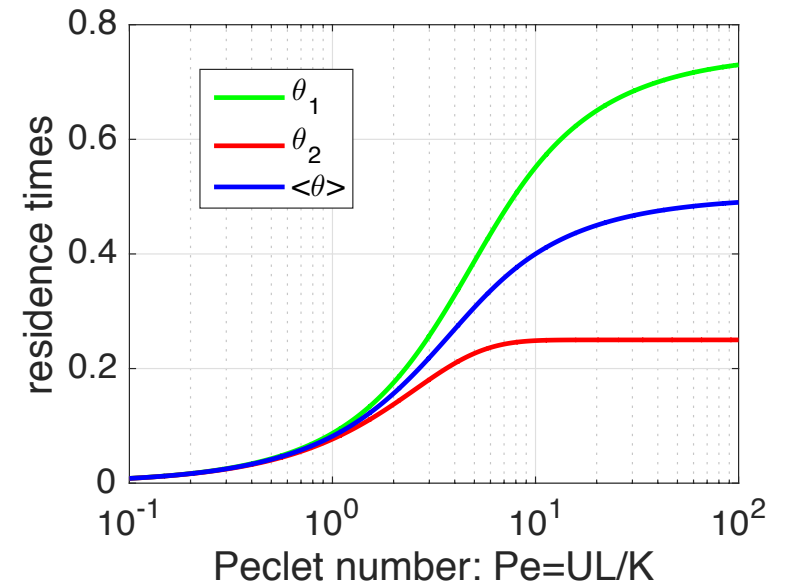
$$\langle \theta \rangle = \int_0^1 \theta(x) dx = \frac{\theta_1 + \theta_2}{2} = \frac{1}{2} + \frac{1}{e^{Pe} - 1} - \frac{1}{Pe} \quad (13)$$

- Residence times (10)-(13) are illustrated in the figure below for various values of the Peclet number.



For large values of the Peclet number, there exists a boundary layer in the vicinity of the incoming boundary ($x = 0$), whose dimensionless thickness is Pe^{-1} — and the corresponding dimensional thickness is K / U (e.g., Delhez and Deleersnijder 2006, Blaise et al. 2010).

- The figure opposite represents the above-mentioned space-averaged residence time for a wide range of values of the Peclet number (Pe).



- If the Peclet number is large, then, the domain-averaged residence time is close to that corresponding to a plug flow (zero diffusivity):

$$\langle \theta \rangle \sim \frac{1}{2} - \frac{1}{Pe}, \quad Pe \rightarrow \infty \quad (14)$$

This is illustrated in Appendix A of Lucas and Deleersnijder (2020). If, on the other hand, diffusion is the dominant process, then the following asymptotic expression holds valid

$$\langle \theta \rangle \sim \frac{Pe}{12} - \frac{Pe^3}{720}, \quad Pe \rightarrow 0 \quad (15)$$

In the latter case, the residence time tends to zero because diffusion causes every water particle to hit very quickly one of the open boundaries of the domain. At the very instant this occurs, the particle is discarded, which is why its residence time (and, hence, the domain-averaged residence time) tends to zero as $Pe \rightarrow 0$.

- Such behaviour is not always deemed to be acceptable. This is why the exposure time (e.g., Delhez 2013) may be worth considering. Additional flexibility is being searched (e.g., Deleersnijder 2020).

Appendix: Illustrating the equivalence between the forward/direct and backward/adjoint approaches

According to the forward approach, for the one-dimensional test case under consideration, the mean residence time of a water type whose concentration is $C(t,x)$ is

$$(A1) \quad \theta = \frac{\int_0^1 \int_0^\infty C(t,x) dx dt}{\int_0^1 C(0,x) dx} = \frac{\int_0^\infty \int_0^1 C(t,x) dt dx}{\int_0^1 C(0,x) dx} = \frac{\int_0^1 \xi(x) dx}{\int_0^1 C(0,x) dx} \quad \text{with} \quad \xi(x) = \int_0^\infty C(t,x) dt$$

In the present context, obtaining the analytical expression of the relevant concentrations is far from straightforward (e.g., Mojtabi and Deville 2015). However, for evaluating the residence time, it is not necessary to determine explicitly the above-mentioned concentrations. Indeed, only variable $\xi(x)$ for every water type needs to be dealt with. Since $[C(t,x)]_{t=\infty} = 0$ (this can be proven rigorously), the integration over time of the advection-diffusion equation and its boundary conditions leads to

$$(A2) \quad \underbrace{\int_0^\infty \frac{\partial}{\partial t} C(t,x) dt}_{C(\infty,x)-C(0,x)=-C(0,x)} = - \underbrace{\frac{\partial}{\partial x} \int_0^\infty C(t,x) dt}_{=\xi(x)} + \frac{1}{Pe} \underbrace{\frac{\partial^2}{\partial x^2} \int_0^\infty C(t,x) dt}_{=\xi(x)}, \quad 0 = \int_0^\infty C(t,0) dt = \xi(0), \quad 0 = \int_0^\infty C(t,1) dt = \xi(1)$$

