Water renewal of a region of freshwater influence (ROFI): mathematical properties of some of the relevant diagnostic variables

Eric Deleersnijder, 20 October 2019

Abstract. We first lay out the partial differential problems governing the concentrations of the water types (the original, river and coastal ocean waters) and their aggregates (the renewing water and the water itself) that help gain insight into the water renewal processes of a generic region of freshwater of influence (ROFI). We establish the mathematical properties of these concentrations, showing that they are well behaved. Then, in the framework of the Constituent-oriented Age and Residence time Theory (CART, www.climate.be/cart), we show how to evaluate the age (time elapsed since leaving the relevant open boundary) of the above water types and their aggregates, which are treated as passive tracers. We demonstrate that the ages satisfy criteria suggesting that the diagnostic strategy outlined herein is well founded. Finally, we set up a highly-idealised, steady-state, one-dimensional illustration, allowing us to obtain closed-form solutions. The age of the river and coastal ocean waters are seen to be symmetric with respect to the centre of the domain of interest. This unexpected property has yet to be explained. We believe that some of the present mathematical developments are part of the activities that should be carried out in order to validate a diagnostic strategy based on time- and position-dependent timescales.

1. Introduction

The concept of water renewal refers to all the processes by which water initially present in the domain of interest is replaced by water originating from its environment. Such phenomena significantly impact ecology, pollutant dispersal, sediment transport, etc. Therefore, quantifying the rate at which water renewal takes place is considered as an important step in many eco-hydrodynamic studies. In this respect, evaluating space and time-dependent timescales is an approach that is becoming increasingly popular (e.g. Shen and Haas 2004, Shen and Lin 2006, Shen and Wang 2007, de Brye et al. 2012, Liu et al. 2012, Radtke et al. 2012, Andutta et al. 2016, Kärnä et al. 2016, Rayson et al. 2016, Liu et al. 2017, Du et al. 2018, Rutherford and Fennel 2018, Grosse et al. 2019, Chen et al. 2019, Cheng et al. 2019, Li et al. 2019, Lin and Liu 2019, Shang et al. 2019, Wang et al. 2019, Yang et al. 2019)

Gourgue et al. (2007) outlined a generic approach to the evaluation of water renewal timescales. It consists in splitting the water present in the domain into two water components, namely the original water and the renewing water, tracking them in a Eulerian or Lagrangian way, and calculating related timescales. The original water refers to the water particles[1] that

[1] Hereinafter, the term "particle" does not refer to a water molecule. Instead, it is to be comprehended in the same way as in Lagrangian models, in which the number of particles is much smaller than the number of molecules of the substance under study because of the limitation of computing power. In other words, a particle encompasses many molecules. It is noteworthy that we will refrain from using the expression "water parcel", which, in our opinion, should exclusively refer to an elemental material control domain, i.e. an elemental control volume whose velocity is that of the water. Though its volume remains constant under the Boussinesq approximation, it does not always contain the same water molecules (or particles) due to the impact of diffusive processes.

are present in the domain of interest at the initial instant. They progressively leave the domain through its open boundaries and are being replaced by renewing water particles, i.e. water originating from its environment. The renewing water may be further divided into several water types, depending on their origins (river, coastal ocean, lock, canal, etc.). To calculate diagnostic timescales related to these water types (or aggregates of them[2]), it is first necessary to evaluate their concentrations. Then, additional variables leading to the sought-after timescales can be computed.

Hereinafter, seeking inspiration in Gourgue et al. (2007) and de Brye et al. (2012), we will present in detail a method for computing diagnostic timescales in a generic region of freshwater influence (ROFI). We will focus on the evaluation of relevant ages, leaving aside all the developments related to residence time and its variants, such as the exposure time (e.g. Monsen et al. 2002, Delhez et al. 2004, de Brauwere et al. 2011, Andutta et al. 2016). Our main objective is to establish rigorously the properties of all the variables involved in the diagnostic process, thereby proving that the partial differential problems obeyed by these variables are well posed.

In the present working note, all the mathematical developments will be carried out in the framework of the Constituent-oriented Age and Residence time Theory (CART[3]) (Delhez et al. 1999, Deleersnijder et al. 2001a).

2. Geometry and hydrodynamics

Domain of interest Ω is a generic ROFI in which water renewal timescales are to be evaluated. The domain boundary, Γ, consists of three components (Figure 1), i.e. Γ^{riv}, the riverine boundary or, equivalently, the upstream boundary of the domain, lying in freshwater, Γ^{oce}, which separates the domain of interest from the coastal ocean, and the impermeable part of the boundary (bottom of the water column and water-air interface), denoted Γ^{imp}. Surfaces Γ^{riv} and Γ^{oce} are open boundaries. Obviously, the open boundary of the domain of interest is the union of the Γ^{riv} and Γ^{oce}, i.e. $\Gamma^{r+o} = \Gamma^{riv} \cup \Gamma^{oce}$.

River runoff, tides and wind stress are time-dependent forcings that are generally significant in ROFIs, which is why the position of the water-air interface depends on time. Therefore, some parts of Γ move freely. This is of a crucial importance for the formulation of the boundary conditions under which the partial differential equations laid out hereinafter are to be solved. Clearly, we must be in a position to evaluate the velocity, $\mathbf{v}^{\Gamma}$, at which every point of the domain boundary moves (e.g. Deleersnijder 2014a).

Due to the movement of a fraction of the domain boundary, the volume of Ω,

$$V = \int_{\Omega} d\Omega \quad , \tag{2.1}$$

is time-dependent. The time rate of change of the domain volume is readily evaluated by having recourse to Reynolds' transport theorem:

[2] The expression "water type" refers to marked water particles belonging to a category that will not be further divided. An aggregate of water types is defined as a group of water types.
[3] http://www.climate.be/cart

$$\frac{dV}{dt} = \frac{d}{dt}\int_{\Omega} d\Omega = \int_{\Gamma} \mathbf{v}^{\Gamma} \bullet \mathbf{n}\, d\Gamma \quad , \tag{2.2}$$

where t and $\mathbf{n}$ denote the time and the outward unit normal to the domain boundary, respectively.

