On the method for estimating the mean property experienced by a tracer pioneered by Gross et al. (2019)

Eric Deleersnijder, 19 May 2021 - 6 June 2021

Contents

Abstract. *Elaborating on equations introduced by Gross et al. (Water, 2019, 11, 2207), a method for estimating the mean property experienced by a passive or reactive tracer is developed in the Eulerian framework by seeking inspiration in the age theory that is part of CART (www.climate.be/cart). The relevant age concentration distribution function is defined, the zero-th and first order moments of which lead to the sought-after diagnosis. All of the relevant variables are the solution of partial differential problems involving reactive transport equations. A simple method for numerically solving the distribution function equation is outlined. The concept of partial property exposure is introduced. The link between age and property exposure related variables is highlighted. Then, three test cases are tackled, leading to results in accordance with elementary physical intuition, contributing to lend credence to the novel diagnostic approach. Generic boundary conditions are introduced (Appendix A). Relevant inequalities are thoroughly derived in the context of a general study of a region of freshwater influence (ROFI) (Appendix B). Time is now ripe to assess the potential of the novel method for diagnosing numerically-simulated realistic (reactive) transport processes taking place in geophysical and environmental flows.*

Keywords: environmental flows, reactive transport, diagnostic variables, property exposure, age, distribution function, CART

1. Introduction

Today's numerical models environmental fluid flows and the associated reactive transport processes, and, to a lesser degree, field data collection systems produce vast amounts of real numbers. Making sense of them (i.e., identifying key processes and establishing causal relationships between them) is no trivial task. Analysing primitive variables (velocity components, pressure, temperature, concentrations, etc.) is not always conducive to the most fruitful interpretations (see, e.g., Lucas and Deleersnijder 2021 and references therein). An option worth considering consists in examining auxiliary variables, e.g., local effective diffusivities estimated *a posteriori* (Petton et al. 2020) or timescales such as the age or the residence/exposure time, introduced for diagnostic purposes (see, e.g., Deleersnijder et al. 2018, Lucas and Deleersnijder 2020, and references therein). Such variables may also be instrumental in designing reduced-dimension models, which may be used as interpretation or simplified prediction tools (see, e.g., Deleersnijder 2009, Mouchet et al. 2012, Lucas and Deleersnijder 2020, and references therein).

The age, one of the diagnostic variables referred to above, is usually defined as the time elapsed since leaving the relevant region of origin (e.g. Bolin and Rodhe 1973, Zimmerman 1976, Takeoka 1984). It has been estimated by means of various techniques. Some of them were inspired by radiocarbon dating (e.g. Doney and Jenkins 1994, Campin et al. 1999, Liu et al. 2020), whilst others consisted in evaluating the time lag between concentration time series (Salomon et al. 1995). These approaches as well as a few others (e.g. Kazemi et al. 2006, Cornaton et al. 2011) yield age values that are not exactly in accordance with the abovementioned definition and, unsurprisingly, are impacted by systematic biases that, in some cases, may be very significant (e.g. Beckers et al. 2001, Delhez et al. 2003, Delhez and Deleersnijder 2008). On the other hand, a number of model studies were based on age equations that were flawless but poorly justified in the related articles (e.g. Thiele and Sarmiento 1990, England 1995, Venkatram et al. 1998, Hirst 1999).

These shortcomings prompted some authors to build theories for evaluating timescales at any time and location that would be in strict accordance with their definitions, i.e. approaches that would not rest on simplifying assumptions that are not always valid. Having recourse to the concept of Green's function has proved to be a fruitful option (e.g. Hall and Plumb 1994, Holzer and Hall 2000, Cornaton and Perrochet 2006, Holzer and Primeau 2006), although it does not allow dealing with tracers subject to non-linear production-destruction processes. The Constituent-oriented Age and Residence time Theory (CART, www.climate.be/cart) (e.g. Delhez et al. 1999, Deleersnijder et al. 2001, Delhez et al. 2004) allows overcoming this problem since it provides partial differential equations aimed at evaluating the age of every constituent or group of constituents (i.e., an aggregate) irrespective of the nature of the reactions it may be involved in. The core variable of CART's age theory is the concentration distribution function, which, in its most general form, depends of five independent variables (i.e., time, three space coordinates, age). Explicitly calculating it is generally uneasy (Delhez and Deleersnijder 2002). However, obtaining the mean age in the sense of the age-averaging hypothesis (Deleersnijder et al. 2001) is much less demanding, for the latter is the ratio of two variables obeying rather classical reactive-transport equations, i.e., the age concentration and the concentration. As was pointed out by Deleersnijder et al. (2020), initial and, above all, boundary conditions must be prescribed with care so as to obtain timescales that are in accordance with the declared objective of the diagnostic strategy.

Several attempts have been made to generalise the concept of the age of a dissolved constituent of a fluid mixture. Suspended and deposited sediment ages were simulated numerically (Mercier and Delhez 2007, Gong and Shen 2010, Ralston and Geyer 2017, Munhoven 2020) as well as the age of substances adsorbed on sediment particles (Delhez and Wolk 2013). Seeking inspiration in Liu et al. (2012), Mouchet et al. (2016) introduced the notion of partial ages, which consists in, schematically speaking, attaching several clocks, rather than a single one, to every particle of the constituent under study. In the framework of CART, various approaches to the evaluation of the age of sea ice have been suggested (e.g., Lietaer et al. 2011, Deleersnijder and Bouillon 2017). Deleersnijder (2008) outlined how CART's methodology could be applied to the evaluation of the age of energy-containing eddies in a turbulent flow and, later on, attempted to generalise this line of reasoning to non-positive definite variables (Deleersnijder et al. 2017), which has met with little success.

Relying on splendid physical intuition and in-depth understanding of CART's age concept, Gross et al. (2019) pioneered a novel approach, eventually yielding the “mean property experienced by a tracer”. This variable does not have the physical dimensional of a timescale. Instead, its physical dimension is that of the property under consideration, which, moreover, is not necessarily positive definite. According to Gross et al. (2019), the new diagnostic quantity is obtained as the ratio of the property-age-concentration to the age-concentration. The latter variable is taken from CART, whereas the former is completely new.

The objective of this working note is to substantiate, document and illustrate (by tackling instructive test cases) the method suggested by Gross et al. (2019). To do so, it is first necessary to return to the fundamentals of CART, which will help unravel the type of averaging lying at the core of the method of Gross et al. (2019).

2. CART's age averaging hypothesis

The core variable of CART is the concentration distribution function[1], $c(t,\mathbf{x},\tau)$, where t, $\mathbf{x}=(x,y,z)$ and τ denote the time, the position-vector and the age (as an independent variable), respectively. In the framework of the Boussinesq approximation, where constant ρ is the reference density of the fluid mixture under consideration, the concentration distribution function of one of its constituents is defined as follows (e.g. Delhez et al., 1999):

> At time t, let $\delta\Omega$ represent the elemental control domain located at point $\mathbf{x}$, whose volume is δV. The mass of the constituent under consideration contained in $\delta\Omega$, whose age lies in the interval $[\tau,\tau+\delta\tau]$, tends to $\rho\, c(t,\mathbf{x},\tau)\delta V\,\delta\tau$ in the limit $\delta V,\delta\tau\rightarrow 0$. The physical dimension of the concentration distribution function is time^{-1}.

The concentration distribution function may be regarded as the histogram of the concentration as a function of the age of the particles of the constituent under consideration that are present

[1] Function $c(t,\mathbf{x},\tau)$ was called “age distribution function” by Delhez et al. (1999) and “concentration distribution function” in Deleersnijder et al. (2001). Considering everything, the second expression should be preferably used, for $c(t,\mathbf{x},\tau)$ quantifies the distribution of the concentration in “age bins”.

in $\delta\Omega$. It can be defined for every constituent, be it passive or not.

Assuming that advection and (turbulent) diffusion proceed independently of the age (this assumption obviously is valid in the vast majority of cases, if not in all of them), the equation governing the evolution of the concentration distribution function was established on the basis of mass budget considerations alone (Delhez et al. 1999, Deleersnijder et al. 2001):

$$\frac{\partial c}{\partial t} = \theta - \nabla\bullet(c\mathbf{v} - \mathbf{K}\bullet\nabla c) - \frac{\partial c}{\partial \tau} \tag{2.1}$$

where $\mathbf{v}(t,\mathbf{x})$ and $\mathbf{K}(t,\mathbf{x})$ denote the velocity field and the eddy diffusivity tensor, respectively; the velocity is divergence-free (Boussinesq approximation) and the diffusivity tensor is symmetric and positive-definite (e.g., Deleersnijder et al. 2001); θ is related to reactions and, hence, is zero if the constituent is passive. The physical dimension of θ is time^{-2}.

Let $C(t,\mathbf{x})$ denote the concentration defined as a mass fraction (i.e., a dimensionless variable). Then, the mass of the constituent present in $\delta\Omega$ is

$$\rho C(t,\mathbf{x})\delta V = \lim_{\delta\tau\to 0}\sum_{\tau=0}^{\infty}\rho c(t,\mathbf{x},\tau)\delta V\,\delta\tau = \int_0^{\infty}\rho c(t,\mathbf{x},\tau)\delta V\,d\tau \tag{2.2}$$

yielding directly

$$C(t,\mathbf{x}) = \int_0^{\infty} c(t,\mathbf{x},\tau)\,d\tau \tag{2.3}$$

meaning that the concentration is the zero-th order moment of the distribution function. Integrating (2.1) over the age leads to the equation satisfied by the concentration:

$$\frac{\partial C}{\partial t} = \int_0^{\infty}\theta\,d\tau - \nabla\bullet(C\mathbf{v} - \mathbf{K}\bullet\nabla C) \tag{2.4}$$

The age content was defined by Deleersnijder et al. (2001) as the sum of the products of the mass and the age of every particle. For the constituent under consideration in elemental control domain $\delta\Omega$, the age content is

$$\rho\alpha(t,\mathbf{x})\delta V = \lim_{\delta\tau\to 0}\sum_{\tau=0}^{\infty}\left[\rho c(t,\mathbf{x},\tau)\delta V\,\delta\tau\right]\tau = \int_0^{\infty}\rho c(t,\mathbf{x},\tau)\,\tau\,\delta V\,d\tau \tag{2.5}$$

where

$$\alpha(t,\mathbf{x}) = \int_0^{\infty} c(t,\mathbf{x},\tau)\,\tau\,d\tau \tag{2.6}$$

is termed the age concentration and is the first-order moment of the concentration distribution function. Like mass, the age content is an additive or extensive quantity. This is why the age concentration satisfies a conservation equation,

$$\frac{\partial \alpha}{\partial t} = \int_0^{\infty}\theta\,\tau\,d\tau + C - \nabla\bullet(\alpha\mathbf{v} - \mathbf{K}\bullet\nabla\alpha) \tag{2.7}$$

which is derived by integrating over the age the product of (2.1) and the age (τ).

Deleersnijder et al. (2001) suggested that the mean age, $a(t,\mathbf{x})$, be evaluated as the mass-weighted average of the relevant particle ages, i.e.,

$$a(t,\mathbf{x}) = \lim_{\delta\tau\to 0} \frac{\sum_{\tau=0}^{\infty} \left[\rho\, c(t,\mathbf{x},\tau)\delta V\,\delta\tau\right] \tau}{\sum_{\tau=0}^{\infty} \left[\rho\, c(t,\mathbf{x},\tau)\delta V\,\delta\tau\right]} = \frac{\int_0^{\infty} \rho\, c(t,\mathbf{x},\tau)\,\tau\,\delta V\, d\tau}{\int_0^{\infty} \rho\, c(t,\mathbf{x},\tau)\delta V\, d\tau} = \frac{\alpha(t,\mathbf{x})}{C(t,\mathbf{x})} \tag{2.8}$$

where the blue and red colours are associated with mass and age, respectively. This type of averaging, which is not the only one that could be contemplated, is the only arbitrary element in CART's age theory. Clearly, the mean age is an intensive variable, which, as a consequence, does not obey a conservative equation (Deleersnijder et al. 2001).

