CHAPTER FIFTEEN

Time Characteristics of Compartmental Systems

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CONTENTS

To understand carbon flows through terrestrial ecosystems, it is very important to use metrics to quantify the time carbon spends in the entire system and in particular compartments. In this chapter, we introduce the concepts of age and transit time as two fundamental metrics that characterize the speed at which carbon flows through ecosystems. Age is defined as the time carbon atoms spend in an ecosystem, from when they enter through photosynthesis until they are observed in a particular compartment. Transit time is defined as the time carbon atoms require to pass through the entire ecosystem, from the time they enter through photosynthesis until they are lost in gas, liquid, or solid form. We review here mathematical formulas for computing age and transit time in compartmental systems, distinguishing between formulas for autonomous systems in equilibrium and nonautonomous systems moving along a known trajectory.

INTRODUCTION

One of the advantages of representing models in the compact form of compartmental systems is that we can derive system-level diagnostics that help to better understand system dynamics. Differences in process representations, parameterizations, or size of compartments required to represent a system, can be compared using simple aggregated metrics at the level of the entire system.

Two important system-level diagnostics for describing compartmental systems are the concepts of system age and transit (residence) time (Bolin and Rodhe 1973; Sierra et al. 2017). We define *system age* as the age of all atoms or particles inside the system, from the time they entered t_e until the time of observation t. *Transit time* is defined as the average time required for atoms or particles to traverse the system from their arrival time until they leave in the output flux. In other words, system age characterizes the age structure of all the atoms or particles in the system, while transit time characterizes the age structure of all atoms or particles in the output flux (Figure 15.1).

It is also possible to characterize the age structure of the atoms or particles inside each pool or compartment. We define *pool age* as the time elapsed since the atoms or particles entered the system until the time of observation t inside a pool i (Figure 15.1). Therefore, the system age is the aggregated result of the pool ages for all pools.

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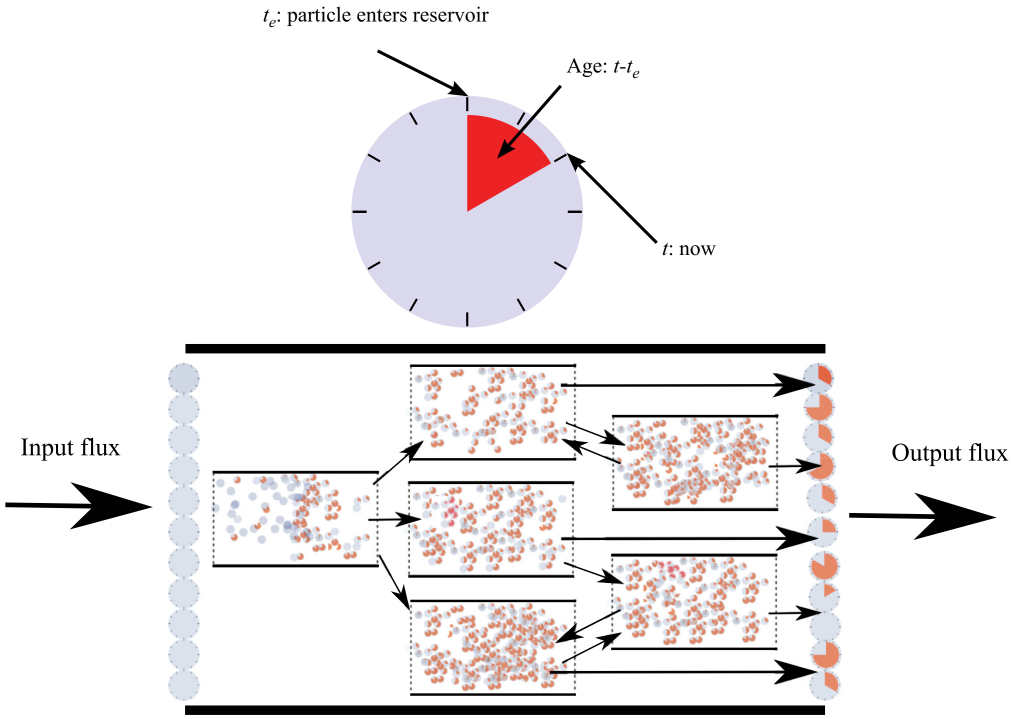

