Management Unit of the North Sea Mathematical Models
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The Constituent-oriented Age and Residence time Theory (CART): a holistic approach to the understanding of the results of complex geophysical and environmental fluid flow models

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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?

Deleersnijder and Delhez, *Estuarine, Coastal and Shelf Science*, 2007

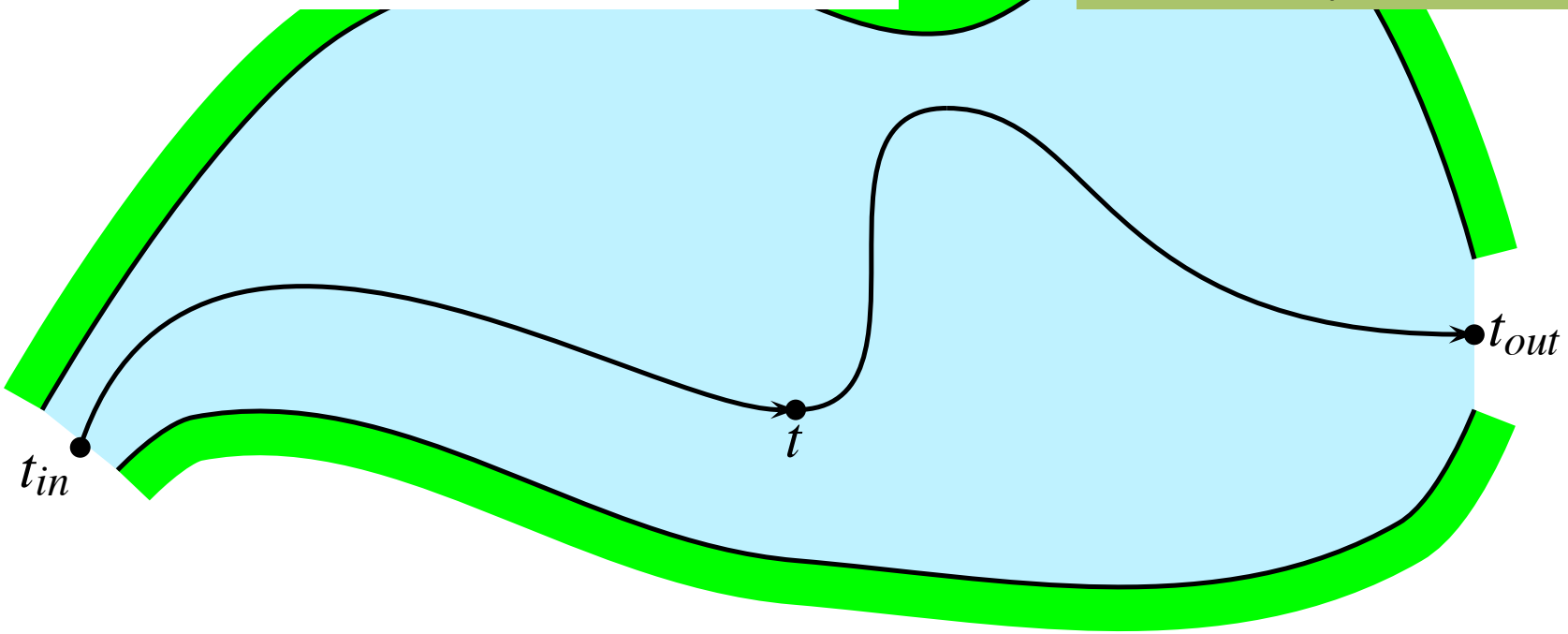
• Methods are needed that drastically reduce the amount of results submitted to the human brain without leaving data aside. Statistics and timescale analyses fall into this class of interpretation methods. These methods are holistic in that all/most of the results are taken into account.

Age and residence time

Deleersnijder et al., *Journal of Marine Systems*, 2001
Delhez et al., *Estuarine, Coastal and Shelf Science*, 2004

Age: forward/direct approach

Residence time: backward/adjoint approach

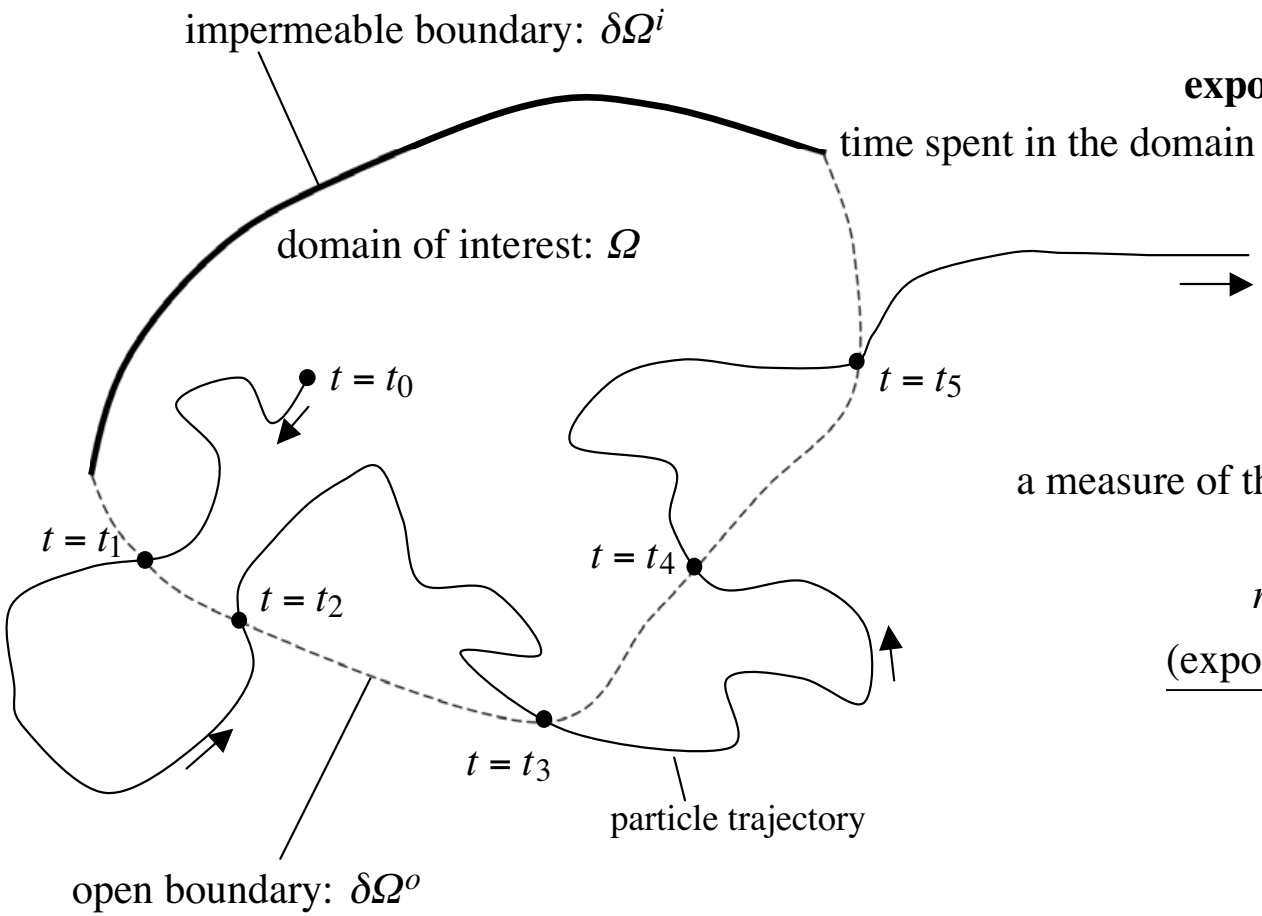


$$age = t - t_{in} \;, \quad residence\ time = t_{out} - t$$

$$transit\ time = age + residence\ time$$

The exposure time, an alternative to the residence time

$t_0 < t_1 < t_2 < t_3 < t_4 < t_5$



residence time:

time to leave the domain for the first time = $t_1 - t_0$

exposure time:

time spent in the domain = $(t_1 - t_0) + (t_3 - t_2) + (t_5 - t_4)$

return coefficient:

a measure of the propensity to return into the domain

$$r = \text{return coefficient} = \frac{(\text{exposure time}) - (\text{residence time})}{(\text{exposure time})}$$

$$0 \le r \le 1$$

$r = 0$: no return

$r = 1$: frequent reentries

de Brauwere et al., *Journal of Marine Systems*, 2011

Age: basic variables and equations

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

- Concentration: $C_i(t,\mathbf{x}) = \int_0^\infty c_i(t,\mathbf{x},\tau)\ d\tau$

- Age concentration: $\alpha_i(t,\mathbf{x}) = \int_0^\infty \tau c_i(t,\mathbf{x},\tau)\ d\tau$

- Mean age: $a_i(t,\mathbf{x}) = \dfrac{\alpha_i(t,\mathbf{x})}{C_i(t,\mathbf{x})}$

Delhez et al., *Ocean Modelling*, 1999

Age: basic variables and equations (continued)

- Simple mass budget considerations yield:

$$\frac{\partial c_i}{\partial t} = \underbrace{p_i - d_i}_{\text{source - sink}} - \nabla \bullet \underbrace{(\mathbf{u}c_i - \mathbf{K} \bullet \nabla c_i)}_{\text{advection + diffusion}} - \underbrace{\frac{\partial c_i}{\partial \boldsymbol{\tau}}}_{\text{ageing}}$$

$$\frac{\partial C_i}{\partial t} = \underbrace{P_i - D_i}_{\text{source - sink}} - \nabla \bullet \underbrace{(\mathbf{u}C_i - \mathbf{K} \bullet \nabla C_i)}_{\text{advection + diffusion}}$$

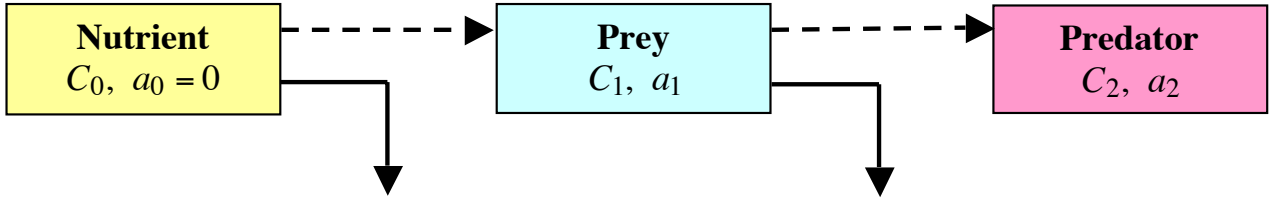
$$\frac{\partial \alpha_i}{\partial t} = \underbrace{C_i}_{\text{ageing}} + \underbrace{\pi_i - \delta_i}_{\text{source - sink}} - \nabla \bullet \underbrace{(\mathbf{u}\alpha_i - \mathbf{K} \bullet \nabla \alpha_i)}_{\text{advection + diffusion}}$$

- All advection-diffusion operators are of the same form: no need to develop new numerical algorithm.

