A probabilistic approach of flow-balanced network

based on Markov chains

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Abstract:

We used Markov chains to assess residence time, first passage time, rate of transfers between compartments, recycling index with a general mathematical formalism. Such a description applies to any flow-balanced system that can be modelled as a series of discrete stages or compartments through which matter flows. We derived a general set of equations from a probabilistic approach and applied them to a food web and a physical system derived from the literature. We therefore analysed preferential pathways of matter and behaviour of these systems and showed how it was possible to build up and exploit indices on the basis of a transition probability matrix describing the network, and to characterize with a generic algorithm: (1) the total indirect relationships between two compartments, (2) the residence time of one compartment and (3) the general recycling pathways including the amount of matter recycling and the implication of each compartment in recycling.

Keywords: Markov chain; Residence time; Transfer rate; Network; Food web model; Box model; First passage time

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Abstract

We used Markov chains to assess residence time, first passage time, rate of transfers between compartments, recycling index with a general mathematical formalism. Such a description
20 applies to any flow-balanced system that can be modelled as a series of discrete stages or compartments through which matter flows. We derived a general set of equations from a probabilistic approach and applied them to a food web and a physical system derived from the literature. We therefore analysed preferential pathways of matter and behaviour of these systems and showed how it was possible to build up and exploit indices on the basis of a transition probability matrix describing the network, and to characterize with a generic algorithm: (1) the total indirect relationships between two compartments, (2) the residence time of one compartment and (3) the general recycling pathways including the amount of matter recycling and the implication of each compartment in recycling.

Introduction

30 Ecosystem behaviour is driven by different temporal and spatial scales of biological and physical processes. Because of the spatial boundaries of a system, any matter (salt or fresh water, carbon, nitrogen or any substance) flowing through it will remain for a period which

depends on the interactions between the process involved and the type of matter. Therefore, assessing matter cycling, pathways and residence time within ecosystem compartments can help in understanding ecosystem properties. For deterministic systems based on interactions between compartments - whether this be matter transfer as described by Guangso et al. 2002, Thompson et al. 2002, Sivakumar et al. 2005, Yu & Wehrby 2004, or changes of the system from one state to another as described by Logofet & Lesnaya 2000 - probability of transition from one compartment to another can be defined during a given time. Assuming that

40   transition probabilities are time-independent, this corresponds to a Markov-chain model, where the state of the system at time $s > t$ can be predicted from the knowledge of the state of the system at time t and does not depend on the situation before t (Markov property, Bailey 1964). Markov-chain models are particularly adapted to the study of succession processes such as forest successions (Logofet & Lesnaya 2000, Benabdellah et al. 2003), metapopulation dynamics (Moilanen 2004), or the evaluation of transit times of tracers in various environments. Examples of transit though environments include: transit in a gasifer (Guangso et al. 2002), of a particle in a tidal mixing estuary (Thompson et al. 2002), of a solute in an aquifer system (Sivakumar et al. 2005) and of drugs within the body (Yu & Wehrby 2004).

50   Description of this type also applies to ecological studies. Odum (1959) defined ecology as "the study of the relationships of organisms with one another and with their non-living environment" and the magnitude of matter and energy flows between the various components of an ecosystem is now regarded as an appropriate measure of such relationships (Szyrmer & Ulanowicz, 1987). A food web is therefore a good method for the quantitative description of an ecosystem (Ulanowicz 1984). The food web can be seen as a graph, with nodes (the compartments) and quantitative links (the trophic fluxes between them). Such a representation might seem static and non-evolutive, as would a still photograph of the ecosystem. Yet trophic dynamic aspects emerge from such representations (Lindeman 1942). Once the food web is drawn, this often complex scheme can be transformed into a more synthetic

60   representation which reveals the emergent properties of the system (Ulanowicz 1986). When studying the interrelations between components of a food web, looking at direct interactions (first passage flows) is not enough and one has also to consider subsequent passage flow from a holistic point of view (Patten, 1995). Hannon (1973) applied Leontief's Input-Output analysis (Leontief, 1936, 1951) to ecology, in order to study the interdependence of organisms in an ecosystem. The central element in this theory is the Leontief structure matrix, which is commonly thought to express the total direct and indirect flows between any two compartments of a system (Szyrmer & Ulanowicz, 1987). Two parallel conceptions can be distinguished in input-output analysis. These are Leontief's backward formalism, which from the outputs of the systems deduces the necessary inputs, and Augustinovicz's forward

70   formalism, which calculates the fate of outputs from the compartments, thus deducing the

transit of the matter from the inputs to the system (Kay et al. 1989). The direct interactions are shown by the two-dimensional matrix of internal exchanges, and much information can be obtained about the indirect links through straightforward operations on the matrix of direct flows (Ulanowicz, 1984). The multiplicity of possible pathways within the food web are translated into indices based on thermodynamics and information theory, such as Ascendency, Redundancy and Overheads (Ulanowicz 1986, Ulanowicz & Norden 1990). By introducing the idea of temporality into this conception, Higashi et al. (1993) gave importance to the biomass of the compartments. In their description, the transfer of matter (energy, carbon, biomass etc.) from one compartment to another can be delayed by storage in the

80   compartments. Hence, each flow is a possible pathway for matter which is taken with a certain probability. This describes a Markov process in which matter is transferred or retained in the food web at each time-step, depending only on its previous trajectories. Markov transition probability matrices can be constructed according to the two conceptions of information theory, backward or forward cases (Kay et al. 1989).

Residence time has received a lot of attention as a useful indicator in physical oceanography. Several definitions of residence time can be found in the literature. According to Takeoka (1984a), transit time should be distinguished from residence time. The first deals with the time water particles take to cross an area from entrance to exit. For the second, all the particles contained in the area are considered. In this case, the residence time corresponds to

90   the mean transit time but depends on the initial location of the particles. Takeoka (1984a) showed that the difference between the two mean temporal characteristics could be defined as the age of the particles retained in the area. In a general approach, Bolin and Rodhe (1972) summarized and compared the basic concepts of age distribution and transit time showing that the mean transit time equals the so-called 'turnover time' (defined as the ratio between the volume and the total inflow). Following Zimmerman (1976), Takeoka (1984b) compared residence and transit time scales. He solved the case of a one-dimensional channel with uniform advection and longitudinal diffusion. Zimmerman (1976) used salinity distribution and a box model to assess the exchange terms between the boxes and the spreading of a tracer in the Wadden Sea, under the assumption of a steady-state. Numerical integration of the

100   transport equation yielded residence time estimations in each spatial box. Dronkers and Zimmerman (1982) derived an estimation of the residence time and the age of fresh water in the Oosterschelde from a steady state unidimensional and dispersive equation. Once again the dispersion coefficients were estimated from salinity distribution. Using a box model and a salt balance equation, Miller and McPherson (1991) computed the residence time in an one-dimensional case through the simulation of the salt transport with different initial conditions corresponding to the initial vector filled with values 0 or 1 in some boxes. Recently, Thompson et al. (2002) used a Markov chain approach combined with a spatial box model to characterise water mixing and transport within a bay.

In our study, we develop Markov chains further to construct a series of indicators: residence
110   time, first passage time, rates of transfer between compartments and number of passages in a
compartment. Since such a description applies to any flow-balanced system that can be
modelled as a series of discrete stages or compartments through which matter flows, we
applied Markov chains to a food web (Takapoto atoll food web, Niquil et al. 2001) and a
physical system (Passamaquoddy Bay tidal mixing model, Thompson et al. 2002). We used
our indicators to analyse preferential pathways of matter and behaviour of these systems.

Methods

Markov transition matrix

Food-web matrix F

The food-web matrix F describes all the flows between N compartments and between
120   compartments and the exterior of the system. Flows are given in matter (energy, carbon,
biomass …) per unit of time (day, year). The formalism is derived from Finn (1976), Patten &
Higashi (1995) and Fath & Patten (1998): elements F_{ij} define the flow going from
compartment j to compartment i. The last column and row give respectively the inputs from
the exterior of the system, and the outputs from the compartments. The internal flow matrix
concerns only the exchanges between compartments of the system. The food web is
described at steady state, which means that the total output from any compartment ($Tout_i$ -
sum of corresponding column) equals the total input to this compartment (Tin_i - sum of the
corresponding row). Each compartment has a known biomass B_i.

Transition matrix P

130   According to the Higashi et al (1993) view of flow temporality, the probability that a particle
which is in compartment j ($j = 1..N$) at time t passes to compartment i ($i = 1..N+1$) during one
time step Δt is equal to:

$$P(j \rightarrow i/j) = P_{ij} = \frac{F_{ij}}{B_j} \cdot \Delta t$$

Probability for a particle that is in i to stay in i during one time step is given by:

$$P(i \rightarrow i/j) = P_{ii} = 1 - \sum_{k \neq i} P_{ki} - P_{N+1,i}$$

Time step Δt must be chosen so that each term of matrix P is positive and less than 1. Any
choice for this time step will lead to the same results, provided that it is small enough to
represent less that the time needed to empty any compartment (the minimum of turnover

times defined as the biomass of a compartment divided by the sum of all its exiting flows).

140 Hence, we chose half the minimum of turnover times computed for all compartments. From here on, time will be expressed as a number of time steps. The matrix P is completed by adding a column for the exterior of the system: a column of zeros, with 1 for the last element which is an absorbing element. This matrix is column-stochastic since the sum of each of its column is one (Bailey 1964). It is the transition matrix of a Markov process, in which the random variable is the concentration C of a tracer in each compartment. Given the initial state C^0 of a particle in the system and C_i^0 the probability that the particle is in compartment i at time 0, the concentration at time $t+\Delta t$ is equal to:

$$C^{t+1} = P \cdot C^t$$

hence

150 $$C^t = P^t \cdot C^0 \qquad (1)$$

Distribution C^{t+1} only depends on state C^t and not on the previous states, which is the characteristic of the Markov property (Bailey 1964). In the following descriptions, C will always be less than 1, and hence represents the probability distribution of a unit of matter within the food web. As time is incremented, one can then compute the probability distribution of a unit of matter, or, as Thompson et al. (2002), compute the probability that a particle stays in a compartment in which it was at time $t = 0$, the probability that a particle is absorbed by the exterior compartment, or the probability that a particle moves from one compartment to another for the first time during time t. With the latest representation, another computation is necessary. For each compartment i we constructed a new matrix Q_i in which i

160 is an absorbing compartment: the ith column is replaced by a column of zeros, with 1 at the ith position. Q_i is also a Markov transition matrix, and we can also compute (see Results):

$$C^t = Q_i^t \cdot C^0$$

Calculation of indices from a Markov transition probability matrix

In the following we will use the Markov transition probability matrix P and generator functions to compute analytically the average passage time and the transfer rate from compartment j to compartment i.

Transfer rate and transit time

Let us define $A_{i,t}$ as the event of being in compartment i at time $t \geq 0$, $C_{i,t}$ as the event of being in compartment i for the first time at time $t>0$ and $C_{i,j,t}$ as the subset of $C_{i,t}$ corresponding to

170   being in j at time 0. We write the conditional probability $c_{i,j,t}$ as $c_{i,j,t} = P(C_{i,t} / A_{j,0})$. We define the average passage time T_{ij} as the expectation of the random variable t associated with the probability distribution $c_{i,j,t}$, and the transfer rate R_{ij} as the average of the probability distribution $C_{i,j,t}$. Using the generator functions $\gamma_{i,j}(s) = \sum_{k=0}^{\infty} c_{i,j,k} \cdot s^k$ and $\alpha_{i,j}(s) = \sum_{k=0}^{\infty} a_{i,j,k} \cdot s^k$, we can write:

$$T_{ij} = \frac{d\gamma_{i,j}}{ds}(s=1) \qquad (2)$$

and

$$R_{ij} = \gamma_{i,j}(1)$$

The conditional probability $a_{i,j,t} = P(A_{i,t} / A_{j,0})$ is easily derived from the transition matrix P using equation (1) and it is easy to show that:

180   $$\alpha_{i,j}(s) = (I - s \cdot P)_{i,j}^{-1}$$

where I is the identity matrix. In the following, we will show how to derive $\gamma_{i,j}(s)$ from $\alpha_{i,j}(s)$.