If the concentration distribution function is available, then the mean age can be calculated as the ratio of the first order moment to the zero-th order one thereof. However, as was pointed out above, evaluating the distribution function is no trivial task, especially for a long-tailed distribution function (Cornaton 2012). Therefore, many authors do not tackle equation (2.1) and, instead, solve the age concentration and concentration equations, and eventually obtain the mean age as the ratio of these variables (see, e.g., Deleersnijder et al. 2020 and references therein). The latter approach is feasible provided the reactive terms in (2.4) and (2.7) can be expressed in terms of the age concentration and concentration, which holds true for radioactive tracers (e.g., Delhez et al. 2003), sediment-related variables (Mercier and Delhez 2007, Gong and Shen 2010, Delhez and Wolk 2013, Ralston and Geyer 2017, Munhoven 2020) or a number of processes taken into account when modelling marine biology or chemistry (e.g., Delhez et al. 2004, Radtke et al. 2012), but is not necessarily beyond reproach (e.g., Deleersnijder 2019a).

Needless to say, none of the developments of this Section is novel. However, reviewing them will help build the theory for evaluating the mean property experienced by a tracer. Accordingly, in the next Section, an attempt will be made to derive the equation introduced by Gross et al. (2019) from that governing the suitable distribution function.

3. Mean property experienced by a tracer

The property to which the mean exposure is to be estimated is denoted $\psi(t,\mathbf{x})$. Its precise physical meaning is unimportant in the present context. It is not necessarily a positive definite quantity: it may be assumed that $\psi(t,\mathbf{x}) \in]-\infty,+\infty[$. Hereinafter, it will be necessary to introduce an independent variable, ξ, that is equivalent to $\psi(t,\mathbf{x})$ in the calculations related to the distribution function (Table 1)

As for CART's age theory, a distribution function is to be introduced. Accordingly, the age concentration distribution function, $\eta(t,\mathbf{x},\xi)$, is defined as follows:

> At time t, let $\delta\Omega$ represent the elemental control domain located at point $\mathbf{x}$, whose volume is δV. The age content of the constituent under consideration contained in $\delta\Omega$, whose property exposure lies in the interval $[\xi,\xi+\delta\xi]$, tends to $\rho\,\eta(t,\mathbf{x},\xi)\delta V\,\delta\xi$ in the limit $\delta V,\delta\xi \to 0$. The physical dimension of the age concentration distribution function is $\text{time}\times[\psi]^{-1}$, where $[\psi]$ denotes the physical dimension of property ψ.

From age content budget considerations, the equation for the above-mentioned distribution function is obtained:

$$\frac{\partial \eta}{\partial t} = \mu + C\delta[\xi - \psi(t,\mathbf{x})] - \nabla \bullet (\eta \mathbf{v} - \mathbf{K} \bullet \nabla \eta) \tag{3.1}$$

where δ is the Dirac delta function[2]. The first term in the right-hand side member of (3.1) is a source-sink term related to the reactions that the tracer might undergo and obviously is zero if the tracer is passive; its physical dimension is the inverse of that of property ψ. The second term is zero except for a value of ξ equal to the local value of property ψ. In other words, this source is active only at the local value of property $\psi(t,\mathbf{x})$, hence the need to have recourse to the Dirac delta function.

For the tracer under consideration, the age content of $\delta\Omega$ is

$$\rho\alpha(t,\mathbf{x})\delta V = \lim_{\delta\xi \to 0} \sum_{\xi=-\infty}^{\infty} \rho\eta(t,\mathbf{x},\xi)\delta V \delta\tau = \int_{-\infty}^{\infty} \rho\eta(t,\mathbf{x},\xi)\delta V \, d\xi \tag{3.2}$$

yielding directly

$$\alpha(t,\mathbf{x}) = \int_{-\infty}^{\infty} \eta(t,\mathbf{x},\xi) \, d\xi \tag{3.3}$$

meaning that the age concentration is zero-th order moment of distribution function $\eta(t,\mathbf{x},\xi)$. Integrating (3.1) over ξ must lead to the equation governing the age concentration, i.e. relation (2.7), which requires that

$$\int_{-\infty}^{\infty} \left[\mu + C\delta[\xi - \psi(t,\mathbf{x})]\right] d\xi = \int_{0}^{\infty} \theta\tau \, d\tau + C \tag{3.4}$$

It is readily seen that

$$\int_{-\infty}^{\infty} C\delta[\xi - \psi(t,\mathbf{x})] \, d\xi = C \tag{3.5}$$

implying that constraint (3.4) actually simplifies to

$$\int_{-\infty}^{\infty} \mu \, d\xi = \int_{0}^{\infty} \theta\tau \, d\tau \tag{3.6}$$

Thus, there must exist a strong link between the age-related variables and those associated with the calculation of the property experienced by a tracer. This issue is briefly addressed below.

At time *t* and location **x**, the mean property experienced by the tracer is defined as the age content weighted average of the relevant particle property exposure, i.e.,

[2] It is worth bearing in mind that the physical dimension of the Dirac delta function is the inverse of the physical dimension of its argument.

Table 1. Brief definition of the variables involved in age and property exposure calculations. The square brackets refer to the physical dimension of the related variable. The property of interest is denoted ψ . It is a function of time t and position vector $\mathbf{x}$. The age concentration is a variable involved in both methods, underscoring the link between them.

age	**property exposure**
τ : age as an independent variable • $[\tau]=T$	ξ : property as an independent variable • $[\xi]=[\psi]$
$c(t,\mathbf{x},\tau)$: concentration distribution function • $[c]=T^{-1}$	$\eta(t,\mathbf{x},\xi)$: age concentration distribution function • $[\eta]=T\times[\psi]^{-1}$
$\theta(t,\mathbf{x},\tau)$: reaction term in the equation governing c • $[\theta]=T^{-2}$	$\mu(t,\mathbf{x},\xi)$: reaction term in the equation governing η • $[\mu]=[\psi]^{-1}$
$C(t,\mathbf{x})=\int_0^\infty c(t,\mathbf{x},\tau)\,d\tau$: tracer concentration • $[C]=1$	$\alpha(t,\mathbf{x}) = \int_{-\infty}^{\infty} \eta(t,\mathbf{x},\xi)\,d\xi$: age concentration • $[\alpha]=T$
$\alpha(t,\mathbf{x})=\int_0^\infty c(t,\mathbf{x},\tau)\,\tau\,d\tau$: age concentration • $[\alpha]=T$	$\beta(t,\mathbf{x}) = \int_{-\infty}^{\infty} \eta(t,\mathbf{x},\xi)\,\xi\,d\xi$: property age concentration • $[\beta]=T\times[\psi]$
$a(t,\mathbf{x})=\dfrac{\alpha(t,\mathbf{x})}{C(t,\mathbf{x})}$: (mean) age • $[a]=T$	$b(t,\mathbf{x})=\dfrac{\beta(t,\mathbf{x})}{\alpha(t,\mathbf{x})}$: mean property experienced by the tracer or (mean) property exposure, for short • $[b]=[\psi]$

$$b(t,\mathbf{x}) = \lim_{\delta\xi\to 0} \frac{\sum_{\xi=-\infty}^{\infty} [\rho\eta(t,\mathbf{x},\xi)\delta V\,\delta\xi]\,\xi}{\sum_{\xi=-\infty}^{\infty} [\rho\eta(t,\mathbf{x},\xi)\delta V\,\delta\xi]} = \frac{\int_{-\infty}^{\infty} \rho\eta(t,\mathbf{x},\xi)\,\xi\,\delta V\,d\xi}{\int_{-\infty}^{\infty} \rho\eta(t,\mathbf{x},\xi)\delta V\,d\xi} = \frac{\int_{-\infty}^{\infty} \eta(t,\mathbf{x},\xi)\,\xi\,d\xi}{\int_{-\infty}^{\infty} \eta(t,\mathbf{x},\xi)\,d\xi}$$

(3.7)

where the blue and red colours are associated with the age content and property value, respectively. This type of averaging, which is not the only one that could be contemplated, is the only arbitrary element introduced in this section. Clearly, the mean property experienced by the tracer is the ratio of the first-order moment of the distribution function to the zero-th order one. The latter is the age concentration, whilst the former was called property age concentration by Gross et al. (2019). It reads

$$\beta(t,\mathbf{x}) = \int_{-\infty}^{\infty} \eta(t,\mathbf{x},\xi)\,\xi\,d\xi \qquad (3.8)$$

so that the mean property experienced by the tracer is to be evaluated as follows

$$b(t,\mathbf{x}) = \frac{\beta(t,\mathbf{x})}{\alpha(t,\mathbf{x})} \qquad (3.9)$$

The property age concentration (resp. the mean property exposure) is an extensive (resp. intensive) variable. This is readily understood.

Taking the first-order moment of (3.1) leads to the equation obeyed by the property age concentration:

$$\frac{\partial\beta}{\partial t} = \int_{-\infty}^{\infty} \mu\xi\,d\xi + C\psi - \nabla\bullet(\beta\mathbf{v} - \mathbf{K}\bullet\nabla\beta) \qquad (3.10)$$

If the tracer is passive ($\mu = 0$), then (3.10) simplifies to an equation equivalent to relation (8) of Gross et al. (2019). The second term in the right-hand side member of (3.10) stems from the first-order moment of the second-term in the right-hand side of equation for the age concentration distribution function (3.1), i.e.,

$$\int_{-\infty}^{\infty} C\delta[\xi - \psi(t,\mathbf{x})]\,\xi\,d\xi = C\int_{-\infty}^{\infty} \delta[\xi - \psi(t,\mathbf{x})]\,\xi\,d\xi = C\psi \qquad (3.11)$$

This source-sink term represents the imprint of the value of property $\psi(t,\mathbf{x})$ on the property age concentration at time t and location $\mathbf{x}$.

For a tracer undergoing a first-order decay at constant rate λ (e.g., a radioactive tracer whose mean life and half-life are λ^{-1} are $(\log 2)\lambda^{-1} \approx 0.7\times\lambda^{-1}$), the reactive terms (2.1) and (3.1) read $\theta = -\lambda c$ and $\mu = -\lambda\eta$, respectively, since, when disintegrating, the tracer particles "take their age or property exposure along with them". For such a tracer, the first term in the right-hand side member of the concentration, age concentration and property age concentration are $-\lambda C$, $-\lambda\alpha$ and $-\lambda\beta$, respectively.

Now consider a tracer produced at rate $\Theta(t,\mathbf{x})$ with the age $A(t,\mathbf{x})$, which should not always be prescribed to be zero (e.g. Delhez et al. 2004). In this case, the reactive term in (2.1) and (3.1) must be $\theta = \Theta\,\delta(\tau - A)$ and $\mu = \Theta\,A\,\delta(\xi - \Xi)$, where $\Xi(t,\mathbf{x})$ is the property exposure at which the tracer is produced, which is not necessarily zero. Then, the first term in the right-hand side member of the concentration, age concentration and property age concentration are Θ , ΘA and $\Theta A \Xi$, respectively.