Diagnosing matter fluxes in ecological models (I)

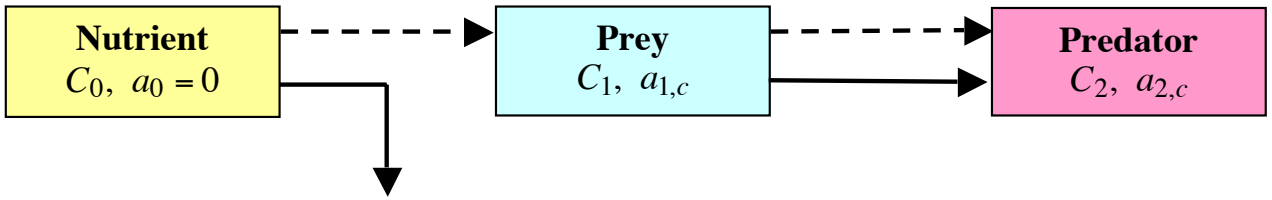
- At least two options, illustrated here in a simple/generic model:

Estimating the age of every compartment



The matter entering each compartment has zero age

Estimating cumulative ages



The prey takes zero-age nutrients.

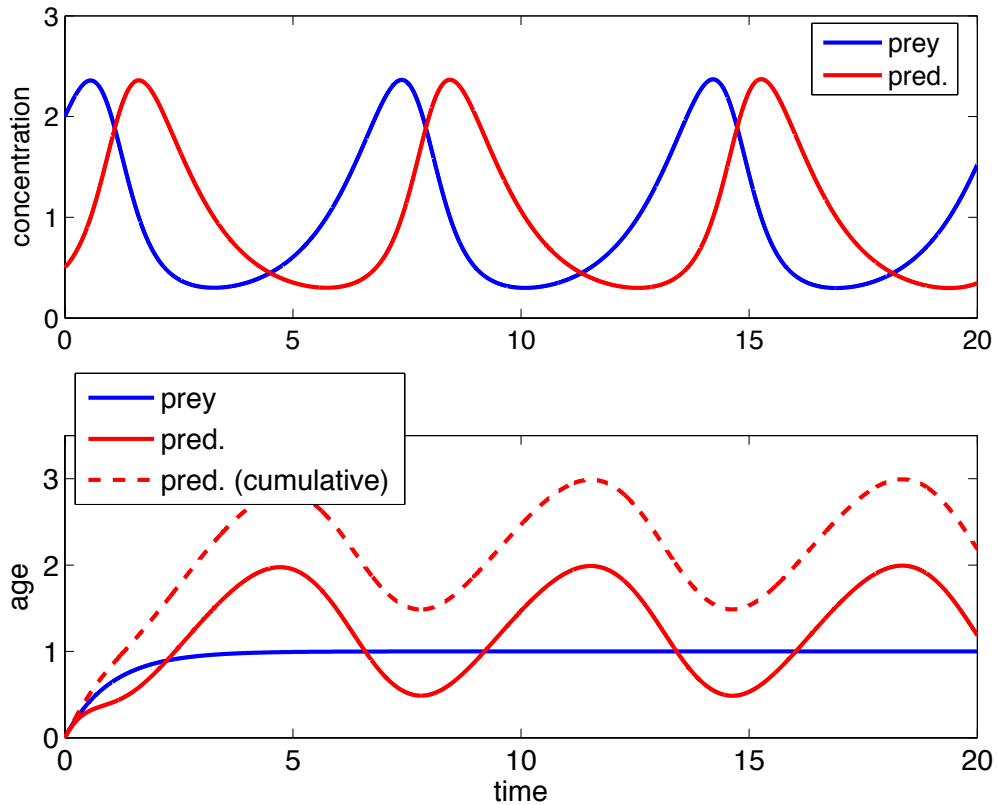
The predator takes the prey "along with its age".

$a_1 = a_{1,c}$

$a_2 < a_{2,c}$

Diagnosing matter fluxes in ecological models (II)

Assuming an infinite stock of nutrients (no nutrient-related limitation to growth), the solutions of a classical two-equation prey-predator model (Lotka-Volterra model) are illustrated in the figure opposite (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:

$$\frac{dC_1}{dt} = \underbrace{\frac{C_1}{\theta}}_{\substack{nutrient\\uptake}} - \underbrace{\frac{C_2}{\theta^*}C_1}_{predation} \quad , \quad \frac{d\alpha_1}{dt} = \underbrace{0}_{\substack{nutrient\\uptake}} - \underbrace{\left(\frac{C_2}{\theta^*}C_1\right)a_1}_{predation} + \underbrace{C_1}_{ageing}$$

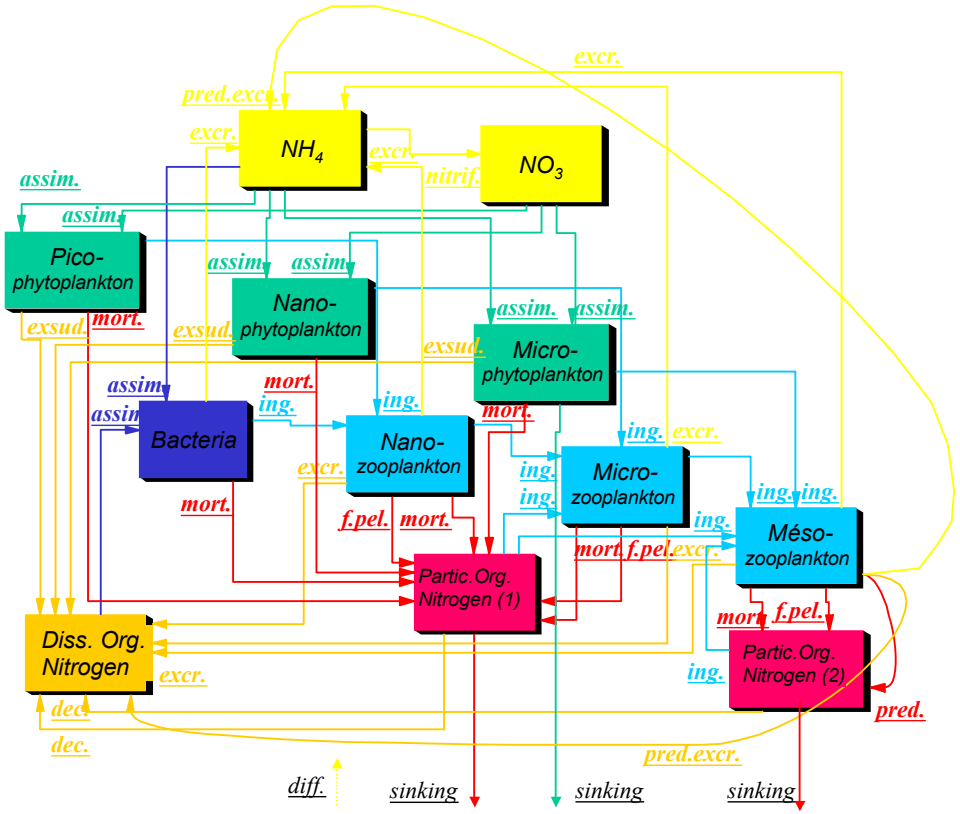
$$\Rightarrow \quad \frac{da_1}{dt} = \underbrace{-\frac{a_1}{\theta}}_{\substack{nutrient\\uptake}} + \underbrace{1}_{ageing} \quad \Rightarrow \quad a_1(t) = \underbrace{[a_1(0)-\theta]e^{-t/\theta}}_{\to 0 \ as \ t/\theta \to \infty} + \theta$$

The prey's age tends to the nutrient uptake timescale, θ, 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)

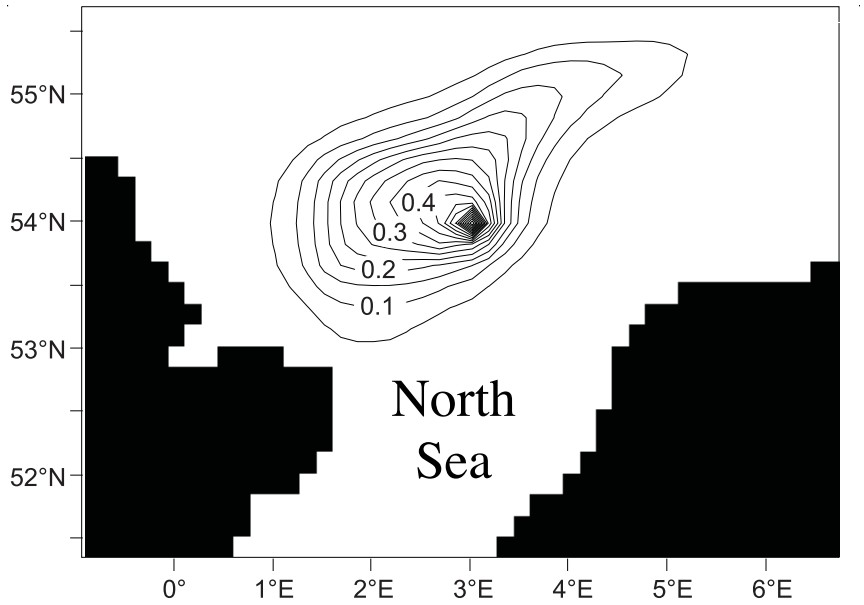
- Delhez et al. applied similar ideas to a sophisticated 1D eco-hydrodynamic model (2004, *Ocean Dynamics*, 54, 221-231).



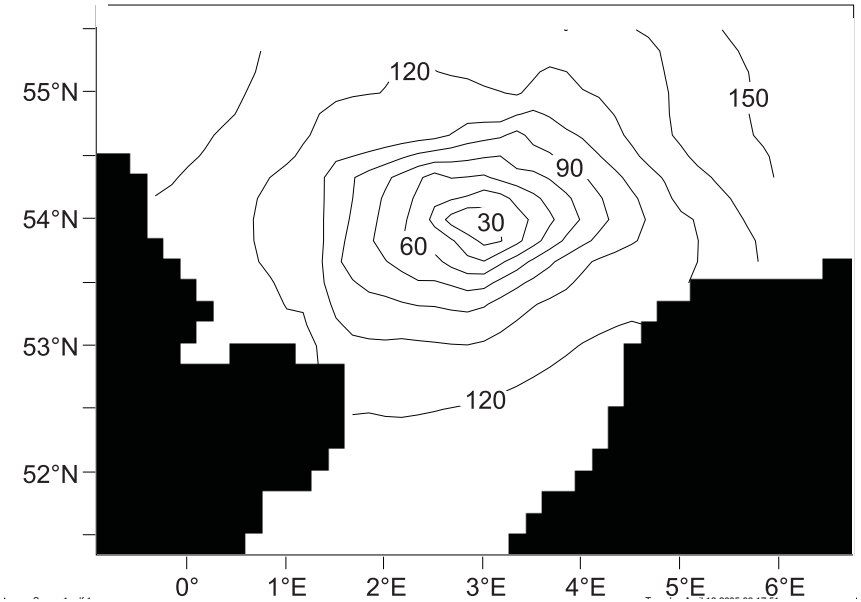
Ages of tracers released by a point-source (I)

- Modelling tracers released by a point source in the North Sea:

passive tracer concentration



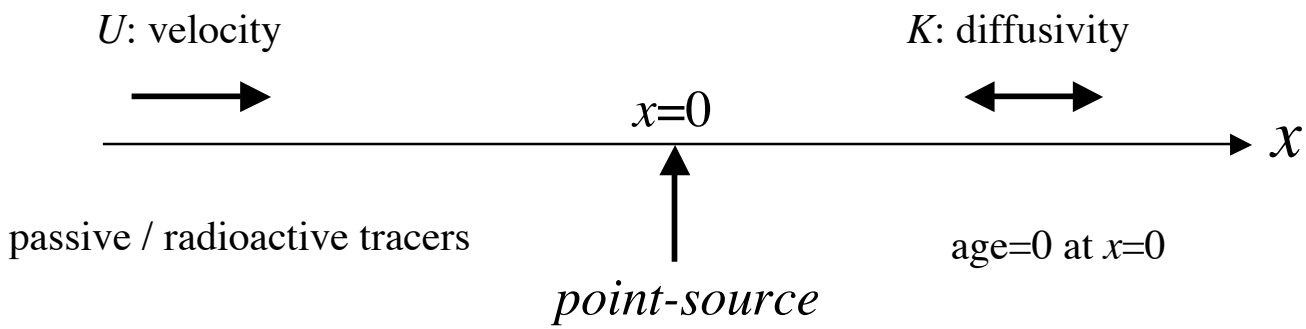
radio-age (i.e. carbon-14 type age)



- The tracer concentration reflects the direction of the advection, but the age does not! A numerical artefact?

