CART: the Constituent-oriented Age and Residence time Theory

A holistic tool to help understand complex reactive transport processes

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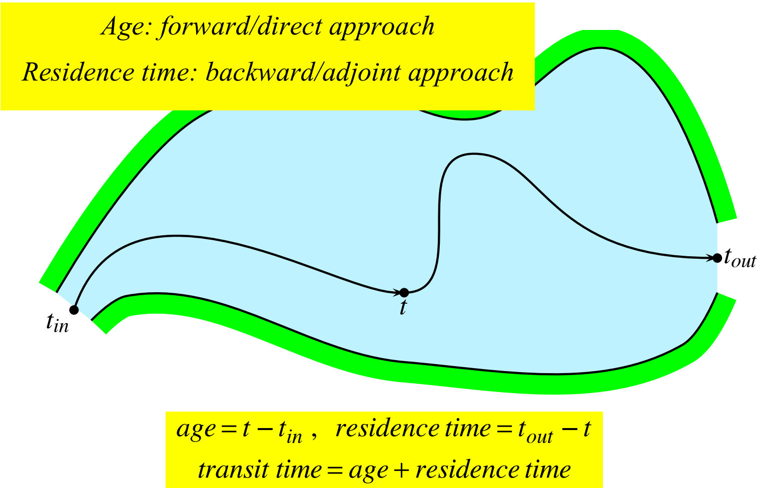


Nowadays marine models routinely produce large amounts of results. Making sense of all these real numbers is not a trivial task. This is why specific interpretation methods are needed. Estimating timescales is one of them. In this respect, a comprehensive theory (CART) is developed that allows for the estimation of timescales such as the age and the residence time from the solution of **partial differential problems**.

At any time and position, the **age** — a measure of the **elapsed time** — of every constituent, or group of constituents, of seawater can be estimated in such a way that **advection**, **diffusion** and **reactions** are properly taken into account. For every constituent, the core variable is the **age distribution function**, $c_i(t,\mathbf{x},\tau)$, where the subscript i identifies the constituent under consideration, whilst t and $\mathbf{x}$ denote the time and the position vector, respectively. For a seawater sample of volume $\delta V \to 0$ taken at time t and location $\mathbf{x}$, the mass of the i-th constituent whose age lies in the interval $[\tau, \tau+\delta\tau]$ tends to $\rho_{\bullet} c_i(t,x,\tau)\delta\tau\,\delta V$ in the limit $\delta\tau \to 0$, where $\rho_{\bullet}$ is the (constant) reference density of seawater (Boussinesq approximation). The age distribution function may be viewed as the histogram of the ages of the particles of the i-th constituent in the aforementioned seawater sample.

Classical mass budget considerations lead to the equation governing the evolution of $c_i(t,\mathbf{x},\tau)$, which is closely related to Green's function when the concentration of the constituent under study obeys a linear equation. Then, the concentration (defined as a mass fraction) and age concentration, $C_i(t,\mathbf{x})$ and $\alpha_i(t,\mathbf{x})$, are the zeroth and first-order moments of the age distribution, respectively (see equations opposite). The mean age, $a_i(t,\mathbf{x})$, is obtained in accordance with the age-averaging hypothesis (Deleersnijder et al. 2001): the mean age is to be evaluated as the mass-weighted mean of the ages of the particles under consideration.

$$\underbrace{\frac{\partial c_i}{\partial t} = \vartheta_i - \nabla\bullet(c_i\mathbf{v} - \mathbf{K}\bullet\nabla c_i) - \frac{\partial c_i}{\partial \tau}}$$

$$\Downarrow$$

$$C_i(t,\mathbf{x}) = \int_0^\infty c_i(t,\mathbf{x},\tau)\,d\tau \ , \quad \alpha_i(t,\mathbf{x}) = \int_0^\infty \tau\, c_i(t,\mathbf{x},\tau)\,d\tau$$

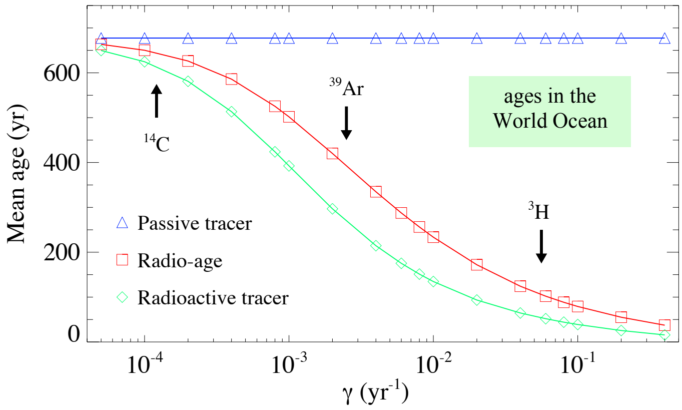
$$a_i(t,\mathbf{x}) = \frac{\alpha_i(t,\mathbf{x})}{C_i(t,\mathbf{x})}$$

