"The Constituent-oriented Age and Residence time Theory (CART) - A holistic approach to the understanding of the results of complex marine results"

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The Constituent-oriented Age and Residence time Theory (CART)
A holistic approach to the understanding of the results of complex marine models

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(with many thanks to Jean-Marie Beckers, Jean-Michel Campin and Anne Mouchet)
The need for holistic interpretation methods

• Today's numerical models produce output files that are so huge that the human brain can “read/peruse” only a tiny fraction of them. Thus, making sense of the results is a great challenge.

• Producing graphs based on space-time slices in the output files amounts to ignoring most of the results and relies on the assumption that the slices are well chosen. But, how can we be sure of that as most of the results are ignored?

• Methods are needed that drastically reduce the amount of results submitted to the human brain without leaving data aside. Statistics and timescale analyses fall into this class of interpretation methods. These methods are holistic in that all/most of the results are taken into account.
Basic timescale definitions

Age: forward/direct approach
Residence time: backward/adjoint approach

\[ \text{age} = t - t_{in}, \quad \text{residence time} = t_{out} - t \]

transit time = age + residence time
Traditional applications of the age

**estimating ocean ventilation rate**

- atmosphere
- ocean mixed layer
- particle trajectory

**inferring shelf sea circulation**

- shelf sea
- particle trajectory
- tracer source
- continent

age = time elapsed since leaving the source

See for instance:


Diffusion paradox of some dating techniques

- Using the radioactive decay as a clock:

  \[
  \text{“radio-age”} = r(t, x) = \gamma^{-1} \log \frac{C_p(t, x)}{C_r(t, x)}
  \]

  \(C_p\) = concentration of a passive — i.e. inert — tracer

  \(C_r\) = concentration of a radioactive tracer (half-life = \(\gamma^{-1} \log 2\))

- The main assumption underlying the concept of radio-age is that diffusion is negligible. However, diffusion cannot be neglected to compute \(C_p\) and \(C_r\). This is somewhat paradoxical...

- Similar problems in other “pragmatic” dating techniques.

- Are we really estimating an elapsed time? Is a single age really relevant for every water parcel?
A general theory of the age

A theory for evaluating the age in **numerical models** such that:

- advection, mixing, and production/destruction processes are properly accounted for;
- age is a time- and position-dependent variable;
- the age of every constituent can be evaluated separately, hence the name CART, i.e. Constituent-oriented Age and...;
- the age may be calculated in the Eulerian formalism;
- CART is intended for numerical models, but some of its aspects may be of use to applications relying on field data only.

Only one arbitrary assumption

• Particles “A” and “B”, mass $m^A$ and $m^B$, age $a^A$ and $a^B$.
• System “A+B”, consisting of particles “A” and “B”.
• Mass of system “A+B”: $m^{A+B} = m^A + m^B$.

  (mass is an additive quantity, i.e. basic physical principle)
• Age of system “A+B”: no underlying physical principle!

Age-averaging hypothesis: mass-weighted arithmetic mean:

$$a^{A+B} = \frac{m^A a^A + m^B a^B}{m^A + m^B}$$

• Age content: $m^{A+B} a^{A+B} = m^A a^A + m^B a^B$ (additive quantity).
Basic variables

• $\rho c_i(t, x, \tau)\delta V\delta \tau$: mass of the $i$-th constituent in $\delta V$, whose age lies in the interval $[\tau - \delta \tau / 2, \tau + \delta \tau / 2]$ ($\delta \tau \to 0$), where $c_i(t, x, \tau)$ is the concentration distribution function.

• Concentration: $C_i(t, x) = \int_{0}^{\infty} c_i(t, x, \tau) \ d\tau$

• Age concentration: $\alpha_i(t, x) = \int_{0}^{\infty} \tau c_i(t, x, \tau) \ d\tau$

• Mean age: $a_i(t, x) = \frac{\alpha_i(t, x)}{C_i(t, x)}$
Basic equations

• Simple mass budget considerations yield:

\[
\frac{\partial c_i}{\partial t} = p_i - d_i - \nabla \cdot (uc_i - K \cdot \nabla c_i) - \frac{\partial c_i}{\partial \tau}
\]

source - sink  

advection + diffusion  

ageing

\[
\frac{\partial C_i}{\partial t} = P_i - D_i - \nabla \cdot (uC_i - K \cdot \nabla C_i)
\]

source - sink  

advection + diffusion

\[
\frac{\partial \alpha_i}{\partial t} = C_i + \pi_i - \delta_i - \nabla \cdot (u \alpha_i - K \cdot \nabla \alpha_i)
\]

ageing  

source - sink  

advection + diffusion

• All advection-diffusion operators are of the same form.
Diagnosing matter fluxes in ecological models (I)