Ages of tracers released by a point-source (II)

- Steady-state, one-dimensional idealised model:



γ^{-1}: mean life of the radioactive tracer

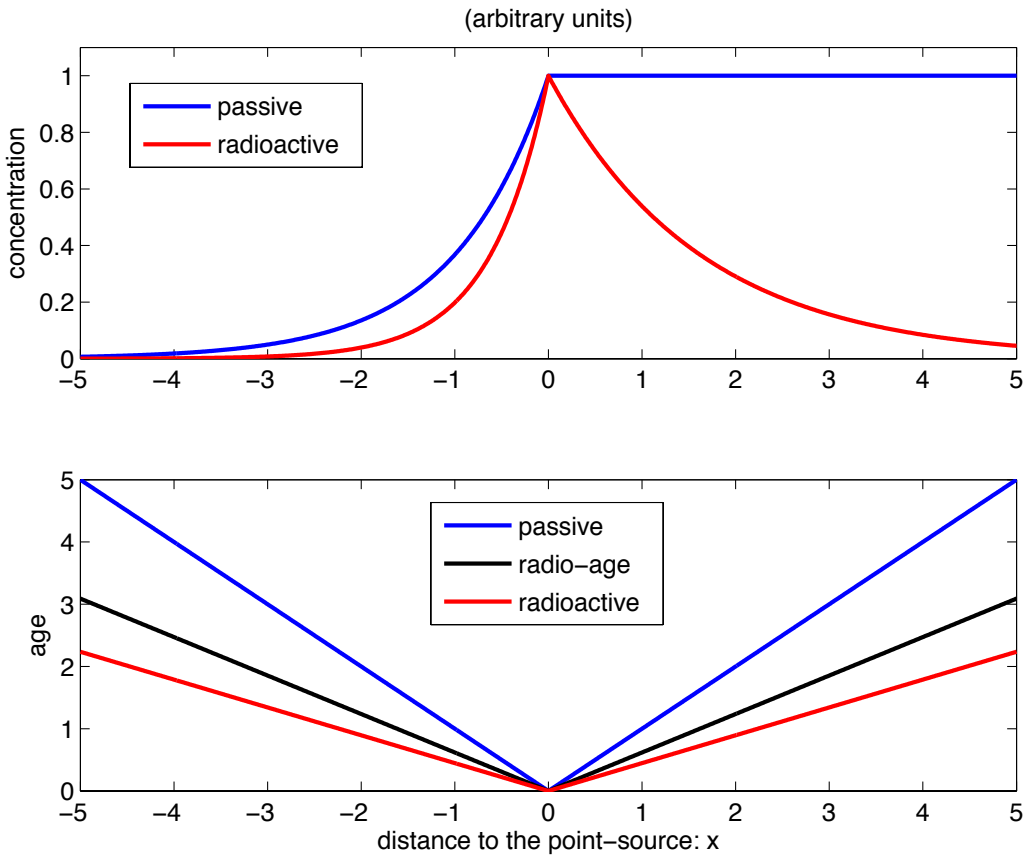
- If K=0: $\begin{cases} x < 0: & \text{no tracer} \\ x > 0: & \begin{cases} C_p = 1,\ C_r = \exp\left[-\dfrac{x}{U\gamma^{-1}}\right] \\ a_p = a_r = r = \dfrac{x}{U}\ , \quad \text{with}\ \ r = \gamma^{-1}\log\dfrac{C_p}{C_r} \end{cases} \end{cases}$

All ages are equal!

Ages of tracers released by a point-source (III)

- If $K \neq 0$, diffusion causes tracer to be present upstream of the source and ages to be all different, but symmetric!

The radioactive tracer age is smaller than that of the passive tracer because of decay+diffusion, rather than decay alone.



See also the Lagrangian approach to this problem by Hall and Haine (2004, *Journal of Marine Systems*, 48, 51-59)

Ages of tracers released by a point-source (IV)

- Scaling of the ages:

$$\begin{cases} a_p = \dfrac{|x|}{U} \quad \text{(passive tracer age)} \\ r = \dfrac{\sqrt{1+4Je^{-1}}-1}{2Je^{-1}} \dfrac{|x|}{U} \quad \text{(radio-age)} \\ a_r = \dfrac{1}{\sqrt{1+4Je^{-1}}} \dfrac{|x|}{U} \quad \text{(radioactive tracer age)} \end{cases}$$

with $Je = \dfrac{U(U/\gamma)}{K} = \dfrac{U^2}{K\gamma}$ (Jenkins number, i.e. Peclet with $L = U/\gamma$)

- Symmetry also arises in transient, multi-dimensional problems by prescribing that either the ages are zero at the source point or the age of the tracers released by the source is zero. A robust property!

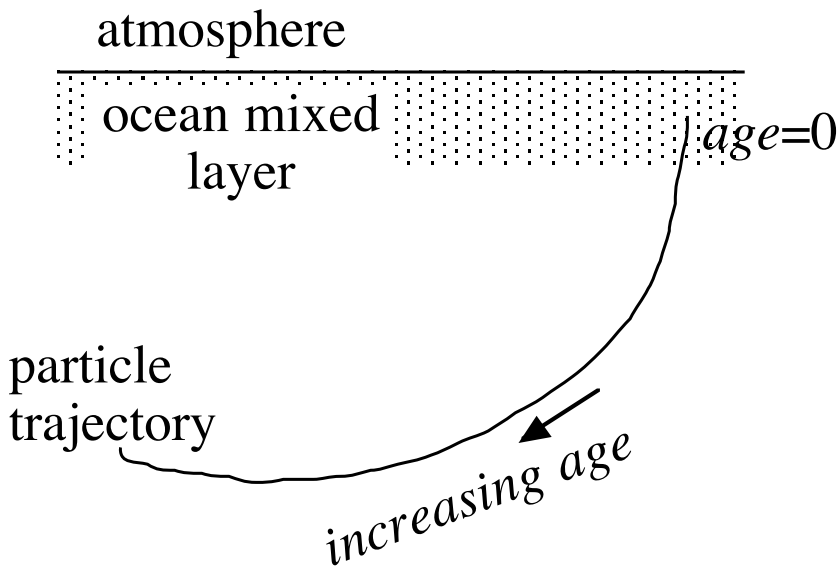
Beckers et al., *SIAM Journal on Applied Mathematics*, 2001

Ventilation of the World Ocean (I)

According to England (JPO, 1995), the "World Ocean circulation at its largest scale can be thought of as a gradual renewal or ventilation of the deep ocean by water that was once at the sea surface."

Therefore, the age, a measure of the time since leaving the ocean upper mixed layer, is a popular diagnostic tool in the World Ocean.

estimating ocean ventilation rate



age = time elapsed since leaving surface mixed layer

Ventilation of the World Ocean (II)

- At a steady state, the *water age distribution* $c(\mathbf{x},\tau)$ is satisfies

$$\frac{\partial c}{\partial \tau} = -\nabla \bullet (\mathbf{u}c - \mathbf{K} \bullet \nabla c) \ , \ \left[c(\mathbf{x},\tau)\right]_{\Gamma} = \delta(\tau - 0) \ , \ \left[c(\mathbf{x},0)\right]_{\Omega} = 0$$

with τ = the age, Γ = the ocean surface and Ω = the ocean interior.

- *Global water age distribution* $\mu(\tau)$: the volume of the water whose age lies in the interval $[\tau, \tau + \Delta\tau]$ $(\Delta\tau \to 0)$ is $\Omega\mu(\tau)\Delta\tau$, with

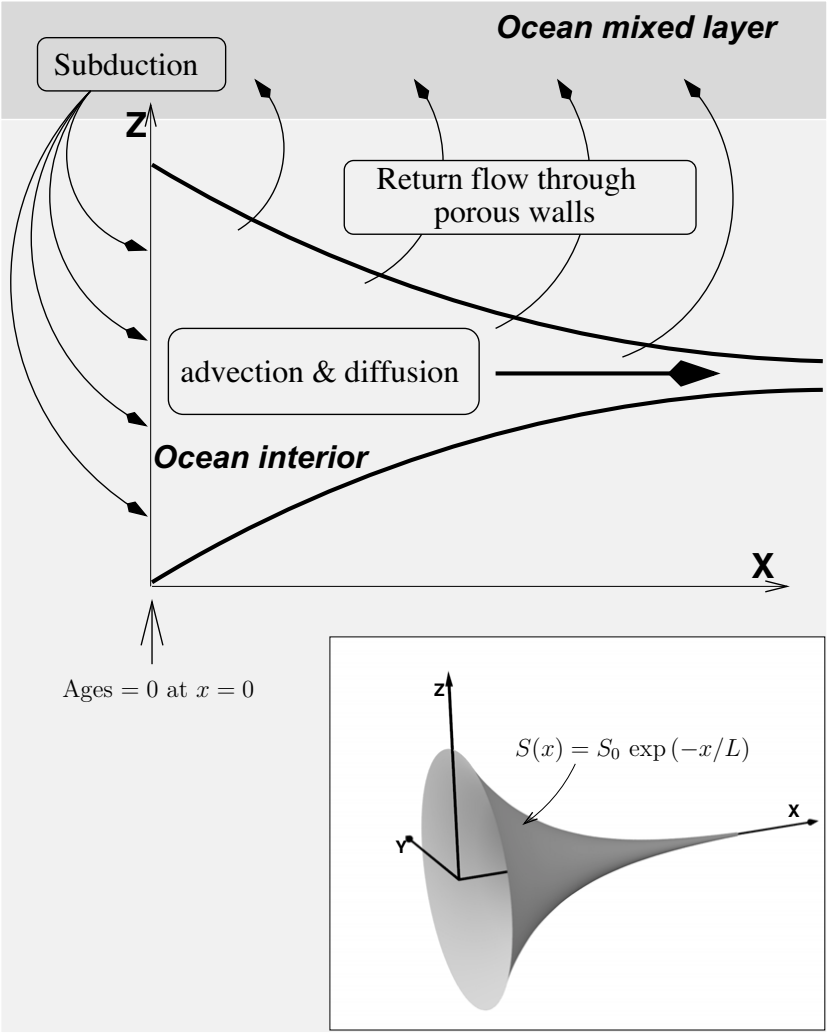
$$\mu(\tau) = \frac{1}{\Omega}\int_{\Omega} c(\mathbf{x},\tau)\, d\mathbf{x} \quad \Rightarrow \quad \boxed{\int_0^{\infty} \mu(\tau)\, d\tau = 1}$$

- *Global mean water age*: $\bar{a} = \int_0^{\infty} \tau\, \mu(\tau)\, d\tau = \frac{1}{\Omega}\int_0^{\infty}\int_{\Omega} \tau\, c(\mathbf{x},\tau)\, d\mathbf{x}\, d\tau$.