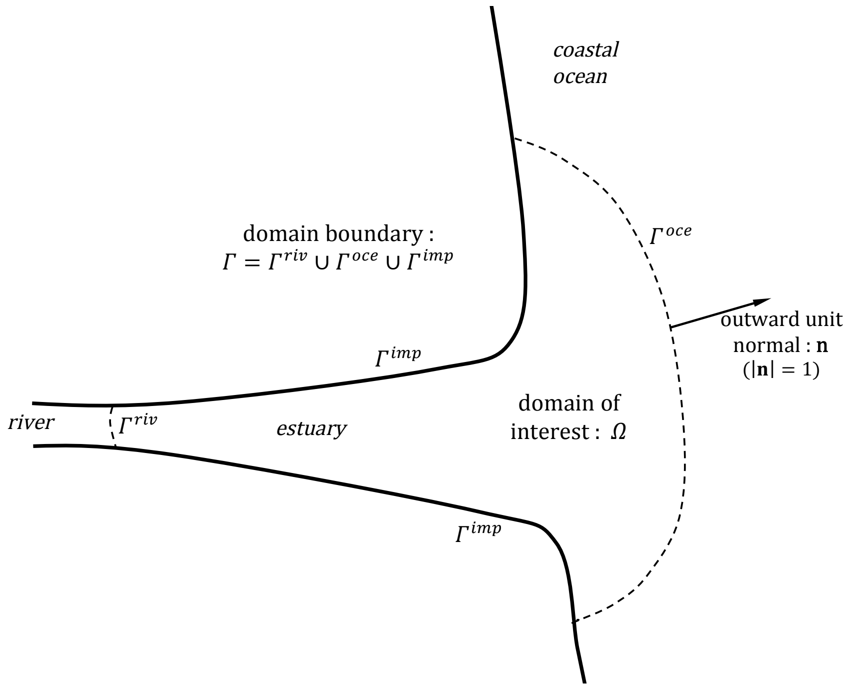

Figure 1. Schematic representation of the generic region of freshwater influence (ROFI) in which water renewal timescales are to be evaluated.

The abovementioned movement of the domain boundary is not arbitrary. In other words, velocity $\mathbf{v}^{\Gamma}$ is not specified by the modeller. Instead, it is determined by water motion. Therefore, some of the properties of water velocity $\mathbf{v}$ must be laid out and, subsequently, employed so as to establish the link between the variation of the domain geometry and the hydrodynamics.

As is usual in studies of flows in rivers, estuaries and shallow marine regions, the Boussinesq approximation is assumed to hold valid. As a consequence, the water velocity is divergence-free, i.e.

$$\nabla \bullet \mathbf{v} = 0 \quad , \tag{2.3}$$

where ∇ is the three-dimensional del operator. On the impermeable part of the boundary, $\mathbf{v}$ satisfies impermeability condition

$$[(\mathbf{v} - \mathbf{v}^{\Gamma}) \bullet \mathbf{n}]_{\mathbf{x} \in \Gamma^{imp}} = 0 \quad , \tag{2.4}$$

where $\mathbf{x}$ denotes the position-vector. The net volumetric flow rate ($\mathrm{m}^3\mathrm{s}^{-1}$) leaving the domain of interest is due to the water parcels crossing open boundaries. It reads

$$Q = \int_{\Gamma^{r+o}} (\mathbf{v} - \mathbf{v}^{\Gamma}) \bullet \mathbf{n}\, d\Gamma^{r+o} \quad . \tag{2.5}$$

Integrating continuity equation (2.3) over the domain, using the divergence theorem as well as (2.4)-(2.5), we obtain

$$Q = -\int_{\Gamma} \mathbf{v}^{\Gamma} \bullet \mathbf{n} \, d\Gamma \quad . \tag{2.6}$$

Finally, combining relation (2.2) and (2.6) yields the sought-after relationship between geometry and hydrodynamics:

$$\frac{dV}{dt} = -Q \quad . \tag{2.7}$$

Thus, the volume of the domain of interest decreases (increases) when the net outgoing water flux is positive (negative), which is in agreement with elementary physical intuition.

3. Concentration of the water types and their aggregates

Following previous diagnostic studies (e.g. Cox 1989, Hirst 1999, Goosse et al. 2001, Deleeersnijder et al. 2002, Haine and Hall 2002, Meier 2005), every water type will be regarded as a passive tracer, whose concentration obeys an advection-diffusion equation. All of the concentrations are defined as pointwise mass fractions, implying that they are dimensionless variables, depending on time and position.

The water types to be considered are identified by subscripts *ori*, *riv* and *oce*, which are associated with the original, river and coastal ocean waters, respectively. Thus, every water type concentration is denoted $C_{\chi}(t,\mathbf{x})$ with $\chi = ori, riv, oce$, and each concentration obeys an advection-diffusion equation,

$$\frac{\partial C_{\chi}}{\partial t} = -\nabla \bullet (C_{\chi}\mathbf{v} - \mathbf{K} \bullet \nabla C_{\chi}) \ , \quad \chi = ori, riv, oce \quad , \tag{3.1}$$

where diffusivity tensor $\mathbf{K}(t,\mathbf{x})$ is symmetric and positive-definite. The initial and boundary conditions must be prescribed in accordance with the above considerations as to the definition of the water types.

The initial conditions are trivial. The Dirichlet boundary conditions prescribed on the open boundaries convey the fact that the original water particles are discarded at the moment they hit Γ^{r+o}, whilst the river (coastal ocean) water particles are discarded at the instant they touch Γ^{oce} (Γ^{riv}). On Γ^{riv} (Γ^{oce}), we prescribe that all the water particles belong to the river (coastal ocean) type. On Γ^{imp}, the normal water type flux must be zero, leading to

$$\left[[C_{\chi}(\mathbf{v} - \mathbf{v}^{\Gamma}) - \mathbf{K} \bullet \nabla C_{\chi}] \bullet \mathbf{n} \right]_{\mathbf{x} \in \Gamma^{imp}} = 0 \ , \quad \chi = ori, riv, oce \quad . \tag{3.2}$$

Then, substituting (2.4) into (3.2) allows simplifying (3.2) to

$$\left[(-\mathbf{K} \bullet \nabla C_{\chi}) \bullet \mathbf{n} \right]_{\mathbf{x} \in \Gamma^{imp}} = 0 \ , \quad \chi = ori, riv, oce \quad . \tag{3.3}$$

Thus, on the impermeable part of the boundary, the normal advective and diffusive fluxes are both zero. The abovementioned initial and boundary conditions are laid out in Table 1.

Table 1. Initial and boundary conditions to be used to simulate the evolution of the concentrations of the original, river and coastal ocean water (i.e. water types) concentrations as well as the concentrations of the relevant aggregates thereof, i.e. the renewing water and the water itself.

designation	initial condition ($t=0$)	boundary conditions		
		Γ^{riv}	Γ^{oce}	Γ^{imp}
original water	$C_{ori}=1$	$C_{ori}=0$	$C_{ori}=0$	$(-\mathbf{K}\bullet\nabla C_{ori})\bullet\mathbf{n}=0$
river water	$C_{riv}=0$	$C_{riv}=1$	$C_{riv}=0$	$(-\mathbf{K}\bullet\nabla C_{riv})\bullet\mathbf{n}=0$
coastal ocean water	$C_{oce}=0$	$C_{oce}=0$	$C_{oce}=1$	$(-\mathbf{K}\bullet\nabla C_{oce})\bullet\mathbf{n}=0$
renewing water	$C_{ren}=0$	$C_{ren}=1$	$C_{ren}=1$	$(-\mathbf{K}\bullet\nabla C_{ren})\bullet\mathbf{n}=0$
water	$C_{wat}=1$	$C_{wat}=1$	$C_{wat}=1$	$(-\mathbf{K}\bullet\nabla C_{wat})\bullet\mathbf{n}=0$