$$\Uparrow$$

$$\overbrace{\begin{aligned} \frac{\partial C_i}{\partial t} &= \Theta_i - \nabla\bullet(C_i\mathbf{v} - \mathbf{K}\bullet\nabla C_i) \\ \frac{\partial \alpha_i}{\partial t} &= C_i + \Pi_i - \nabla\bullet(\alpha_i\mathbf{v} - \mathbf{K}\bullet\nabla\alpha_i) \end{aligned}}$$

$$(\Theta_i, \Pi_i) = \int_0^\infty (\vartheta_i, \tau\vartheta_i)\,d\tau$$

The form of (resolved and unresolved) transport terms is identical in the equation governing the concentration and in that for the age concentration. Therefore, the mean age, $a_i(t,\mathbf{x})$, provides diagnoses fully consistent with the model whose results are to be interpreted. Another advantage of the present Eulerian approach is that



theoretical results are easier to obtain than in the Lagrangian formalism. For instance, the biases of the age derived from radioactive tracers (see figure opposite) or from the time lag method have been uncovered and investigated in depth. The age also turned out to be of use to diagnose reaction rates in ecosystem models, i.e. in models in which the reaction terms are non-linear. On the other hand, the age of tracers released by a point source in a number of shallow water domains has been simulated numerically and investigated in a theoretical manner, leading to the discovery of an intriguing symmetry property (Beckers et al. 2001).

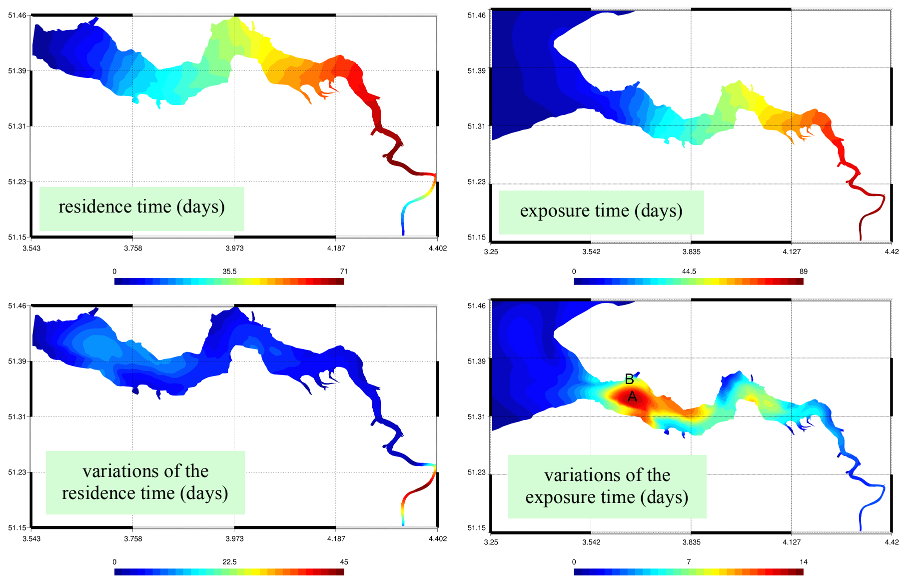
The **residence time** is defined as the time needed for a particle to hit for the first time an open boundary of the domain. To account for the fact that particles may re-enter the domain of interest after leaving it, the concept of **exposure time** was introduced. The propensity of particles to re-enter the domain may be evaluated by means of the **return coefficient**. The residence time and the exposure time, $\eta(t,\mathbf{x})$, are the solution of an adjoint equation (Delhez et al. 2004), which is to be integrated backward in time,

$$\frac{\partial \eta}{\partial t} = -\omega - \nabla \bullet (\eta \mathbf{v} + \mathbf{K} \bullet \nabla \eta) \ , \quad \omega(\mathbf{x}) = \begin{cases} 1 & \text{if } \ \mathbf{x} \in \text{domain of interest} \\ 0 & \text{if } \ \mathbf{x} \notin \text{domain of interest} \end{cases}$$

In the framework of idealised flow studies, it was seen that the residence/exposure time of sinking particles (e.g. diatoms) in the upper mixed layer is an increasing function of the eddy diffusivity. A generalisation of this approach allowed for the evaluation of the amount of light such particles are exposed to. Relevant inequalities and seemingly counterintuitive results were established and discussed.

The abovementioned time-scales proved to be particularly useful for investigating the **water renewal** of semi-enclosed domains. A general method was developed, which suggests that the age of the renewing water be estimated as well as the residence/exposure time of the water originally present in the domain of interest (de Brye et al 2012). Several estuaries share the same property (see figure opposite): the variability of the residence and exposure time is much more pronounced at the period of the dominant tidal component than at the timescale of the spring-neap cycle though these diagnostic timescales are usually significantly longer than the duration of a spring-neap cycle.

Scheldt Estuary water renewal timescales



The concept of age is being generalised, leading to the notion of **partial age** (Mouchet et al. 2016). The domain of interest is split into several subdomains and every constituent particle is henceforth “equipped” with several clocks (rather than only one), allowing for the time spent in each subdomain to be evaluated. This way, information about pathways is obtained without having recourse to Lagrangian calculations.

Publications related to the development and application of the

Constituent-oriented Age and Residence time Theory (CART)

http://www.climate.be/cart

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