Ventilation of the World Ocean (III)

The leaky-funnel model
a World Ocean idealization,
is based on the following
key assumption:

The horizontal circulation in the actual ocean may be thought to be a consequence of ***localized sinking*** *and* ***generalized upwelling***.
(Warren, 1981)



Mouchet and Deleersnijder, *Tellus*, 2008 — Mouchet et al., *Tellus*, 2012

Ventilation of the World Ocean (IV)

- Parameters of the leaky funnel model:

U = water velocity, K = diffusivity

L = e-folding length scale for the section: $S(x) = S_0\, e^{-x/L}$

L is also the mean length of the water parcel trajectories in the funnel

- The leaky funnel water age distribution is

$$\mu(\tau) = \sqrt{\frac{K}{\pi L^2 \tau}} \exp\left(-\frac{U'^2 \tau}{4K}\right) + \frac{1}{\theta}\left[1 + \mathrm{erf}\left(\frac{1}{\theta}\sqrt{\frac{L^2 \tau}{K}}\right)\right] \exp\left(-\frac{U\tau}{L}\right)$$

with $Pe = UL/K$, $\frac{1}{\theta} = \frac{U'}{2L}\left(1 - \frac{2}{Pe'}\right)$, $Pe' = U'L/K$ and $U' = U + K/L$.

- The leaky funnel mean age is $\bar{a} = \dfrac{L}{U + K/L}$.

Ventilation of the World Ocean (V)

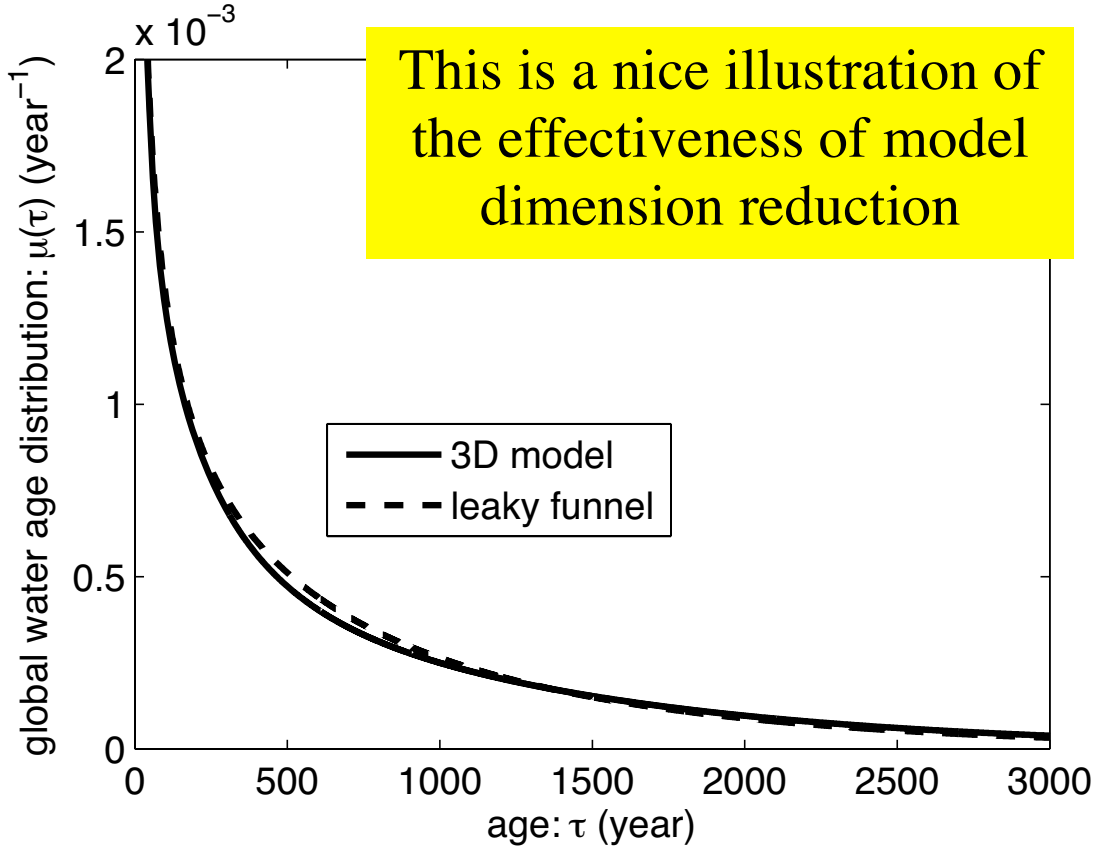
• The leaky funnel age distribution compares very well with that obtained from a 3D OGCM:

The parameters of the leaky funnel are optimised so as to minimise the difference between $\mu^{3D}(\tau)$ and $\mu(\tau)$

$$U \approx 3\times10^{-3}\,\mathrm{ms^{-1}} \;,\quad L \approx 10^{8}\,\mathrm{m}$$

$$K \approx 1.4\times10^{5}\,\mathrm{m^2\,s^{-1}}$$

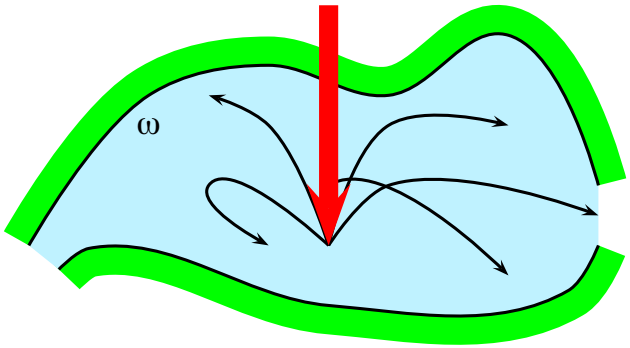
$$\bar{a}^{3D} = 764\,\mathrm{y} \;,\quad \bar{a} = 721\,\mathrm{y}$$



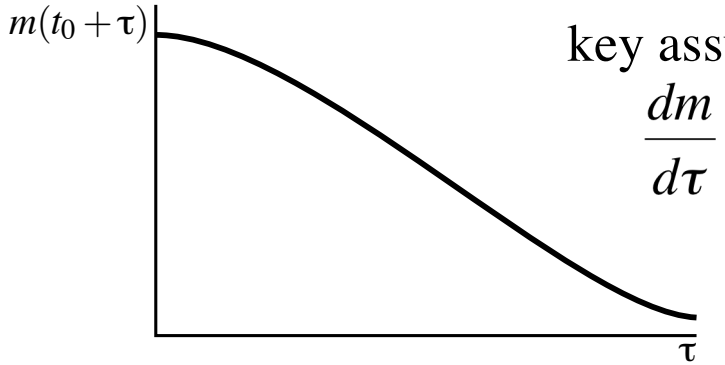
This is a nice illustration of the effectiveness of model dimension reduction

Residence time: the forward/direct procedure

unit mass released
at $(t_0, \mathbf{x}_0)$



$$m(t_0+\tau) = \int_\omega C(t_0+\tau, \mathbf{x})\, d\mathbf{x}$$



key assumption:

$$\frac{dm}{d\tau} \leq 0$$

1. Introduce unit mass of passive tracer at time t_0 and location $\mathbf{x}_0$;
2. Calculate the mass $m(t_0+\tau)$ of the tracer in the domain ω;
3. Residence time: $\theta(t_0, \mathbf{x}_0) = -\int_1^0 \tau\, dm = \int_0^\infty m(t_0+\tau)\, d\tau$.

Tartinville et al., *Coral Reefs*, 1997 — Deleersnijder et al., *Applied Mathematics Letters*, 1997
Deleersnijder et al., *Continental Shelf Research*, 1998

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 $\mathbf{x}_0$ at which the residence time is to be estimated.

  $\Rightarrow$ CPU cost can be prohibitive!

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

- The residence time $\theta(t,\mathbf{x})$ is the solution of

$$\frac{\partial \theta}{\partial t} = -1 - \nabla \bullet (\mathbf{u}\theta + \mathbf{K} \bullet \nabla \theta)$$

Residence time: the backward/adjoint procedure (II)

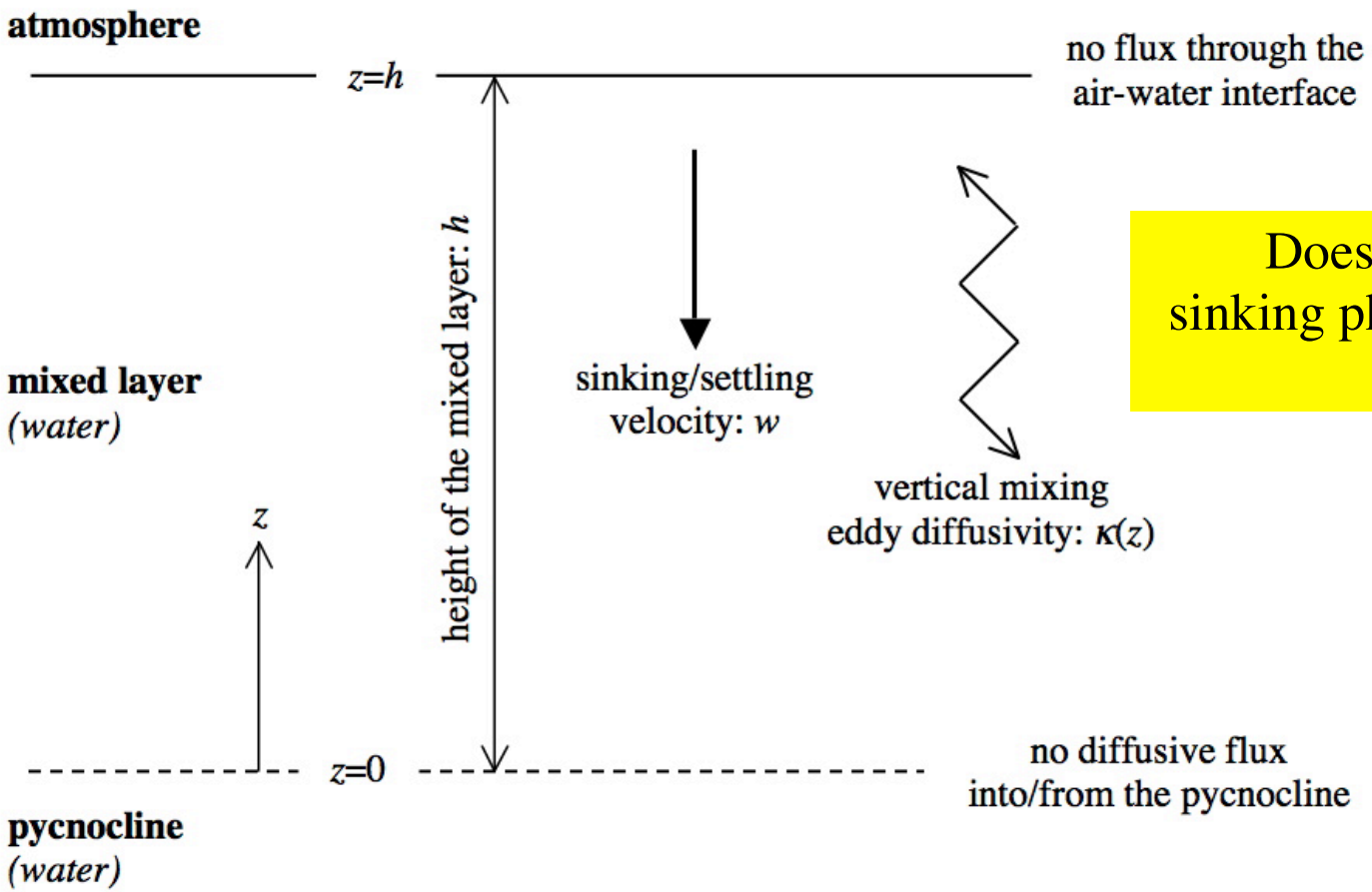
- The equation governing $\theta(t,\mathbf{x})$ is to be integrated backward in time from $t = T$, with $\theta(T,\mathbf{x}) = 0$ and $T \rightarrow \infty$.

