Age structure of well-mixed compartmental systems

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Overview

We find general formulas for the transit time and age distributions in well-mixed compartmental systems. As an example we consider a simple three-pool global carbon model with nonlinearities in two different scenarios:

steady state	pre-industrial system before 1765
perturbed	adding fossil fuels to the atmosphere, considering land use change, 1765-2500

Main quantities of interest

transit time	time that a particle needs to travel through the system exit time − entry time
system age	for particles in the system current time − entry time
compartment age	system age of particles in a compartment

Mathematical description

Well-mixed compartmental systems can be descibed by a system of generally **nonlinear** ordinary differential equations of the form

$$\frac{d}{dt}\,\mathbf{x}(t) = \mathrm{A}(\mathbf{x}(t),t)\,\mathbf{x}(t) + \mathbf{u}(t), \quad t > t_0, \tag{1}$$

with a given initial value $\mathbf{x_0}$.

Reduction to linear nonautonomous systems

We assume to know (at least numerically) the unique solution of (1) and denote it by $\mathbf{x}$. We then plug it into $\mathrm{A}(\mathbf{x}(t),t)$ and obtain the **linear** system of ordinary differential equations

$$\frac{d}{dt}\,\mathbf{x}(t) = \mathrm{A}(t)\,\mathbf{x}(t) + \mathbf{u}(t), \quad t > t_0.$$

This equation has the general solution formula

$$\mathbf{x}(t) = \underbrace{\Phi(t,t_0)\,\mathbf{x_0}}_{\text{age}(t)=t-t_0+\text{initial age}} + \int_{t_0}^{t} \underbrace{\Phi(t,\tau)\,\mathbf{u}(\tau)}_{\text{age}(t)=t-\tau}\,d\tau,$$

where Φ is the so-called state transition matrix. This leads immediately to the vector of age densities

$$\mathbf{p}(a,t) = \begin{cases} \Phi(t,t_0)\,\mathbf{p_0}(a-(t-t_0)), & a \geq t-t_0, \\ \Phi(t,t-a)\,\mathbf{u}(t-a), & a < t-t_0, \end{cases}$$

where $\mathbf{p_0}$ is the initial age distribution.

Pre-industrial (<1765), system in steady state

Transit time density

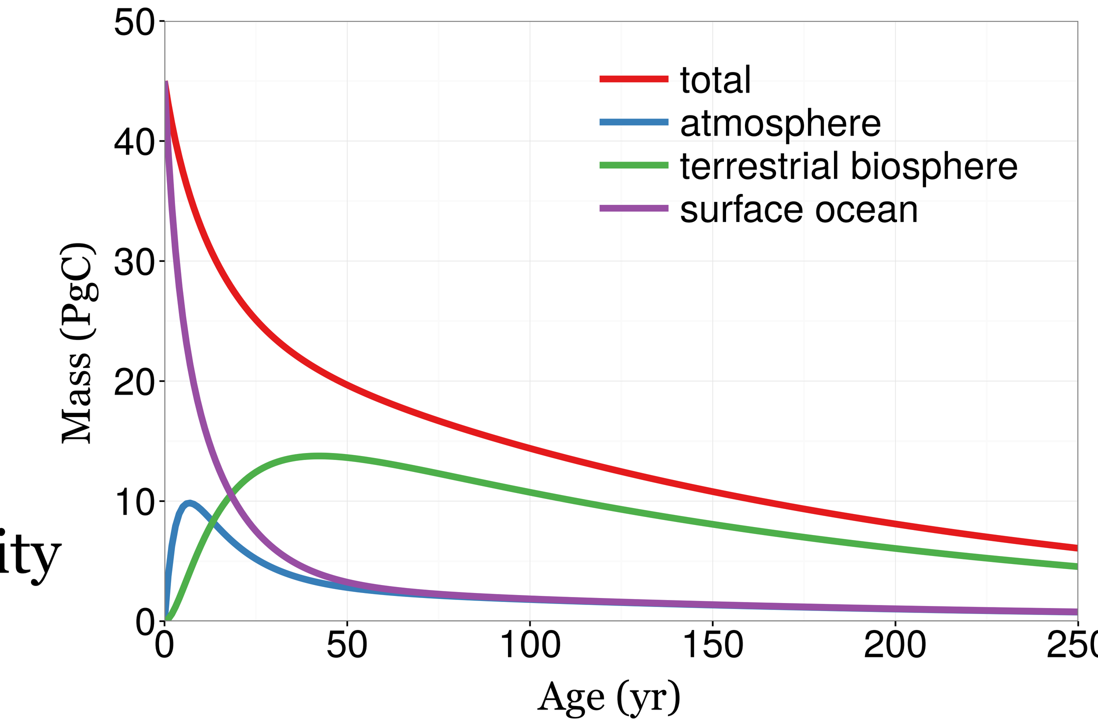
$$p_T(t) = \mathbf{z}^T\,e^{t\,\mathrm{A}}\,\mathbf{u}$$