Multiplying the equation governing C_{ori} by C_{ori} and taking into account continuity equation (2.3), we get after some manipulations the equation governing C_{ori}^2:

$$\frac{\partial C_{ori}^2}{\partial t} = -\nabla\bullet(C_{ori}^2\mathbf{v} - 2C_{ori}\mathbf{K}\bullet\nabla C_{ori}) - 2\nabla C_{ori}\bullet\mathbf{K}\bullet\nabla C_{ori} \quad . \tag{3.4}$$

Then, integrating (3.4) over the domain of interest, using the divergence and Reynolds' transport theorems, taking into account the relevant boundary conditions (Table 1), we obtain

$$\begin{aligned}
\frac{d}{dt}\overbrace{\int_{\Omega}(C_{ori})^2\,d\Omega}^{=L^2\text{-norm of }C_{ori}} = &-\overbrace{\int_{\Gamma^{riv}}(C_{ori})^2(\mathbf{v}-\mathbf{v}^{\Gamma})\bullet\mathbf{n}\,d\Gamma}^{=0,\text{ since }C_{ori}=0\text{ on }\Gamma^{riv}} - \overbrace{\int_{\Gamma^{oce}}(C_{ori})^2(\mathbf{v}-\mathbf{v}^{\Gamma})\bullet\mathbf{n}\,d\Gamma}^{=0,\text{ since }C_{ori}=0\text{ on }\Gamma^{oce}} - \overbrace{\int_{\Gamma^{imp}}(C_{ori})^2(\mathbf{v}-\mathbf{v}^{\Gamma})\bullet\mathbf{n}\,d\Gamma}^{=0,\text{ since }(\mathbf{v}-\mathbf{v}^{\Gamma})\bullet\mathbf{n}=0} \\
&+ \underbrace{\int_{\Gamma^{riv}}2C_{ori}(\mathbf{K}\bullet\nabla C_{ori})\bullet\mathbf{n}\,d\Gamma}_{=0,\text{ since }C_{ori}=0\text{ on }\Gamma^{riv}} + \underbrace{\int_{\Gamma^{oce}}2C_{ori}(\mathbf{K}\bullet\nabla C_{ori})\bullet\mathbf{n}\,d\Gamma}_{=0,\text{ since }C_{ori}=0\text{ on }\Gamma^{oce}} + \underbrace{\int_{\Gamma^{imp}}2C_{ori}(\mathbf{K}\bullet\nabla C_{ori})\bullet\mathbf{n}\,d\Gamma}_{=0,\text{ since }(\mathbf{K}\bullet\nabla C_{ori})\bullet\mathbf{n}=0} \\
&+ \underbrace{\int_{\Omega}(-2\nabla C_{ori}\bullet\mathbf{K}\bullet\nabla C_{ori})\,d\Omega}_{\le 0,\text{ since }\mathbf{K}\text{ is positive definite}}
\end{aligned}$$

(3.5a)

which simplifies to

$$\frac{d}{dt}\underbrace{\int_{\Omega}C_{ori}^2\,d\Omega}_{=L^2\text{-norm of }C_{ori}} = \underbrace{\int_{\Omega}(-2\nabla C_{ori}\bullet\mathbf{K}\bullet\nabla C_{ori})\,d\Omega}_{<0\text{ if }\nabla C_{ori}\neq 0;\ =0\text{ if }\nabla C_{ori}=0} \le 0 \tag{3.5b}$$

Thus the L^2-norm of the original water concentration, which is equal to the volume of the domain at $t=0$, will decrease monotonically until $\nabla C_{ori}=0$, in which case C_{ori} must be identically zero since this concentration is prescribed to be zero on the open boundaries. As a consequence, the following limit holds valid:

$$\lim_{t\to\infty} C_{ori}(t,\mathbf{x}) = 0 \tag{3.6}$$

As expected, the original water progressively leaves the domain and, in the limit $t\to\infty$, no particle of this water is left in the ROFI under consideration.

The renewing water, identified below by subscript *ren*, is the aggregate of the river and coastal ocean water. Accordingly, its concentration is $C_{ren} = C_{riv} + C_{oce}$. The water is the aggregate of all water types, implying that its concentration reads

$$C_{wat}(t,\mathbf{x}) = C_{ori}(t,\mathbf{x}) + \underbrace{C_{riv}(t,\mathbf{x}) + C_{oce}(t,\mathbf{x})}_{=C_{ren}(t,\mathbf{x})} \quad . \tag{3.7}$$

Since all the equations introduced above are linear, the partial differential problems governing the concentration of the renewing water and that of the water (i.e. the aggregate of all water types) are easily derived from appropriate sums of the abovementioned advection-diffusion equations, initial and boundary conditions. Accordingly, the advection-diffusion equation obeyed by C_{ren} and C_{wat} read

$$\frac{\partial C_\chi}{\partial t} = -\nabla\bullet(C_\chi \mathbf{v} - \mathbf{K}\bullet\nabla C_\chi) \ , \quad \chi = ren, wat \quad . \tag{3.8}$$

The relevant auxiliary conditions are listed in Table 1.

It is straightforward to show that the concentration of the water is equal to unity at any time and location,

$$C_{wat}(t,\mathbf{x}) = 1 \tag{3.9}$$

which immediately implies that the renewing water concentration obeys

$$C_{ren}(t,\mathbf{x}) = 1 - C_{ori}(t,\mathbf{x}) \tag{3.10}$$

Finally, combining (3.6) and (3.10) yields

$$\lim_{t\to\infty} C_{ren}(t,\mathbf{x}) = 1 \tag{3.11}$$

Clearly, the ROFI under study progressively fills with renewing water and, in the long run, there is only renewing water in the domain of interest.

4. Upper and lower bounds of the concentrations

The concentration properties derived in the previous Section do not suffice to convince us that the concentrations are well behaved. It must also be seen that, at any time and position, concentrations C_{ori}, C_{riv} and C_{oce} are non-negative and smaller than or equal to unity.

In order to produce the necessary demonstrations, it is convenient to first establish a theorem from which all the sought-after results will be deduced. If function $\varsigma(t,\mathbf{x})$ is the solution of reactive-transport equation

$$\frac{\partial \varsigma}{\partial t} = \Pi - \nabla\bullet(\varsigma\mathbf{v} - \mathbf{K}\bullet\nabla\varsigma) \ , \tag{4.1}$$

with $\Pi(t,\mathbf{x}) \ge 0$, under initial condition

$$\varsigma(t,\mathbf{x}) = \varsigma^0 \ge 0 \tag{4.2}$$

and boundary conditions

$$[\varsigma(t,\mathbf{x})]_{\mathbf{x}\in\Gamma^{riv}} = \varsigma^{riv} \geq 0 \quad , \tag{4.3}$$

$$[\varsigma(t,\mathbf{x})]_{\mathbf{x}\in\Gamma^{oce}} = \varsigma^{oce} \geq 0 \tag{4.4}$$

and

$$\left[(-\mathbf{K}\bullet\nabla\varsigma)\bullet\mathbf{n}\right]_{\mathbf{x}\in\Gamma^{imp}} = 0 \quad , \tag{4.5}$$

then

$$\varsigma(t,\mathbf{x}) \geq 0 \tag{4.6}$$

Hereinafter, this theorem will be referred to as the "positivity theorem".