Thus, $\xi(x)$ is the solution of the following ordinary differential problem

$$(A3) \quad \frac{1}{Pe} \frac{d^2 \xi}{dx^2} - \frac{d\xi}{dx} = -C(0,x), \quad \xi(0) = 0 = \xi(1)$$

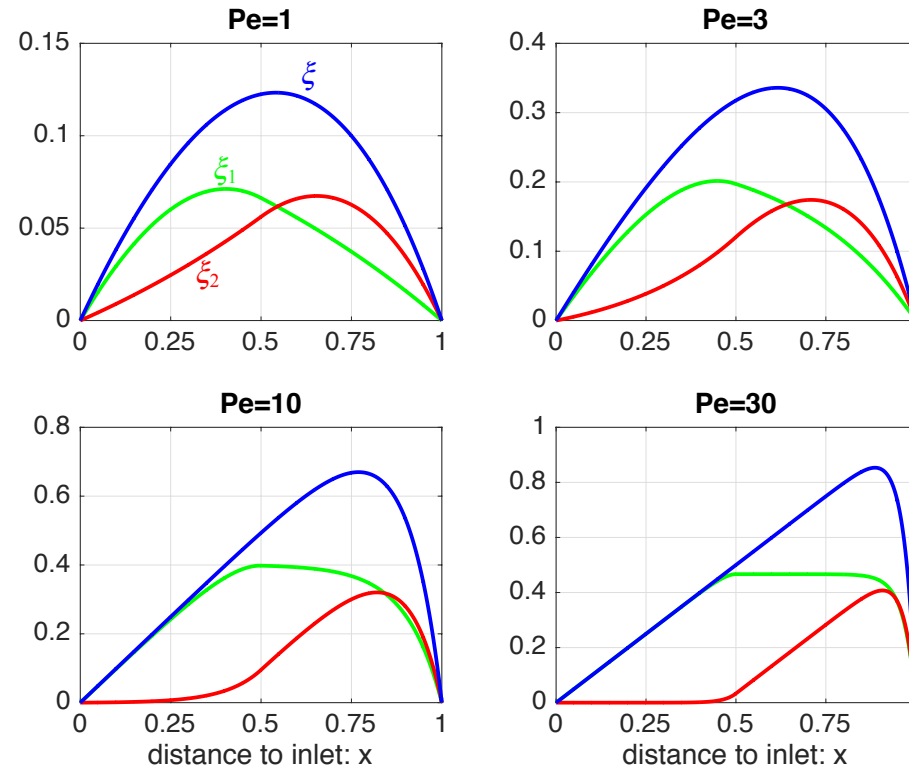
As for the residence time averaged over box Ω_1 , $\xi_1(x)$ must be continuously differentiable. Then, one obtains

$$(A4) \quad \xi_1(x) = \begin{cases} \frac{2 - Pe - 2e^{Pe/2}}{2Pe(e^{Pe} - 1)} (e^{Pe x} - 1) + x, & 0 \leq x < 1/2 \\ \frac{2 - Pe - 2e^{-Pe/2}}{2Pe(e^{Pe} - 1)} (e^{Pe x} - e^{Pe}) , & 1/2 < x \leq 1 \end{cases}$$

and it may be seen that

$$(A5) \quad \theta_1 = \frac{1}{1/2} \int_0^1 \xi_1(x) dx = \frac{3}{4} + \frac{1}{e^{Pe} - 1} - \frac{2}{Pe} \frac{1}{e^{-Pe/2} + 1}$$

as expected.



As for the residence time averaged over box Ω_2 , $\xi_2(x)$ must be continuously differentiable. Then, one obtains

$$(A6) \quad \xi_2(x) = \begin{cases} \frac{2e^{Pe/2} - Pe - 2}{2Pe(e^{Pe} - 1)} (e^{Pe x} - 1) , & 0 \leq x < 1/2 \\ \frac{2e^{-Pe/2} - Pe - 2}{2Pe(e^{Pe} - 1)} (e^{Pe x} - e^{Pe}) + x - 1 , & 1/2 < x \leq 1 \end{cases}$$

and it may be seen that

$$(A7) \quad \theta_2 = \frac{1}{1/2} \int_{1/2}^2 \xi_2(x) dx = \frac{1}{4} + \frac{1}{e^{Pe} - 1} - \frac{2}{Pe} \frac{1}{e^{Pe/2} + 1}$$

as expected.