System age density

$$p_A(a) = \sum_j \left(e^{a\,\mathrm{A}}\,\mathbf{u}\right)_j$$

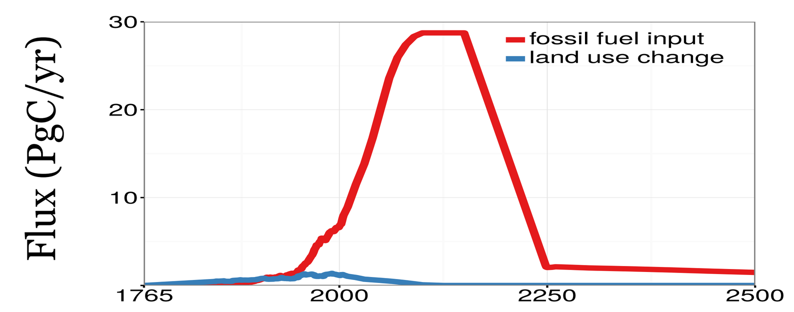
Compartment age density

$$p_j(a) = \left(e^{a\,\mathrm{A}}\,\mathbf{u}\right)_j$$

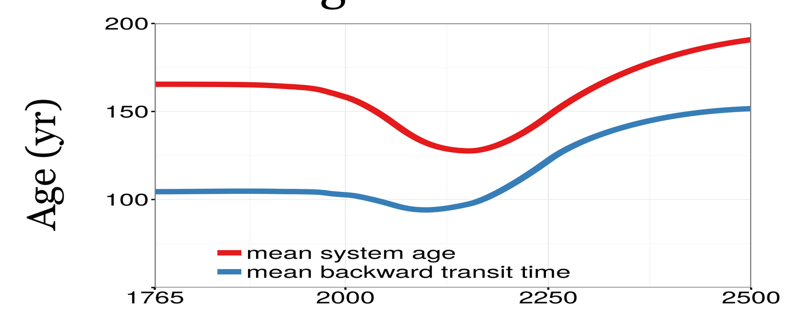


Perturbed (1765-2500)