- 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 (*Ocean Science*, 2006).

- Some examples of boundary conditions:

direct problem	adjoint problem
$C = 0$	$\theta = 0$
$(\mathbf{K} \bullet \nabla C) \bullet \mathbf{n} = 0$	$(\mathbf{u}\theta + \mathbf{K} \bullet \nabla \theta) \bullet \mathbf{n} = 0$
$(\mathbf{u}C - \mathbf{K} \bullet \nabla C) \bullet \mathbf{n} = 0$	$(\mathbf{K} \bullet \nabla \theta) \bullet \mathbf{n} = 0$

Residence time in the upper mixed layer (I)



Does turbulence help sinking phytoplankton species to survive?

Key assumptions: horizontal homogeneity and hydrodynamics at a steady state.

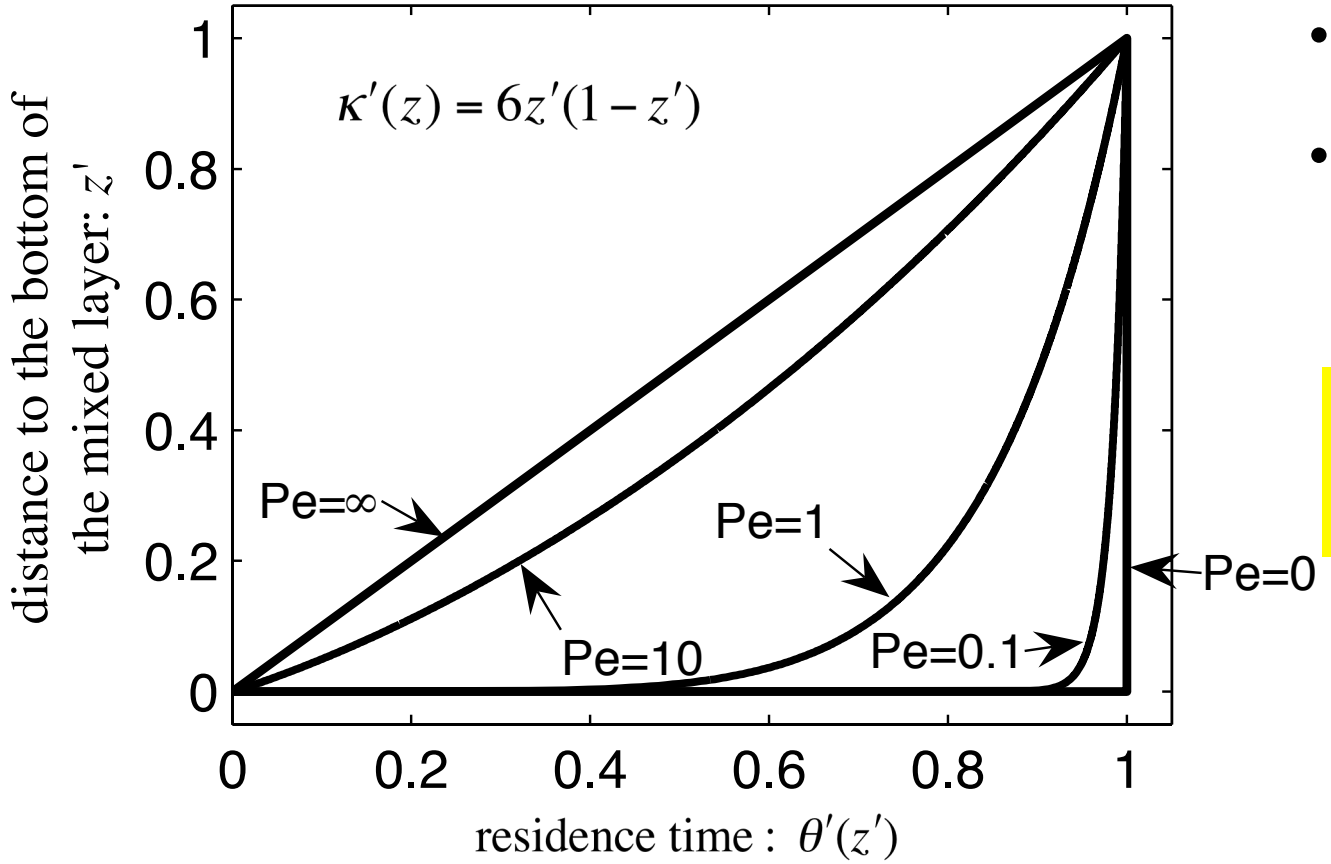
Deleersnijder et al., *Environmental Fluid Mechanics*, 2006a & 2006b
Delhez and Deleersnijder, *Journal of Theoretical Biology*, 2010

Residence time in the upper mixed layer (II)

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

$\theta\uparrow$ if $h\uparrow$, $\kappa\uparrow$, $w\downarrow$

Residence time in the upper mixed layer (III)



- Peclet number: $Pe = \dfrac{wh}{\bar{\kappa}}$
- Dimensionless variables:

$$z' = \frac{z}{h}\ ,\quad \kappa' = \frac{\kappa}{\bar{\kappa}}\ ,\quad \theta' = \frac{\theta}{h/w}$$

$$z' \ \leq\ \theta'(z')\ \leq\ 1$$

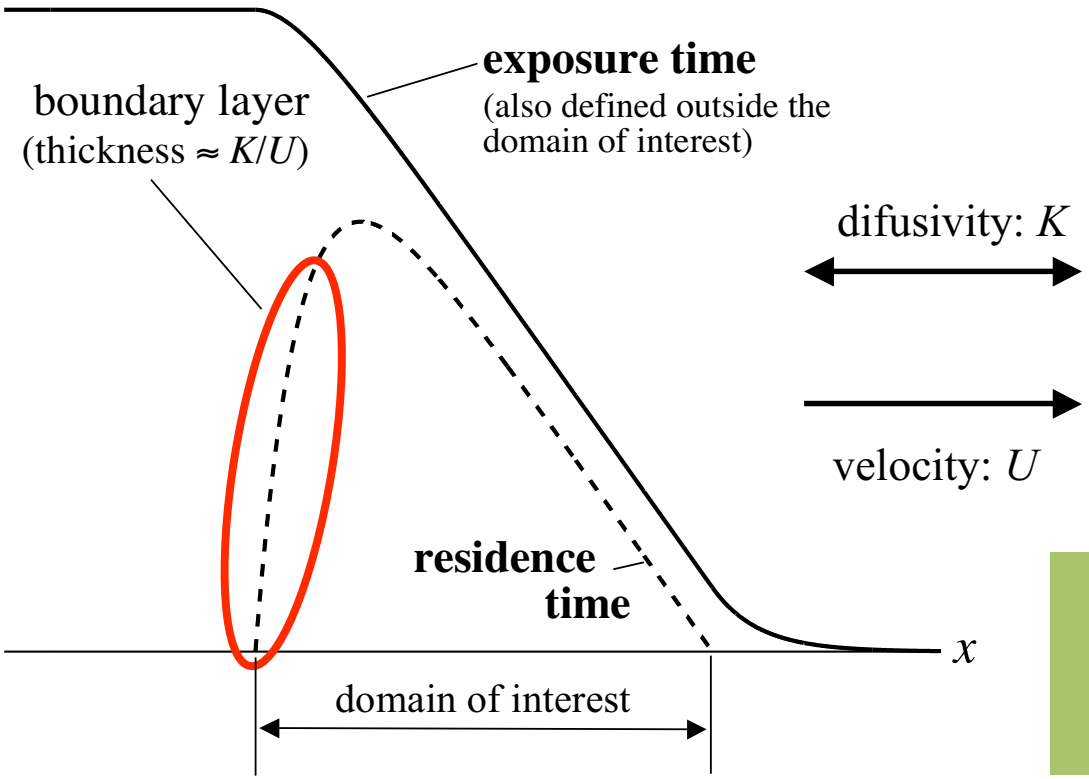
$\theta'(1)$ independent of $\kappa'(z')$!

Delhez and Deleersnijder, *Ocean Dynamics*, 2012

Turbulence does help sinking phytoplankton species to survive, by increasing the residence in the upper mixed layer (and the exposure time in the euphotic layer)

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*.



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

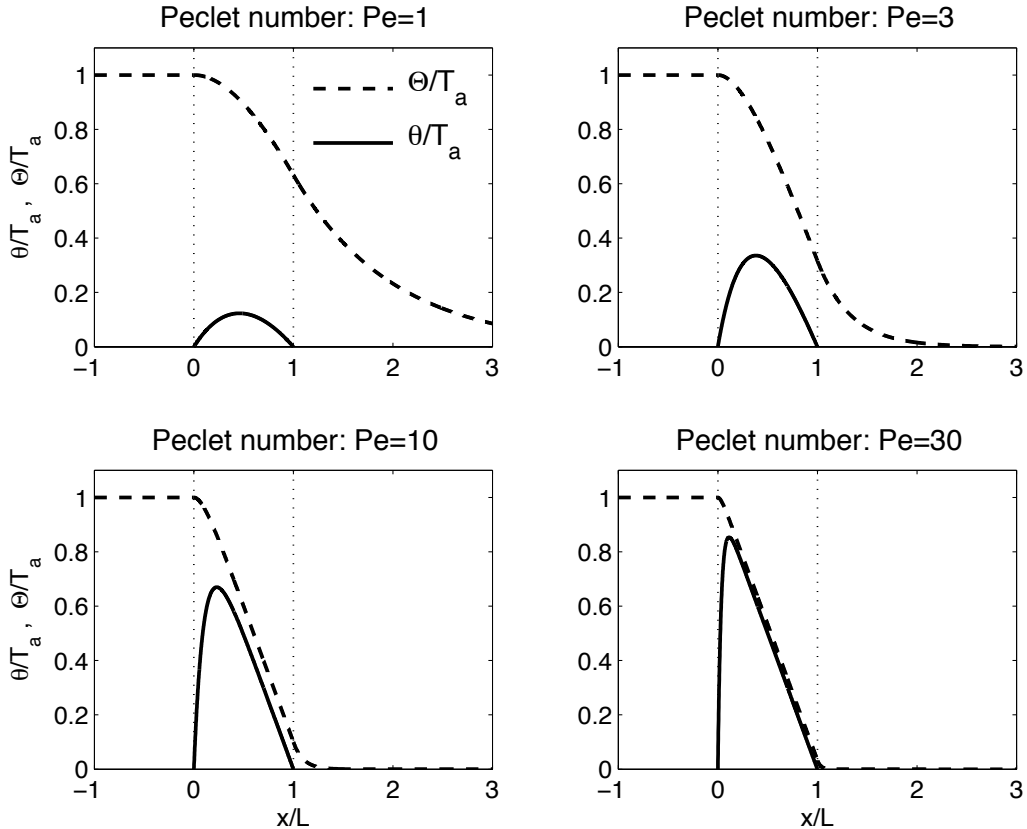
Delhez and Deleersnijder, *Ocean Dynamics*, 2006

Blaise et al., *Ocean Dynamics*, 2010

Residence time *vs* exposure time (continued)

- Illustration of the residence time, exposure time and return coefficient in a 1D flow (in a unbounded domain) with constant velocity U and diffusivity K.