Proving that $\varsigma(t,\mathbf{x})$ is non-negative is tantamount to showing that the negative part of $\varsigma(t,\mathbf{x})$,

$$\varsigma^{-}(t,\mathbf{x}) = \frac{\varsigma(t,\mathbf{x})-|\varsigma(t,\mathbf{x})|}{2} = \begin{cases} 0\,, \text{ if } \varsigma(t,\mathbf{x})\geq 0 \\ \varsigma(t,\mathbf{x})\,, \text{ if } \varsigma(t,\mathbf{x})<0 \end{cases} \quad , \tag{4.7}$$

is zero at any time and position. Then, we multiply (4.1) by ς^{-} and, after lengthy manipulations, we obtain

$$\begin{aligned}
\frac{d}{dt}\overbrace{\int_{\Omega}(\varsigma^{-})^2\,d\Omega}^{=L^2\text{-norm of }\varsigma^{-}} &= \overbrace{\int_{\Omega}2\varsigma^{-}\Pi\,d\Omega}^{\leq 0,\text{ since }\varsigma^{-}\leq 0\text{ and }\Pi\geq 0} \\
&- \overbrace{\int_{\Gamma^{riv}}(\varsigma^{-})^2(\mathbf{v}-\mathbf{v}^{\Gamma})\bullet\mathbf{n}\,d\Gamma}^{=0,\text{ since }\varsigma=\varsigma^{riv}\geq 0\Rightarrow\varsigma^{-}=0} - \overbrace{\int_{\Gamma^{oce}}(\varsigma^{-})^2(\mathbf{v}-\mathbf{v}^{\Gamma})\bullet\mathbf{n}\,d\Gamma}^{=0,\text{ since }\varsigma=\varsigma^{oce}\geq 0\Rightarrow\varsigma^{-}=0} - \overbrace{\int_{\Gamma^{imp}}(\varsigma^{-})^2(\mathbf{v}-\mathbf{v}^{\Gamma})\bullet\mathbf{n}\,d\Gamma}^{=0,\text{ since }(\mathbf{v}-\mathbf{v}^{\Gamma})\bullet\mathbf{n}=0} \\
&+ \underbrace{\int_{\Gamma^{riv}}2\varsigma^{-}(\mathbf{K}\bullet\nabla\varsigma)\bullet\mathbf{n}\,d\Gamma}_{=0,\text{ since }\varsigma=\varsigma^{riv}\geq 0\Rightarrow\varsigma^{-}=0} + \underbrace{\int_{\Gamma^{oce}}2\varsigma^{-}(\mathbf{K}\bullet\nabla\varsigma)\bullet\mathbf{n}\,d\Gamma}_{=0,\text{ since }\varsigma=\varsigma^{oce}\geq 0\Rightarrow\varsigma^{-}=0} + \underbrace{\int_{\Gamma^{imp}}2\varsigma^{-}(\mathbf{K}\bullet\nabla\varsigma)\bullet\mathbf{n}\,d\Gamma}_{=0,\text{ since }(\mathbf{K}\bullet\nabla\varsigma)\bullet\mathbf{n}=0} + \underbrace{\int_{\Omega}(-2\nabla\varsigma^{-}\bullet\mathbf{K}\bullet\nabla\varsigma^{-})\,d\Omega}_{\leq 0,\text{ since }\mathbf{K}\text{ is positive definite}}
\end{aligned} \tag{4.8a}$$

This relation simplifies to

$$\frac{d}{dt}\underbrace{\int_{\Omega}(\varsigma^{-})^2\,d\Omega}_{=L^2\text{-norm of }\varsigma^{-}} = \underbrace{\int_{\Omega}2\varsigma^{-}\Pi\,d\Omega}_{\leq 0,\text{ since }\varsigma^{-}\leq 0\text{ and }\Pi\geq 0} + \underbrace{\int_{\Omega}(-2\nabla\varsigma^{-}\bullet\mathbf{K}\bullet\nabla\varsigma^{-})\,d\Omega}_{\leq 0,\text{ since }\mathbf{K}\text{ is positive definite}} \leq 0 \quad . \tag{4.8b}$$

Since ς^{0} is non-negative, the L^2-norm of ς^{-} is zero at the initial instant ($t=0$). Furthermore, this L^2-norm cannot increase, as indicated in (4.8b). Therefore, the L^2-norm of ς^{-} will remain zero as time progresses, implying that $\varsigma(t,\mathbf{x})$ is a non-negative function. QED.

The mathematical developments leading to (4.8a) require the application of the divergence and Reynolds' transport theorems in a manner that is not as straightforward as we might think at first glance. This is because function ς^{-}, though continuous, is not differentiable at every point of the domain of interest. On the surface separating the region where $\varsigma(t,\mathbf{x})$ is positive from that in which this function is negative, the derivatives of $\varsigma(t,\mathbf{x})$ in the direction normal to that interface are not defined. Additional pieces of information may be found in Appendix C of Deleersnijder et al. (2001a) and references therein, in particular Lewandowski (1997).

If we set $\Pi=0$, $\varsigma^{0}=1$, $\varsigma^{riv}=0$ and $\varsigma^{oce}=0$, then $\varsigma(t,\mathbf{x})$ will be equal to the original water concentration. To obtain the concentration of the other two water types, we can resort to a somewhat similar approach. The values to be prescribed are listed in Table 2. Then, by virtue of the positivity theorem, we can say for certain that the original, river and coastal ocean water concentrations are non-negative. Furthermore, by having recourse to a similar method, we can demonstrate that $1-C_{\chi}(t,\mathbf{x})$, with $\chi = ori, riv, oce$, is non-negative. The relevant values are laid out in Table 2. As a consequence, the concentrations of the three water types under consideration as well as the relevant aggregates (i.e. the renewing water and the water itself) satisfy inequalities

$$0 \le C_{\chi}(t,\mathbf{x}) \le 1 \ , \quad \chi = ori, riv, oce, ren, wat \tag{4.9}$$

The properties of the concentrations established above lead us to conclude that the partial differential problems governing the concentrations under study are well posed. In other words, the concentrations are well-behaved, i.e. their behaviour is in accordance with physical intuition and elementary mathematical requirements.