The equation for the concentration distribution function encompasses first order derivative $\partial c / \partial \tau$. This term requires an appropriate discretization and a sufficient resolution in the age direction, which likely leads to a high computational cost. In contrast, the equation obeyed by the age concentration distribution function encompasses no derivative in the ξ-direction, implying that tackling it could be much more feasible. Distribution function η may be split into unrelated discrete variables $\eta_j(t,\mathbf{x})$, where subscript "*j*" refers to interval $[\xi_j, \xi_{j+1}]$, with $j \in [1, J]$. Then, the equations to be solved are

$$\frac{\partial \eta_j}{\partial t} = \mu_j + C\delta[\xi - \psi(t,\mathbf{x})]_j - \nabla \bullet (\eta_j \mathbf{v} - \mathbf{K} \bullet \nabla \eta_j) \; , \quad j = 1, J \tag{3.12}$$

where μ_j is a suitable discrete form of source-sink term μ in the *j*-th interval, whilst

$$\delta[\xi - \psi(t,\mathbf{x})]_j = \begin{cases} (\xi_{j+1} - \xi_j)^{-1} \text{ , if } \psi(t,\mathbf{x}) \in [\xi_j, \xi_{j+1}] \\ 0 \text{ , if } \psi(t,\mathbf{x}) \notin [\xi_j, \xi_{j+1}] \end{cases} \tag{3.13}$$

is the (simplest) discrete form of Dirac impulse function $\delta[\xi - \psi(t,\mathbf{x})]$. If it is acceptable to deal with a small number of property intervals, solving equations (3.12) may be achieved at a reasonable computational cost.

The mean property exposure may be obtained from the first two moments of the distribution function. The latter may be computed explicitly from the solution of (3.12). However, the mean property experienced by a tracer may also be derived from the ratio of the solutions of the property age concentration and age concentration equations. They must be solved under initial and boundary condition that are not independent of each other. As for age calculations (Deleersnijder et al. 2020), the initial and boundary condition should be prescribed first for the age concentration distribution function (even if the associated equation is not solved explicitly). Then, the zero-th and and first order moments of them should be evaluated, yielding the auxiliary conditions under which the age concentration and property age concentration equations should be solved (Appendix A).

It is believed that, as in most age studies relying partly or entirely on CART's diagnostic tools (e.g., Tang et al. 2021, Hong et al. 2020, Pinilla et al. 2020, Pham Van et al. 2020, Wang and Shen 2020, Grosse et al. 2019, Du et al. 2018, Liu et al. 2017, Kärnä and Baptista 2016, and references therein), the equation governing the distribution function will rarely be solved explicitly. Instead, the mean property experienced by the tracer will likely be obtained from the solution of the age concentration and property age concentration equations as was suggested in Gross et al. (2019).

Partial property exposures may be introduced by seeking inspiration in the concepts of partial ages (Mouchet et al. 2016) and partial residence/exposure times (Lin and Liu 2019). First, the domain of interest is split into non-overlapping subdomains (e.g., hydrodynamic provinces, or habitats in an ecological study), which are denoted Ω_i ($i = 1, I$). Then, if no reactions are to be taken into account, the equations for the partial property age concentrations, $\beta_i(t,\mathbf{x})$, are

$$\frac{\partial \beta_i}{\partial t} = C\psi\,\delta_{\Omega_i} - \nabla \bullet (\beta_i \mathbf{v} - \mathbf{K} \bullet \nabla \beta_i) \;, \quad i = 1, I \tag{3.14}$$

where δ_{Ω_i} denotes the characteristic function of the i-th subdomain, i.e.,

$$\delta_{\Omega_i}(\mathbf{x}) = \begin{cases} 1 \text{ if } \mathbf{x} \in \Omega_i \\ 0 \text{ if } \mathbf{x} \notin \Omega_i \end{cases} \tag{3.15}$$

The partial property exposures are then

$$b_i(t,\mathbf{x}) = \frac{\beta_i(t,\mathbf{x})}{\alpha(t,\mathbf{x})} \tag{3.16}$$

Since

$$\sum_{i=1}^{I} \delta_{\Omega_i}(\mathbf{x}) = 1 \tag{3.17}$$

the partial property age concentrations satisfy

$$\beta(t,\mathbf{x}) = \sum_{i=1}^{1} \beta_i(t,\mathbf{x}) \tag{3.18}$$

implying that

$$b(t,\mathbf{x}) = \frac{\beta(t,\mathbf{x})}{\alpha(t,\mathbf{x})} = \sum_{i=1}^{I} \frac{\beta_i(t,\mathbf{x})}{\alpha(t,\mathbf{x})} = \sum_{i=1}^{I} b_i(t,\mathbf{x}) \tag{3.19}$$

Partial property exposure may turn out to be of use in connectivity studies (among others).

4. Test cases

An open question is as follows: how should diagnostic approaches be validated prior to applying them to realistic model results? As far as diagnostic timescales and variables of a similar nature are concerned, this issue is particularly challenging: comparison with field data is intrinsically questionable, for, to put it simply and perhaps crudely, tracer particles do not wear a clock or any other measuring instrument[3]. Nonetheless, validation activities should be carried out. Potentially interestingly lines of thought about validation in general may be found in Oreskes et al. (1994), Dee (1995), Deleersnijder (1996), or Lane and Richards (2001).

Although a comprehensive methodology for validating studies using diagnostic timescales has yet to be set out, it is noteworthy that some authors made attempts to check, by means of analytical developments, the inner consistency of the partial differential problems that were dealt with. For instance, it was seen that the diagnostic tracer concentrations are well behaved and that their ages are positive definite and smaller than or equal to the elapsed time (e.g., Deleersnijder et al. 2001, de Brye et al. 2012, Deleersnijder 2019b).

A positive point for the theory of property exposure is that, in the preceding Section, no

[3] Of course, it is possible to compare numerically simulated diagnostic quantities with their counterparts evaluated from relevant *in situ* tracer measurements (e.g., Downing et al. 2016, Gross et al. 2019, Lucas and Deleersnijder 2020 and references therein). However, except in very special cases (e.g., Deleersnijder 2011, Deleersnijder 2014), these quantities usually are inherently different and, hence, for the comparison to be meaningful, the order or magnitude of the related systematic bias must also be estimated, which is rarely done.

insurmountable hurdle has been found when expressing the reactive terms for a tracer undergoing a first-order decay process and a tracer being produced at an arbitrary rate. This does not imply that the theory is correct; it simply means that no blatant inner inconsistency has been uncovered thus far.

Hereinafter, seeking inspiration in the aforementioned validation activities, idealized flows will be tackled in which the mean property experienced by a tracer can be evaluated unquestionably without having recourse to the diagnostic strategy of Gross et al. (2019). Then, the latter will be seen to yield similar results, helping to lend credence to the novel diagnostic method.

4.1. Time-dependent property in an isolated domain

Let Ω, Γ and $\mathbf{n}$ denote the domain of interest, its boundary, which is impermeable, and the outward unit normal to the boundary, respectively (Figure 1). Assume that a tracer, whose concentration is $C(t,\mathbf{x})$, is present in the domain. It undergoes a first-order decay characterized by (constant) timescale λ^{-1}, so that the reaction term in the concentration distribution function equation reads $\theta = -\lambda c$. The property to which the mean exposure is to be estimated is independent of the position and, hence, is denoted $\psi(t)$. If the initial mean property exposure is zero, then physical intuition suggests that the mean property experienced by the tracer must be equal to the time mean of $\psi(t)$, i.e.,

$$b(t,\mathbf{x}) = \frac{1}{t}\int_0^t \psi(t')\,dt' \tag{4.1.1}$$

Is this result consistent with the equations laid out in Section 3?

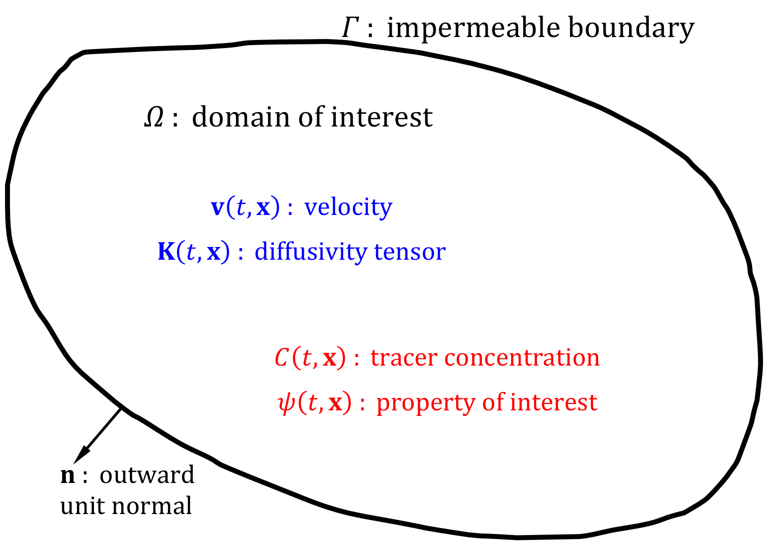

Figure 1. Illustration of the domain of interest (Ω) limited by impermeable boundary Γ in which a time-dependent, position-dependent property experienced by a tracer undergoing a first-order decay is evaluated.

Concentration $C(t,\mathbf{x})$ and age concentration $\alpha(t,\mathbf{x})$ are the solutions of the following partial differential problems:

$$\begin{cases} \dfrac{\partial C}{\partial t} = -\lambda C - \nabla \bullet (C\mathbf{v} - \mathbf{K} \bullet \nabla C) \\ C(0,\mathbf{x}) = C^0(\mathbf{x}) , \ \left[(C\mathbf{v} - \mathbf{K} \bullet \nabla C) \bullet \mathbf{n} \right]_{\mathbf{x} \in \Gamma} = 0 \end{cases} \tag{4.1.2}$$

and

$$\begin{cases} \dfrac{\partial \alpha}{\partial t} = -\lambda \alpha + C - \nabla \bullet (\alpha\mathbf{v} - \mathbf{K} \bullet \nabla \alpha) \\ \alpha(0,\mathbf{x}) = 0 , \ \left[(\alpha\mathbf{v} - \mathbf{K} \bullet \nabla \alpha) \bullet \mathbf{n} \right]_{\mathbf{x} \in \Gamma} = 0 \end{cases} \tag{4.1.3}$$

It is readily seen that

$$\alpha(t,\mathbf{x}) = C(t,\mathbf{x})t \tag{4.1.4}$$

so that the age is equal to the elapsed time,

$$a(t,\mathbf{x}) = \frac{\alpha(t,\mathbf{x})}{C(t,\mathbf{x})} = t \tag{4.1.5}$$

Although the concentration and age concentration depend on the rate of decay, λ, the mean age does not. This is because the domain is limited by impermeable boundaries and the tracer particles "take their age along with them at the instant they decompose". Accordingly, the concentration and age concentration satisfy $(C,\alpha) = e^{-\lambda t}(C_p,\alpha_p)$, where subscript "$p$" refers to the variables that would be obtained by setting $\lambda = 0$ (passive tracer) without modifying any other aspect of the problem under consideration.

The property age concentration obeys

$$\begin{cases} \dfrac{\partial \beta}{\partial t} = -\lambda \beta + C\psi - \nabla \bullet (\beta\mathbf{v} - \mathbf{K} \bullet \nabla \beta) \\ \beta(0,\mathbf{x}) = 0 , \ \left[(\beta\mathbf{v} - \mathbf{K} \bullet \nabla \beta) \bullet \mathbf{n} \right]_{\mathbf{x} \in \Gamma} = 0 \end{cases} \tag{4.1.6}$$

yielding

$$\beta(t,\mathbf{x}) = C(t,\mathbf{x}) \int_0^t \psi(t')\, dt' \tag{4.1.7}$$

so that (4.1.1) is correct. QED.

Irrespective of its time variations, the mean property experienced by the tracer does not depend on the rate of decay of the tracer, λ. This is because the property age concentration satisfies $\beta = e^{-\lambda t}\beta_p$, where β_p is the property age concentration that would be obtained if the tracer were passive ($\lambda = 0$), implying that

$$b(t,\mathbf{x}) = \frac{\beta(t,\mathbf{x})}{\alpha(t,\mathbf{x})} = \frac{e^{-\lambda t}\,\beta_p(t,\mathbf{x})}{e^{-\lambda t}\,\alpha_p(t,\mathbf{x})} = \frac{\beta_p(t,\mathbf{x})}{\alpha_p(t,\mathbf{x})} \tag{4.1.8}$$

In other words, expression (4.1.1) remains valid for a passive tracer ($\lambda = 0$).