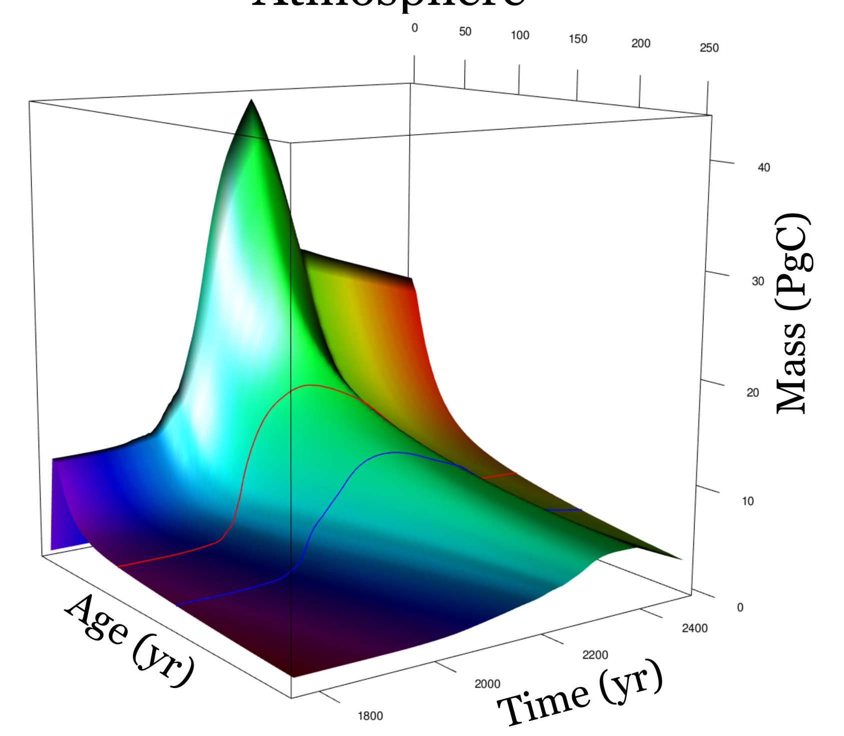
Anthropogenic perturbations



Mean age and transit time

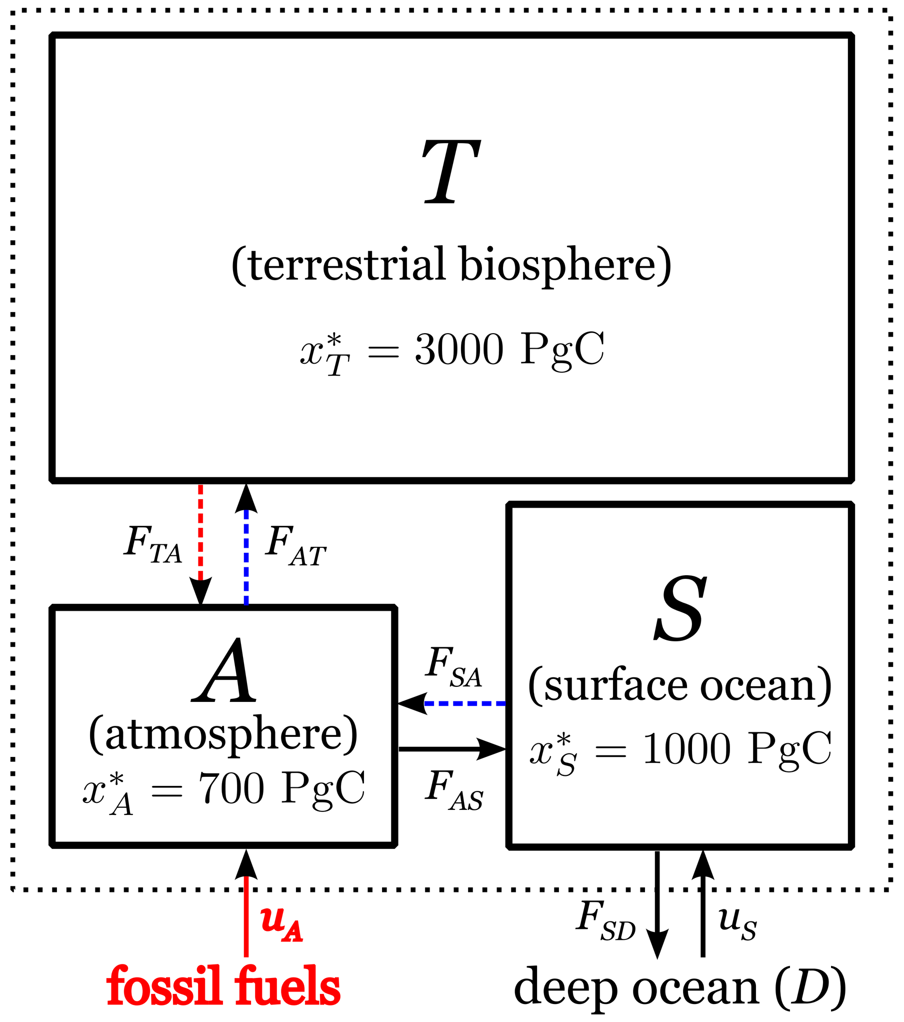


Atmosphere



Model

Pre-industrial (<1765) + perturbed (1765-2500)



External input fluxes

$u_S = 45$, $\quad u_A(t) = \text{fossil-fuels}(t)$

Internal fluxes

$F_{AT} = 60\,(x_A/700)^{0.2}$

$F_{TA}(t) = 60\,x_T/3000 + \text{land-use-change}(t)$

$F_{AS} = 100\,x_A/700$

$F_{SA} = 100\,(x_S/1000)^{10}$

External output flux

$F_{SD} = 45\,x_S/1000$

State transition matrix

one-dimensional	$\Phi(t,t_0) = \exp\left[(t-t_0)\,A(t)\right]$	exponential function
multi-dimensional, autonomous	$\Phi(t,t_0) = \exp\left[(t-t_0)\,\mathrm{A}(t)\right]$	matrix exponential
multi-dimensional, nonautonomous	$\frac{d}{dt}\,\Phi(t,t_0) = \mathrm{A}(t)\,\Phi(t,t_0)$	only numerical solution

Transit time

If we define the (backward) transit time of a particle as the age of the particle at the time when it exits the system, we can easily derive explicit formulas for its distribution from the age distribution.

The simple approach stock/flux for the transit time is valid only for a system in steady state. Out of steady state, stock(t)/flux(t) cannot be interpreted as a transit time.

Evolution of explicit age formulas

Year	Author	System	Quantity	Geometric structure	Example
1983	Anderson	steady state	mean	point	
2009	Manzoni et al.	steady state (simple structure)	density	curve over age	