Table 2. Source term, initial condition and boundary conditions on Γ^{riv} and Γ^{oce} to be implemented in order to obtain the functions used to demonstrate, by having recourse to the positivity theorem, that inequalities (4.9) hold valid.

source term $\Pi(t,x)$	initial condition ς^0	boundary conditions		solution $\varsigma(t,\mathbf{x})$
		ς^{riv}	ς^{oce}	
0	1	0	0	$\varsigma = C_{ori}$
0	0	1	0	$\varsigma = C_{riv}$
0	0	0	1	$\varsigma = C_{oce}$
0	0	1	1	$\varsigma = 1 - C_{ori}$
0	1	0	1	$\varsigma = 1 - C_{riv}$
0	1	1	0	$\varsigma = 1 - C_{oce}$

5. Ages: definitions, governing equations and properties

In line with Deleersnijder (2019), we define the age of a particle of a water type as the time that has elapsed since it began to be taken into consideration. It is also necessary to define the moment at which a particle will cease to be taken into consideration, otherwise the age of certain particles, if not all of them, will grow unboundedly. Finally, the age calculations must be in agreement with the fact that there is no crossing of the impermeable boundary of the domain.

Since the overall objective of the present study is to obtain water renewal timescales, in view of the above considerations, we define the age of a particle of river (coastal ocean) water as the time elapsed since it left domain boundary Γ^{riv} (Γ^{oce}) given that such a particle is discarded at the moment it hits Γ^{oce} (Γ^{riv})[4]. Since an original water particle is to be discarded at the moment it touches an open boundary, the age of the original water must be equal to the elapsed time (*t*). This provides no insight into water renewal processes, but is a validation element for the equations developed herein.

The fate of a single particle is rather irrelevant: a sufficiently large number of particles must be taken into consideration. In accordance with the age-averaging hypothesis[5] (Deleersnijder et al. 2001a), the mean age is defined as follows: the mean age of a sufficiently large number of particles is the mass weighted average of their individual ages. This definition paves the way for the calculation at every time and position of the mean age of water types as well as that of the relevant aggregates of them, i.e. the renewing water and the water itself.

Delhez et al. (1999) developed in the Eulerian framework the general theory of the age, according to which, in the present context, the mean age of a water type is

$$a_\chi(t,\mathbf{x}) = \frac{\alpha_\chi(t,\mathbf{x})}{C_\chi(t,\mathbf{x})} \ , \ \chi = ori, riv, oce \ , \tag{5.1}$$

where $\alpha_\chi(t,\mathbf{x})$ is called "age concentration". This function is governed by partial differential equation

$$\frac{\partial \alpha_\chi}{\partial t} = C_\chi - \nabla \bullet (\alpha_\chi \mathbf{v} - \mathbf{K} \bullet \nabla \alpha_\chi) \ , \ \chi = ori, riv, oce \ . \tag{5.2}$$

The initial and boundary conditions under which the age concentration equations must be solved are

$$\alpha_\chi(0,\mathbf{x}) = 0 \ , \ [\alpha_\chi(t,\mathbf{x})]_{\mathbf{x}\in\Gamma^{r+o}} = 0 \ , \ \left[(-\mathbf{K} \bullet \nabla C_\chi) \bullet \mathbf{n}\right]_{\mathbf{x}\in\Gamma^{imp}} = 0 \quad (\chi = ori, riv, oce) \tag{5.3}$$

Then, the age concentration of the original water is readily seen to be $\alpha_{ori} = t\, C_{ori}$, yielding

$$a_{ori}(t,\mathbf{x}) = t \tag{5.4}$$

as expected.

In accordance with the abovementioned age-averaging hypothesis, the age of the renewing

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[4] The time elapsed since leaving an open boundary is not equivalent to the time elapsed since crossing an open boundary. The Dirichlet boundary conditions implemented in this working note are appropriate for evaluating the previous type of timescale, whilst, to evaluate the latter, a more sophisticated diagnostic strategy would be necessary.

[5] Consider, for instance, two particles that are identified by means of subscripts "A" and "B". Their mass and age are denoted m^X and a^X, respectively, with *X=A,B*. The mass of the system "A+B" obvioulsy is $m^{A+B} = m^A + m^B$. This is in agreement with basic physical principles that stipulate that mass is an additive quantity. No such principle exists for the age. Therefore, to obtain the mean age of system "A+B", an arbitrary decision is to be made. The latter was formulated as the so-called age-averaging hypothesis (Deleersnijder et al., 2001a), which is the only arbitrary element of CART's age. It stipulates that the mean age of a system made up of various particles is the mass-weighted average of the ages of the particles. Accordingly, the mean age of the system "A+B", a^{A+B}, satisfies the follow relation: $m^{A+B}a^{A+B} = m^A a^A + m^B a^B$. Clearly, the age is not an additive quantity, but the age content is — the age content of a particle being defined as the product of its mass and its age. Ages other than CART's, such as the carbon-14 age, implicitly or explicitly rely on an age-averaging hypothesis (Deleersnijder et al., 2001a). However, it is believed that CART's age-averaging hypothesis is the simplest one could think of.

water and that of the water are as follows:

$$a_{ren} = \frac{\overbrace{\alpha_{riv} + \alpha_{oce}}^{=\alpha_{ren}}}{\underbrace{C_{riv} + C_{oce}}_{=C_{ren}}} = \frac{\alpha_{ren}}{C_{ren}} \tag{5.5}$$

and

$$a_{wat} = \frac{\overbrace{\alpha_{ori} + \alpha_{ren}}^{=\alpha_{wat}}}{\underbrace{C_{ori} + C_{ren}}_{=C_{wat}}} = \frac{\alpha_{wat}}{C_{wat}} \quad . \tag{5.6}$$

Clearly, the age concentration of these aggregates satisfy

$$\frac{\partial \alpha_\chi}{\partial t} = C_\chi - \nabla \bullet (\alpha_\chi \mathbf{v} - \mathbf{K} \bullet \nabla \alpha_\chi) \ , \quad \chi = ren, wat \quad . \tag{5.7}$$

The relevant initial and boundary conditions are easily derived from those obeyed by the water types. They are as follows:

$$\alpha_\chi(0,\mathbf{x}) = 0 \ , \ \ [\alpha_\chi(t,\mathbf{x})]_{\mathbf{x}\in\Gamma^{r+o}} = 0 \ , \ \ \left[(-\mathbf{K} \bullet \nabla C_\chi) \bullet \mathbf{n}\right]_{\mathbf{x}\in\Gamma^{imp}} = 0$$
$$(\chi = ren, wat) \tag{5.8}$$

As $\alpha_{ori} = t\,C_{ori}$ and $C_{wat} = 1$, (5.6) transforms to

$$a_{wat} = t\,C_{ori} + a_{ren}\,C_{ren} \quad . \tag{5.9}$$

Since $1 - C_{ori} = C_{ren} << 1$ in the limit $t \to 0$ and $1 - C_{ren} = C_{ori} << 1$ in the limit $t \to \infty$, relation (5.6) admits the following asymptotic expansions

$$a_{wat} \sim \begin{cases} t \ , & t \to 0 \\ a_{ren} \ , & t \to \infty \end{cases} \tag{5.10}$$