Figure 15.1. Graphical representation of the concepts of system age, transit time, and pool age. Mass entering a compartmental system can be conceptualized as being composed of small particles or atoms, each of them with a 'clock' that measures the time they have been in the system since they entered. All particles in the input fluxes have an age of zero. If we collect all particles inside the system at any given time and organize this information as a distribution of ages, we obtain the system age distribution of particles inside the system. If we collect the particles inside a specific pool and organize particles according to their age, we obtain the pool age distribution. Collecting particles in the output flux and organizing this information as a distribution of ages provides the transit time distribution. Figure extracted from Sierra et al. (2017).

Since the age and transit time concepts are defined for all individual atoms or particles inside a system, we can also think about them in terms of distributions that quantify the proportional distribution of the mass in age classes. Therefore, these distributions can be characterized by statistics such as the mean, standard deviation, and quantiles such as the median.

In the following sections, we will introduce mathematical formulas to quantify age and transit time distributions for two separate cases, (1) autonomous systems in equilibrium and (2) nonautonomous systems. Note that we will not be making a distinction between linear and nonlinear, because for case (1), linear and nonlinear systems in equilibrium can be treated similarly since the vector of states does not change once the equilibrium is reached and the system behaves similarly as a linear system. For case (2), the formulas rely on a linearization of the specific trajectory of a nonlinear system, therefore we will first introduce the linearization strategy and then provide the formulas for the linear nonautonomous case.

AGE AND TRANSIT TIME DISTRIBUTIONS FOR AUTONOMOUS SYSTEMS IN EQUILIBRIUM

The derivation of the formulas for age and transit time distribution of linear autonomous systems in equilibrium was originally introduced in Metzler and Sierra (2018). For their derivation, we were able to show that linear compartmental systems are analogous to absorbing continuous-time Markov chains. This means that linear compartmental systems can also be interpreted in a stochastic sense, with the deterministic system of differential equations representing the macroscopic behavior of entire masses, and the absorbing Markov chains representing the stochastic behavior of individual atoms of particles with respect to their age. For details about the stochastic process and derivation of formulas, interested readers can refer to Metzler and Sierra (2018) for additional details.

Let's consider linear autonomous systems introduced in Chapter 7, of the form of equation 7.2, with an equilibrium point given by equation 7.4. Let's also consider the 1-norm of a vector, defined as $\|\mathbf{v}\|_1 = \|\mathbf{v}\| := \sum_{i=1}^{n} |v_i|$, which is simply the sum of all the elements in the vector. We say that the random variable age a that measures age of atoms or particles in the system is distributed according to a Phase-Type (PH) distribution of the form:

$$f(a) = \mathbf{z}^{\mathsf{T}} e^{a\mathbf{B}} \eta = \mathbf{z}^{\mathsf{T}} e^{a\mathbf{B}} \frac{\mathbf{x}^*}{\|\mathbf{x}^*\|}, \quad a \geq 0.$$

Note that this density distribution is composed of three terms: the vector of fractional release coefficients, the matrix exponential of the compartmental matrix evaluated at each value of age, and the proportional distribution of mass at steady state. Since the fractional release coefficients can be computed directly from $\mathbf{B}$, we can say that the system age distribution follows a Phase Type distribution with two parameters: the probability vector of mass at steady state, and the transition rate matrix generated by the compartmental matrix. This can be abbreviated as $a \sim \mathrm{PH}(\boldsymbol{\eta}, \mathbf{B})$.