It is worth underscoring that it is not necessary that property ψ be positive definite. Assume, for instance, that $\psi = \cos(\omega t)\Psi$, where Ψ is a constant (whose physical dimension is unimportant in the present context) and ω is the appropriate angular frequency. Unsurprisingly, the mean property exposure is

$$b(t) = \frac{1}{t}\int_0^t \cos(\omega t')\Psi\, dt' = \frac{\sin(\omega t)}{\omega t}\Psi \tag{4.1.9}$$

which illustrates that the sign changes of the property under consideration cause no problem to the calculation of the mean exposure to it. In the present case, the oscillatory nature of the property implies that the mean property experienced by the tracer tends to zero as time progresses, i.e.,

$$\lim_{t\to\infty} b(t) = \lim_{t\to\infty} \frac{\sin(\omega t)}{\omega t}\Psi = 0 \tag{4.1.10}$$

4.2. Position-dependent property in a one-dimensional, steady-state flow

Consider a semi-infinite channel for which space coordinate x denotes the distance to the entrance, with $0 \le x < \infty$ (Figure 2). Let $S(x)$ and $U(x)$ represent the cross-sectional area and the velocity, which are such that volumetric flow rate $Q = S(x)U(x)$ is constant. All variables are at a steady state. Along-flow diffusive processes are neglected. The property of interest is time-independent and is a function only of along-flow coordinate x. The age and the property exposure are assumed to be zero at the channel entrance ($x = 0$).

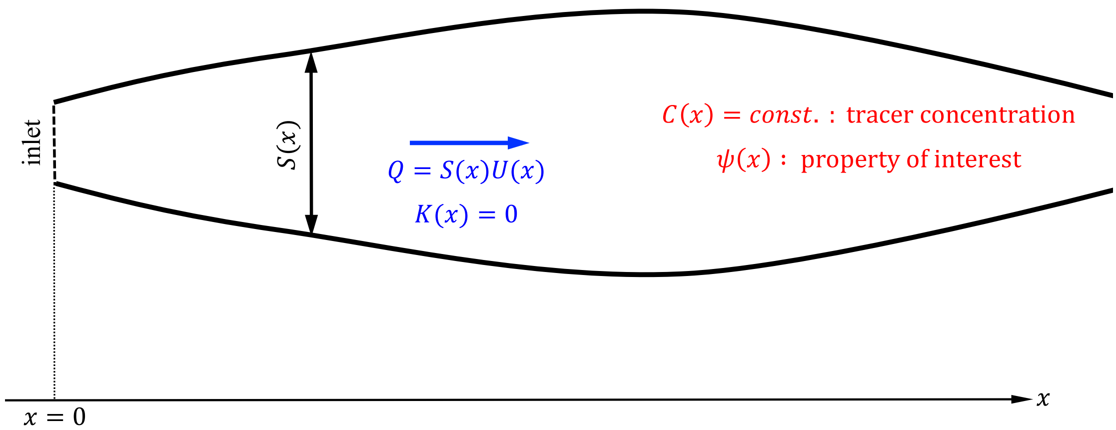

Figure 2. Illustration of the one-dimensional domain of interest, i.e., a semi-infinite channel with a variable cross-sectional area, $S(x)$. The volumetric flow rate (Q) is constant and diffusive processes are ignored. The tracer concentration is constant. The property of interest, ψ , is time-independent and is a function of the distance to the channel entrance ($x = 0$).

The time-spent by tracer particles in the space interval $[x, x+\delta x]$ tends to $U^{-1}(x)\delta x$ in the limit $\delta x \to 0$. Therefore, if the tracer concentration is constant, the mean property experienced by the tracer should be

$$b(x) = \frac{\int_0^x \psi(x')U^{-1}(x')\,dx'}{\int_0^x U^{-1}(x')\,dx'} \tag{4.2.1}$$

It will be shown that this expression can also be obtained by means of the method pioneered by Gross et al. (2019).

Concentration $C(x)$ of a passive tracer obeys

$$0 = \frac{d}{dx}(QC) \ , \quad C(0) = C_0 \tag{4.2.2}$$

so that

$$C(x) = C_0 \tag{4.2.3}$$

The corresponding age concentration satisfies

$$0 = SC + \frac{d}{dx}(Q\alpha) \ , \quad \alpha(0) = 0 \tag{4.2.4}$$

yielding

$$\alpha(x) = C_0 \int_0^x U^{-1}(x')\,dx' \tag{4.2.5}$$

Then, the mean age reads

$$a(x) = \frac{\alpha(x)}{C(x)} = \int_0^x U^{-1}(x')\,dx' \tag{4.2.6}$$

as expected.

The property age concentration satisfies

$$0 = SC\psi - \frac{d}{dx}(Q\beta) \ , \quad \beta(0) = 0 \tag{4.2.7}$$

leading to

$$\beta(x) = C_0 \int_0^x \psi(x')U^{-1}(x')\,dx' \tag{4.2.8}$$

Dividing (4.2.8) by (4.2.5) yields (4.2.1), as expected. QED.

If the cross-sectional area of the channel and property ψ are constant, then the velocity is also constant, and it is readily seen that $\alpha = C_0\, x / U$ and $\beta = C_0 \psi\, x / U$, yielding $b = \psi$, which is in agreement with elementary physical intuition.

4.3. Light exposure in a water column model

Evaluating the amount of light energy that phytoplankton cells are exposed to is a crucial ingredient in many marine ecology studies (e.g., Huisman et al. 2002, Huisman et al. 2004, Delhez and Deleersnijder 2010, and references therein). Accordingly, it will be examined whether or not the method dealt with herein is of any use in this respect.

Consider a water column to which vertical coordinate z is associated, with $z = -h$ (resp.

$z=0$) at the seabed (resp. the water-air interface) (Figure 3). Assuming that extinction coefficient k (m^{-1}) is a constant, the solar irradiance ($\mathrm{Watt/m^{-2}}$) is (Beer-Lambert law)

$$I(z) = I_0 e^{kz} \tag{4.3.1}$$

where I_0 is the irradiance just below the water surface ($z \to 0^-$). Obviously, the property of interest is the solar irradiance, i.e., $\psi(z)=I(z)$. If the upper and lower boundaries of the domain are impermeable and if the tracer under consideration is passive, the concentration of the latter will tend to a constant. Therefore, the mean solar irradiance experienced by the tracer must satisfy asymptotic expression

$$b(t,z) \sim \overline{I} \quad , \quad t \to \infty \tag{4.3.2}$$

where $\overline{I}$ is the depth-averaged solar irradiance, i.e.,

$$\overline{I} = \frac{1}{h} \int_{-h}^{0} I(z)\, dz = \frac{1-e^{-kh}}{kh} I_0 \tag{4.3.3}$$

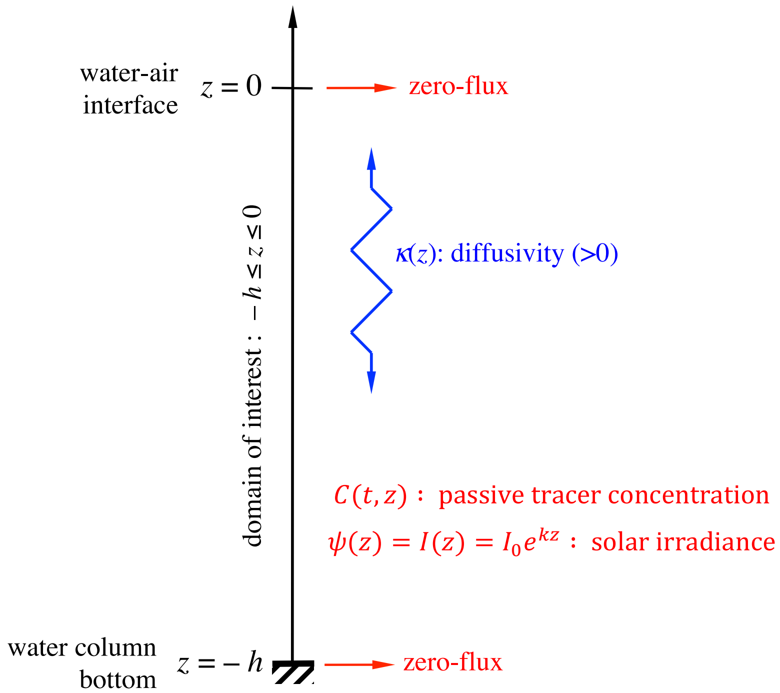

Figure 3. Illustration of the domain in which the solar irradiance experienced by a passive tracer is to be estimated. All variables are assumed to be horizontally homogeneous. The eddy diffusivity, $\kappa(z)$, is positive and depends on the vertical coordinate, z. The solar irradiance is an exponentially decreasing function of the distance to the surface.

Concentration $C(t,z)$ of the passive tracer to be taken into consideration is the solution of the following partial differential problem:

$$\begin{cases} \dfrac{\partial C}{\partial t} = \dfrac{\partial}{\partial z}\left[\kappa \dfrac{\partial C}{\partial z}\right] \\ C(0,z) = C^0(z)\,, \ \left[\kappa \dfrac{\partial C}{\partial z}\right]_{z=-h} = 0 = \left[\kappa \dfrac{\partial C}{\partial z}\right]_{z=0} \end{cases} \tag{4.3.4}$$

where $\kappa(z)$ (>0) is the eddy coefficient, which, for simplicity, is taken to be time-independent. Owing to the abovementioned impermeability conditions, it is readily seen that the depth mean of the concentration remains constant:

$$\bar{C} = \frac{1}{h}\int_{-h}^{0} C^0(z)\,dz = \frac{1}{h}\int_{-h}^{0} C(t,z)\,dz \tag{4.3.5}$$

The concentration is

$$C(t,z) = \sum_{n=0}^{\infty} \chi_n\, e^{-\gamma_n t}\, \varphi_n(z) \tag{4.3.6}$$

where γ_n (with $\gamma_n < \gamma_{n+1}$) and $\varphi_n(z)$ are the eigenvalues and eigenfunctions of the diffusion operator, i.e.,

$$\frac{d}{dz}\left[\kappa \frac{d\varphi_n}{dz}\right] = -\gamma_n \varphi_n \ , \quad \left[\kappa \frac{d\varphi_n}{dz}\right]_{z=-h} = 0 = \left[\kappa \frac{d\varphi_n}{dz}\right]_{z=0} \tag{4.3.7}$$

It is convenient to render the eigenfunctions orthonormal:

$$\frac{1}{h}\int_{-h}^{0} \varphi_m(z)\,\varphi_n(z)\,dz = \begin{cases} 1 \ \text{if} \ m = n \\ 0 \ \text{if} \ m \neq n \end{cases} \tag{4.3.8}$$

In addition, it is readily seen that $\gamma_0 = 0$ and $\varphi_0(z) = 1$, so that

$$\int_{-h}^{0} \varphi_n(z)\,dz = 0 \ , \quad n = 1, 2, 3, \ldots \tag{4.3.9}$$

As a result, concentration (4.3.6) may be rewritten as follows:

$$C(t,z) = \bar{C} + \sum_{n=1}^{\infty} \chi_n\, e^{-\gamma_n t}\, \varphi_n(z) \tag{4.3.10}$$

with

$$\chi_n = \frac{1}{h}\int_{-h}^{0} C^0(z)\,\varphi_n(z)\,dz \ , \quad n = 1, 2, 3, \ldots \tag{4.3.11}$$

which is agreement with constraint (4.3.5).