2016	Rasmussen et al.	linear time dependent	mean	curve over time	
2016	Metzler & Sierra	steady state (all structures)	density	curve over age	
2017	Metzler et al.	linear/nonlinear time dependent	density	surface over age and time	

increasing information

System classification

$\mathrm{A}(\mathbf{x}(t),t)$ $\mathrm{A}(\mathbf{x}(t)),\mathbf{u}(t)$	nonlinear, nonautonomous
$\mathrm{A}(\mathbf{x}(t)),\mathbf{u}$	nonlinear, autonomous
$\mathrm{A}(t),\mathbf{u}$ $\mathrm{A},\mathbf{u}(t)$ $\mathrm{A}(t),\mathbf{u}(t)$	linear, nonautonomous
$\mathrm{A},\mathbf{u}$	linear, autonomous

Notation

$\mathbf{x}(t)$	vector of compartment content (e.g. C) at time t
A	compartmental matrix, describes fluxes between compartments
$\mathbf{z}(t)$	external outflux vector at time t
$\mathbf{u}(t)$	external input vector at time t

Anderson DH (1983) Compartmental modeling and tracer kinetics, vol 50. Springer Science & Business Media

Manzoni S, Katul GG, Porporato A (2009) Analysis of soil carbon transit times and age distributions using network theories. Journal of Geophysical Research 114(G4):1–14, DOI10.1029/2009JG001070

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Rasmussen M, Hastings A, Smith MJ, Agusto FB, Chen-Charpentier BM, Hoffman FM, Jiang J, Todd-Brown KEO, Wang Y, Wang YP, Luo Y (2016) Transit times and mean ages for nonautonomous and autonomous compartmental systems. J Math Biol

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