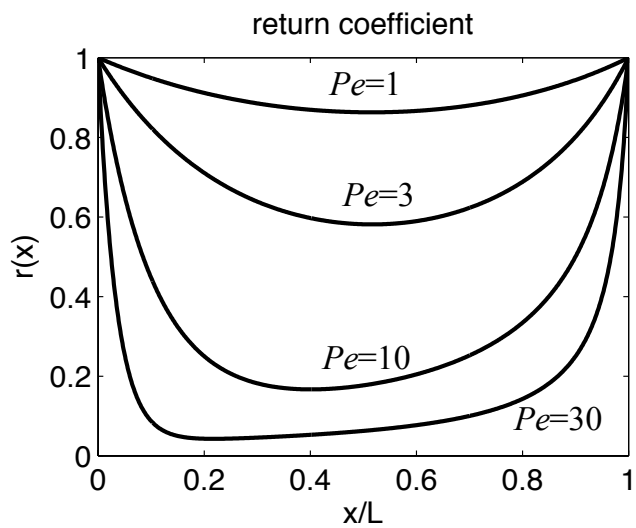
$T_a = \frac{L}{U}$ = advective timescale



θ : residence time , Θ: exposure time

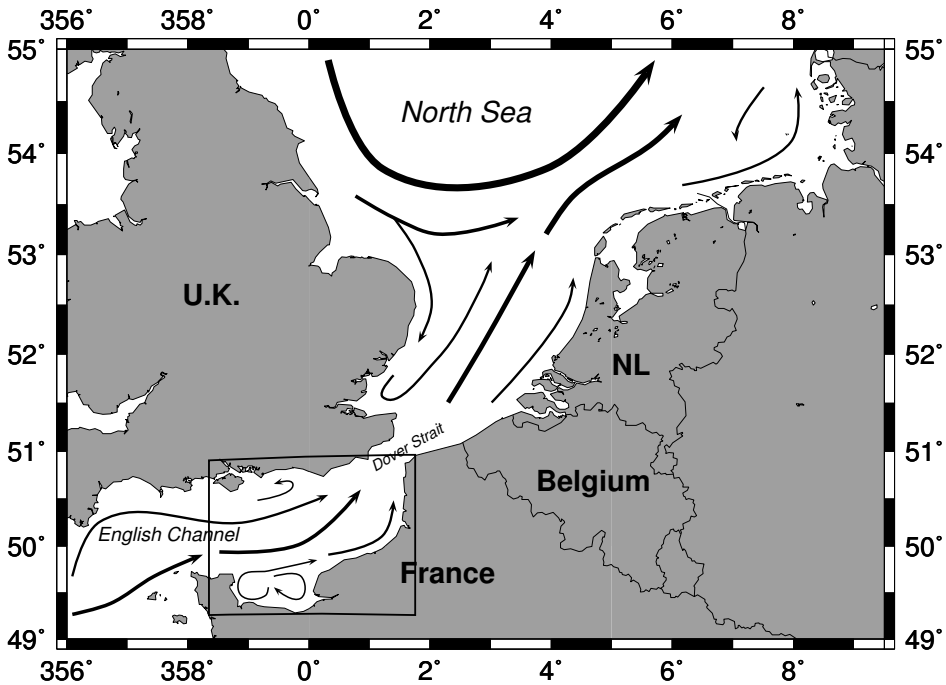
Peclet number: $Pe = \frac{UL}{K}$

return coefficient: $r = \frac{\Theta - \theta}{\Theta}$



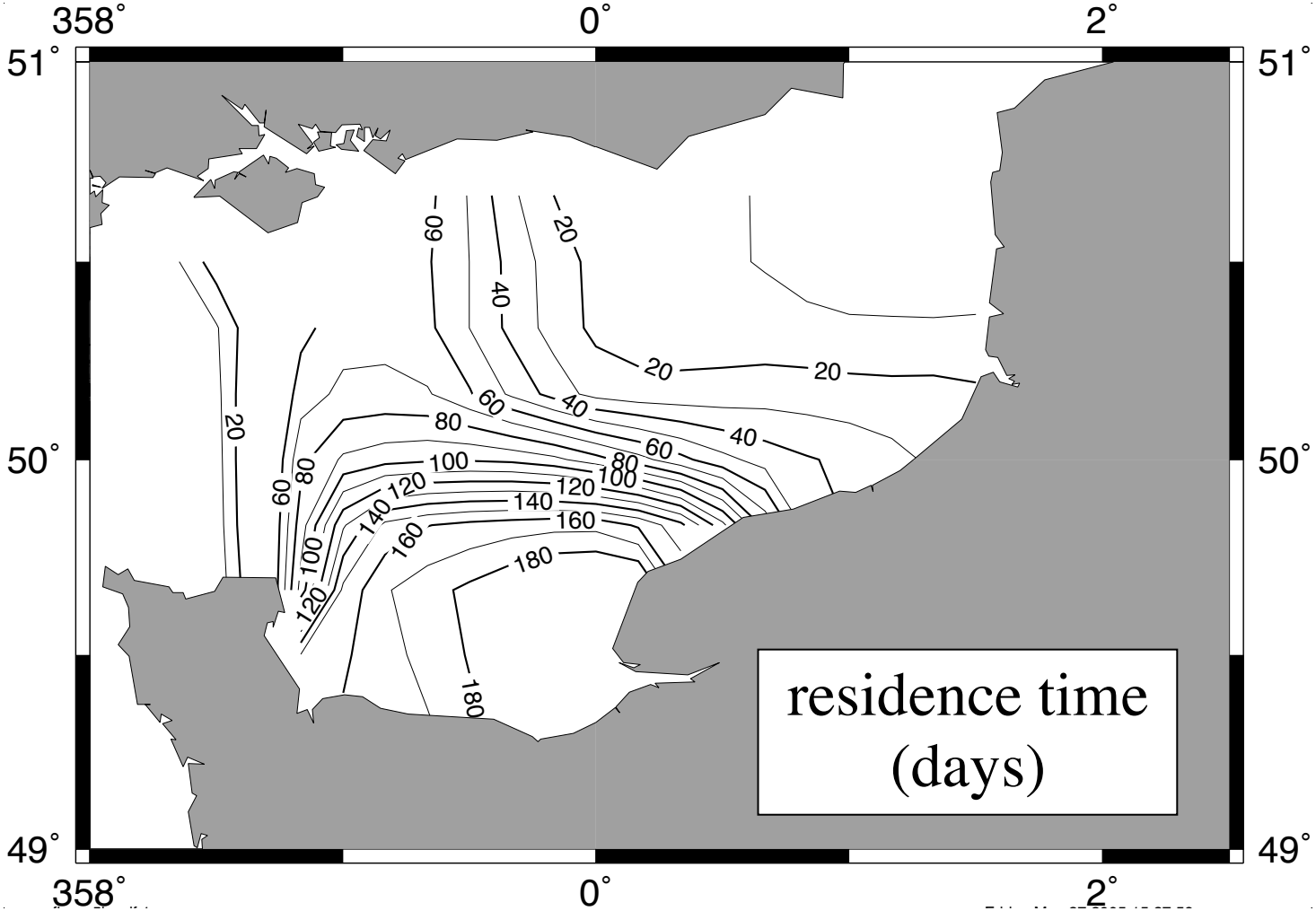
Residence/exposure time in the English Channel (I)

- Horizontal resolution: 10'; 10 σ-levels.
- Free-surface; baroclinic; *k* turbulence closure model.
- Forcings: 10 tidal constituents and NCEP reanalysis met. data.

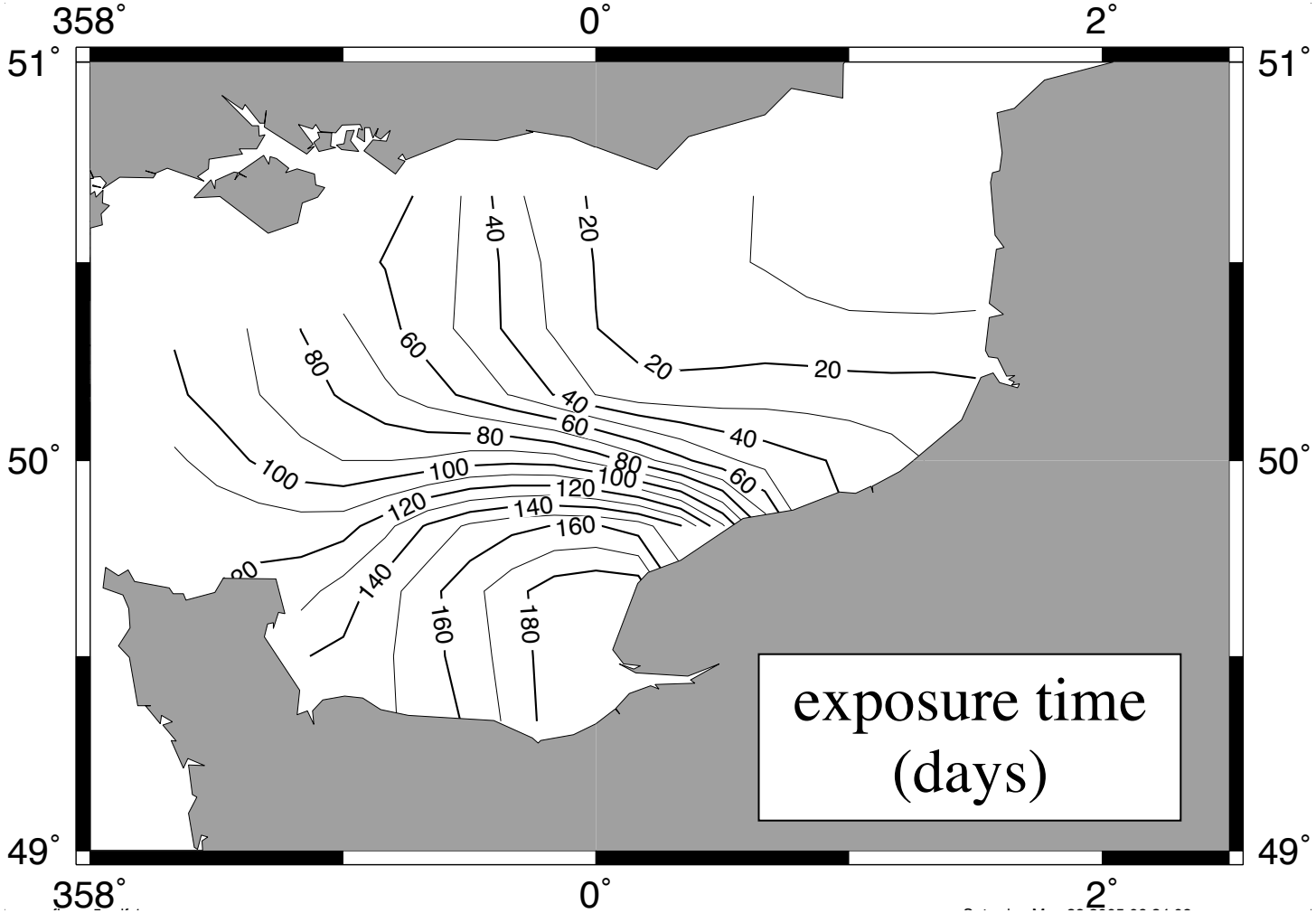


Numerical results from
E.J.M. Delhez's model
(Liège University, Belgium)