The mean or expected value $\mathbb{E}$ of the system age distribution can be obtained as:

$$\mathbb{E}[a] = -\mathbf{1}^{\mathsf{T}} \mathbf{B}^{-1} \eta = \frac{\|\mathbf{B}^{-1}\mathbf{x}^*\|}{\|\mathbf{x}^*\|},$$

where $\mathbf{1}$ is a vector containing ones, and T is the transpose operator.

To obtain the pool-age density distribution, we define first a diagonal matrix with the steady-state values for each compartment as $\mathbf{X}^* := diag(x_1^*, \ldots, x_n^*)$. The vector-valued function that returns the age distribution for each pool is then given by:

$$\mathbf{f}(a) = (\mathbf{X}^*)^{-1} e^{a\mathbf{B}} \mathbf{u}, \quad a \geq 0,$$

and the mean age for each pool:

$$\mathbb{E}[\mathbf{a}] = -(\mathbf{X}^*)^{-1} \mathbf{B}^{-1} \mathbf{x}^*.$$

The density distribution of the random variable transit time τ is also Phase-Type distributed, with the probability vector given by the proportional distribution of the input flux $\boldsymbol{\beta}$, and the compartmental matrix as the transition rate matrix; i.e. $\tau \sim \mathrm{PH}(\boldsymbol{\beta}, \mathbf{B})$. It can be obtained as:

$$f(\tau) = \mathbf{z}^{\mathsf{T}} e^{t\mathbf{B}} \beta = \mathbf{z}^{\mathsf{T}} e^{t\mathbf{B}} \frac{\mathbf{u}}{\|\mathbf{u}\|}, \quad \tau \geq 0,$$

with mean transit time given by:

$$\mathbb{E}[\tau] = \|\mathbf{B}^{-1} \beta\| = \frac{\|\mathbf{x}^*\|}{\|\mathbf{u}\|}.$$

Notice that the mean transit time is given by the ratio between the total mass at steady state and the total input flux.

AGE AND TRANSIT TIME DISTRIBUTIONS FOR NONAUTONOMOUS SYSTEMS

We consider now the nonlinear nonautonomous compartmental system introduced in Chapter 7 of the form of equation 7.9, for which we can always find a unique numerical solution of the form $\mathbf{x}(t, t_0, \mathbf{x}_0)$. To obtain time-dependent age and transit time distributions for this system, we will use the known solution to construct an equivalent linear nonautonomous system with the exact same solution. Details about the approach are presented in Metzler, Müller, and Sierra (2018).

Plugging in the known solution $\mathbf{x}(t) = \mathbf{x}(t, t_0, \mathbf{x}_0)$ into a new linear version of the system, we can define a new vector of inputs as $\tilde{\mathbf{u}}(t) := \mathbf{u}(\mathbf{x}(t), t)$, and a new compartmental matrix as $\tilde{\mathbf{B}}(t) := \mathbf{B}(\mathbf{x}(t), t)$. Then, we obtain a linear nonautonomous compartmental system of the form:

$$\dot{\mathbf{y}}(t) = \tilde{\mathbf{u}}(t) + \tilde{\mathbf{B}}(t) \cdot \mathbf{y}(t), \quad t > t_0, \quad \mathbf{y}(t_0) = \mathbf{x}_0,$$

which has a unique solution $\mathbf{y}(t, t_0, \mathbf{y}_0)$. Since we assume that the original nonlinear system of equation 7.9 also has a unique solution, both solutions must be identical; i.e. $\mathbf{y}(t, t_0, \mathbf{y}_0) = \mathbf{x}(t, t_0, \mathbf{x}_0)$. We can then use the solution of a nonlinear nonautonomous system to construct an equivalent linear nonautonomous compartmental system of the general form of equation 7.7, which has a general solution given by equation 7.8.

Age Distributions

We assume now that the initial content $\mathbf{x}_0$ has an initial age distribution $\mathbf{f}_0(a)$ such that $\mathbf{x}_0 = \int_0^\infty \mathbf{f}_0(a)\,da$. This initial age distribution is then perturbed by the time-dependent mass inputs and process rates of the system, generating a time-dependent age distribution of the form

$$\mathbf{f}(a,t) = \mathbf{g}(a,t) + \mathbf{h}(a,t),$$

where the term $\mathbf{g}(a,t)$ is the time evolution of the age distribution of the initial mass in the system, and $\mathbf{h}(a,t)$ is the time evolution of the age distribution of mass that enters the system after t_0.