The age properties derived above do not suffice to convince us that the ages are well-behaved. It must also be seen that, at any time and position, ages a_{riv} and a_{oce} are non-negative and smaller than or equal to the elapsed time. For $\chi = riv, oce$, if we set $\Pi = C_\chi$, $\varsigma^0 = 0$, $\varsigma^{riv} = 0$ and $\varsigma^{oce} = 0$, then $\varsigma(t,\mathbf{x})$ will be equal to α_χ, which, by virtue of the positivity theorem, must be non-negative. Similarly, if we set $\Pi = 0$, $\varsigma^0 = 0$, $\varsigma^{riv} = t$ and $\varsigma^{oce} = 0$, then $\varsigma(t,\mathbf{x})$ will be equal to $C_{riv}(t - a_{riv})$, which, by virtue of the positivity theorem, must be non-negative. Finally, to show that $C_{oce}(t - a_{oce})$ is non-negative, we set $\Pi = 0$, $\varsigma^0 = 0$, $\varsigma^{riv} = 0$ and $\varsigma^{oce} = t$. As a consequence, inequalities $0 \le a_{riv} \le t$ and $0 \le a_{oce} \le t$ hold valid. Finally, bearing in mind relations (5.1) and (5.4)-(5.6), we obtain

$$0 \le a_\chi(t,\mathbf{x}) \le t \ , \quad \chi = ori, riv, oce, ren, wat \tag{5.11}$$

The properties of the ages established in this Section lead us to conclude that the partial differential problems from which we derive the ages of the water types and their aggregates are well posed. In other words, the behaviour of the ages is in accordance with physical intuition and elementary mathematical requirements.

6. One-dimensional illustration

To illustrate some of the above developments, we will consider a one-dimensional, highly idealised configuration. The velocity and diffusivity are positive constants, denoted U and K, respectively. If space coordinate x and constant L denote the distance to the upstream boundary and the length of the domain, then the domain of interest is defined by inequalities $0 \le x \le L$. All variables are assumed to be at a steady state, which is obtained in the limit $t \to \infty$. Therefore, there is no original water in the domain any more and, hence, the renewing water concentration is equal to unity. As a consequence, we will focus exclusively on diagnostic variables related to the renewing water and its components (river and coastal ocean waters).

It is convenient to introduce the following dimensionless variables (identified by tildes),

$$\tilde{x} = \frac{x}{L} , \quad \tilde{\alpha}_\chi = \frac{\alpha_\chi}{L/U} , \quad \tilde{a}_\chi = \frac{a_\chi}{L/U} \quad , \quad \chi = riv, oce, ren \quad , \tag{6.1}$$

as well as the Peclet number,

$$Pe = \frac{UL}{K} \quad . \tag{6.2}$$

The larger this dimensionless parameter, the greater the impact of advection with respect to that of diffusion.

From here on, we will deal only with dimensionless variables. Therefore, for notational simplicity, the tildes will be systematically omitted.

Table 3. Boundary conditions to be used to solve the one-dimensional, highly idealised equations governing the steady-state river, coastal ocean and renewing water concentrations and age concentrations in the domain defined by inequalities $0 \le x \le 1$. Dimensionless variables are used in accordance with (6.1).

designation	boundary conditions	
	Γ^{riv} (x=0)	Γ^{oce} $(x=1)$
river water	$C_{riv} = 1$ $\alpha_{riv} = 0$	$C_{riv} = 0$ $\alpha_{riv} = 0$
coastal ocean water	$C_{oce} = 0$ $\alpha_{oce} = 0$	$C_{oce} = 1$ $\alpha_{oce} = 0$
renewing water	$C_{ren} = 1$ $\alpha_{ren} = 0$	$C_{ren} = 1$ $\alpha_{ren} = 0$

The concentration and age concentration of the river, coastal ocean and renewing waters obey steady-state equations

$$\frac{1}{Pe}\frac{d^2C_\chi}{dx^2} - \frac{dC_\chi}{dx} = 0 \ , \quad \chi = riv, oce, ren \tag{6.3}$$

and

$$\frac{1}{Pe}\frac{d^2\alpha_\chi}{dx^2} - \frac{d\alpha_\chi}{dx} = -C_\chi \ , \quad \chi = riv, oce, ren \quad , \tag{6.4}$$

which must be solved under boundary conditions listed in Table 3.

The renewing water concentration, age concentration and age are (Figures 2, 3, 4)

$$C_{ren} = 1 \, , \quad \alpha_{ren} = x - \frac{e^{Pe\,x} - 1}{e^{Pe} - 1} = a_{ren} \quad . \tag{6.5}$$

If the Peclet number is small, the impact of diffusion is very significant, which is why the age is approximately symmetrical with respect to the centre of the domain ($x = 1/2$). By contrast, if the Peclet number is large, the advection is the dominant transport process in most of the domain. This is why the age is close to x, except in a boundary layer adjacent to the outgoing boundary ($x = 1$), whose length is of the order of Pe^{-1}.

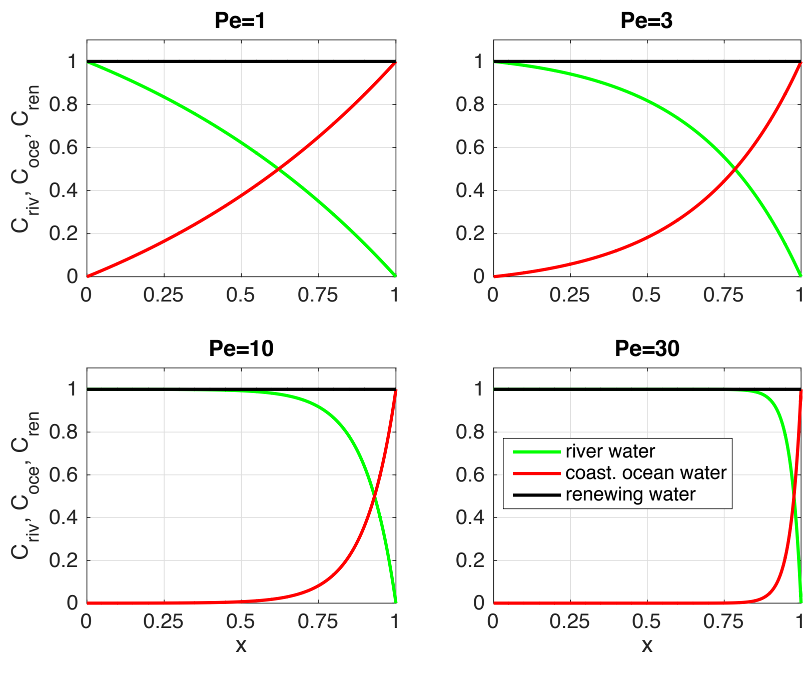

Figure 2. Steady-state river, coastal ocean and renewing water concentrations in the one-dimensional, highly idealised ROFI model for various values of the Peclet number. Dimensionless variables are used in accordance with (6.1).