When one lists all the elements of $C_{i,j,t}$, all the events where i has been reached at least once before time t must be excluded. The product $a_{i,j,t-k} \cdot c_{i,i,k}$ gives the probability of being in i at time t-k and coming again to compartment i after exactly k steps. Therefore we can write:

$$c_{i,j,t} = a_{i,j,t} - \sum_{k=1}^{t-1} a_{i,j,t-k} \cdot c_{i,i,k}$$

We will see below that it is necessary to extend the summation from $k = 0$ up to t. We introduce the new element $c_{i,i,0}$, which can be arbitrarily chosen, and write:

$$c_{i,j,t} = a_{i,j,t} - \sum_{k=0}^{t} a_{i,j,t-k} \cdot c_{i,i,k} + a_{i,j,t} \cdot c_{i,i,0} + a_{i,j,0} \cdot c_{i,i,t}$$

190   If $i{\neq}j$, $a_{i,j,0} = 0$ and the equation becomes:

$$c_{i,j,t} = a_{i,j,t} - \sum_{k=0}^{t} a_{i,j,t-k} \cdot c_{i,i,k} + a_{i,j,t} \cdot c_{i,i,0} \qquad (3)$$

and is valid for $t>0$. To extend the above equation to the case $t = 0$, we must define a new term $c_{i,j,0} = 0$ and it is valid for all t.

In the following explanations, we will simplify the notations by writing $\gamma_{i,j}(s) = \gamma_{i,j}$ and $\alpha_{i,j}(s) = \alpha_{i,j}$. We have:

$$\alpha_{i,j} \cdot \gamma_{i,i} = \sum_{p=0}^{\infty} a_{i,j,p} \cdot s^p \cdot \sum_{q=0}^{\infty} c_{i,i,q} \cdot s^q = \sum_{t=0}^{\infty} \left(\sum_{k=0}^{t} a_{i,j,t-k} \cdot c_{i,i,k} \right) \cdot s^t$$

Using equation (3), we can write:

$$\sum_{k=0}^{t} a_{i,j,t-k} \cdot c_{i,i,k} = -c_{i,j,t} + a_{i,j,t} \cdot \left(1 + c_{i,i,0}\right)$$

and therefore:

$$\alpha_{i,j} \cdot \gamma_{i,i} = -\gamma_{i,j} + \alpha_{i,j} \cdot \left(1 + c_{i,i,0}\right) \tag{4}$$

A similar equation is obtained for $t>0$ and $I = j$. We have:

$$c_{i,i,t} = a_{i,i,t} - \sum_{k=1}^{t-1} a_{i,i,t-k} \cdot c_{i,i,k}$$

and we extend the summation again from 0 to t:

$$c_{i,i,t} = a_{i,i,t} - \sum_{k=0}^{t} a_{i,i,t-k} \cdot c_{i,i,k} + a_{i,i,t} \cdot c_{i,i,0} + a_{i,i,0} \cdot c_{i,i,t}$$

Here $a_{i,i,0} = 1$ yields:

$$0 = a_{i,i,t} - \sum_{k=0}^{t} a_{i,i,t-k} \cdot c_{i,i,k} + a_{i,i,t} \cdot c_{i,i,0} = a_{i,i,t} \cdot \left(1 + c_{i,i,0}\right) - \sum_{k=0}^{t} a_{i,i,t-k} \cdot c_{i,i,k}$$

or

$a_{i,i,t} \cdot \left(1 + c_{i,i,0}\right) = \sum_{k=0}^{t} a_{i,i,t-k} \cdot c_{i,i,k}$. Note however that this equation does not stand for $t = 0$.

Using $\alpha_{i,i} \cdot \gamma_{i,i} = \sum_{t=0}^{\infty} \left(\sum_{k=0}^{t} a_{i,i,t-k} \cdot c_{i,i,k} \right) \cdot s^t$, we get:

$$\alpha_{i,i} \cdot \gamma_{i,i} = \sum_{t=1}^{\infty} \left(\sum_{k=0}^{t} a_{i,i,t-k} \cdot c_{i,i,k} \right) \cdot s^t + a_{i,i,0} \cdot c_{i,i,0} = \sum_{t=1}^{\infty} \left(\sum_{k=0}^{t} a_{i,i,t-k} \cdot c_{i,i,k} \right) \cdot s^t + c_{i,i,0}$$

and

$$\alpha_{i,i} \cdot \gamma_{i,i} = \left(1 + c_{i,i,0}\right) \cdot \alpha_{i,i} + c_{i,i,0} \tag{5}$$

Equations (4) and (5) can be simplified if we choose $c_{i,i,0} = -1$. We therefore get:

$$\begin{cases} \gamma_{i,i} = -\dfrac{1}{\alpha_{i,i}} \\ \gamma_{i,j} = -\dfrac{\alpha_{i,j}}{\alpha_{i,i}} \end{cases}$$

The average passage time T_{ij} is the first order derivate of the generator function $\gamma_{i,j}(s)$ for $s = 1$ (equation (2)). It may be proved (not shown) that this derivative always exists even in cases where $\gamma_{i,j}(1)$ is not finite. It was computed as the limit:

$$T_{ij} = \lim_{\varepsilon \to 0} \frac{\gamma_{i,j}(1 - 2 \cdot \varepsilon) - \gamma_{i,j}(1 - \varepsilon)}{\varepsilon}$$

and the transfer rate R_{ij} as the value:

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$$R_{ij} = \gamma_{i,j}(1)$$

Adaptation to various issues

Conditional probabilities

The T_{ij} and R_{ij} ($i = 1..N$, $j = 1..N$, N+1 being the exterior compartment) coefficients computed from the paragraph above represent the time taken to reach the compartment i and the amount of matter that will reach the compartment i, when one unit of matter is in compartment j at $t = 0$. In this calculation we can split the matter into two categories, matter which leaves j within the first time step and matter which stays longer in j. When we want to calculate transit time and transfer rate for the first category of matter therefore, we consider the fate of matter depending on whether it leaves compartment j at time 0.

230   We define two sets of conditional probabilities. P'_{kj} is the probability that a particle living j arrives to compartment k within one time step ($k = 1..N+1$, $k \neq j$), and P''_{kj} is the probability that a particle leaving j arrives to compartment k with the additional condition that the particle stays within the system ($k = 1..N$, $k \neq j$).

A planktonic theoretical food web provides a small theoretical example for an explanation. The example food web has 4 compartments: 'phytoplankton' ("phyto", compartment n°1), 'bacteria' ("bact", n°2), 'zooplankton' ("zoo", n°3), and 'detritus' ("det", n°4) (Figure 1). Assuming that the transition probability matrix P has been defined on the basis of the food-web matrix and considering the case of bacteria compartment (n°2), we defined conditional probabilities as following:

240

$$
\begin{cases}
P'_{12} = \dfrac{P_{12}}{P_{12} + P_{32} + P_{42} + P_{ext2}} \\[2ex]
P'_{32} = \dfrac{P_{32}}{P_{12} + P_{32} + P_{42} + P_{ext2}} \\[2ex]
P'_{42} = \dfrac{P_{42}}{P_{12} + P_{32} + P_{42} + P_{ext2}}
\end{cases}
\text{ and }
\begin{cases}
P''_{12} = \dfrac{P_{12}}{P_{12} + P_{32} + P_{42}} \\[2ex]
P''_{32} = \dfrac{P_{32}}{P_{12} + P_{32} + P_{42}} \\[2ex]
P''_{42} = \dfrac{P_{42}}{P_{12} + P_{32} + P_{42}}
\end{cases}
$$

Conditional transfer rates

Transfer rate is defined as the fraction of matter leaving compartment *j* that will reach the compartment *i*. Supposing that a particle has left the compartment *j* between time $t = 0$ and Δt (during the first step). *P'* represents the probability that the particle either reached another compartment or left the system. Then, at each time step, matter can exit the system, be transferred to another compartment, or stay where it is. The conditional transfer rates RC_{ij} from the bacterial compartment ($j = 2$) to other compartments $i \neq j$ were derived from R_{ij} as following:

$$RC_{42} = R_{41} \cdot P'_{12} + R_{43} \cdot P'_{32} + 1 \cdot P'_{42}$$

For $i = j = 2$, we write:

$$RC_{22} = R_{21} \cdot P'_{12} + R_{23} \cdot P'_{32} + R_{24} \cdot P'_{42}$$

Conditional transit times

Conditional transit time TC_{ij} is the time taken by a particle that leaves compartment *j* between $t = 0$ and $t = \Delta t$ to reach the target compartment *i*. Two cases must be distinguished: the transit time from one compartment to another is computed using *P''* probability, and the transit time from one compartment to outside (residence time of the compartment) is not changed, because it represents the residence time of one compartment, i.e. the time taken to get out of the system assuming that the matter is in the compartment at time $t = 0$. As above conditional transit times TC_{ij} were derived from T_{ij} for $i = 4$ and $j = 2$ as following:

$$TC_{42} = T_{41} \cdot P''_{12} + T_{43} \cdot P''_{32} + 1 \cdot P''_{42}$$

For $i = j = 2$ we write:

$$TC_{22} = T_{21} \cdot P''_{12} + T_{23} \cdot P''_{32} + T_{24} \cdot P''_{42}$$

Return time and number of passages

R_{ii} defines the return rate to compartment *i* and corresponds to the fraction of biomass that comes back for the first time to compartment *i*. The average number of passages N_{ii} can easily be derived from the successive fractions R_{ii}, R_{ii}^2, R_{ii}^3, ..., R_{ii}^k, ... We write:

$$N_{ii} = \sum_{k=1}^{\infty} R_{ii}^k \cdot k$$

Since $\sum_{k=1}^{\infty} R_{ii}^k \cdot k = R_{ii} \cdot \sum_{k=1}^{\infty} R_{ii}^{k-1} \cdot k = R_{ii} \cdot \dfrac{d}{dR_{ii}} \left(\sum_{k=0}^{\infty} R_{ii}^k \right)$ and $\sum_{k=0}^{\infty} R_{ii}^k = \dfrac{1}{1 - R_{ii}}$, we get:

$$N_{ii} = \frac{R_{ii}}{\left(1 - R_{ii}\right)^2}$$

Applications

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The first application was made to Takapoto lagoon (TA) pelagic food-web model analysed by Niquil et al. (2001) who aggregated organic carbon stocks into eight living and two non-living compartments (Table 1), which structure the ecosystem on the basis of processes and sizes (Figure 2a). The compartments were: bacteria (BAC), phytoplankton < 1 µm (PH1), phytoplankton from 1 to 3 µm (PH2), phytoplankton > 3 µm (PH3), protozoa < 35 µm (PZ1), protozoa > 35 µm (PZ2), microzooplankton < 250 µm (MIC) and mesozooplankton from 250 to 2000 µm (MES), dissolved organic carbon (DOC) and particulate organic carbon (POC). Flows between planktonic compartments (Table 2a) were partly determined by field experiments and completed by inverse analysis (Vézina & Platt 1988). The second application

280

concerns Passamaquoddy Bay (PB) box model developed by Thompson et al. (2002) who characterised water mixing with a discrete-time, finite-state Markov Chain model. The bay was divided into 15 homogeneous regions ('boxes') (Figure 2b) and transition probabilities were estimated by computing a lot of trajectories by the means of two-dimensional hydrodynamic model (Table 3). Initially the time unit was the tidal cycle (one flow and one ebb). In the following we have used day units by considering that 2 tidal cycles occurred during one day.