The nonautonomous age distribution of the initial mass is given by:

$$\mathbf{g}(a,t) = 1_{[t-t_0,\infty)}(a) \cdot \Phi(t,t_0) \cdot f_0(a-(t-t_0))$$

where the indicator function $1_S(a)$ of a set S equals 1 if $a \in S$, or zero otherwise. The state transition operator $\Phi(t,t_0)$ is defined as in Chapter 7.

The nonautonomous age distribution of the mass that enters the system after t_0 is given by:

$$\mathbf{h}(a,t) = 1_{[0,t-t_0)}(a) \cdot \Phi(t,t-a) \cdot u(t-a)$$

To obtain the age distribution of the entire system, we simply sum the densities over all pools as:

$$f(a,t) = \|\mathbf{f}(a,t)\|.$$

Transit Time Distributions

To obtain transit time distributions in the nonautonomous case, it is necessary to distinguish between the concepts of backward versus forward transit times. The backward transit time is defined as the age of particles in the output flux at the time of release from the system t_r. Using the fractional release coefficients, it is possible to obtain the vector of outflow rates at time t_r as:

$$z_j(t_r) = -\sum_{i=1}^{n} B_{ij}(t_r), \quad j = 1, 2, \ldots, n.$$

The backward transit time distribution can be obtained as:

$$f_{BTT}(a,t_r) = \mathbf{z}^T(t_r) \cdot \mathbf{f}(a,t_r) \quad t_r \geq t_0.$$

Now, the forward transit time is defined as the age of an atom or particle that enters the system at an entering time $t_e > t_0$ and exits at time $t_r = t_e + a$. The forward transit time distribution can be obtained as:

$$f_{FTT}(a,t_e) = \mathbf{z}^T(t_e + a) \cdot \mathbf{f}(a,t_e + a).$$

Both distributions are tightly connected, with the forward transit time distribution of particles entering at time t_e being equal to the backward transit time distribution of the particles being released from the system at time t_r, i.e.:

$$f_{FTT}(a,t_e) = f_{BTT}(a,t_r).$$

FINAL REMARKS

The compartmental system representation also unveils analogies between deterministic systems that conserve mass with stochastic systems that conserve probabilities. This stochastic representation can be used to obtain formulas for the age of particles or atoms in the compartmental systems. With this approach, we derived formulas for the age of mass inside a compartmental system (system age), and the age of mass in the output flux (transit time). The concept of age can be very valuable to assess how old carbon and biogeochemical elements can be in an ecosystem. The concept of transit time can be very useful to understand how fast biogeochemical elements are processed inside an ecosystem, integrating all transfers and transformations that may take place.

There are other opportunities to further explore carbon cycle models in a stochastic setting. This could be particularly useful for studying, for example, the macroscopic properties at larger scales where patterns emerge by the action of microorganisms acting at microscopic scales. Also, the compartmental system representation may help to integrate concepts from other disciplines such as graph theory or control theory to address a number of questions not being explored yet in carbon cycle science.

SUGGESTED READING

A general introduction to the concepts of ages and transit times can be found in Bolin and Rodhe (1973). More specific results for the derivation of formulas and the computation of ages and transit times can be found in Rasmussen et al. (2016) for the mean of their distributions in nonautonomous systems, and for complete distributions in autonomous systems in Metzler and Sierra (2018), and for complete distributions in nonautonomous systems in Metzler, Müller, and Sierra (2018).

QUIZZES

1. Give examples of systems where the mean transit time is higher than the mean system age.
2. Give examples where the mean system age is higher than the mean transit time.
3. In what type of systems are the mean system age, the mean transit time, and the turnover time equal?