The age concentration obeys

$$\begin{cases} \dfrac{\partial \alpha}{\partial t} = C + \dfrac{\partial}{\partial z}\left[\kappa \dfrac{\partial \alpha}{\partial z}\right] \\ \alpha(0,z) = 0\,, \ \left[\kappa \dfrac{\partial \alpha}{\partial z}\right]_{z=-h} = 0 = \left[\kappa \dfrac{\partial \alpha}{\partial z}\right]_{z=0} \end{cases} \tag{4.3.12}$$

leading to

$$\alpha(t,z) = C(t,z)t = \bar{C}t + \left[\sum_{n=1}^{\infty} \chi_n e^{-\gamma_n t} \varphi_n(z)\right] t \quad (4.3.13)$$

The irradiance age concentration, $\beta(t,z)$, is governed by the relations

$$\begin{cases} \dfrac{\partial \beta}{\partial t} = CI + \dfrac{\partial}{\partial z}\left[\kappa \dfrac{\partial \beta}{\partial z}\right] \\ \beta(0,z) = 0 \, , \left[\kappa \dfrac{\partial \beta}{\partial z}\right]_{z=-h} = 0 = \left[\kappa \dfrac{\partial \beta}{\partial z}\right]_{z=0} \end{cases} \quad (4.3.14)$$

The analytical solution to (4.3.14) is likely to be rather intricate. Fortunately, the following asymptotic expansion is readily derived

$$\beta(t,z) \sim \bar{C}\bar{I}t + \sum_{n=1}^{\infty} \frac{\bar{C}I_n}{\gamma_n} \varphi_n(z) \, , \quad t \to \infty \quad (4.3.15)$$

with

$$I_n = \frac{1}{h} \int_{-h}^{0} I(z)\, \varphi_n(z)\, dz \, , \quad n = 1, 2, 3, \ldots \quad (4.3.16)$$

All of the terms omitted in the above relation decrease exponentially as time progresses.

The ratio of the irradiance age concentration (4.3.15) to the age concentration (4.3.13) leads to

$$b(t,z) \sim \frac{\bar{C}\bar{I}t}{\bar{C}t} + O(t^{-1}) \sim \bar{I} + O(t^{-1}) \, , \quad t \to \infty \quad (4.3.17)$$

which is equivalent to (4.3.2), as expected. QED.

The irradiance age concentration represents the amount of light energy received by the tracer particles ($\mathrm{Joule/m^2}$), which, unsurprisingly, tends to increase linearly in time as time progresses, i.e., $\beta(t,z) \sim \bar{C}\bar{I}t$ as $t \to \infty$.

5. Conclusion and outlook

Gross et al. (2019) outlined and briefly applied a method for evaluating the mean property experienced by a tracer, which is meant to hold valid irrespective of the very nature of the property of interest, which, for instance, can be a non-positive definite variable. Herein, an attempt has been made to give this method solid foundations by seeking inspiration in the theoretical developments that led to CART's age concept. Specifically, a distribution function has been introduced, the zero-th and first order moments of which are CART's age concentration and the property age concentration. The ratio of the latter to the former yields the sought-after mean property experienced by the tracer under study.

It must be stressed that the methodology developed in this working note is not restricted to passive tracers. It is believed that tracers undergoing reactions can be dealt with. This was illustrated by cursorily considering two types of reactions, i.e., first-order decay and production at a prescribed rate.

The age concentration is a variable common to CART's age theory and the property exposure theory. Whether or not this would handicap the definition and use of the property experienced by a tracer has yet to be investigated. Of particular interest is the definition of the initial and, above all, boundary conditions. The latter cannot be prescribed independently for all the variables involved. They must be consistent with each other as is the case for the age-related variables (Deleersnijder et al. 2020). This is outlined in Appendix A.

Test cases were considered for which the mean property exposure can be reliably evaluated *a priori*. The method pioneered by Gross et al. (2019) was seen to lead to similar values of the property exposure, contributing to lend credence to the novel diagnostic approach. Thus far, no inner inconsistencies have been found in it. Therefore, time is probably ripe for applying this method to a number of realistic problems, which would allow assessing to what degree it can help understand complex processes taking place in the aquatic environment and help develop reduced-dimension models of them.

In this working note all of the mathematical developments are carried out in the Eulerian framework, although, for the sake of simplicity, most literal explanations are formulated by having recourse to the Lagrangian vocabulary. Having recourse to the Eulerian formalism has three distinct advantages. First, establishing properties of the diagnostic variables as part of the validation activities (for the novel diagnoses, an immense amount of work still remains to be done) is generally easier to do by manipulating Eulerian equations than dealing with Lagrangian ones, partly because the latter encompass stochastic terms for representing diffusive processes (e.g. Hall and Haine 2004, Delhez and Deleersnijder 2006, Delhez and Deleersnijder 2012). Second, the numerical models for which the diagnoses dealt with above could be of use are likely equipped with a reactive transport equation solver, which can be taken advantage of to solve the property exposure related equations. Accordingly, it is not necessary to achieve significant numerical developments to utilize the novel diagnoses. Finally, Eulerian numerical schemes are generally better than Lagrangian ones at handling diffusive operators, especially when eddy coefficients exhibit very steep gradients (e.g. Spivakovskaya et al. 2007a, Gräwe et al. 2012, van Sebille et al. 2018, and references therein).

Needless to say, computing the property experienced by tracer particles is certainly more natural in a Lagrangian model. Thus, employing such type of models should also be contemplated whenever possible and appropriate. Lagrangian methods are generally superior to Eulerian ones for the representation of advection. They also allow representing rather easily dispersive phenomena others than those modelled by means of harmonic diffusion (e.g. Visser 2008, van Sebille et al. 2018). However, a poorly-documented shortcoming of Lagrangian methods lies in the fact that a large number of particles must be seeded into the domain of interest to obtain accurate concentration fields, possibly requiring greater computational resources than their Eulerian counterparts to achieve the same level of accuracy. What is worse, estimating a priori the minimum number of particles needed is not as straightforward as one would like. Useful guidelines, however, exist (Silverman 1986, Spivakovskaya et al. 2007b).

It must be borne in mind that “well designed Eulerian and Lagrangian schemes converge to the exact solution as the space and time increments decrease for the former methods, and as the time resolution and the number of particles are increased for the latter. Therefore, discrepancies between Eulerian and Lagrangian simulation results are always due to numerical inaccuracies (or an erroneous implementation) and, hence, must not be ascribed to supposedly irreconcilable differences between the two approaches" (adapted from Deleersnijder 2020).

Appendix A: generic boundary conditions

In Appendix D of Deleersnijder et al. (2020), a generic boundary condition for the concentration distribution function is provided, which reads[4]

$$\left[\mathbf{d}\bullet\nabla c+\varsigma c+\upsilon\right]_{\mathbf{x}\in\Gamma} = 0 \tag{A.1}$$

where $\mathbf{d}(t,\mathbf{x})$ is an appropriate vector, whilst $\varsigma(t,\mathbf{x})$ and $\upsilon(t,\mathbf{x},\tau)$ are relevant scalar functions. Then, by taking the zero-th and first order moments of (A.1), the boundary conditions for the concentration and age concentration are obtained, i.e.,

$$\left[\mathbf{d}\bullet\nabla C+\varsigma C+\int_0^\infty \upsilon(t,\mathbf{x},\tau)\,d\tau\right]_{\mathbf{x}\in\Gamma} = 0 \tag{A.2}$$

and

$$\left[\mathbf{d}\bullet\nabla \alpha+\varsigma \alpha+\int_0^\infty \upsilon(t,\mathbf{x},\tau)\tau\,d\tau\right]_{\mathbf{x}\in\Gamma} = 0 \tag{A.3}$$

Depending on the values of functions $\mathbf{d}$, ς and υ, the above generic expressions may yield Dirichlet, Neumann or Robin boundary conditions.

The generic boundary condition for the age concentration distribution function is of the form

$$\left[\mathbf{d}\bullet\nabla \eta+\varsigma \eta+\iota\right]_{\mathbf{x}\in\Gamma} = 0 \tag{A.4}$$

where $\iota(t,\mathbf{x},\xi)$ must satisfy constraint

$$\int_0^\infty \upsilon(t,\mathbf{x},\tau)\tau\,d\tau = \int_{-\infty}^\infty \iota(t,\mathbf{x},\xi)\,d\xi \tag{A.5}$$

for boundary condition for the age concentration (A.3) to be equivalent to that derived in the framework of the property exposure assessment. The latter is the zero-th order moment of (A.4):

$$\left[\mathbf{d}\bullet\nabla \alpha+\varsigma \alpha+\int_{-\infty}^\infty \iota(t,\mathbf{x},\xi)\,d\xi\right]_{\mathbf{x}\in\Gamma} = 0 \tag{A.6}$$

Finally, the property age concentration boundary condition reads

$$\left[\mathbf{d}\bullet\nabla \beta+\varsigma \beta+\int_{-\infty}^\infty \iota(t,\mathbf{x},\xi)\xi\,d\xi\right]_{\mathbf{x}\in\Gamma} = 0 \tag{A.7}$$

[4] Here, notations different from those of Deleersnijder et al. (2020) are used in order to ensure consistency with those of the present working note.

which is the first-order moment of (A.4).

The age concentration is common to the age and property exposure diagnostic approaches. Accordingly, there is a link between them through the reactive terms (see Section 3) and the boundary conditions as is expressed in constraint (A.5). Failing to satisfy these constraints will yield inconsistent diagnoses.

A specific case is worth investigating herein. If the age concentration distribution function is prescribed to be zero on a portion of the domain boundary, denoted Γ^a below, then the age concentration and property age concentration must also be zero on Γ^a. Therefore, on this portion of the boundary, the mean property exposure is the ratio of two variables that are both zero, which may cast doubt over the well-foundedness of the boundary conditions.

This difficulty is not an insurmountable one. To convince oneself of this, it is first necessary to write the equation obeyed by the mean property exposure. This is achieved by manipulating (2.7), (3.9) and (3.10)[5], eventually leading to

$$\frac{\partial b}{\partial t} = -\frac{b-\psi}{\alpha} - \nabla \bullet (b\mathbf{v} - \mathbf{K} \bullet \nabla b) + \frac{2}{\alpha} \nabla \alpha \bullet \mathbf{K} \bullet \nabla b \qquad \text{(A.8)}^{6}$$

The first term in the right-hand side member of (A.8) tends to locally nudge mean property exposure $b(t,\mathbf{x})$ toward value of the property $\psi(t,\mathbf{x})$ with relaxation timescale $\alpha(t,\mathbf{x})$. This is far from counterintuitive. Because of the last term of (A.8), this equation is not in conservative form (and cannot be cast into such a form) unlike the equations for the age concentration and property age concentration. This is no surprise: as was seen in Sections 2 and 3, the mean property exposure is an intensive variable, whereas $\alpha(t,\mathbf{x})$ and $\beta(t,\mathbf{x})$ are extensive ones.

The second step consists in rewriting (A.8) as follows:

$$\nabla \alpha \bullet \mathbf{K} \bullet \nabla b - \frac{b-\psi}{2} = \frac{\alpha}{2}\left[\frac{\partial b}{\partial t} + \nabla \bullet (b\mathbf{v} - \mathbf{K} \bullet \nabla b)\right] \qquad \text{(A.9)}$$

As the age concentration is zero on Γ^a, (A.9) simplifies to

$$\left[\nabla \alpha \bullet \mathbf{K} \bullet \nabla b - \frac{b-\psi}{2}\right]_{\mathbf{x} \in \Gamma^a} = 0 \qquad \text{(A.10)}$$

Since α is zero on Γ^a and positive in the interior of the domain, (A.10) transforms to the following Robin boundary condition

$$\left[\mathbf{n} \bullet \mathbf{K} \bullet \nabla b - \frac{b-\psi}{2\alpha_n}\right]_{\mathbf{x} \in \Gamma^a} = 0 \qquad \text{(A.11)}$$

with[7]

$$\alpha_n = \mathbf{n} \bullet \nabla \alpha < 0 \qquad \text{(A.12)}$$

The "flux of b" through the boundary, $[-\mathbf{n} \bullet \mathbf{K} \bullet \nabla b]_{\mathbf{x} \in \Gamma^a}$, is directed toward the exterior (resp.