From here on, T and R will refer to the final computed transit time and transfer rate (after use of conditional probabilities).

Results and discussion

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Tracking a particle within the ecological network

P matrix structure

The elements of the P matrices generally correspond to direct links between compartments of the systems. However, some unusual values should be mentioned. In the PB model, some probabilities existed between zones that are not physically linked (which can be seen on the map, Figure 2b, in Thompson et al. 2002), due to the fact that transition probabilities are based on simulations (with a hydrodynamical model) of particle trajectories which may cross several spatial compartments within one day. Therefore the probability that a particle exiting

the system from compartment 7 or 8, for example, is not zero even though 7 and 8 are not physically linked to the boundary of the system. For the TA model, the method of P matrix

300 construction did not allow this to happen. Another unusual compartment is zone 9 in the PB system, which only receives matter from itself, making it impossible to compute any transfer rate or time to this compartment. Physically, this means that matter flowing to this compartment during one day does not stay inside it and is quickly expelled (this can be seen on the figure 4 in Thompson et al. (2002), where this zone does not change colour, there is no overall mixing with adjacent compartments). Although this could seem troublesome from a mass conservation point of view, the evolution of the systems only shows probabilities of presence, i.e. not the entire flow of matter in the system. Considering these probabilities as amounts of labelled matter, and the exterior is an absorbing state, the amount of matter in the system globally decreases.

310 *Direct use of P matrices*

The first application of a Markov transition probability matrix is generally to follow the evolution of a system step by step (Baltzer 2000, Logofet & Lesnaya 2000, Thompson et al. 2002, Benabdellah et al. 2003, Sivakumar et al. 2005). Here, we applied a conception like this to the tracing of a particle flowing through a network (Table 2b & Table 3). Thompson et al. (2002) chose 3 possible representations of this, and over the course of time followed: (1) the probability that a particle was still in the source compartment, (2) the probability that the released particle was absorbed by the boundary state, and (3) the probability that the particle had reached the target. The evolution of this system was tracked by computing the components of the probability vector C described above (see Methods) and plotting the

320 component corresponding to the source compartment for the first probability and to the target compartment for the two others. Apart from the second case, where the target compartment was already an absorbing state, the P matrix was transformed into the Q_i matrix described in the Methods, in which the target compartment column i was that of a sink compartment. We verified that we obtained the same results as Thompson et al. (2002) in their figures 5b, 6b and 7b. In the present study, with the TA and PB models, we represented the latest case from the initial condition that «at time $t = 0$, one unit of matter has left the source compartment (j)», i.e. the initial concentration was the jth column of the probability matrix P'' described in the Methods section. Using the representation of the probability that a particle leaving a source compartment (j) has reached an identified sink compartment (i) after a time t, we

330 observed different types of comportment, and represented four extreme cases, which we will

refer to by the «source, target» pairs they describe. As these curves grew uniformly and increased (by 100%), they reached an upper limit, and therefore an asymptote. The values for these asymptotes and the way in which they were approached defined the different evolution types. The probabilities could reach high values or remain low, and the evolution could be rapid (the asymptote was quickly approached) or slow (the asymptote appeared much later). The time it took to approach the asymptotes defined two types of behaviour: «fast» pairs and «slow» pairs. The transfer rates between source and sink defined the pairs as «strong» or «weak» depending on their intensity. The examples shown in Figures 3a and 4a respectively represent the strong pairs (PH3,DOC) (fast) and (PH3,BAC) (slow) for TA, and (6,8) (fast)

340 and (1,10) (slow) for PB. Figures 3b and 4b present the weak pairs, which were (BAC,MIC) (fast) and (POC,BAC) (slow) for TA, and (13,12) (fast) and (1,5) (slow) for PB. The simulations were conducted for one year for both TA and PB so that the asymptotes were approached. The values that can be read on the graphs correspond to the computed rates of Tables 4 and 5. For example, the asymptote for the pair (POC,BAC) had a value of 4.2%, meaning that at the most, 4.2% of the matter leaving the bacterial compartment would, in the end and by all possible pathways, reach the zooplankton compartment. These direct observations of the evolution of the system thus allow a new type of relation between compartments to emerge, which goes beyond the direct absolute values of flows to describe their interdependency.

350 ## *Interpretation of indices*

Indices based on transit times and transfer rates quantify previous relational observations by integrating all possible pathways between the sources and the targets and considering transfers related to first passage times.

From one compartment to another: transfer rate and transit time

To compute the transfer rates, the initial condition was that the particle had left the compartment at time $t = 0$, whether it be going to the exterior of the system, or to another compartment. Hence, the transit time is the average time needed to reach a target compartment for a particle that has just left the source compartment. To compute the transit times, the initial condition was that one unit of matter had left the source compartment but not

360 the system at time $t = 0$. Whether one takes the conditional probability P' or P'', the result does not change. Indeed, whatever the amount leaving the source at time $t = 0$ or thereafter, what counts is the relative quantity eventually reaching the target.

From one compartment to itself: return rate, return time and number of passages

The rate of return to one compartment reflects its implication in matter recycling, it represents the amount of matter that will cycle back to the compartment once having left it. From this amount the number of passages through this compartment (i.e. the average number of times that a particle which left this compartment will enter it again over the course of time) can be computed. The higher the return rate, the more matter cycles back, and the more will cycle back yet again. This index reveals the intensity of recycling in the web. Like transfer rates, return rates are associated with return times, which complete the description. The return times indicate how long it takes to a unit of matter that has left the source compartment to return. It reveals the number of links there is in the associated cycle, or the complexity of the return pathways.

From one compartment to exterior: residence time

As previously mentioned, the rate of transfer to the exterior is of no interest here. As there is no accumulation in the systems, all the matter will exit in the end. The residence time of the compartments is more interesting, as this describes the transit time from the source compartment to the exterior of the system. The initial condition was that one unit of matter was in the source compartment at time $t = 0$.

Transfer indices and simplified networks

Plotting transfer rates vs. transit times between paired compartments characterises integrated links between compartments (Figure 5 gives the result for TA model as an example). Dividing the space (Transit times, Transfer rates) into 4 zones, one can see the intuitive characterization described above. On the left hand side, the transit time is short and the "fast pairs" are plotted. Here one can note that these are not only the directly linked ones. On the upper side, the links are strong, and are once more not necessarily direct links, nor necessarily important ones (in absolute value) either. Hence, we can draw integrated networks, in which links reveal the intensity and speed of the flows between compartments (Figures 6a & 7a for TA and PB respectively). The choice of the limits between strong and weak (up and down a horizontal limit) and fast and slow (left and right along a vertical limit) can seem subjective. In the present case, as the two systems presented are very different, we chose to fix relative limits. The strong links would correspond to the first 15% highest transfer rates among all existing links, and the fast ones to those faster than the mean transit time.

From the representation of all the main links, one can see that some patterns emerge, and thus draw simplified integrated networks (Figure 6b for TA & Figure 7b for PB), by grouping together the compartments which have the same comportment, and keeping only the strongest links.

Takapoto Lagoon

For the TA model, we constructed a simplified network on the basis of the links between compartments (Figure 6). When the transfer rate was more than 29%, the link was considered strong, when it was between 19% and 29%, it was considered an average link. Weak links (less than 19%), were not studied further. On this basis, compartments were grouped according to their behaviour towards other compartments, sometimes associating average and strong links, in particular when the average link was a fast one (Transit time less than 10 days). The distinction between 'strong', 'average' and 'weak' was chosen so that 15% of all possible links (100 links can exist between 10 compartments) were «strong», and 20% were «average». From this representation, it appears that the most important compartments are all strongly linked with the DOC compartment, which is a central element of the network. The primary producers can be grouped, as can the two metazoan protozoa groups and the two zooplankton groups. Most of the strong and fast links flow through the DOC compartment which appears to be a key compartment in the system. The DOC receives carbon from various sources, though mostly from phytoplankton, and transfers this matter to heterotrophs, especially bacteria and protozoa, which were considered as potential direct users of DOC. Bacteria appear to be a dead-end compartment for carbon flows, leading mainly to dissipation by respiration. The zooplankton is an exit pathway for carbon coming mainly from protozoa and transfers most of this to the detritus compartments. The POC compartment is primarily an exit pathway for the whole system and cycles with the zooplankton compartments whose diet is mainly composed of non-living compartments. It appears that very few links exceed 50%, the maximum values being obtained for important direct links from primary producers to non living (POC and DOC) compartments. These low rates could be due to the fact that many components are directly linked to the exterior. In fact, all the compartments except the DOC are physically exported, and all the living compartments loose matter by respiration. The observation of return rates and residence times emphasises these observations (Table 6). Indeed, the shortest residence time is that of the bacteria and not of the POC (as the main exit pathway, it would have been expected to have the shortest residence time), the link between these two is average (13% from BAC to POC) but fast (0.5 days). The return rates do not

exceed 10%, and the number of returns to one compartment does thus not exceed 0.16. The residence times are short overall, less than 50 days and around 12 days on average. The shortest residence times, 2.3 and 7 days for bacteria and POC respectively, suggest that the system is an open one, through which matter flows. These values are very low, especially when compared to the high residence time of the lagoon water mass which was estimated as around 4 years (Sournia & Ricard 1976). This can be explained by the fact that the planktonic system described here is open to the macroscopic communities with very high carbon flow values compared to low biomass. This highly rapid system concerns all the carbon flows and results in large scale carbon dissipation by respiration. The dominance of small organisms emphasises these high respiration rates. Hence, we can describe TA as a system through which matter flows, transiting in the DOC compartment, not being transferred to the higher trophic levels (zooplankton), but being quickly expelled from the system.

Passamaquoddy Bay

With the same method, we kept the strong and average links between compartments for the intermediate simplified network, i.e. 35% of the 210 (source, target) pairs composed of the first 15% - 32 strongly linked pairs (R>63%) and the following 20% - 42 averagely linked pairs (R>29%). We then separated slow and fast pairs as having more or less than 57 days. In contrast to links in TA, many were higher than 50% on PB and the boundary between average and strong links was much higher (63% vs. 25%). Like with the TA system, the scheme of all average and strong links can be simplified and some compartments grouped. Analogies can be found between the groups (1, 2, 3), (5, 6) and (11, 12, 15). The grouping of compartments 1, 2 and 3 is obvious and the fact that any pairs from 1 to other compartments are slower than those from 2, and that those from 2 are slower than those from 3, comes from the physical structure of the web where water flows firstly from 1 to 2, then to 3, then to 4 and then to other compartments. The links between 1, 2 and 3 and other compartments of the system are indirect links, but they can be strong and/or fast. Going further, zone 10 could be grouped with zones 7 and 8 making a new aggregated compartment analogous to the POC compartment in TA, because these compartments (7, 8, 10) receive matter from all groups, but scarcely recycle it to the system. This is an "exit point" and also a "compulsory path" for the matter.