The river and coastal ocean water concentrations read (Figure 2)

$$C_{riv} = \frac{e^{Pe} - e^{Pe\,x}}{e^{Pe} - 1} \, , \quad C_{oce} = \frac{e^{Pe\,x} - 1}{e^{Pe} - 1} \quad . \tag{6.6}$$

It is readily seen that their sum is $C_{riv}+C_{oce}=C_{ren}=1$, as it should be. As is depicted in Figure 2, for a large value of the Peclet number, the river water concentration is close to unity in most of the domain, except in a thin boundary layer adjacent to the downstream boundary. This is because the advection is the dominant transport process. This is much less so if the Peclet number is of order unity. In this case, the amount of coastal ocean water present in the domain is much greater. Unsurprisingly, the age concentrations,

$$\alpha_{riv}=x\,\frac{e^{Pe}+e^{Pe\,x}}{e^{Pe}-1}-\frac{2\,e^{Pe}\,(e^{Pe\,x}-1)}{\left(e^{Pe}-1\right)^2}\,,\quad \alpha_{oce}=-x\,\frac{e^{Pe\,x}+1}{e^{Pe}-1}+\frac{(e^{Pe}+1)(e^{Pe\,x}-1)}{\left(e^{Pe}-1\right)^2}\,, \tag{6.7}$$

exhibit a somewhat similar sensitivity to the value of the Peclet number (Figure 3).

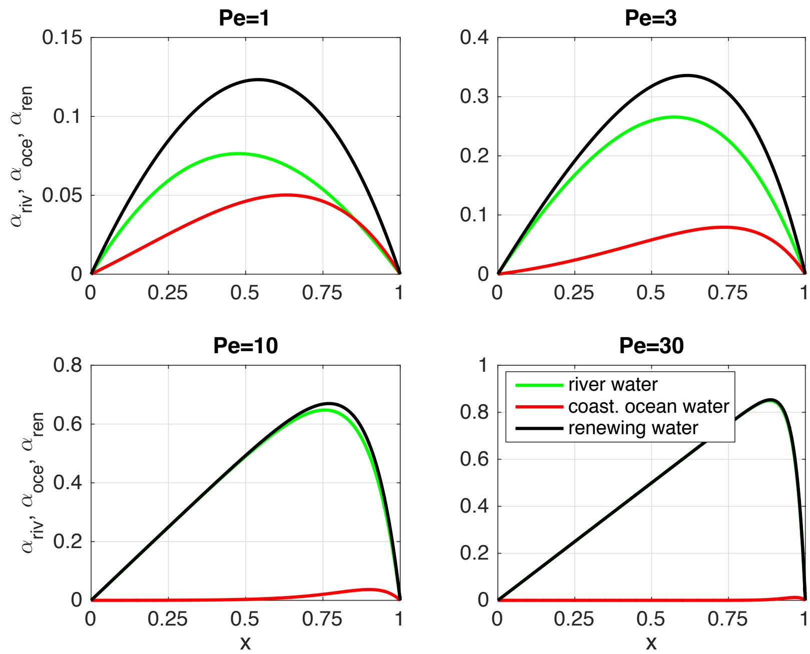

Figure 3. Steady-state river, coastal ocean and renewing water age concentrations in the one-dimensional, highly idealised ROFI model for various values of the Peclet number. Dimensionless variables are used in accordance with (6.1).

The river water age (Figure 4),

$$a_{riv}(x) \;=\; x\,\frac{e^{Pe}+e^{Pe\,x}}{e^{Pe}-e^{Pe\,x}}\;-\;\frac{2\,e^{Pe}\,(e^{Pe\,x}-1)}{(e^{Pe}-1)(e^{Pe}-e^{Pe\,x})} \tag{6.8}$$

admits the following asymptotic expressions

$$a_{riv}(x)\;\sim\;\begin{cases}\dfrac{e^{2Pe}-2\,Pe\,e^{Pe}-1}{(e^{Pe}-1)^2}\,x\,, & x\to 0\\[2ex] \dfrac{(Pe-2)e^{Pe}+Pe+2}{Pe(e^{Pe}-1)}-\dfrac{Pe}{6}\,(1-x)^2\,, & x\to 1\end{cases} \tag{6.9}$$

Unsurprisingly, the river water age is zero at the upstream boundary ($x=0$). This age has a finite, non-zero value at the downstream boundary ($x=1$), though the associated concentration and age concentration are both zero. Furthermore, the age gradient is zero at $x=1$. On the other hand, the age of the coastal ocean water reads (Figure 4)

$$a_{oce}(x) = -x\,\frac{e^{Pe\,x}+1}{e^{Pe\,x}-1} + \frac{e^{Pe}+1}{e^{Pe}-1} \tag{6.10}$$

In the vicinity of the domain boundaries, the following asymptotic expansions hold valid:

$$a_{oce}(x) \sim \begin{cases} \dfrac{(Pe-2)e^{Pe}+Pe+2}{Pe(e^{Pe}-1)} - \dfrac{Pe}{6}x^2\,, & x\to 0 \\ \dfrac{e^{2Pe}-2\,Pe\,e^{Pe}-1}{(e^{Pe}-1)^2}(1-x)\,, & x\to 1 \end{cases} \tag{6.11}$$

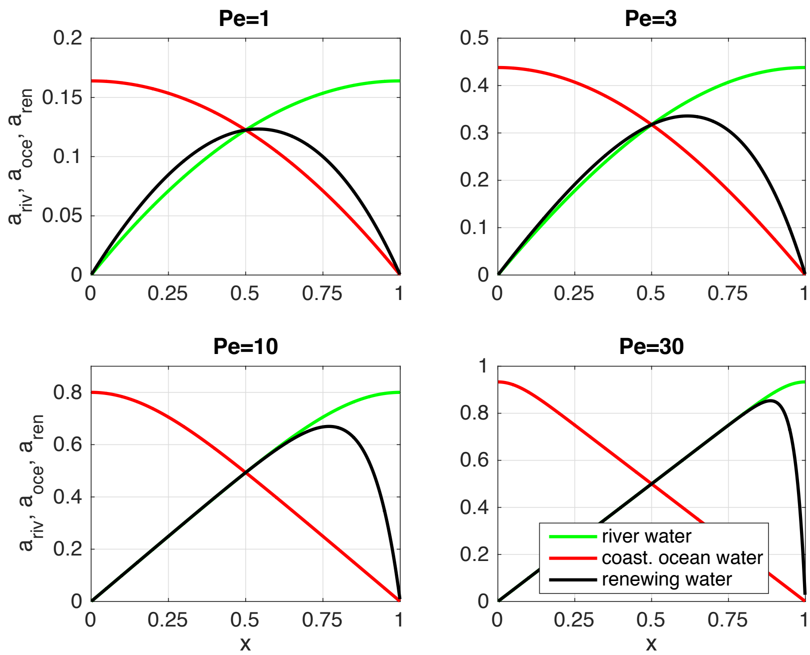

Figure 4. Steady-state river, coastal ocean and renewing water ages in the one-dimensional, highly idealised ROFI model for various values of the Peclet number. Dimensionless variables are used in accordance with (6.1).