• At least two options, illustrated here in a simple/generic model:

Estimating the age of every compartment

Nutrient \( C_0, \ a_0 = 0 \)  
Prey \( C_1, \ a_1 \)  
Predator \( C_2, \ a_2 \)

The matter entering each compartment has zero age

Estimating cumulative ages

Nutrient \( C_0, \ a_0 = 0 \)  
Prey \( C_1, \ a_{1,c} \)  
Predator \( C_2, \ a_{2,c} \)

The prey takes zero-age nutrients.  
The predator takes the prey “along with its age”.

\[ a_1 = a_{1,c} \]
\[ a_2 < a_{2,c} \]
Assuming an infinite stock of nutrients (no nutrient-related limitation to growth), the solutions of a classical two-equation Lotka-Volterra model are (in dimensionless variables):

- The prey and predator concentrations exhibit periodic oscillations and, yet, the age of the prey tends to a constant!
Diagnosing matter fluxes in ecological models (III)

- The equations for the prey concentration and age are:

\[
\frac{dC_1}{dt} = \frac{C_1}{\theta} - \frac{C_2}{\theta^*} C_1, \quad \frac{d\alpha_1}{dt} = \frac{0}{\text{nutrient uptake}} - \left(\frac{C_2}{\theta^*} C_1\right) a_1 + \frac{C_1}{\text{ageing}}
\]

\[\Rightarrow \quad \frac{da_1}{dt} = -\frac{a_1}{\theta} + 1\Rightarrow a_1(t) = [a_1(0) - \theta]e^{-t/\theta} + \theta \to 0 \text{ as } t/\theta \to \infty\]

The prey's age tends to the nutrient uptake timescale, \(\theta\), because the predation term is age-independent.

- Valid for any predation term of the form \(f(t,C_1,C_2)C_1\).
Diagnosing matter fluxes in ecological models (IV)

Renewal of Lake Tanganyika's epilimnion water (I)

Meromictic lake that lies between Congo, Burundi, Tanzania and Zambia. Its hypolimnion is the second largest anoxic water body in the world.

The water fluxes (entrainment) through the permanent thermocline are the main source of “new” water and nutrients for the epilimnion.

Finite-element, reduced-gravity model of the epilimnion that distinguishes between original epilimnion water and renewing water — from lower layer.
Renewal of Lake Tanganyika's epilimnion water (II)

• Epilimnion water concentration: $C_e(t, x)$, with $0 \leq C_e(t, x) \leq 1$
  Hypolimnion water concentration: $C_h(t, x)$, with $0 \leq C_h(t, x) \leq 1$

\[
C_e(0, x) = 1 \quad C_e(\infty, x) = 0
\]

with

\[
C_h(0, x) = 0 \quad C_h(\infty, x) = 1
\]

\[
C_e(t, x) + C_h(t, x) = 1
\]

• Two seasons:
  dry season (April-August) with strong winds from south-east;
  wet season (September-March) with weak winds.
  Dry season: thermocline is deeper in the north and oscillates;
  Wet season: thermocline oscillations get progressively damped.
Residence time: the forward/direct procedure

1. Introduce unit mass of passive tracer at time $t_0$ and location $x_0$;
2. Calculate the mass $m(t_0 + \tau)$ of the tracer in the domain $\omega$;
3. Residence time: $\theta(t_0, x_0) = -\int_{0}^{\infty} \tau \ dm = \int_{0}^{\infty} m(t_0 + \tau) \ d\tau$. 

\[ m(t_0 + \tau) = \int_{\omega} C(t_0 + \tau, x) \ dx \]

Key assumption: $\frac{dm}{d\tau} \leq 0$. 

Unit mass released at $(t_0, x_0)$
Residence time: the backward/adjoint procedure (I)

• Using the direct procedure, the number of models runs that are needed is equal to the number of \( t_0 \) and \( x_0 \) at which the residence time is to be estimated.

\[ \Rightarrow \text{CPU cost can be prohibitive!} \]

• Delhez et al. (2004, *Estuarine, Coastal and Shelf Science*, 61, 691-702) developed an adjoint model that is potentially much more efficient, but requires backward integration in time.

• The residence time \( \theta(t, x) \) is the solution of

\[
\frac{\partial \theta}{\partial t} = -1 - \nabla \cdot (u \theta + K \cdot \nabla \theta)
\]
Residence time: the backward/adjoint procedure (II)

• The equation governing $\theta(t,x)$ is to be integrated backward in time from $t = T$, with $\theta(T,x) = 0$ and $T \to \infty$.