The return times and rates (Table 7) confirmed the position of the "exit compartments" as the ones which have the shortest residence times: 15, 7, 9 and 10. The return rates are much higher than in TA model, where they did not exceed 10%. The return rates of compartments

460 1, 2 and 3 are unusual because they are linked together only amongst themselves, meaning that this return only creates a delay in the transfer to other zones. As for the other compartments, the numbers 4, 14 and 13 appear to recycle the most, and compartments 5, 6 and 9 the least, this is in agreement with the aggregated description of figure 7b. The residence times are longer than those of the TA model compartments, the shortest (20 days) is that of the exit compartment (10). The compartments with the longest residence times are, as expected, 1, 2 and 3 in that order (157, 107, 73 days), and also compartments 11 and 12 (111 and 61 days). The first three compartments are the ones at the 'beginning' of the water flow path, and the other two can be considered as a kind of dead end. Globally, the mean residence time of 57 days situates the Bay between highly flushed systems such as Marennes-Oléron

470 Bay (France, Bacher 1989) and very closed ones such as lagoons.

Links between compartments: sensitivity indicators

Such simplified networks can be used as qualitative indicators of the reactions systems have to perturbations, in the place of more complicated calculus approaches. Indeed, simplified networks offer clues about possible propagation of a perturbation from a particular location across the rest of a web.

For example, in PB model, any perturbation occurring in the system will have consequences for the compartments 4, 13, 14, 7, 8 and 10, because they are linked to all other compartments and matter cycles within them. Depending on which compartment was disturbed, the system would be more or less affected. A perturbation in compartment 1, 2, 3, 5, or 6 would therefore

480 affect the whole system, whereas a perturbation in compartment 7, 8, 9, 0, 11, 12 or 15 would have less influence. Due to the high cycling rates, any perturbation will have a long-lasting effect, which will not disappear for another 10 days. In contrast, in the TA model, a perturbation in the primary production would affect all the compartments of the system, but would certainly disappear quickly because the return times are long (more than 40 days, apart from the DOC compartment). As the return rates are low, any occasional perturbation would most likely not last and might not even propagate to the zooplankton compartments. A perturbation in the zooplankton compartments (occasional high mortality for example) would scarcely have any effect on overall functioning of the system.

Such descriptions do not, of course, replace the dynamic models that describe the evolution of

490 a system more precisely, but they are much simpler and might be used for initial predictions and system diagnoses on responses to occasional perturbation. An example of such a perturbation might be pollution spreading in a physical system, or a phytoplankton bloom or,

constrastingly, an isolated mortality episode in an ecosystem model. Applying this idea to these two systems has shown, without heavy and time-consuming simulations, that any disturbance in the TA ecosystem would most certainly affect the DOC compartment, but would quickly disappear. A perturbation in PB however, might propagate and stay within the compartments surrounding the central island.

Transfer rates therefore give the total portion of the matter leaving the source that will arrive in the sink. This is also the definition of contribution coefficients, defined from a forward case point of view in flow network analysis (Kay et al. 1989). We have compared the values of transfer rates and contribution coefficients and obtained, as expected, the same results. Only for the return rates were they different, as our method allows a correction of the artificially augmented contribution of one compartment to itself. Indeed, contribution coefficients lead to consider as returning material the matter that has not left the compartment. With the present computation, we consider only the portion of matter that has left a compartment and returns to the same compartment. These coefficients also describe integrated links between compartments and are described as "integrative diets" of the compartments (Field et al. 1989, Kay et al. 1989, Baird & Ulanowicz 1989). The present study however also takes delay into account, by means of storage consideration in the computation of indices. The construction of Markov chains based on source compartment biomass makes the present computation a forward case as described by Kay et al. (1989) and further studied by Higashi et al. (1993). These authors showed the relationship that exists between the Markov transition probability matrix and the total flow matrices (Szyrmer & Ulanowicz 1987). They observed general properties of ecosystems and individual properties of their compartments based on infinite sums of powers of this matrix. Here, we use the same Markov transition probabilities to compute pairs of source and sink indices in a generalised mathematical algorithm. The transit time and transfer rate of one pair (source, sink) defines the integrated link between these two compartments as strong or weak and as fast or slow. The 2D space (Rates/Times) can thus be divided into four regions that classify the pairs (Figures 4 & 5).

Conclusion

Many indices have been developed in Network Analysis on the basis of economic studies by Leontief (1951) and Augustinovicz (1970), and applied in the ecological domain by Hannon (1973) and Finn (1976) and Patten (1985). The first formalism (output analysis, or backward point of view) is used to study the demand for matter, knowing the output of a system. The second formalism (input analysis, or forward point of view) studies the fate of system inputs.

The present study is of this second type (the forward case). Classical indices are based on the fractional outflow matrix, which is obtained by dividing each flow by the total output of the source compartment. It is used to compute contribution coefficients (Kay et al. 1989, Baird & Ulanowicz 1989), which describe the amount of matter flowing out of a compartment that

530   will eventually contribute to the diet of the consumer. Such indices integrate direct and indirect effects and are the classical network analysis equivalent of the transfer rates defined here. The use of Markov chains adds the notion of delay to the storage and flows. This is done by normalizing the flows by the biomass of the source compartments instead of by their outputs. In this way, at each step, matter can remain in its compartment. Then all possible pathways between compartments and delays due to the storage in compartments are taken into account in the computation of transit time and transfer rates.

Application of Markov Chains to describe flow-balanced network have already been published (Thompson et al. 2002, Higashi et al. 1993) but, to our knowledge, no general algorithm was previously presented to assess transit time, return time, first passage time and

540   transfer rate. In our paper we developed a general algorithm applicable to any flow-balanced ecological or physical network, using Markov transition probabilities and conditional probabilities. With two real case applications, we have shown that it is possible to build and exploit these indices to characterise: (1) the total indirect relationships between two compartments, (2) the residence time in one compartment and (3) the general recycling pathways, amount of matter recycling, and implication of each compartment in this phenomenon. We also gave some clues on how such holistic indices could be a substitute for more sophisticated models to assess system behaviour.

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Tables

Table 1: Takapoto model (Niquil et al. 2001). The abbreviations given in the 2nd column are used in the other results.

Compartments *in* Niquil et al. (2001)	Abbreviation used	Biomass (mgC/m²)
Cyanobacteria, assimilated to phytoplankton < 1 µm	PH1	308
Picoeukaryotes, or phytoplankton from 1 to 3 µm	PH2	126
Phytoplankton > 3 µm	PH3	323
Heterotrophic bacteria	BAC	477
Protozoa < 35 µm	PZ1	307
Protozoa > 35 µm	PZ2	498
Metazoan zooplankton < 250 µm	MIC	54
Metazoan zooplankton > 250 µm	MES	165
Detritus (non living carbon > 0.7 µm)	DOC	2789
Dissolved organic Carbon (< 0.7 µm)	POC	33400

Table 2: Food-web F and transition P matrices for Takapoto model. F_{ij} gives, in gC.m^{-2}.d^{-1}, the trophic flow from compartment j to compartment i (from Niquil *et al.* 2001), and P_{ij} gives, in percentage, the probability that a particle in j at t arrives in i at $t+\Delta t$. The arrows symbolize the source and target compartments of the links. In F matrix, the "gpp" column represents the gross primary production and "input" column the migrating inputs to the system. The "out" and "resp" lines represent respectively the output of matter from the system and the respiration losses. Compartments abbreviations used in the two matrices are explained in Table 1. In P matrix, the 11th compartment represents the exterior of the system (which is an absorbing state: $P_{11\,11} = 1$).

2a

F	gpp	input	PH1	PH2	PH3	BAC	PZ1	PZ2	MIC	MES	DOC	POC
PH1	768											
PH2	390											
PH3	407											
BAC											449	
PZ1			105	19	59	19	0				299	29
PZ2				33	73		78				313	43
MIC							56	39				93
MES		659		45	17		147	131	72			185
DOC			262	195	204		48.4	78	16	259		0
POC			363	0.03	0.51	55	53.5	53.4	51.9	299		0
out			0.03	0.03	0.51	0.01	0.49	0.79	0.09	263		526
resp			38.4	97.8	53.7	375	147	238	48	435		

2b

P	PH1	PH2	PH3	BAC	PZ1	PZ2	MIC	MES	DOC	POC	out
PH1	83.6										83.6
PH2		79.7									
PH3			91.7						0		
BAC				93.8					0.09		
PZ1	2.24	0.99	1.2	0.26	88.7				0.06	0.07	2.24
PZ2		1.72	1.48		1.67	92.9			0.06	0.1	
MIC					1.2	0.51	77.1			0.22	

MES		2.35	0.35		3.15	1.73	8.76	50		0.44	
DOC	5.58	10.2	4.14		1.04	1.03	1.95	10.3	99.8		5.58
POC	7.74		0.01	0.76	1.15	0.7	6.31	11.9		97.9	7.74
out	83.6										83.6

Table 3: *P* matrix for Passamaquoddy Bay system (from Thompson et al. 2002). P_{ij} gives, in percentage, the probability that a particle in *j* at *t* arrives in *i* at $t+\Delta t$, Δt being one day (the arrow indicates the source and target compartments). The 16th compartment is the exterior of the system.

P	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	99	1														
2	1	96	3													
3		3	91	3				1								
4			6	89				5					3			
5					96	2	2									
6						97	3									
7						1	70	5	2	10						
8				4	4		9	82		1			2			
9									93							
10							9	5	3	78			3	12	1	
11											99	1				
12											1	96		1	6	
13				4									75	13		
14										3			17	72	4	
15												3		2	80	
16							7	2	2	8					9	100

Table 4: Transit times (T, in days) and Transfer rates (R, in percent) for TA model from sources (columns) to targets (lines). The last line of the Transit times matrix gives the Residence times of the compartments, '-' signs mean that no transit time can be computed because no matter is transferred to those compartments. Compartment abbreviations are given in Table 1. Fast transit times (less than 10 days) are coloured in dark grey, and strong (15% of the highest transfer rates) and mean (20 following percent) transfer rates are coloured in dark and light grey, respectively.

T (d)	PH1	PH2	PH3	BAC	PZ1	PZ2	MIC	MES	DOC	POC
PH1	-	-	-	-	-	-	-	-	-	-
PH2	-	-	-	-	-	-	-	-	-	-
PH3	-	-	-	-	-	-	-	-	-	-
BAC	36.7	36.3	36.4	38.9	36.8	36.5	36.9	36.6	4.7	37.0
PZ1	15.5	26.6	18.8	2.7	31.2	31.7	29.2	31.1	2.6	14.5
PZ2	26.0	22.8	16.6	12.6	10.2	30.3	27.0	29.5	2.2	11.0
MIC	13.7	27.8	21.9	5.1	4.5	6.7	12.6	17.1	6.2	1.9
MES	13.4	16.1	17.2	3.9	3.1	4.3	2.2	17.4	4.4	0.9
DOC	0.5	0.1	0.2	2.7	0.6	0.3	0.7	0.4	1.4	0.8
POC	4.7	24.8	22.3	0.5	5.5	6.8	3.0	5.4	5.4	5.0
Out	18.1	21.9	23.6	2.3	9.9	10.2	9.2	9.7	38.3	7.0

R (%)	PH1	PH2	PH3	BAC	PZ1	PZ2	MIC	MES	DOC	POC
PH1	0	0	0	0	0	0	0	0	0	0
PH2	0	0	0	0	0	0	0	0	0	0
PH3	0	0	0	0	0	0	0	0	0	0
BAC	19.9	26.9	28.1	1.0	10.5	10.8	9.5	11.0	48.5	4.2
PZ1	27.7	22.8	32.5	5.0	7.8	7.9	7.6	8.2	32.6	6.2
PZ2	19.7	29.0	40.0	2.0	22.6	9.2	9.2	9.6	36.7	8.7
MIC	11.0	6.5	8.7	2.2	15.5	10.9	6.0	4.8	8.5	12.7
MES	28.1	28.8	28.8	5.4	43.1	34.2	48.5	12.0	24.5	29.4
DOC	41.1	55.5	58.1	2.0	21.6	22.2	19.6	22.7	13.5	8.7
POC	57.8	16.4	19.2	13.4	27.2	22.4	40.0	27.9	19.9	12.1
Out	100	100	100	100	100	100	100	100	100	100

Table 5: Transit times (*T*, in days) and transfer rates (*R*, in percent) for PB model from sources (columns) to targets (lines). The last line of the transit times matrix gives the residence times of the compartments, '-' signs mean that no transit time can be computed because no matter is transferred to those compartments. Compartment abbreviations are given in Table 1. Fast transit times are coloured in dark grey, and strong (15 first percents of the pairs) and mean (20 following percent) transfer rates are coloured in dark and light grey, respectively.