[5] For the sake of simplicity, reactive processes are ignored in this Appendix. Taking them into account on a general basis is likely to be difficult. Presumably, the impact of reactions on boundary conditions should be done on a case by case basis.

[6] To obtain this equation, it was necessary to take into account the following constraints (which were introduced in Section 2): the velocity is divergence-free and the diffusivity tensor is symmetric.

[7] The age concentration exhibits no variation along the boundary: its gradient is parallel to **n** and points in the opposite direction.

the interior) of the domain if $b > \psi$ (resp. $b < \psi$) on Γ^a, thereby tending to nudge the value of b toward that of ψ on boundary Γ^a.

The above considerations show that, unsurprisingly, the value of the property exposure tends to be nudged toward the value of the property of interest both in the interior of the domain (see A.8) and on its boundary (see A.11-12).

Appendix B: upper and lower bounds of the property age concentration

Deleersnijder et al. (2001), de Brye et al. (2012) and Deleersnijder (2019b) thoroughly established inequalities satisfied by CART-related variables as part of the assessment of the inner consistency of the considered diagnostic approaches. It is believed that a similar approach should be applied to property exposure investigations. A cursory illustration thereof is provided below.

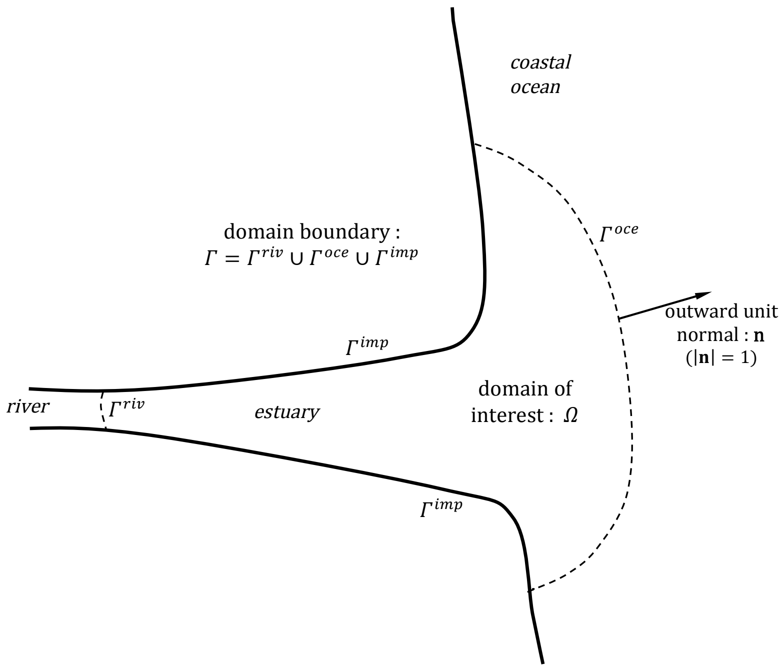

Figure B1. Schematic representation of the generic region of freshwater influence (ROFI) in which diagnostic variables are to be evaluated.

As in Deleersnijder (2019b), the domain of interest Ω (Figure B1) is a generic region of freshwater influence (ROFI). The domain boundary, Γ, consists of three components, 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 (river banks, coastline, bottom of the water column and water-air interface), denoted Γ^{imp}. Surfaces Γ^{riv} and Γ^{oce} are open boundaries. As opposed to what is done in Deleersnijder (2019b), the domain boundaries are, for the sake simplicity, assumed to be time-independent hereinafter, but the flow is not assumed to be at a steady state.

The velocity and diffusivity tensor are time- and position-dependent. The former is divergence-free (Boussinesq approximation), whilst the latter is symmetric and positive-definite. These constraints are crucial for the theoretical developments carried out below.

Following the ideas of Gourgue et al. (2007) and de Brye et al. (2012), Deleersnijder (2019b) performed theoretical developments related to water renewal assessment in the abovementioned generic ROFI. The first step consisted in tracking several water types, which were treated as passive tracers as has been done in many previous water tracking studies (e.g. Cox 1989, Hirst 1999, Goosse et al. 2001, Deleeersnijder et al. 2002, Haine and Hall 2002, Meier 2005, de Brye et al. 2012). They were the original water (i.e., the water present in the domain at the initial time) and the renewing water, which is progressively replacing the former water particles by entering the domain through the open boundaries. The renewing water was split into two water types according to their boundaries of origin. Here, only the riverine water is taken into consideration.

Table B1. Boundary conditions satisfied by the age and property exposure related diagnostic variables. These boundary conditions are consistent with each other in the sense of the theoretical results established by Deleersnijder et al. (2020).

	portion of the domain boundary		
	$\mathbf{x} \in \Gamma^{riv}$: river-estuary boundary	$\mathbf{x} \in \Gamma^{imp}$: impermeable boundary	$\mathbf{x} \in \Gamma^{oce}$: ROFI-coastal ocean boundary
age	$c(t,\mathbf{x},\tau) = \delta(\tau - 0)$	$(-\mathbf{K} \bullet \nabla c) \bullet \mathbf{n} = 0$	$c(t,\mathbf{x},\tau) = 0$
age	$C(t,\mathbf{x}) = \int_0^\infty \delta(\tau - 0)\, d\tau = 1$	$(-\mathbf{K} \bullet \nabla C) \bullet \mathbf{n} = \int_0^\infty 0\, d\tau = 0$	$C(t,\mathbf{x}) = \int_0^\infty 0\, d\tau = 0$
age	$\alpha(t,\mathbf{x}) = \int_0^\infty \delta(\tau - 0)\tau\, d\tau = 0$	$(-\mathbf{K} \bullet \nabla \alpha) \bullet \mathbf{n} = \int_0^\infty 0 \times \tau\, d\tau = 0$	$\alpha(t,\mathbf{x}) = \int_0^\infty 0 \times \tau\, d\tau = 0$
property exposure	$\eta(t,\mathbf{x},\xi) = 0$	$(-\mathbf{K} \bullet \nabla \eta) \bullet \mathbf{n} = 0$	$\eta(t,\mathbf{x},\xi) = 0$
property exposure	$\alpha(t,\mathbf{x}) = \int_{-\infty}^\infty 0\, d\xi = 0$	$(-\mathbf{K} \bullet \nabla \alpha) \bullet \mathbf{n} = \int_{-\infty}^\infty 0\, d\xi = 0$	$\alpha(t,\mathbf{x}) = \int_{-\infty}^\infty 0\, d\xi = 0$
property exposure	$\beta(t,\mathbf{x}) = \int_{-\infty}^\infty 0 \times \xi\, d\xi = 0$	$(-\mathbf{K} \bullet \nabla \beta) \bullet \mathbf{n} = \int_{-\infty}^\infty 0 \times \xi\, d\xi = 0$	$\beta(t,\mathbf{x}) = \int_{-\infty}^\infty 0 \times \xi\, d\xi = 0$

On the impermeable portion of the boundary, the velocity satisfies

$$\left[\mathbf{v}(t,\mathbf{x}) \bullet \mathbf{n}\right]_{\mathbf{x} \in \Gamma^{imp}} = 0 \tag{B.1}$$

As advocated by Deleersnijder et al. (2020), the initial and boundary conditions for the concentration and age concentration are derived from those applied to the concentration distribution function, implying that all the auxiliary conditions are consistent with each other. At the initial instant ($t = 0$), the riverine water related variables are

$$[c(t,\mathbf{x},\tau)]_{t=0} = 0 \quad \Rightarrow \quad \begin{cases} [C(t,\mathbf{x})]_{t=0} = \int_0^\infty c(0,\mathbf{x},\tau)\, d\tau = 0 \\ [\alpha(t,\mathbf{x})]_{t=0} = \int_0^\infty c(0,\mathbf{x},\tau)\tau\, d\tau = 0 \end{cases} \tag{B.2}$$

The boundary conditions are laid out in Table B1. Then, according to Deleersnijder (2019b), the concentration and age concentration may be seen to obey inequalities

$$0 \le C(t,\mathbf{x}) \le 1 \ , \quad 0 \le \alpha(t,\mathbf{x}) \le C(t,\mathbf{x})t \tag{B.3}$$

so that the age is no larger than elapsed time t as it must be.

The riverine water is treated as a passive tracer, which is why the reactive term in the equation for the property age concentration is zero. Accordingly, this relation is

$$\frac{\partial \beta}{\partial t} = C\psi - \nabla \bullet (\beta \mathbf{v} - \mathbf{K} \bullet \nabla \beta) \tag{B.4}$$ [8]

Here, the very nature of property $\psi(t,\mathbf{x})$ is unimportant. It is, however, necessary to prescribe the initial values of the related variables. As will probably be the case in many studies, the age concentration distribution function is taken to be zero at the initial instant:

$$[\eta(t,\mathbf{x},\xi)]_{t=0} = 0 \quad \Rightarrow \quad \begin{cases} [\alpha(t,\mathbf{x})]_{t=0} = \int_{-\infty}^{\infty} \eta(0,\mathbf{x},\xi)\, d\xi = 0 \\ [\beta(t,\mathbf{x})]_{t=0} = \int_{-\infty}^{\infty} \eta(0,\mathbf{x},\tau)\xi\, d\xi = 0 \end{cases} \tag{B.5}$$

Consistent boundary conditions may be found in Table B1.

A simple inspection of (B.4) and elementary considerations on the initial and boundary conditions suggest that the property age concentration should obey inequalities

$$(C\psi)_{\min} \le \frac{\beta}{t} \le (C\psi)_{\max} \tag{B.6}$$

where

$$(C\psi)_{\min} = \min_{t\ge 0,\, \mathbf{x}\in\Omega} [C(t,\mathbf{x})\psi(t,\mathbf{x})] \ , \quad (C\psi)_{\max} = \max_{t\ge 0,\, \mathbf{x}\in\Omega} [C(t,\mathbf{x})\psi(t,\mathbf{x})] \tag{B.7}$$

To prove that (B.6) holds valid, it is convenient to first introduce the following variable:

$$\hat{\beta}(t,\mathbf{x}) = (C\psi)_{\max} t - \beta(t,\mathbf{x}) \tag{B.8}$$

The negative part thereof,

$$\hat{\beta}^-(t,\mathbf{x}) = \frac{\beta(t,\mathbf{x}) - |\beta(t,\mathbf{x})|}{2} \tag{B.9}$$

is identically zero if $\hat{\beta}(t,\mathbf{x})$ is positive and is equal to $\hat{\beta}(t,\mathbf{x})$ otherwise. Then, multiplying (B.4) by $\hat{\beta}^-$ and integrating over the domain of interest, the following integral relation is

[8] Obviously, relation (B.4) is obtained by setting $\mu = 0$ in (3.10).

obtained after some manipulations[9]:

$$\frac{d}{dt}\int_{\Omega}\left(\hat{\beta}^{-}\right)^{2} d\Omega = -\overbrace{\int_{\Omega} 2\left[C\psi-(C\psi)_{\max}\right]\hat{\beta}^{-}\, d\Omega}^{\geq 0,\ \text{since } C\psi\leq(C\psi)_{\max} \text{ and } \hat{\beta}^{-}\leq 0} - \overbrace{\int_{\Gamma^{riv}\cup\Gamma^{oce}} \hat{\beta}^{-}(\hat{\beta}^{-}\mathbf{v}-2\mathbf{K}\cdot\nabla\hat{\beta}^{-})\cdot\mathbf{n}\, d\Gamma}^{=0,\ \text{since } \beta=0 \text{ on } \Gamma^{riv}\cup\Gamma^{oce}}$$
$$-\underbrace{\int_{\Gamma^{imp}} \hat{\beta}^{-}(\hat{\beta}^{-}\mathbf{v}-2\mathbf{K}\cdot\nabla\hat{\beta}^{-})\cdot\mathbf{n}\, d\Gamma}_{=0,\ \text{since } \mathbf{v}\cdot\mathbf{n}=0 \text{ and } (\mathbf{K}\cdot\nabla\hat{\beta})\cdot\mathbf{n}=0 \text{ on } \Gamma^{imp}} - \underbrace{\int_{\Omega} 2\nabla\hat{\beta}^{-}\cdot\mathbf{K}\cdot\nabla\hat{\beta}^{-}\, d\Omega}_{\geq 0,\ \text{since } \mathbf{K} \text{ is positive definite}} \leq 0$$

(B.10)

Thus, the L^2-norm of $\hat{\beta}^{-}$ cannot increase. As $\hat{\beta}^{-}$ is zero at $t=0$, $\hat{\beta}^{-}$ is zero at any time and position, implying that $\hat{\beta}(t,\mathbf{x})$ is non-negative, so that $(C\psi)_{\max} t \geq \beta(t,\mathbf{x})$ or, equivalently, $(C\psi)_{\max} \geq \beta(t,\mathbf{x})/t$. Similar developments allow proving that $(C\psi)_{\min} \leq \beta(t,\mathbf{x})/t$. As a consequence, inequalities (B.6) hold valid. QED.