As for the residence time averaged over domain of interest Ω , one obtains

$$(A8) \quad \xi(x) = x - \frac{e^{Pe x} - 1}{e^{Pe} - 1}$$

and it may be seen that

$$(A9) \quad \langle \theta \rangle = \int_0^1 \xi(x) dx = \frac{\theta_1 + \theta_2}{2} = \frac{1}{2} + \frac{1}{e^{Pe} - 1} - \frac{1}{Pe}$$

as expected.

A rather similar forward/direct method may be resorted to in order to derive the pointwise residence time. In this case, it might not be appropriate to use the term ‘‘concentration’’. Instead, it is presumably more relevant to refer to the Green's function of the one-dimensional advection-diffusion problem under consideration. The latter, $\mathcal{G}(x, t', x')$, is the solution of the following partial differential problem:

$$(A10) \quad \frac{\partial \mathcal{G}}{\partial t'} = - \frac{\partial \mathcal{G}}{\partial x'} + \frac{1}{Pe} \frac{\partial^2 \mathcal{G}}{\partial x'^2} , \quad [\mathcal{G}(x, t', x')]_{t'=0} = \delta(x - x') , \quad [\mathcal{G}(x, t', x')]_{x'=0} = 0 = [\mathcal{G}(x, t', x')]_{x'=1}$$

where $\delta(x - x')$ denotes the Dirac delta function, whose integral over space is identically equal to unity. Clearly, this is meant to evaluate the residence time of water particles initially located at distance x to the inlet. Then, in accordance with (A1), the (pointwise) residence time is

$$(A11) \quad \theta(x) = \frac{\int_0^{\infty} \int_0^1 \mathcal{G}(x, t', x') dx' dt'}{\int_0^1 \mathcal{G}(x, 0, x') dx'} = \frac{\int_0^1 \int_0^{\infty} \mathcal{G}(x, t', x') dt' dx'}{\underbrace{\int_0^1 \delta(x - x') dx'}_{=1}}$$

Function $\mathcal{G}(x, t', x')$ is a series (e.g., Mojtabi and Deville 2015) that is difficult to deal with. Fortunately, as for the preceding illustrations, it is not necessary to explicit evaluate this function. Only its integral over time is needed, i.e.,

$$(A12) \quad G(x, x') = \int_0^{\infty} \mathcal{G}(x, t', x') dt' \Rightarrow \theta(x) = \int_0^1 G(x, x') dx'$$

Function $G(x, x')$ is the solution of the following differential problem

$$(A13) \quad \frac{1}{Pe} \frac{\partial^2 G}{\partial x'^2} - \frac{\partial G}{\partial x'} = [\mathcal{G}(x, t', x')]_{t'=0} = -\delta(x - x')$$

which is obtained by integrating (A10) over time. Obviously, $G(x, x')$ may also be regarded as a Green's function, which at $x = x'$, must satisfy matching conditions

$$(A14) \quad \lim_{\varepsilon \rightarrow 0} [G(x, x')]_{x'=x-\varepsilon}^{x'=x+\varepsilon} = 0, \quad \lim_{\varepsilon \rightarrow 0} \left[\frac{\partial}{\partial x'} G(x, x') \right]_{x'=x-\varepsilon}^{x'=x+\varepsilon} = -1$$

After some calculations, one obtains

$$(A15) \quad G(x, x') = \begin{cases} \frac{1 - e^{Pe(1-x)}}{1 - e^{Pe}} (e^{Pex'} - 1), & x' < x \\ \frac{1 - e^{-Pex}}{1 - e^{Pe}} (e^{Pex'} - e^{Pe}), & x < x' \end{cases}$$

which, by having recourse to (12), eventually yields the pointwise residence time, i.e.,

$$(A16) \quad \theta(x) = \int_0^1 G(x, x') dx' = 1 - x - \frac{e^{-Pe x} - e^{-Pe}}{1 - e^{-Pe}}$$

As expected, this result is identical to that easily derived from the adjoint model.

Acknowledgements. The method aimed at deriving the residence time by means of the forward/direct approach without solving explicitly the related advection-diffusion problem was first suggested to me by Jean-Marie Beckers (personal communication, 2005). It was subsequently employed in Deleersnijder et al. (2006).

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