T (days)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	25	13	31	43	51	63	59	48	62	60	114	101	56	61	78
2	0	28	6	18	26	38	34	23	36	35	89	76	31	36	53
3	34	21	23	6	14	26	22	12	25	23	77	64	20	24	41
4	59	46	20	19	12	23	19	9	22	20	71	58	12	18	35
5	108	95	69	45	33	2	16	30	20	21	81	69	33	30	45
6	101	88	62	38	26	26	9	23	13	13	74	62	26	23	38
7	90	78	51	27	15	15	15	12	2	3	64	51	16	13	28
8	80	67	41	17	0	12	8	18	11	10	68	56	15	16	32
9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10	90	78	52	28	20	27	14	17	5	14	59	46	11	8	23
11	119	106	80	56	64	73	63	61	55	46	18	5	35	29	19
12	101	88	62	38	46	56	46	43	37	29	0	27	17	11	1
13	82	70	43	19	32	43	36	29	31	25	60	47	12	5	24
14	88	75	49	25	33	43	33	30	24	16	52	40	4	10	17
15	111	98	72	48	56	65	55	53	47	38	34	21	27	21	32
16	157	107	74	49	46	56	26	33	23	20	111	61	33	30	28

R (%)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	38.1	38.1	17.5	7.2	4.0	3.4	2.3	4.0	1.3	1.5	0.7	0.7	2.7	2.0	0.7
2	100	59.5	46.0	18.9	10.5	9.0	5.9	10.5	3.3	3.9	1.7	1.7	7.1	5.1	1.7
3	100	100	60.8	41.2	22.9	19.6	12.9	22.9	7.3	8.4	3.8	3.8	15.4	11.1	3.8
4	100	100	100	56.0	45.1	38.5	25.4	45.1	14.5	16.9	8.0	8.0	33.8	23.8	8.0
5	12.4	12.4	12.4	12.4	13.5	73.9	21.7	13.5	11.3	11.9	3.9	3.9	11.4	10.8	3.9
6	9.4	9.4	9.4	9.4	10.2	12.3	16.5	10.2	8.6	9.1	3.0	3.0	8.6	8.2	3.0
7	57.3	57.3	57.3	57.3	62.2	74.8	46.8	62.2	52.2	55.1	18.2	18.2	52.4	49.9	18.2
8	73.6	73.6	73.6	73.6	100	85.2	55.7	49.8	31.0	35.1	13.5	13.5	47.1	38.4	13.5
9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	78.6	78.6	78.6	78.6	71.5	68.7	63.1	71.5	60.9	43.7	31.7	31.7	85.6	86.0	31.7
11	2.1	2.1	2.1	2.1	1.2	1.1	0.8	1.2	0.6	0.9	33.0	33.0	3.0	3.7	10.7
12	6.3	6.3	6.3	6.3	3.6	3.2	2.5	3.6	1.9	2.8	100	49.3	9.1	11.3	32.4
13	66.5	66.5	66.5	66.5	33.0	28.9	20.5	33.0	13.8	18.5	17.4	17.4	51.1	56.2	17.4
14	56.0	56.0	56.0	56.0	31.8	28.5	22.0	31.8	17.0	25.1	30.4	30.4	80.3	51.3	30.4
15	11.5	11.5	11.5	11.5	6.5	5.9	4.5	6.5	3.5	5.2	100	100	16.5	20.6	34.4
16	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100

Table 6: Return times, return rates, average number of passages and residence times of TA compartments. Compartments are ordered by decreasing return rates.

Compartment	Return Time (d)	Return Rate (%)	Number of passages	Residence Time (d)
DOC	1.4	13.5	0.18	38.3
POC	5.0	12.1	0.16	7.0
MES	17.4	12.0	0.15	9.7
PZ2	30.3	9.2	0.11	10.2
PZ1	31.2	7.8	0.09	9.9
MIC	12.6	6.1	0.07	9.2
BAC	38.9	1.0	0.01	2.3
PH1	-	-	-	18.1
PH2	-	-	-	21.9
PH3	-	-	-	23.6

Table 7: Return times, return rates, average number of passages and residence times of PB compartments. Compartments are ordered by decreasing return rates. The return times are given in days.

Compartment	Return Time (d)	Return Rate (%)	Number of passages	Residence Time (d)
3	46	60.8	4.0	73.8
2	55	59.5	3.6	107.1
4	37	55.9	2.9	48.8
14	20	51.3	2.2	29.8
13	23	51.1	2.1	33.1
8	36	49.8	2.0	33.2
12	54	49.3	1.9	61.1
7	30	46.8	1.7	26.2
10	28	43.7	1.4	19.7
1	50	38.2	1.0	157.1
15	64	34.4	0.8	27.8
11	35	33	0.7	111.1
5	65	13.5	0.2	45.7
6	51	12.3	0.2	55.8
9	-	0	0.0	23.1

Figure 1: Theoretical example used for the explanation of the indices computation. This example counts 4 compartments, which can be compartments of a trophic web: 1 for phytoplankton, 2 for bacteria, 3 for detritus and 4 for zooplankton.

Figure 2: Presentation of the two case studies. 2a) Graph of Takapoto ecological network (Niquil et al., 2001). PH1: cyanobacteria, assimilated to phytoplankton < 1 μm, PH2: picoeukaryotes, or phytoplankton from 1 to 3 μm, PH3: phytoplankton > 3 μm, BAC: heterotrophic bacteria, PZ1: protozoa < 35 μm, PZ2: protozoa > 35 μm, MIC: metazoan zooplankton < 250 μm, MES: metazoan zooplankton > 250 μm, DOC: detritus (non living carbon > 0.7 μm), POC: dissolved organic carbon (< 0.7 μm). 2b) Boundaries of the 16 regions of Passamaquody Bay. Region 16 represents the adjacent open ocean and is an absorbing boundary state for the Markov Chain (Thompson et al. 2002).

Figure 3: Probability that a particle leaving a source compartment has reached the target compartment in TA model after the time delay given in abscissa (in days). Figure 3a represents the strong pairs: (PH3, DOC) (fast) and (PH3, BAC) (slow), and Figure 3b represents the weak pairs: (BAC, MES) (fast) and (MES, MIC) (slow). See Figure 2a for the abbreviations.

Figure 4: Probability that a particle leaving a source compartment has reached the target compartment in PB model after the time delay given in abscissa (in days). Figure 4a represent the strong pairs: (6, 8) (fast) and (1, 10) (slow), and Figure 4b represents the weak pairs: (13, 12) (fast) and (1, 5) (slow). The region numbers are given in Figure 2a.

Figure 5: Representation of transfer rate vs. transit times for TA pairs. The space can be divided into various regions: low/mean/strong pairs according to the value of the transfer rate, and slow/fast couple according to the value of the transit times. See Figure 2a for the abbreviations.

Figure 6: Integrated network based on strong and mean links between compartments of TA model. The strong links are represented in bold, fast ones in lines, and slow ones in dashed lines. In Figure 6a, all the mean links are represented in dotted lines (see Figure 2a for the

abbreviations). Figure 6b represents the simplified network, and only the mean fast links are represented in dotted lines.

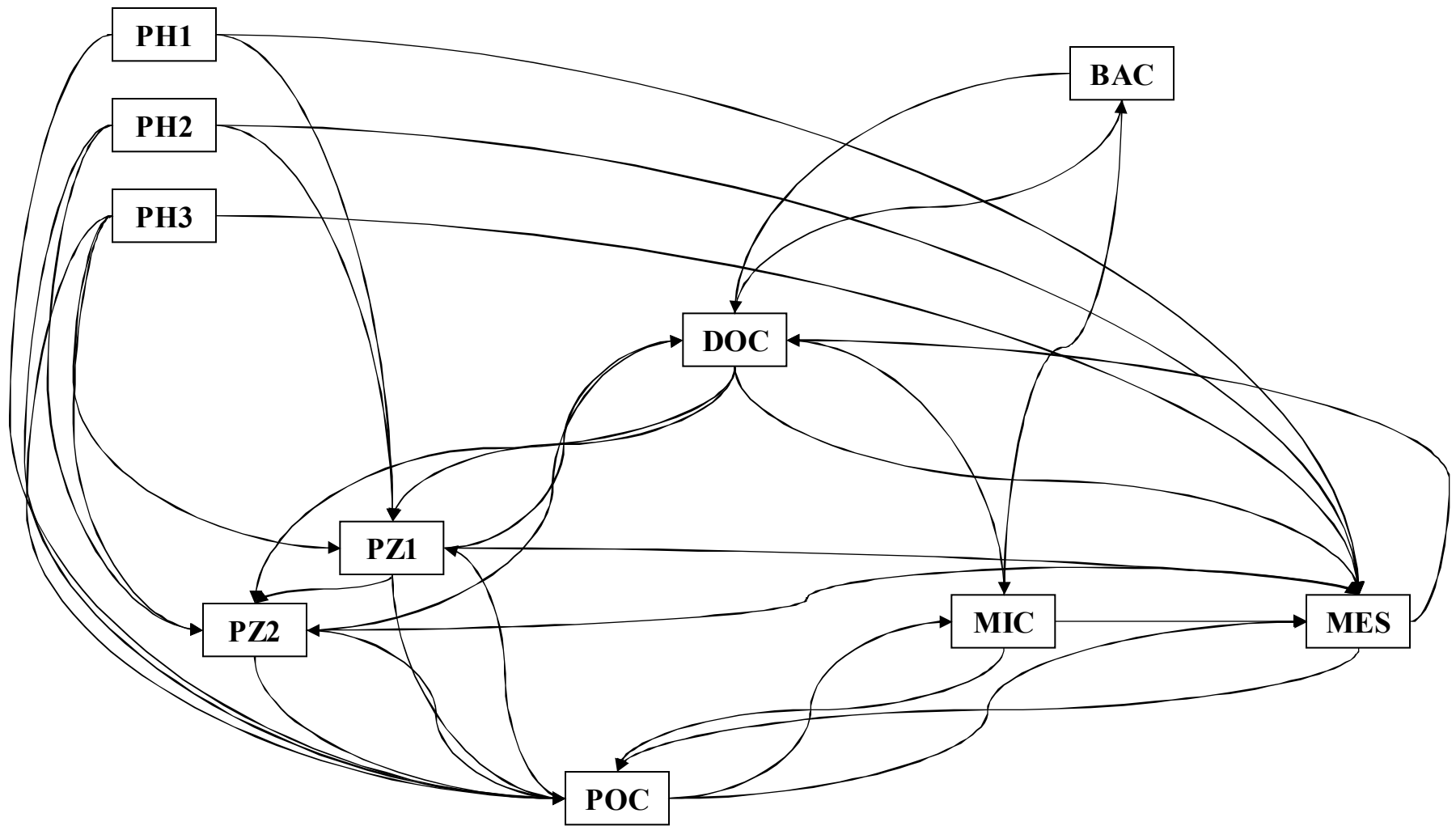**Figure 7:** Integrated network based on strong and mean links between compartments of PB model. The strong links are represented in bold, fast ones in lines, and slow ones in dashed lines. In Figure 7a, all the mean links are represented in dotted lines. Figure 7b represents the simplified network, and only the mean fast links are represented in dotted lines.