Residence/exposure time in the English Channel (II)



Residence/exposure time in the English Channel (III)



A generic method for quantifying water renewal rates

- A loose definition of **water renewal**:

the processess by which water originally inside the domain of interest is progressively replaced by water originally outside the domain of interest

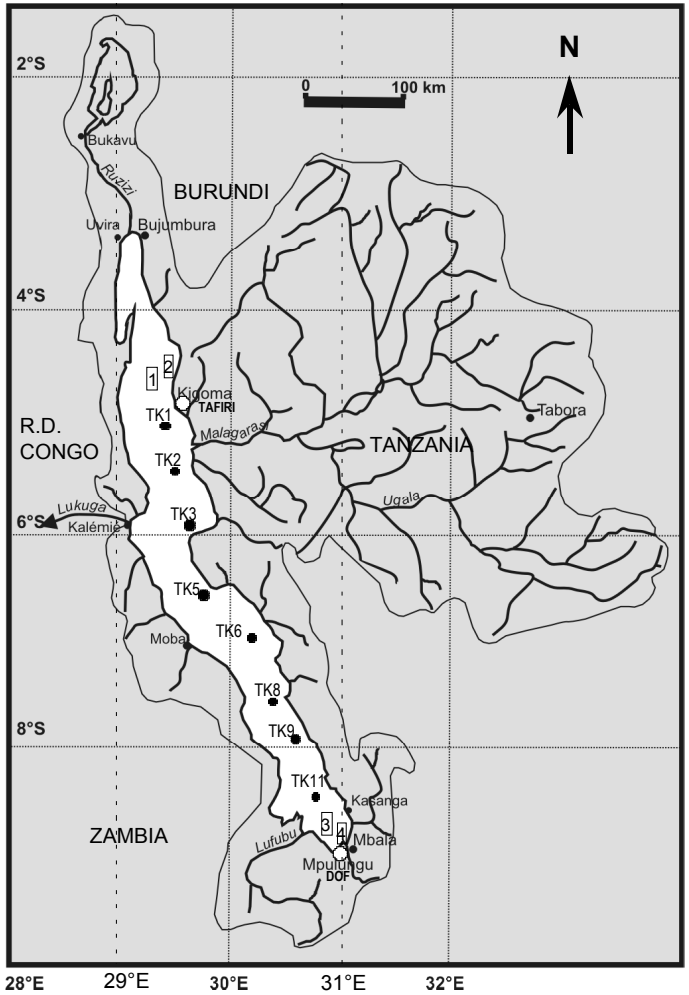
- Outline of a method for assessing the **rate(s)** of **water renewal**:

1. split the water into **original water** and **renewing water**, both of which being regarded as passive tracers;
2. calculate the **time** needed for the **original** water to **leave** the domain of interest;
3. calculate the **time** needed for the **renewing** water to **fill** the domain of interest.

Gourgue et al., *Estuarine, Coastal and Shelf Science*, 2007

de Brye et al., *Journal of Marine Systems*, 2012

Renewal of Lake Tanganyika's epilimnion water



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 renewing 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 (continued)

- Epilimnion water concentration: $C_e(t,\mathbf{x})$, with $0 \le C_e(t,\mathbf{x}) \le 1$
  Hypolimnion water concentration: $C_h(t,\mathbf{x})$, with $0 \le C_h(t,\mathbf{x}) \le 1$

$$\text{with} \quad \begin{cases} C_e(0,\mathbf{x}) = 1 \quad C_e(\infty,\mathbf{x}) = 0 \\ C_h(0,\mathbf{x}) = 0 \quad C_h(\infty,\mathbf{x}) = 1 \\ C_e(t,\mathbf{x}) + C_h(t,\mathbf{x}) = 1 \end{cases}$$

=> movie1

Gourgue et al.,
Estuarine, Coastal and Shelf Science, 2007

- Two seasons:
  dry season (April-August) with strong winds from south-east;
  wet season (September-March) with weak winds.

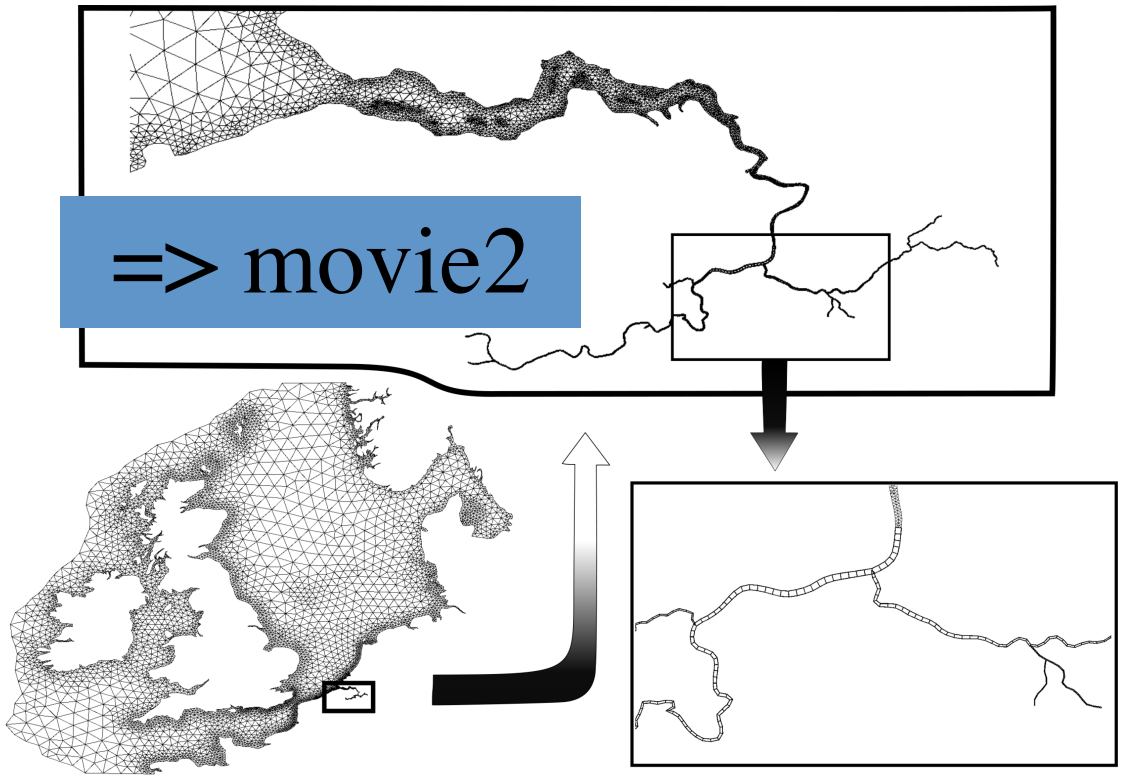
  Dry season: thermocline is deeper in the north and oscillates;
  Wet season: thermocline oscillations get progressively damped.

Water renewal in the Scheldt Estuary (I)

• A finite-element, unstructured-mesh, depth-averaged model of the Scheldt tributaries, River, Estuary, with 2D elements in the sea and estuary and 1D elements in the riverine part.

• 40% of the meshes in the estuary, which represents 0.3% of the computational domain.

• No major problem with open boundary conditions (for tides, storms, river discharge).

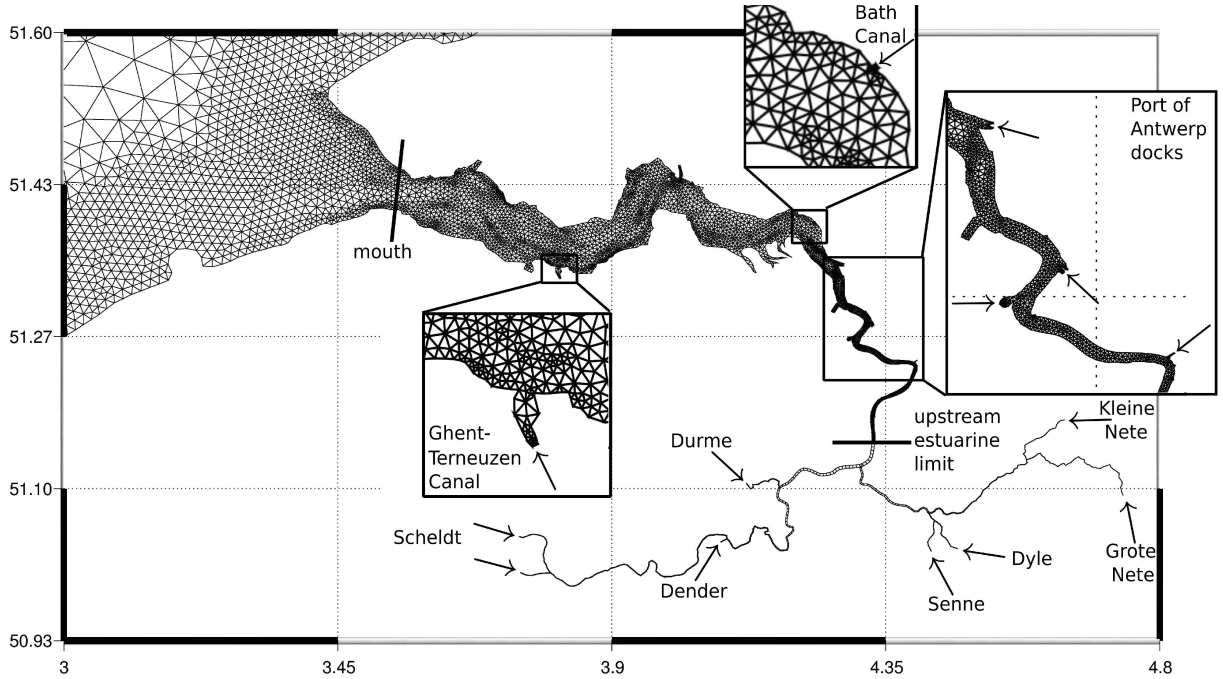


Gourgue et al., *Advances in Water Resources*, 2009 — de Brye et al., *Coastal Engineering*, 2010
Kärnä et al., *Computer Methods in Applied Mechanics and Engineering*, 2011

Water renewal in the Scheldt Estuary (II)

- A detailed water renewal study is carried out.

- The water is divided into the **original water** (present in the estuary at the initial time) and the **renewing water**, which is made up of water originating from the sea, the upstream riverine limits and "spillways" (Ghent-Terneuzen Canal, Bath Canal and docks in Antwerp port) injecting freshwater into the domain of interest.