Acknowledgements. I am indebted to Edward Gross and Insaf Draoui for their useful comments on an early version of this working note.

References

Beckers J.-M., E.J.M. Delhez and E. Deleersnijder, 2001, Some properties of generalised age-distribution equations in fluid dynamics, *SIAM Journal on Applied Mathematics*, 61, 1526-1544, doi: 10.1137/S0036139999363810

Bolin B. and H. Rodhe, 1973, A note on the concepts of age distribution and transit time in natural reservoirs, *Tellus*, 25, 58-62, doi: 10.3402/tellusa.v25i1.9644

Campin J.M., T. Fichefet and J.C. Duplessy, 1999, Problems with using radiocarbon to infer ocean ventilation rates for past and present climate, *Earth and Planetary Science Letters*, 165, 17-24, doi: 10.1016/s0012-821x(98)00255-6

Cornaton F., 2012, Transient water age distributions in environmental flow systems: the time-marching Laplace transform solution technique, *Water Resources Research*, 48, W03524, doi: 10.1029/2011WR010606

Cornaton F. and P. Perrochet, 2006, Groundwater age, life expectancy and transit time distributions in advective-dispersive systems: 1. Generalized reservoir theory, *Advances in Water Resources*, 29, 1267-1291, doi: 10.1016/j.advwatres.2005.10.009

Cornaton F.J., Y.-J. Park and E. Deleersnijder, 2011, On the biases affecting water ages inferred from isotopic data, *Journal of Hydrology*, 410, 217-225, doi: 10.1016/j.jhydrol.2011.09.024

[9] At first glance, these manipulations seem to be based on a straightforward application of the divergence theorem. That is not the case, as may be seen in Appendix C of Deleersnijder et al. (2001). The relevant mathematical developments are inspired by Lewandowski (1997). The difficulty lies in the fact that $\hat{\beta}^{-}$ is not continuously differentiable in space.

Cox M.D., 1989, An idealized model of the World Ocean. Part I: The global-scale water masses, *Journal of Physical Oceanography*, 19, 1730-1752, doi: 10.1175/1520-0485(1989)019<1730:aimotw>2.0.co;2

de Brye B., A. de Brauwere, O. Gourgue, E.J.M. Delhez and E. Deleersnijder, 2012, Water renewal timescales in the Scheldt Estuary, *Journal of Marine Systems*, 94, 74-86, doi: 10.1016/j.jmarsys.2011.10.013

Dee D.P., 1995, A pragmatic approach to model validation, in: D.R. Lynch and A.M. Davies (eds.), *Quantitative Skill Assessment for Coastal Ocean Models*, Coastal and Estuarine Studies (vol. 47), American Geophysical Union, Washington, D.C., pages 1-13, doi: 10.1029/CE047

Deleersnijder E., 1996, On model validation, sensitivity, and intercomparison, in: *Progress in Belgian Oceanographic Research*, National Committee of Oceanology, Royal Academy of Belgium, pp. 43-46, available on the web at URL http://hdl.handle.net/2078.1/155075

Deleersnijder E., 2008, *Can we use CART to evaluate the age of energy-containing eddies in a turbulent flow?*, Université catholique de Louvain, Louvain-la-Neuve, 5 pages, available on the web at URL http://hdl.handle.net/2078.1/155240

Deleersnijder E., 2009, *The unreasonable effectiveness of dimension reduction in complex geophysical flow modelling*, Working note, Université catholique de Louvain, Louvain-la-Neuve, 25 pages, available on the web at URL http://hdl.handle.net/2078.1/154174

Deleersnijder E., 2011, *Exact age from two passive tracer concentrations*, Working note, Université catholique de Louvain, Louvain-la-Neuve, 6 pages, available on the web at URL http://hdl.handle.net/2078.1/155255

Deleersnijder E., 2014, *Exact tracer age from two passive tracer concentrations and ventilation timescales: analytical solutions from a highly-idealised water-column model*, Working note, Université catholique de Louvain, Louvain-la-Neuve, 15 pages, available on the web at URL http://hdl.handle.net/2078.1/155258

Deleersnijder E., 2019a, *On the mean age of the population of preys in a prey-predator model*, Working note, Université catholique de Louvain, Louvain-la-Neuve, 3 pages, available on the web at URL http://hdl.handle.net/2078.1/217778

Deleersnijder E., 2019b, *Water renewal of a region of freshwater influence (ROFI): mathematical properties of some of the relevant diagnostic variables*, Working Note, Université catholique de Louvain, Louvain-la-Neuve, Belgium, 19 pages, available on the web at URL http://hdl.handle.net/2078.1/220841

Deleersnijder E., 2020, *The uneasy collaboration of Leonhard Euler (1707-1783) and Joseph Louis de Lagrange (1736-1813) in environmental fluid mechanics*, Working Note, Université catholique de Louvain, Louvain-la-Neuve, Belgium, 5 pages, available on the web at URL http://hdl.handle.net/2078.1/229071

Deleersnijder E. and S. Bouillon, 2017, *The equation governing the evolution of the surface age distribution function of sea ice*, Working Note, Université catholique de Louvain, 11 pages, available on the web at URL http://hdl.handle.net/2078.1/183042

Deleersnijder E., H. Burchard, P. Delandmeter, E. Delhez, E. Hanert, A. Mouchet and L. Umlauf, 2017, Using the age to diagnose the evolution of turbulence kinetic energy and, possibly, other variables unrelated to the concentration of a constituent, Poster, 49th International Liège Colloquium on Ocean Dynamics & 8th Warnemünde Turbulence Days (Liège, Belgium, 22-26 May 2017), available on the web at URL http://hdl.handle.net/2078.1/185078

Deleersnijder E., J.-M. Campin and E.J.M. Delhez, 2001, The concept of age in marine modelling: I. Theory and preliminary model results, *Journal of Marine Systems*, 28, 229-267, doi: 10.1016/s0924-7963(01)00026-4

Deleersnijder E., I. Draoui, J. Lambrechts, V. Legat and A Mouchet, 2020, Consistent boundary conditions for age calculations, *Water*, 12, 1274, doi: 10.3390/w12051274

Deleersnijder E., A. Mouchet and E.J.M. Delhez, 2018, *Diagnostic timescales in fluid flows: from the Tower of Babel to partial differential equations*, Working note, Université catholique de Louvain, Louvain-la-Neuve, Belgium, 26 pages, available on the web at URL http://hdl.handle.net/2078.1/196273

Deleersnijder A., A. Mouchet, E.J.M. Delhez and J.-M. Beckers, 2002, Transient behaviour of water ages in the World Ocean, *Mathematical and Computer Modelling*, 36, 121-127, doi: 10.1016/s0895-7177(02)00108-5

Delhez E.J.M., J.-M. Campin, A.C. Hirst and E. Deleersnijder, 1999, Toward a general theory of the age in ocean modelling, *Ocean Modelling*, 1, 17-27, doi: 10.1016/S1463-5003(99)00003-7

Delhez E.J.M. and E. Deleersnijder, 2002, The concept of age in marine modelling: II. Concentration distribution function in the English Channel and the North Sea, *Journal of Marine Systems*, 31, 279-297, doi: 10.1016/s0924-7963(01)00066-5

Delhez E.J.M. and E. Deleersnijder, 2006, The boundary layer of the residence time field, *Ocean Dynamics*, 56, 139-150, doi: 10.1007/s10236-006-0067-0

Delhez E.J.M. and E. Deleersnijder, 2008, Age and the time lag method, *Continental Shelf Research*, 28, 1057-1067, doi: 10.1016/j.csr.2008.02.003

Delhez E.J.M. and E. Deleersnijder, 2010, Residence and exposure time of sinking phytoplankton in the euphotic layer, *Journal of Theoretical Biology*, 262, 505-516, doi: 10.1016/j.jtbi.2009.10.004

Delhez E.J.M. and E. Deleersnijder, 2012, Residence and exposure times: when diffusion does not matter, *Ocean Dynamics*, 62, 1399-1407, doi: 10.1007/s10236-012-0568-y

Delhez E.J.M., E. Deleersnijder, A. Mouchet, and J.-M. Beckers, 2003, A note on the age of radioactive tracers, *Journal of Marine Systems*, 38, 277-286, doi: 10.1016/s0924-7963(02)00245-2

Delhez E.J.M., G. Lacroix and E. Deleersnijder, 2004, The age as a diagnostic of the dynamics of marine ecosystem models, *Ocean Dynamics*, 54, 221-231, doi: 10.1007/s10236-003-0075-2

Delhez E.J.M. and F. Wolk, 2013, Diagnosis of the transport of adsorbed material in the Scheldt estuary: a proof of concept, *Journal of Marine Systems*, 128, 17-26, doi: 10.1016/j.jmarsys.2012.01.007

Doney S.C. and W.J. Jenkins, 1994, Ventilation of the deep western boundary current and abyssal western North Atlantic: estimates from tritium and ^{3}He distributions, *Journal of*

Physical Oceanography, 24, 638-659, doi: 10.1175/1520-0485(1994)024%3C0638:VOTDWB%3E2.0.CO;2

Downing B.D., B.A. Bergamashi, C. Kendall, T.E.C. Kraus, K.J. Dennis, J.A. Carter and T.S. Von Dessonneck, 2016, Using continuous underway isotope measurements to map water residence time in hydrodynamically complex tidal environments, *Environmental Science & Technology*, 50, 13387-13396, doi: 10.1021/acs.est.6b05745

Du J., K. Park, J. Shen, B. Dzwonkowski, X. Yu and B.I. Yoon, 2018, Role of baroclinic processes on flushing characteristics in a highly stratified estuarine system, Mobile Bay, Alabama, *Journal of Geophysical Research*, 123, 4518-4537, doi: 10.1029/2018jc013855

England M.H., 1995, The age of water and ventilation timescales in a Global Ocean model, *Journal of Physical Oceanography*, 25, 2756-2777, doi: 10.1175/1520-0485(1995)025<2756:taowav>2.0.co;2

Gong W. and J. Shen, 2010, A model diagnostic study of age of river-borne sediment transport in the tidal York River Estuary, *Environmental Fluid Mechanics*, 10, 177-196, doi: 10.1007/s10652-009-9144-5

Goosse H., J.-M. Campin and B. Tartinville, 2001, The source of Antarctic bottom water in a global ice-ocean model, *Ocean Modelling*, 3, 51-65, doi: 10.1016/s1463-5003(00)00017-2