Figure

1a

1

R_{41}

P'_{12}

P'_{42}

4

2

P'_{ext2}

R_{43}

P'_{32}

3
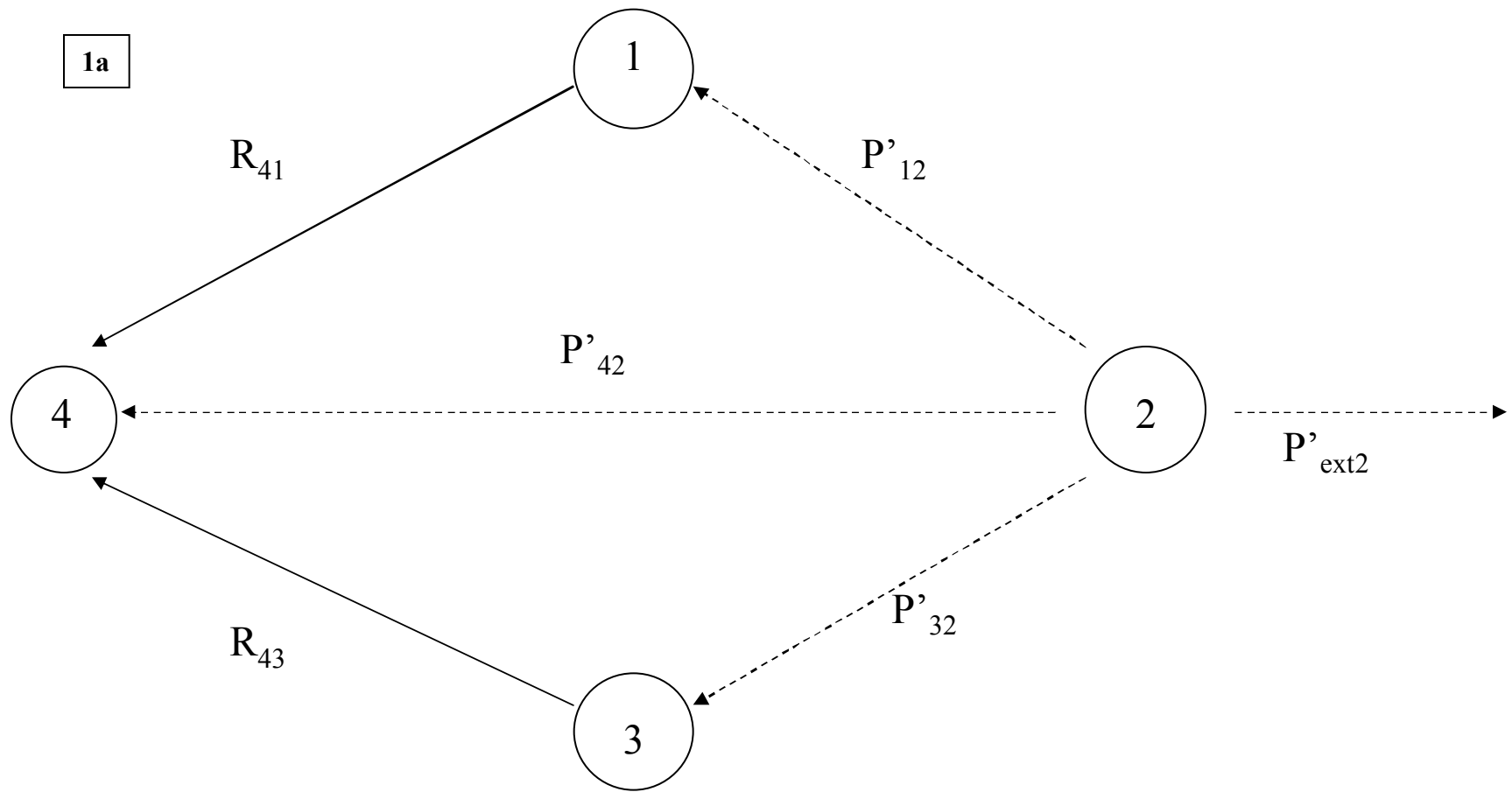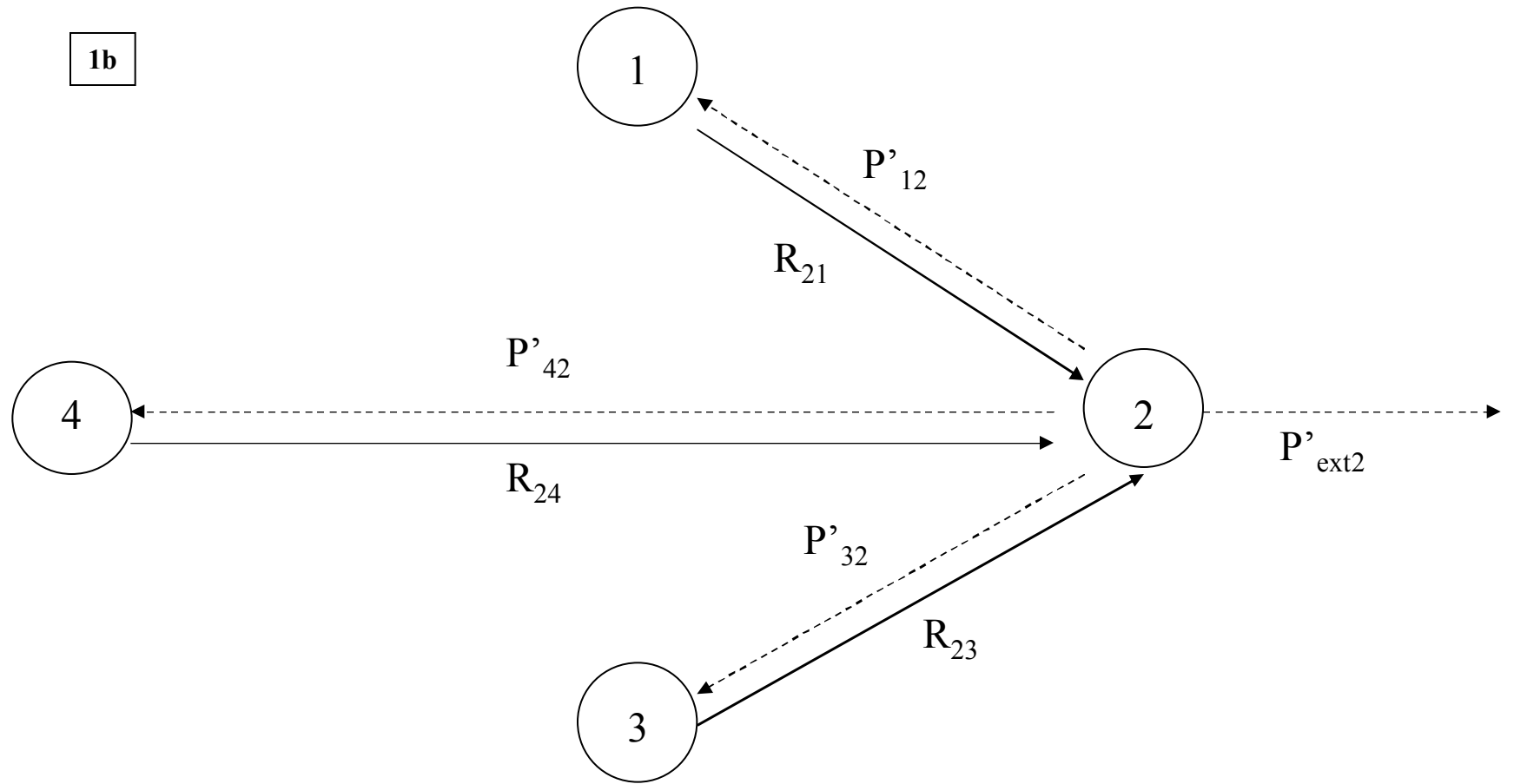
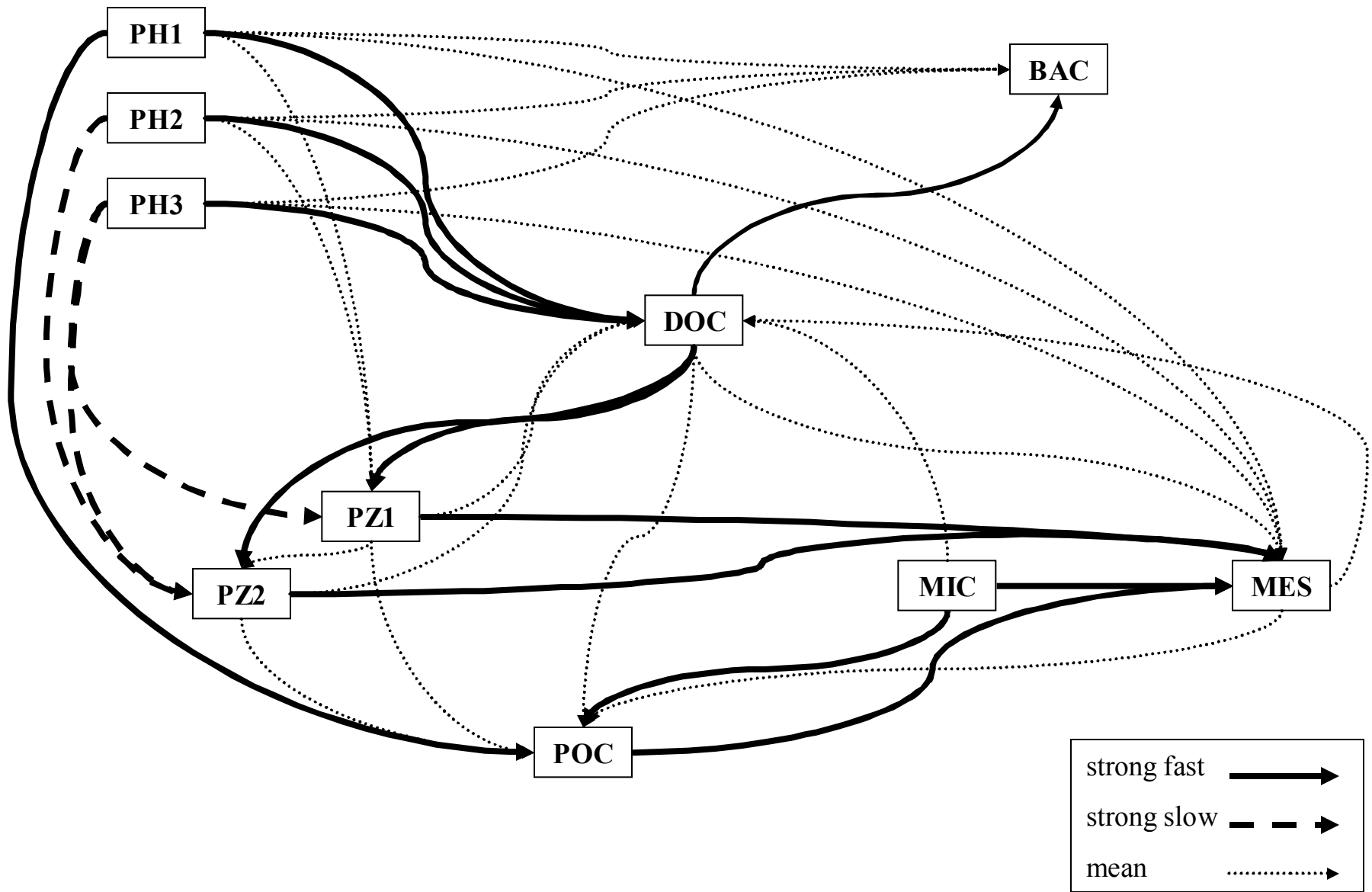Figure 1a