The direction of the water velocity has an unmistakable impact (especially when the Peclet number is large) on the concentrations and age concentrations as well as on the renewing water age (Figures 2, 3, 4). This is not the case, however, for the river and coastal ocean water ages. Indeed, the latter ages satisfy the following symmetry property

$$a_{riv}(x) = a_{oce}(1-x) \tag{6.12}$$

The differential equation obeyed by the ages is of the form

$$\underbrace{\frac{1}{Pe}\frac{d^2 a_\chi}{dx^2}}_{\text{diffusion}} - \underbrace{U_\chi^{eq}\frac{da_\chi}{dx}}_{\substack{\text{equivalent}\\ \text{advection}}} = \underbrace{-1}_{\text{ageing}}\,, \quad \chi = riv, oce, ren\,, \tag{6.13}$$

where

$$U_\chi^{eq} = 1 - \frac{2}{PeC_\chi}\frac{dC_\chi}{dx} \quad , \quad \chi = riv, oce, ren \quad , \tag{6.14}$$

is the (dimensionless) equivalent velocity. The latter is equal to unity for the renewing water and, for the river and coastal ocean waters, it satisfies the following antisymmetry property

$$U_{riv}^{eq}(x) = \frac{e^{Pe} + e^{Pex}}{e^{Pe} - e^{Pex}} = -U_{oce}^{eq}(1-x) \quad . \tag{6.15}$$

These velocities satisfy

$$U_{riv}^{eq}(0) = \frac{e^{Pe}+1}{e^{Pe}-1}, \quad U_{oce}^{eq}(1) = -\frac{e^{Pe}+1}{e^{Pe}-1} \tag{6.16}$$

and

$$\lim_{x\to 1} U_{riv}^{eq}(x) = +\infty, \quad \lim_{x\to 0} U_{oce}^{eq}(x) = -\infty \quad . \tag{6.17}$$

It is also readily seen that U_{riv}^{eq} (U_{oce}^{eq}) tends to +1 (-1) as the Peclet number increases, except in a boundary layer adjacent to the downstream (upstream) boundary. The length of this boundary layer is of the order of Pe^{-1}.

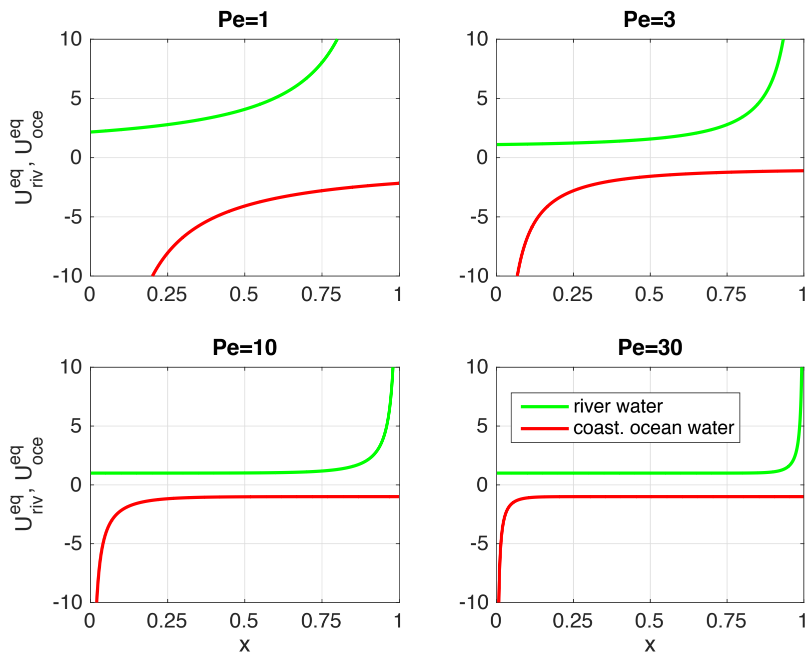

Figure 5. Illustration of (dimensionless) equivalent velocities U_{riv}^{eq} and U_{oce}^{eq} (6.15) for various values of the Peclet number.

As a consequence of the above developments, the differential problems satisfied by the river and coastal ocean water ages may be cast into the same form, i.e.

$$\begin{cases} \dfrac{1}{Pe}\dfrac{d^2 a_{riv}}{dx^2} - U_{riv}^{eq}(x)\dfrac{da_{riv}}{dx} = -1 \\ \left[a_{riv}(x)\right]_{x=0} = 0 \,,\ \left[\dfrac{da_{riv}}{dx}\right]_{x=1} = 0 \end{cases} \tag{6.18}$$

and

$$\begin{cases} \dfrac{1}{Pe}\dfrac{d^2 a_{oce}}{d\hat{x}^2} - U_{riv}^{eq}(\hat{x})\dfrac{da_{oce}}{d\hat{x}} = -1 \\ \left[a_{oce}(\hat{x})\right]_{\hat{x}=0} = 0 \,,\ \left[\dfrac{da_{oce}}{d\hat{x}}\right]_{\hat{x}=1} = 0 \end{cases} \tag{6.19}$$

with $\hat{x} = 1 - x$. The boundary condition at $x = 0 = \hat{x}$ is easily comprehended. However, the very reason why the gradient of the ages is zero at $x = 1 = \hat{x}$ remains somewhat elusive. A simple inspection of (6.18) and (6.19) suggests that symmetry property (6.12) essentially is a consequence of the behaviour of equivalent velocities (6.15).

The physical interpretation of this symmetry property has yet to be built. It is noteworthy that this is not the only intriguing symmetry property that the diagnostic timescale theory led to (e.g. Beckers et al. 2001, Deleersnijder et al. 2001b, Deleersnijder and Delhez 2004, Hall and Haine 2004, Deleersnijder 2014b).

7. Discussion and conclusion

The boundary conditions for the diagnostic variables have been derived from seemingly straightforward physical and mathematical considerations. This is why it was deemed unnecessary, perhaps wrongly, to have recourse to the more elaborate, but presumably more thorough, procedure advocated by Deleersnijder and Mouchet (2017). If we had used Neumann or Robin conditions on the open boundaries, it would certainly have been preferable to have recourse to this method.

On the oceanic (riverine) open boundary, the concentration and the age concentration of the river (coastal ocean) water are both prescribed to be zero. However, the related age is believed to have a finite, non-zero limit, as is illustrated by the highly-idealised, steady-state, one-dimensional solutions derived in Section 6. A theoretical and sufficiently general approach to this issue has yet to be developed.

The symmetry of the idealised ages of the river and coastal ocean water is as yet unexplained. Building a physical interpretation of this surprising result is a challenge worth taking up. If this symmetry property turns out to be a mere laboratory curiosity, then there is little possibility that it will ever be observed in numerical results. By contrast, if it turns out to be robust (i.e. numerical results for several ROFIs yield ages that are approximately symmetric), then it would be all the more important to develop a thorough understanding of this property.

The mathematical developments carried out in Sections 2 to 5 were aimed at showing that the diagnostic variables under consideration are well behaved. The list of criteria considered might well be incomplete. Although the above developments suggest that the partial differential problems dealt with herein are well posed, we must not forget that the design of the validation activities of a diagnostic strategy based on time- and position-dependent timescales is a research field that is still in its infancy.

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