In practice, $T$ is taken to be sufficiently large, so that the residence time is hopefully accurate for $t << T - O(\theta)$. For more details, see Delhez (2005, *Ocean Science Discussions*, 2, 247-265, available on the web).

• Some examples of boundary conditions:

<table>
<thead>
<tr>
<th>direct problem</th>
<th>adjoint problem</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C = 0$</td>
<td>$\theta = 0$</td>
</tr>
<tr>
<td>$(K \cdot \nabla C) \cdot n = 0$</td>
<td>$(u\theta + K \cdot \nabla \theta) \cdot n = 0$</td>
</tr>
<tr>
<td>$(uC - K \cdot \nabla C) \cdot n = 0$</td>
<td>$(K \cdot \nabla \theta) \cdot n = 0$</td>
</tr>
</tbody>
</table>
Residence time in the upper mixed layer (I)

Key assumptions: horizontal homogeneity and hydrodynamics at a steady state.
Residence time in the upper mixed layer (II)

<table>
<thead>
<tr>
<th></th>
<th>direct/forward problem</th>
<th>adjoint problem</th>
</tr>
</thead>
<tbody>
<tr>
<td>unknown</td>
<td>concentration: $C(t,z)$</td>
<td>residence time: $\theta(z)$</td>
</tr>
<tr>
<td>governing equation</td>
<td>$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(wC + \kappa \frac{\partial C}{\partial z}\right)$</td>
<td>$\frac{d}{dz}\left(w\theta - \kappa \frac{d\theta}{dz}\right) = 1$</td>
</tr>
<tr>
<td>initial condition</td>
<td>$C(0,z) = \delta(z-z_0)$</td>
<td>not applicable</td>
</tr>
<tr>
<td>boundary conditions</td>
<td>$\left[wC + \kappa \frac{\partial C}{\partial z}\right]_{z=h} = 0$</td>
<td>$\left[\kappa \frac{d\theta}{dz}\right]_{z=h} = 0$</td>
</tr>
<tr>
<td></td>
<td>$\left[\kappa \frac{\partial C}{\partial z}\right]_{z=0} = 0$</td>
<td>$\left[w\theta - \kappa \frac{d\theta}{dz}\right]_{z=0} = 0$</td>
</tr>
<tr>
<td>solution</td>
<td>$C(t,z) = \text{?}$</td>
<td>$\theta(z) = \frac{z}{w} + \frac{1}{w} \int_z^h \exp\left[-w \int_z^\xi \frac{d\xi}{\kappa(\xi)}\right] d\xi$</td>
</tr>
</tbody>
</table>

$\theta \uparrow$ if $h \uparrow$, $\kappa \uparrow$, $w \downarrow$
Residence time in the upper mixed layer (III)

\[ \kappa'(z) = 6z'(1 - z') \]

- Peclet number: \( Pe = \frac{wh}{K} \)
- Dimensionless variables:

\[ z' = \frac{z}{h}, \quad \kappa' = \frac{K}{\kappa}, \quad \theta' = \frac{\theta}{h/w} \]

\( z' \leq \theta'(z') \leq 1 \)
\( \theta'(1) \) independent of \( \kappa'(z') \)!

(Deleersnijder et al., 2006, *Environmental Fluid Mechanics*)
Residence time vs exposure time

- Particles that left the domain can enter it again at some later time. This can be taken into account by means of the exposure time, i.e. *the time spent in the domain of interest* — whereas the residence time is the time needed to leave it for the first time.

\[
\begin{align*}
\kappa &= \text{Const.} \\
u &= \text{Const.} (> 0)
\end{align*}
\]

To obtain the exposure time, the same adjoint model equations are to be solved, but in a different domain and with different boundary conditions.

(DeHeuvel and Deleersnijder, 2006, *Ocean Dynamics*)
Residence/exposure time in the English Channel (I)

• Horizontal resolution: 10'; 10 σ-levels.
• Free-surface; baroclinic; $k$ turbulence closure model.
• Forcings: 10 tidal constituents and NCEP reanalysis met. data.
Residence/exposure time in the English Channel (II)

Residence time (days)
Residence/exposure time in the English Channel (III)
Concluding remarks

- A general theory of the age has been developed, from which the age of any seawater constituent or group of constituents, passive or not, can be estimated.

- A general theory of the residence/exposure time is being developed. Open questions pertain to boundary conditions and tracers with non-linear source/sink terms.

- Age and residence/exposure times are easy to estimate numerically, are of use in a number of applications, and there is no shortage of surprising results.

- CART can be applied outside the realm of oceanography as long as the Boussinesq approximation remains valid (e.g. industrial chemistry paper by Jongen, 2004, *AICHE*, 50).
For additional information about CART, see
http://www.climate.be/CART