Figure 1b

Figure 2a
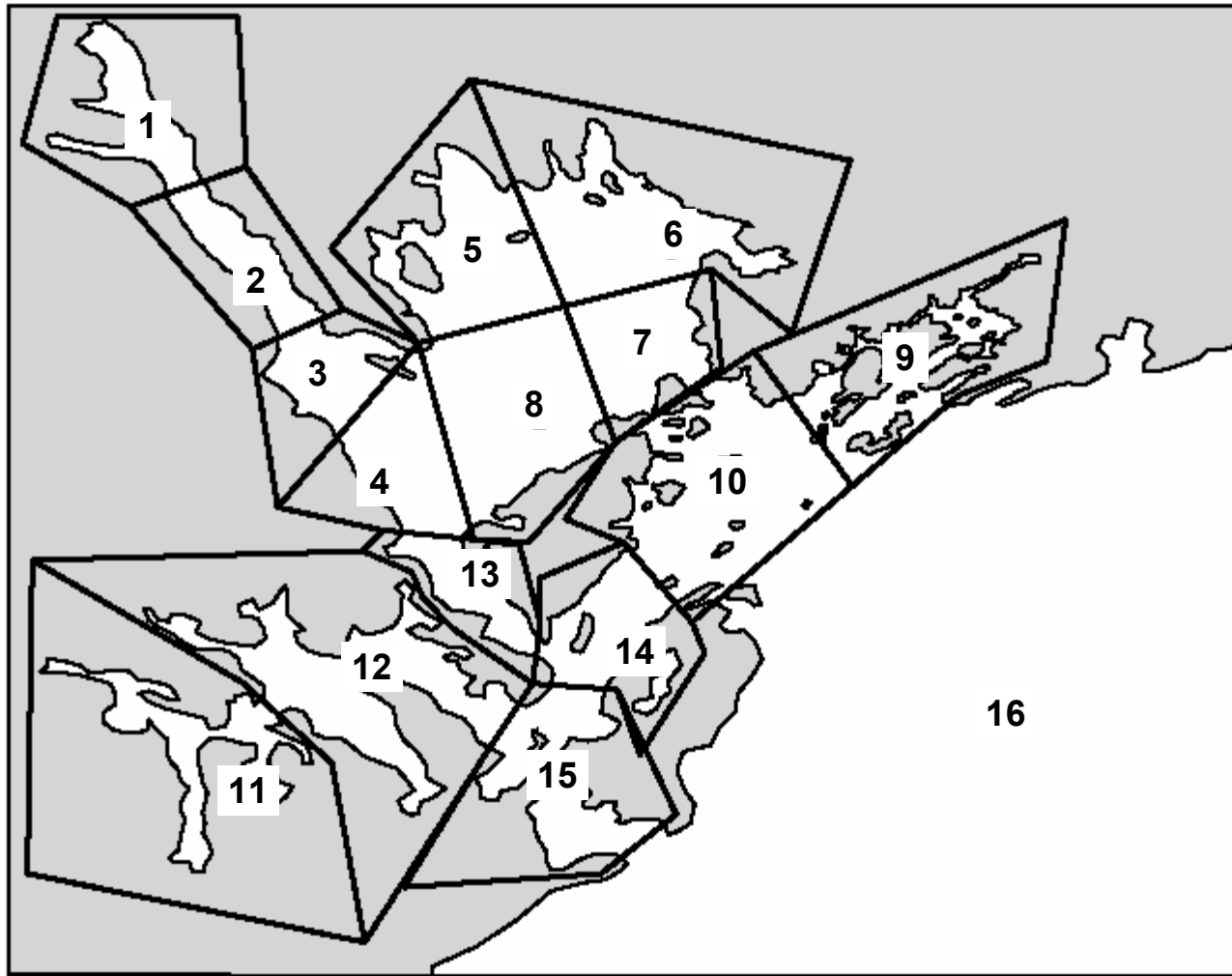
Figure 2b
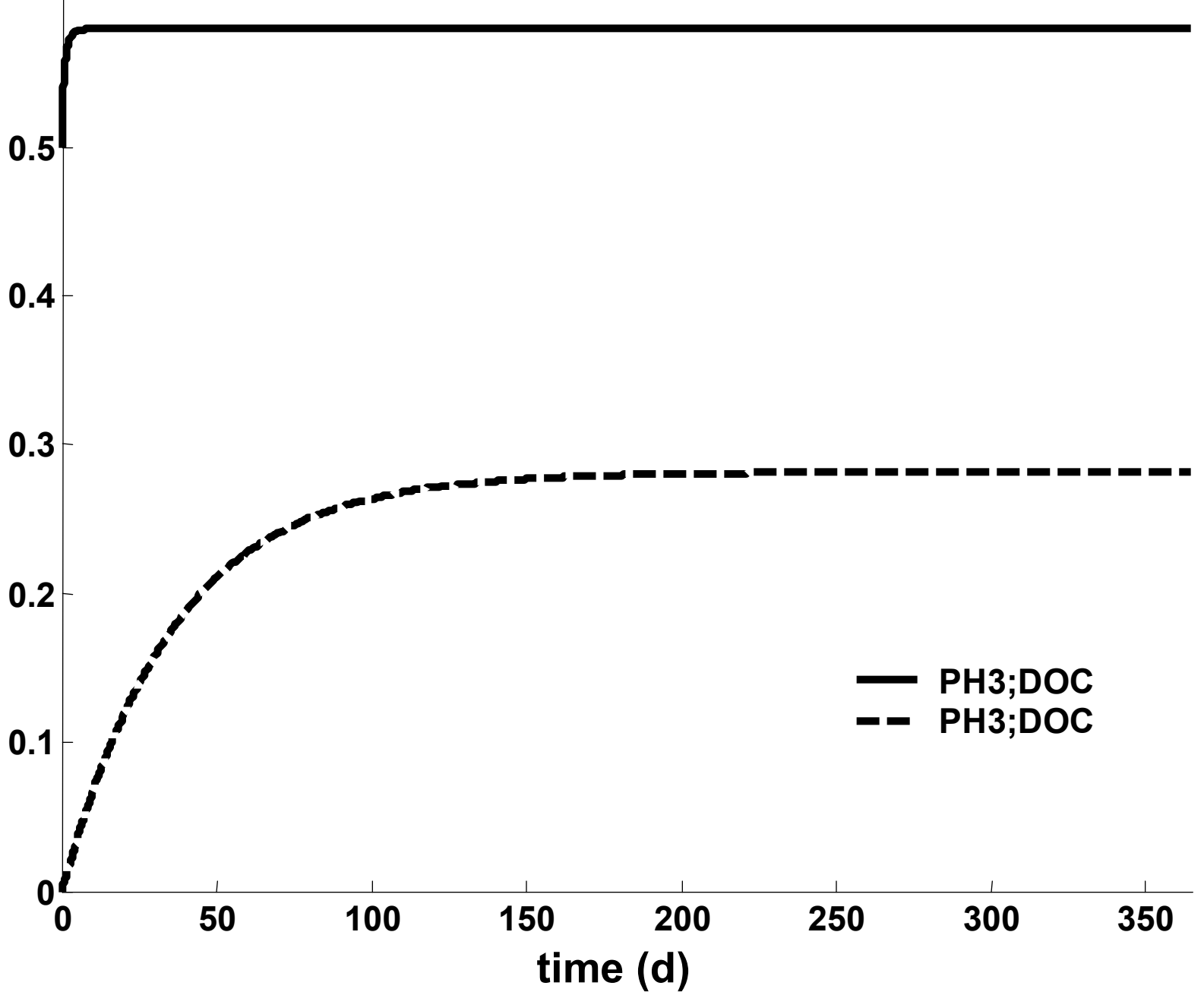
Figure 3a
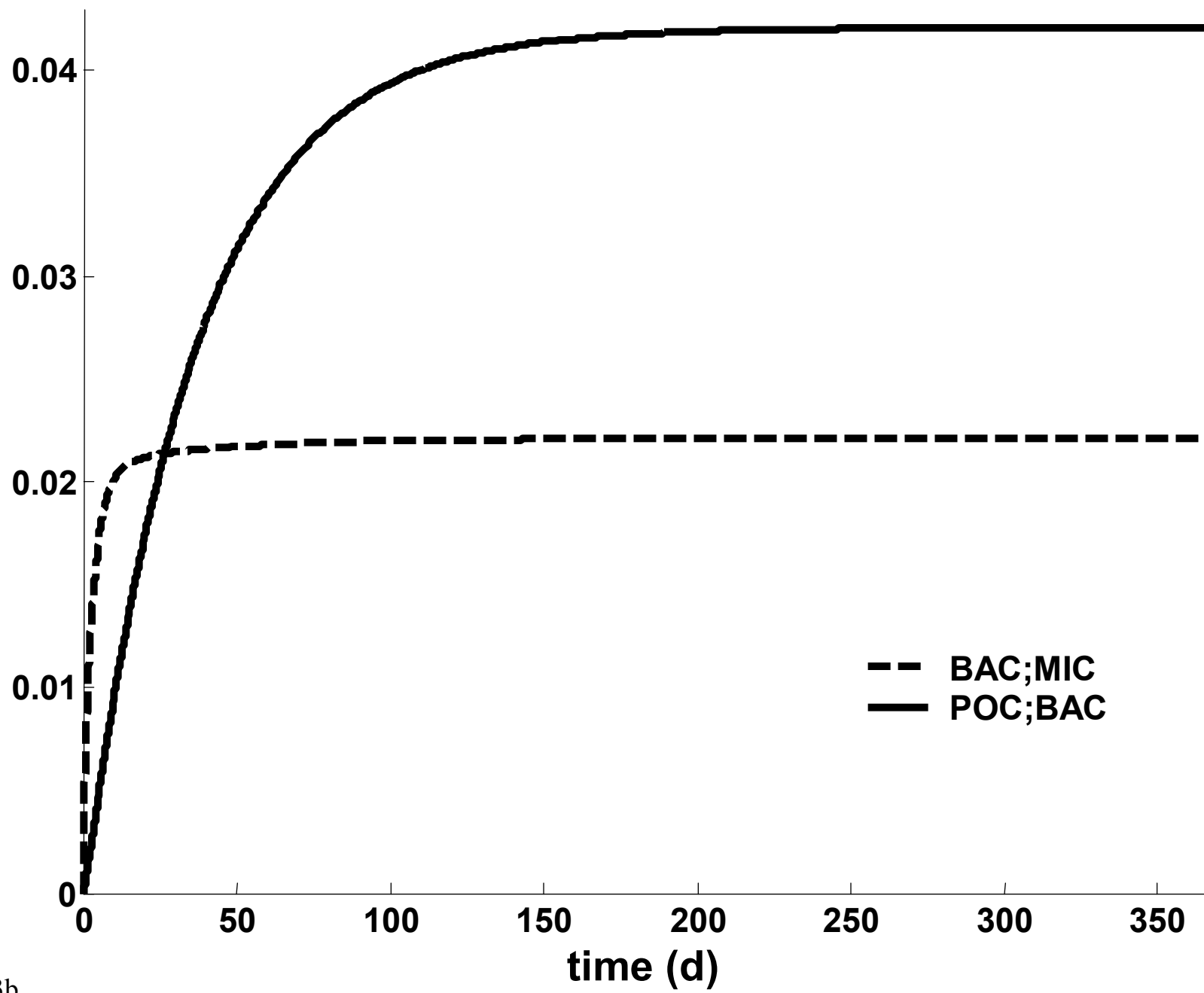
Figure 3b
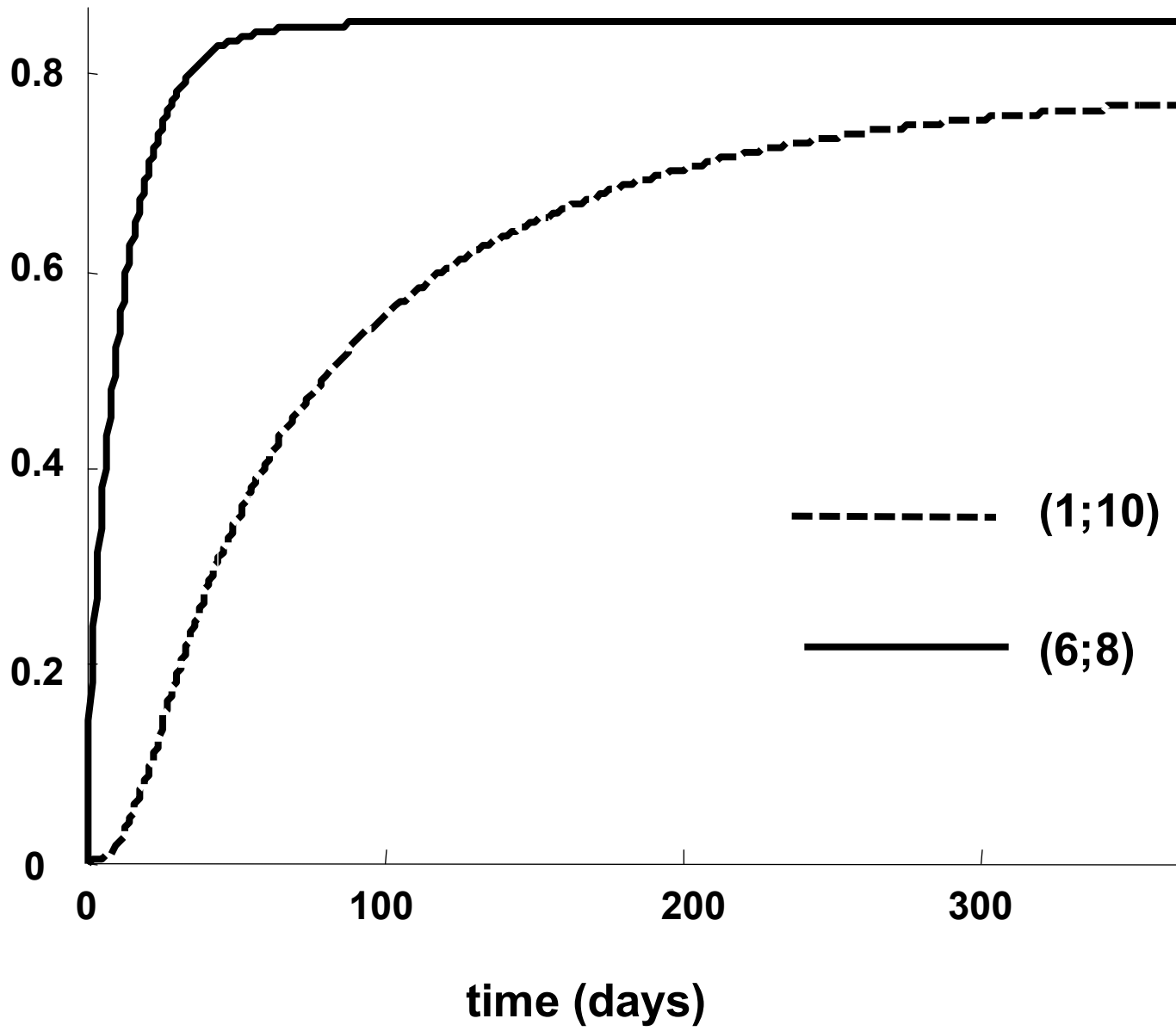
Figure 4a
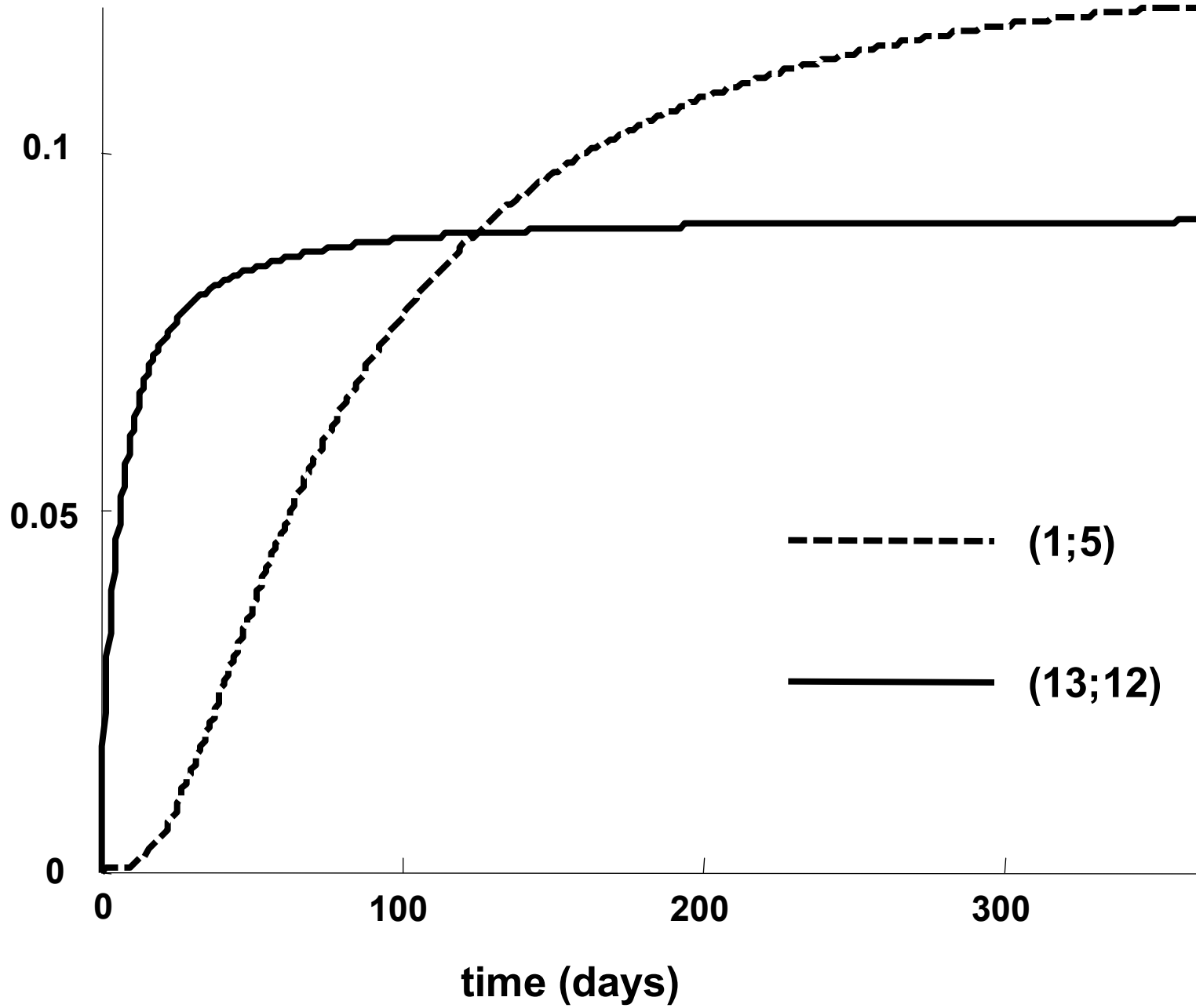
Figure 4b