Gourgue O., E. Deleersnijder and L. White, 2007, Toward a generic method for studying water renewal, with application to the epilimnion of Lake Tanganyika, *Estuarine, Coastal and Shelf Science*, 74, 628-640, doi: 10.1016/j.ecss.2007.05.009

Gräwe U., E. Deleersnijder, S.H.A.M. Shah and A.W. Heemink, 2012, Why the Euler-scheme in particle-tracking is not enough: the shallow-sea pycnocline test case, *Ocean Dynamics*, 62, 501-514, doi: 10.1007/s10236-012-0523-y

Gross E., S. Andrews, B. Bergamashi, B. Downing, R. Holleman, S. Burdick and J. Durand, 2019, The use of stable isotope-based water age to evaluate a hydrodynamic model, *Water*, 11, 2207, doi: 10.3390/w11112207

Grosse F., K. Fennel and A. Laurent, 2019, Quantifying the relative importance of riverine and open-ocean nitrogen sources for hypoxia formation in the northern Gulf of Mexico, *Journal of Geophysical Research*, 124, 5451-5467, doi: 10.1029/2019jc015230

Haine T.W.N. and T.M. Hall, 2002, A generalized transport theory: water-mass composition and age, *Journal of Physical Oceanography*, 32, 1932-1946, doi: 10.1175/1520-0485(2002)032<1932:agttwm>2.0.co;2

Hall T.M. and T.W.N. Haine, 2004, Tracer age symmetry in advective-diffusive flows, *Journal of Marine Systems*, 48, 51-59, doi: 10.1016/j.jmarsys.2003.01.001

Hall T.M. and R.A. Plumb, 1994, Age as a diagnostic of stratospheric transport, *Journal of Geophysical Research*, 99, 1059-1070, doi: 10.1029/93jd03192

Hirst A.C., 1999, Determination of water component age in ocean models: application to the fate of North Atlantic Deep Water, *Ocean Modelling*, 1, 81-94, doi: 10.1016/s1463-5003(99)00010-4

Holzer M. and T.M. Hall, 2000, Transit-time and tracer-age distributions in geophysical flows, *Journal of the Atmospheric Sciences*, 57, 3539-3558, doi: 10.1175/1520-0469(2000)057<3539:ttatad>2.0.co;2

Holzer M. and F. Primeau, 2006, The diffusive ocean conveyor, *Geophysical Research Letters*, 33, L14618, doi: 10.1029/2006GL026232

Hong B., G. Wang, H. Xu and D. Wang, 2020, Study on the transport of terrestrial dissolved substances in the Pearl River Estuary using passive tracers, *Water*, 12, 1235, doi: 10.3390/w12051235

Huisman J., M. Arrayas, U. Ebert and B. Sommeijer, 2002, How do sinking phytoplankton species manage to persist?, *The American Naturalist*, 159, 245-254, doi: 10.1086/338511

Huisman J., J. Sharples, J.M. Stroom, P. M. Visser, W.E.A. Kardinaal, J.M.H. Verspagen and B. Sommeijer, 2004, Changes in turbulent mixing shift competition for light between phytoplankton species, *Ecology*, 85, 2960-2970, doi: 10.1890/03-0763

Kärnä T. and A.M. Baptista, 2016, Water age in the Columbia River estuary, Estuarine, *Coastal and Shelf Science*, 183, 249-259, doi: 10.1016/j.ecss.2016.09.001

Kazemi G.H., J.H. Lehr and P. Perrochet, 2006, *Groundwater Age*, Wiley, 325 pages, doi: 10.1002/0471929514

Lane S.N. and K.S. Richards, 2001, The 'validation' of hydrodynamic models: some critical perspectives, in: M. Anderson and P. Bates (eds.), *Model Validation: Perspectives in Hydrological Science*, Wiley, Chichester, pages 413-438

Lewandowski R., 1997, *Analyse Mathématique et Océanographie*, Masson, Paris, 304 pages, isbn-10: 2225852332, isbn-13 : 9782225852336

Lietaer O., E. Deleersnijder, T. Fichefet, M. Vancoppenolle, R. Comblen, S. Bouillon and V. Legat, 2011, The vertical age profile in sea ice: theory and numerical results, *Ocean Modelling*, 40, 211-226, doi: 10.1016/j.ocemod.2011.09.002

Lin L. and Z. Liu, 2019, Partial residence times: determining residence time composition in different subregions, *Ocean Dynamics*, 69, 1023-1036, doi: 10.1007/s10236-019-01298-8

Liu Z., H. Wang, X. Guo, Q. Wang and H. Gao, 2012, The age of Yellow River water in the Bohai Sea, *Journal of Geophysical Research*, 117, C11006, doi: 10.1029/2012JC008263

Liu S., Q. Ye, S. Wu and M.J.F. Stive, 2020, Wind effects on the water age in a large shallow lakes, *Water*, 12, 1246, doi: 10.3390/w12051246

Liu R., X. Zhang, B. Liang, L. Xin and Y. Zhao, 2017, Numerical study on the influences of hydrodynamic factors on water age in the Liao River Estuary, China, *Journal of Coastal Research*, 80, 98-107, doi: 10.2112/si80-014.1

Lucas L.V. and E. Deleersnijder, 2020, Timescale methods for simplifying, understanding and modeling biophysical and water quality processes in coastal aquatic ecosystems: a review, *Water*, 12, 2717, doi: 10.3390/w12102717

Lucas L. and E. Deleersnijder, 2021, Diagnostic timescales: old concepts, new methods, and the ageless power of simplification, *CERF's Up!*, 47(1), 14-15 (+references)[10]

Meier H.E.M., 2005, Modeling the age of Baltic Seawater masses: Quantification and steady state sensitivity experiments, *Journal of Geophysical Research*, 110, C02006, doi: 10.1029/2004JC002607

Mercier C. and E.J.M. Delhez, 2007, Diagnosis of the sediment transport in the Belgian

[10] Available on the web at URL https://cerf.memberclicks.net/assets/bulletin/2021/CERF%2047-1.pdf

Coastal Zone, *Estuarine, Coastal and Shelf Science*, 74, 670-683, doi: 10.1016/j.ecss.2007.05.010

Mouchet A., F. Cornaton, E. Deleersnijder and E.J.M. Delhez, 2016, Partial ages: diagnosing transport processes by means of multiple clocks, *Ocean Dynamics*, 66, 367-386, doi: 10.1007/s10236-016-0922-6

Mouchet A., E. Deleersnijder and F. Primeau, 2012, The leaky funnel model revisited, *Tellus*, 64A, 19131, doi: 10.3402/tellusa.v64i0.19131

Munhoven G., 2020, Model of Early Diagenesis in the Upper Sediment with Adaptable complexity – MEDUSA (v. 2): a time-dependent biogeochemical sediment module for Earth System Models, process analysis and teaching, *Geoscientific Model Development* (accepted for publication), doi: 10.5194/gmd-2020-309

Oreskes N., K. Shrader-Frechette and K. Belitz, 1994, Verification, validation, and confirmation of numerical models in the Earth sciences, *Science*, 263, 641-646, doi: 10.1126/science.263.5147.641

Petton S., S. Pouvreau and F. Dumas, 2020, Intensive use of Lagrangian trajectories to quantify coastal area dispersion, *Ocean Dynamics*, 70, 541-559, doi: 10.1007/s10236-019-01343-6

Pham Van C., B. de Brye, A. de Brauwere, A.J.F. Hoitink, S. Soares-Frazao and E. Deleersnijder, 2020, Numerical simulation of water renewal timescales in the Mahakam Delta, Indonesia, *Water*, 12, 1017, doi: 10.3390/w12041017

Pinilla E., M.J. Castillo, I. Perez-Santos, O. Venegas and A. Valle-Levinson, 2020, Water age variability in a Patagonian fjord, *Journal of Marine Systems*, 210, 103376, doi: 10.1016/j.jmarsys.2020.103376

Radtke H., T. Neumann, M. Voss and W. Fennel, 2012, Modeling pathways of riverine nitrogen and phosphorus in the Baltic Sea, *Journal of Geophysical Research*, 117, C09024, doi: 10.1029/2012JC008119

Ralston D.K. and W.R. Geyer, 2017, Sediment transport time scales and trapping efficiency in a tidal river, *Journal of Geophysical Research*: *Earth Surface*, 122, 2042-2063, doi: 10.1002/2017JF004337

Salomon J.C., M. Breton and P. Gueguениat, 1995, A 2D long term advection-dispersion model for the Channel and southern North Sea. Part B: transit time and transfer function for Cap de la Hague, *Journal of Marine Systems*, 6, 515-527, doi: 10.1016/0924-7963(95)00021-G

Silverman B.W., 1986, *Density Estimation for Statistics and Data Analysis*, Chapman & Hall, London, 175 pages

Spivakovskaya D., A.W. Heemink and E. Deleersnijder, 2007a, The backward Ito method for the Lagrangian simulation of transport processes with large space variations of the diffusivity, *Ocean Science*, 3, 525-535, doi: 10.5194/os-3-525-2007

Spivakovskaya D., A.W. Heemink and E. Deleersnijder, 2007b, Lagrangian modelling of multi-dimensional advection-diffusion with space-varying diffusivities: theory and idealized tests cases, *Ocean Dynamics*, 57, 189-203, doi: 10.1007/s10236-007-0102-9

Takeoka H., 1984, Fundamental concepts of exchange and transport time scales in a coastal sea, *Continental Shelf Research*, 3, 311-326, doi: 10.1016/0278-4343(84)90014-1

Tang C., C. He, Y. Li and K. Acharya, 2021, Diverse responses of hydrodynamics, nutrients and algal biomass to water diversion in a eutrophic shallow lake, *Journal of Hydrology*, 593, 125933, doi: 10.1016/j.jhydrol.2020.125933

Thiele G. and J.L. Sarmiento, 1990, Tracer dating and ocean ventilation, *Journal of Geophysical Research*, 95 (C6), 9377-9391, doi: 10.1029/JC095iC06p09377

van Sebille E., S.M. Griffies, R. Abernathey, T.P. Adams, P. Berloff, A. Biastoch, B. Blanke, E.P. Chassignet, Y. Cheng, C.J. Cotter, E. Deleersnijder, K. Döös, H. Drake, S. Drijfhout, S.F. Gary, A.W. Heemink, J. Kjellsson, I.M. Koszalka, M. Lange, C. Lique, G.A. MacGilchrist, R. Marsh, C.G. Mayorga Adame, R. McAdam, F. Nencioli, C.B. Paris, M.D. Piggott, J.A. Polton, S. Rühs, S.H.A.M. Shah, M.D. Thomas, J. Wang, P.J. Wolfram, L. Zanna and J.D. Zika, 2018, Lagrangian ocean analysis: fundamentals and practices, *Ocean Modelling*, 121, 49-75, doi: 10.1016/j.ocemod.2017.11.008

Venkatram A., S. Du, R. Hariharan, W. Carter and R. Goldstein, 1998, The concept of species age in photochemical modelling, *Atmospheric Modelling*, 32, 3403-3413, doi: 10.1016/S1352-2310(98)00032-6

Visser A.W., 2008, Lagrangian modelling of plankton motion: from deceptively simple random walks to Fokker-Planck and back again, *Journal of Marine Systems*, 70, 287-299, doi: 10.1016/j.jmarsys.2006.07.007

Wang Y. and J. Shen, 2020, A modeling study on the influence of sea-level rise and channel deepening on estuarine circulation and dissolved oxygen concentration levels in the tidal James River, Virginia, USA, *Journal of Marine Science and Engineering*, 8, 950, doi: 10.3390/jmse8110950

Zimmerman J.T.F., 1976, Mixing and flushing of tidal embayments in the western Dutch Wadden Sea. Part I: Distribution of salinity and calculation of mixing time scales, *Netherlands Journal of Sea Research*, 10, 149-191, doi: 10.1016/0077-7579(76)90013-2