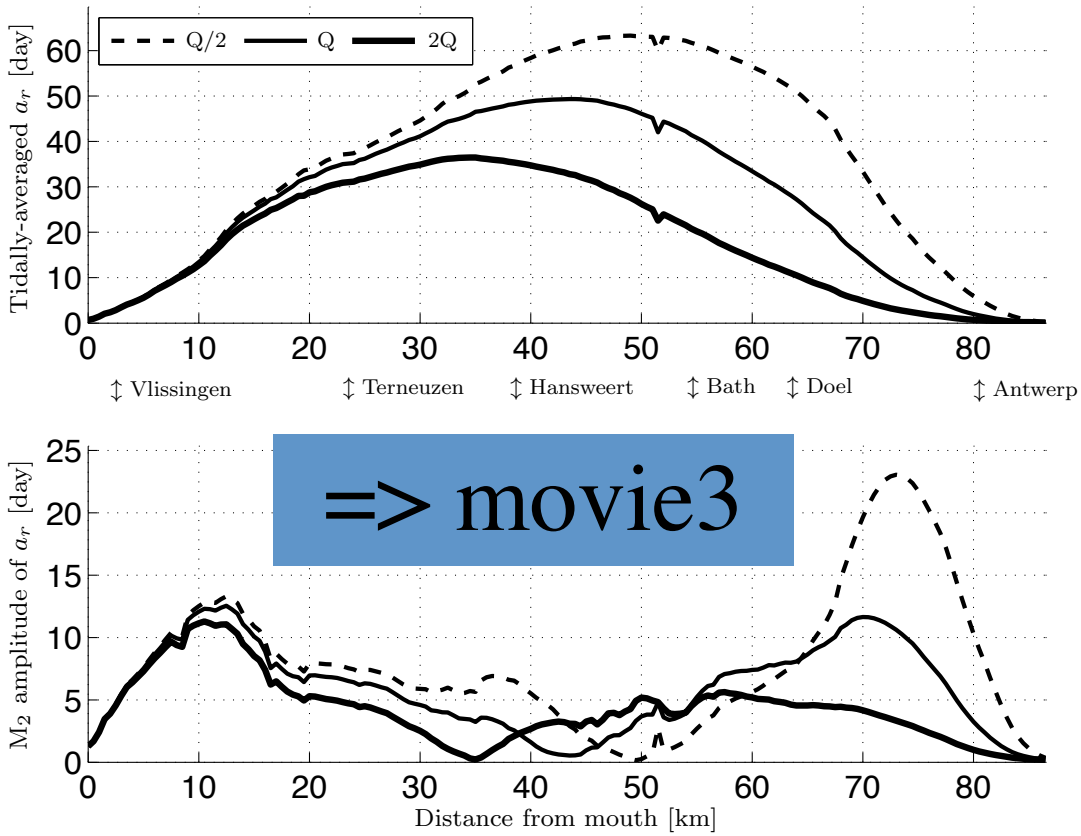


de Brye et al.,
Journal of Marine Systems, 2012

Water renewal in the Scheldt Estuary (III)

- The age of the renewing water (days) is simulated for three discharge scenarios ($Q/2, Q, 2Q$).

The variability of the age (lower panel) of the renewing water is rather high as compared with the age averaged over a tidal cycle (upper panel).

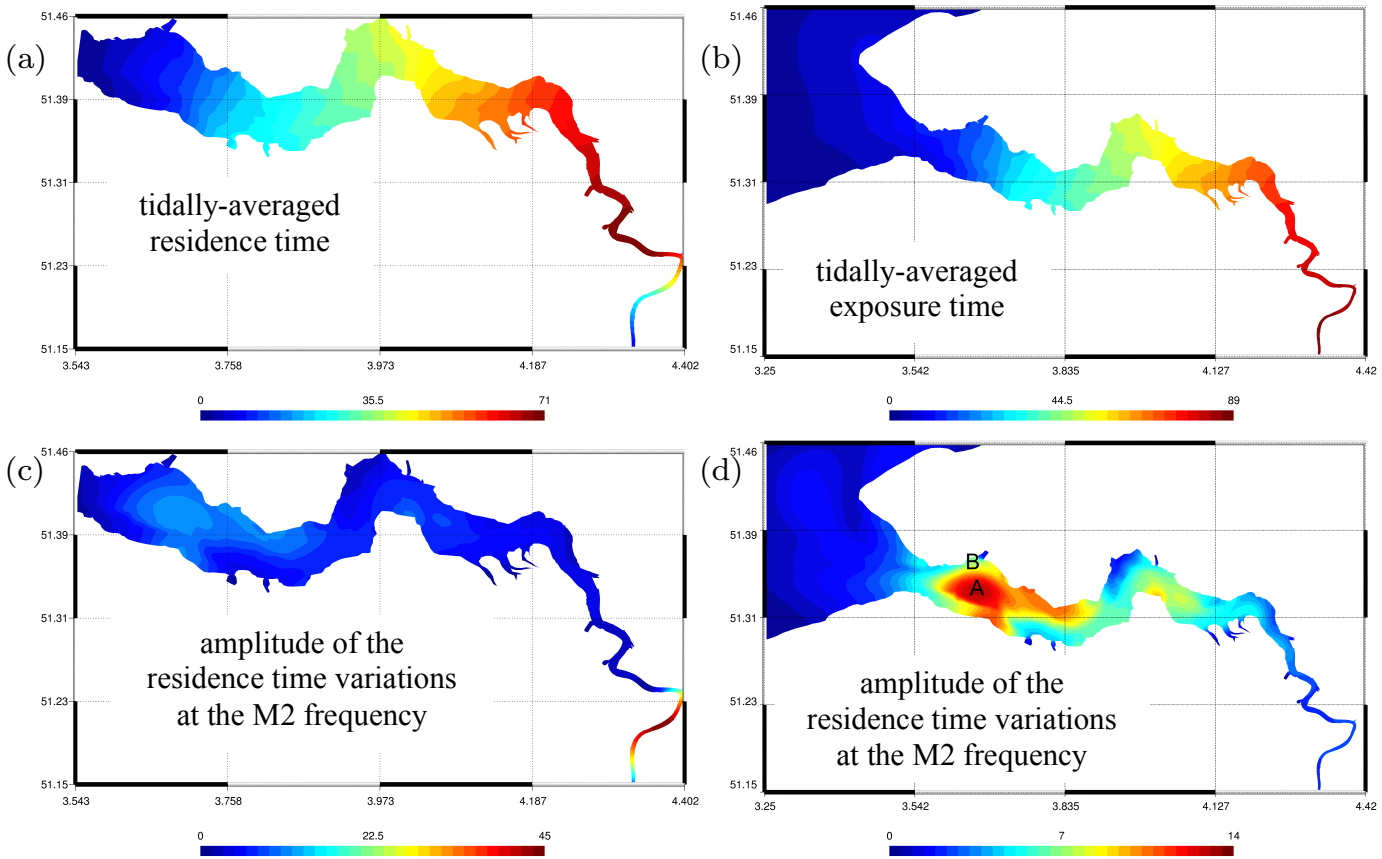


Water renewal in the Scheldt Estuary (IV)

- Residence and exposure times (days) of the original water are simulated for the average discharge scenario (Q).

The variability of the exposure time of the original water is surprisingly high.

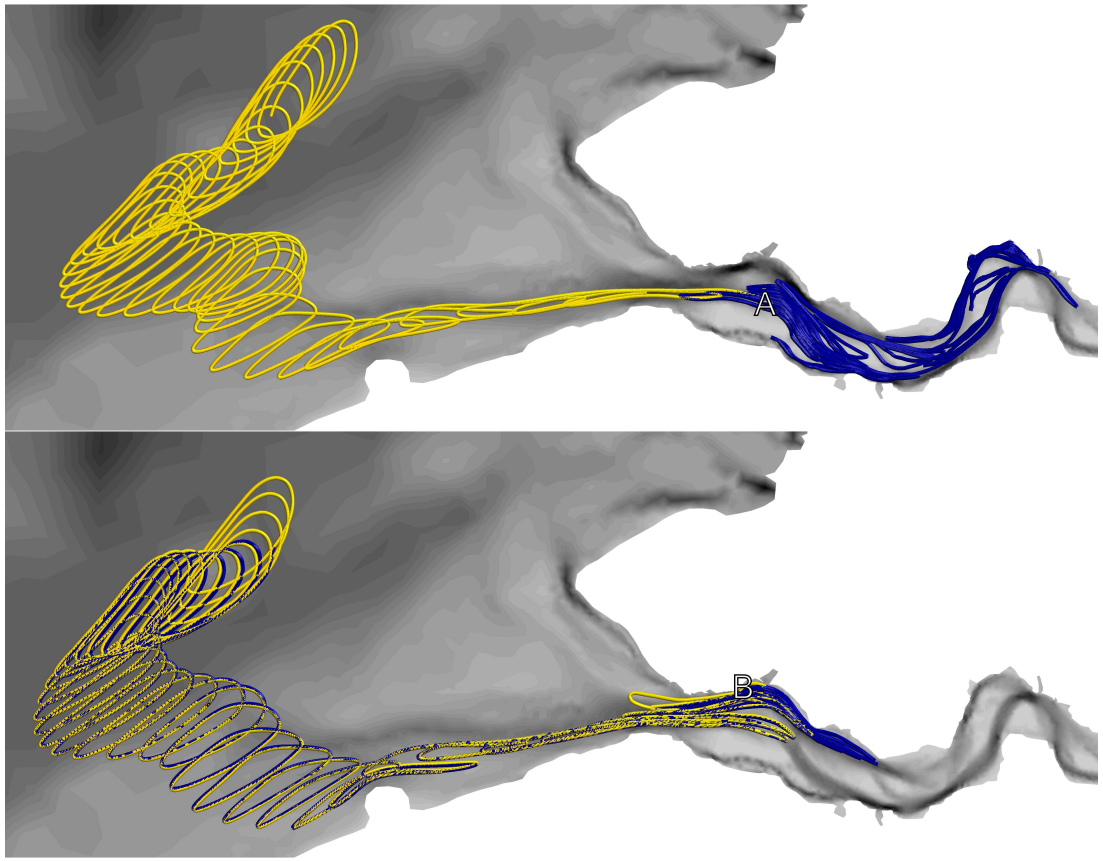
=> movie4
=> movie5



Water renewal in the Scheldt Estuary (V)

- Trajectories of particles released at high tide (yellow) and low tide (blue) at points A (upper panel) and B (lower panel).

The trajectories displayed in the figure opposite are in accordance with the high space/time variability of the exposure time. However, the very reason thereof remains elusive.



Conclusion

- Using simulated velocity and diffusivity fields, it is possible to compute, at any time and position, the age and residence/exposure time of any constituent, including the original or renewing water.
- Age and residence/exposure time are of use for assessing the rate at which the water of a wide variety of domains is renewed.
- Timescales paint a picture of the functioning of (the model of) a system that is different from that obtained by analysing primitive variables, i.e. velocity, surface elevation, temperature, etc. There is no shortage of surprising results!
- Timescales are of use for designing reduced-dimension models, thereby helping in the interpretation of complex flows (e.g. leaky funnel metaphor).

Possible future developments

- Design a generic method for studying ***connectivity*** by having recourse to the concept of exposure time and network science tools.
- Assess a new age concept, namely the ***exposure age***, for evaluating the time spent by constituent particles in various subdomains.
- Introduce into CART ***non-harmonic diffusion*** operators (i.e. fractional diffusion) that are related to non-Brownian motion.
- Investigate the potential of dimension reduction methods so as to produce ***reduced complexity models*** that will help understanding complex flows.
- Assess the potential of the ***inverted leaky funnel*** for developing reduced dimension models of the progressive dilution of freshwater into seawater in a delta, an estuary or the costal zone.

For additional information about:

- timescales, see **www.climate.be/cart**
- the Louvain-la-Neuve, unstructured-mesh, finite-element model, see **www.climate.be/slim**
- model dimension reduction & tracers, see **www.astr.ucl.ac.be/users/ericd/doc/DimensionReduction.pdf**
- network science tools, see e.g. **sites.uclouvain.be/networks**

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