Figure 5

Figure 6a

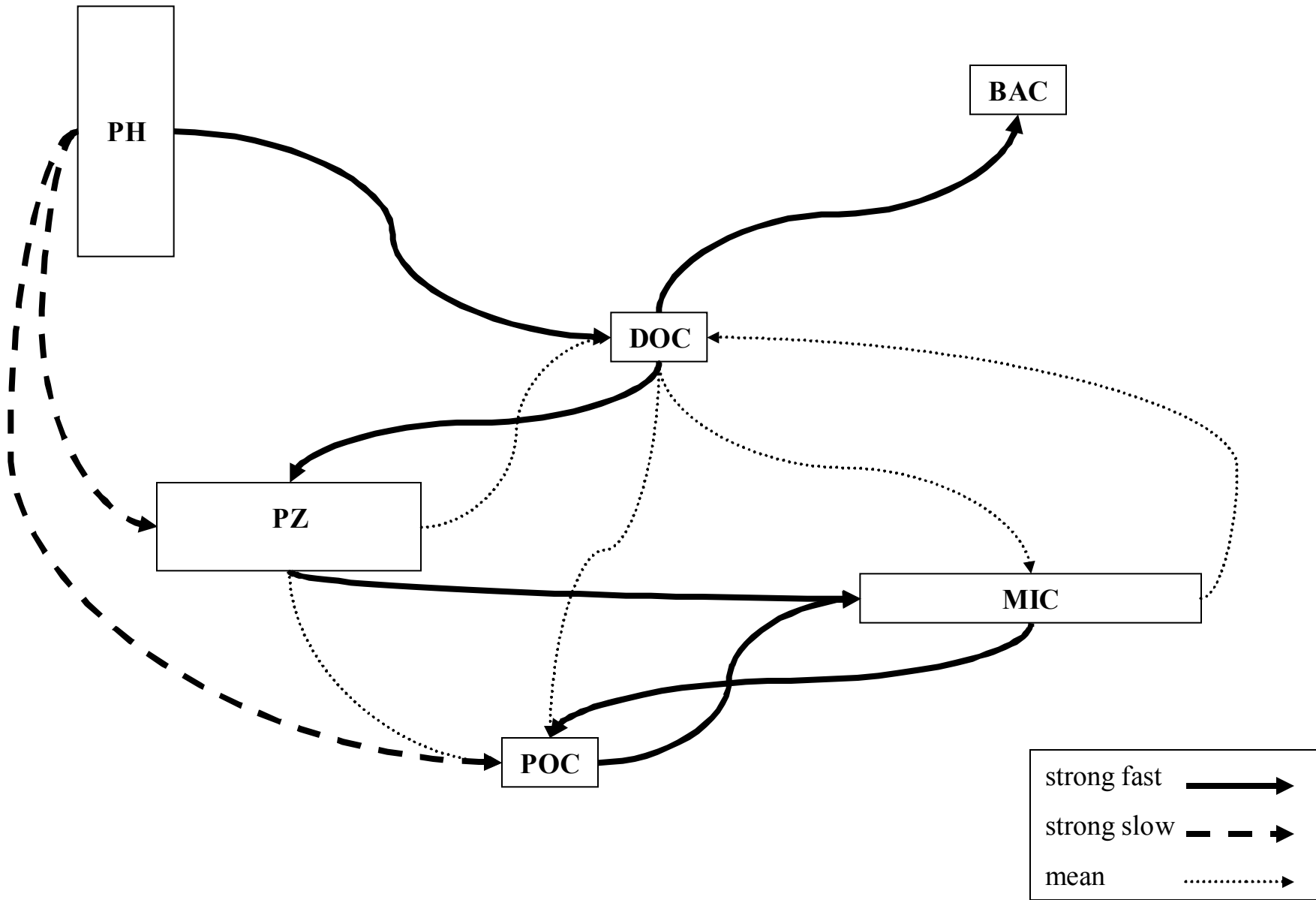PH

BAC

DOC

PZ

MIC

POC

strong fast
strong slow
mean

Figure 6b

Figure 7a

strong fast
strong slow
mean

Figure 7b