# Time Integrated Compartment Models

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## 1 INTRODUCTION

A compartment is defined as a well-delineated biotic or abiotic entity, e.g., the A-horizon of the soil, the canopy in a forest, or the sediment of a lake. In the following discussion, models will be presented that conform to this definition by providing a mathematically simple treatment of the very complex flow of a pollutant through an ecosystem.

The simplification of compartment models exists because distribution inside a compartment is not included. The basic assumption is that a chemical will be homogeneously mixed inside a compartment, resulting in knowing everything about a system's behavior, when the inflow and outflow for each compartment are identified.

In working with compartment models, two fundamental problems need to be addressed: (1) the identification of each relevant compartment; and (2) estimation of flows among compartments.

The second issue, namely the estimation of the flows between compartments, is usually the most difficult to resolve, since data often are so scarce as to give unreliable estimations of the parameters in a model. A method to overcome this problem is to indicate that the dynamic behavior of the system is unimportant, and that the total loading or intake during all times in each compartment are deterministic. This approach is called time-integration, or dose-commitment.

The dose-commitment method was originally proposed by Lindell (1960; 1978) in connection with prediction of radioactive fall-out from nuclear bomb testing. This method was also used by UNSCEAR (1977). Later this method was developed into a more general approach for chemicals introduced in the environment (MARC, 1977; Barry, 1979; O'Brien, 1979; Miller and Buchanen, 1979).

The objective of the dose-commitment method is to estimate the total loading of a pollutant in each compartment of the system under consideration.

If the input flux from the environment at a given time $t$ to compartment $j$ is given by $F_{0j}(t)$, and if it is assumed that the compartment does not receive any amount of a pollutant from any other compartment in the system, then the total loading or intake to the compartment is given by

$$I_j = \int_0^\infty F_{0j}(t)\,dt \qquad (1)$$

If the concentration in compartment $j$ is given by $x_j(t)$, then the exposure in compartment $j$ is given by

$$E_j = \int_0^\infty X_j(t)\,dt \qquad (2)$$

Consider the following simple compartmental system. The amount injected into compartment 2 at a small time interval $dt$ is given by $F_{12}(t)dt$. Focusing on this increment of loading into compartment 2, then at a given time later than $t$, (e.g., $t + s$, $s \geq 0$), the following is obtained

$$R_2(s)\, F_{12}(t)\,dt \qquad (3)$$

where $R_2(s)$ is called the retention function of compartment 2. This function is defined for each compartment and fulfills the following conditions:

(a)  $R_j(u) = 0$ for $u < 0$ $\qquad\qquad$ (4)

(b)  $R_j(0) = 1$

(c)  $R_j(u) \leq R_j(v)$ if $u > v$

(d)  $R_j(+\infty) = 0$ if and only if $C_j$ is not a sink

By using the flux into compartment 2 and the retention function of compartment 2, the amount of pollutant in compartment 2 at a given time $t$ is calculated as

$$Q_2(t) = \int_0^t R_2(t-s)F_{12}(s)\,ds \qquad (5)$$

The concentration in compartment 2 is denoted $X_2(t)$, and this can accordingly be calculated as

$$X_2(t) = Q_2(t)/M_2 \qquad (6)$$

where $M_2$ is defined as the mass of compartment 2, which then gives

$$X_2(t) = M_2 \int_0^t R_2(t-s)F_{12}(s)\,ds \qquad (7)$$

If the flux from compartment 1 to compartment 2 is linear and donor controlled then

$$F_{12}(t) = K_{12}Q_1(t) = K_{12}\frac{X_1(t)}{M_1} \tag{8}$$

which gives

$$X_2(t) = \frac{M_2 K_{12}}{M_1} = \int_0^t R_2(t-s)X_1(s)ds \tag{9}$$

If we define the following as the transfer function between compartments 1 and 2:

$$T_{12}(t) = \frac{M_2 K_{12}}{M_1} R_2(t) \tag{10}$$

then

$$X_2(t) = \int_0^t T_{12}(t-s)X_1(s)ds \tag{11}$$

From these preliminary formulas, the formulas for exposure and intake into the compartments can be defined. The exposure in compartment 1 is defined as

$$E_1 = \int_0^\infty X_1(t)dt \tag{12}$$

while the intake from compartment 1 to compartment 2 is given by

$$I_{12} = \int_0^\infty F_{12}(t)dt \tag{13}$$

By using equation (9), the exposure commitment to compartment 2 is found to be

$$E_2 = \int_0^\infty X_2(t) = \int_0^\infty \int_0^t T_{12}(t-s)X_1(s)ds\,dt \tag{14}$$

if the integration variables are shifted to $u = t-s$, $v = s$, and if it is noted that $T_{12}(t-s) = 0$ for $s > t$ which permits integration to infinity in the inner integration we obtain:

$$E_2 = \int_0^\infty \int_0^\infty T_{12}(u)X_1(v)dv\,du \tag{15}$$

$$= \int_0^\infty T_{12}(u)\mathrm{d}u \int_0^\infty X_1(v)\mathrm{d}v$$

$$= T_{12}E_1$$

where the transfer coefficient $T_{12}$ is defined as

$$T_{12} = \int_0^\infty T_{12}(u)\mathrm{d}u \tag{16}$$

As defined earlier, the transfer function is up to a proportionality constant identical to the retention function. In other words, if the retention coefficient is defined as

$$R_2 = \int_0^\infty R_2(s)\mathrm{d}s \tag{17}$$

then the following relation between the transfer coefficient and the retention coefficient is found:

$$T_{12} = \frac{M_2 K_{12}}{M_1} R_2 \tag{18}$$

The retention coefficient has a well-defined physical interpretation, since it is the mean residence time in the compartment (O'Brien, 1979).

By integrating the formulas and shifting the integration variables, the following formula is derived:

$$E_2 = \int_0^\infty X_2(t)\mathrm{d}t \tag{19}$$

$$= \frac{1}{M_2} \int_0^\infty \int_0^t R_2(t-s)F_{12}(s)\mathrm{d}s$$

$$= \frac{1}{M_2} \int_0^\infty R(u)\mathrm{d}u \int_0^\infty F_{12}(s)\mathrm{d}s$$

$$= \frac{R_2 I_{12}}{M_2}$$

By means of this formula, a relation between the exposure commitment and the intake commitment is established.

In a steady state situation, when $X_i(t) = X_i t$, equation (13) cannot be used, since the integration in both numerator and denominator will take the value $+\infty$. If equation (9) is used, one obtains

$$X_2^* = \int_0^t T_{12}(t-s)X_1^* ds \tag{20}$$

and if $t \to +\infty$ in this equation, the following relation is obtained for the transfer coefficient in the steady state situation:

$$T_{12} = X_2^*/X_1^* \tag{21}$$

The underlying assumption during the calculations leading to the formulas (14), (16), (17), and (19) is that the compartmental model is linear and donor controlled.

For a longer sequence of compartments, it is possible to derive transfer coefficients, according to the means of connecting individual compartments. The following three examples illustrate this point. For example, under steady state assumptions and by repetitive use of equation (19), it is possible to derive the following formula:

$$T_{ij} = T_{j-1j}\, T_{j-2j-1} \ldots T_{i+1,i+2}\, T_{i,i+1} \text{ for } i<j \tag{22}$$

which works as a definition for the transfer coefficient between compartment $i$ and compartment $j$, when the compartments are connected in a chain. The transfer coefficient between compartment 1 and compartment $n$ can be estimated if the steady state concentrations of the two compartments are known.

In the second example, a more complicated compartmental structure is introduced. A situation is examined where some of the material between compartments 2 and 3 is going through another compartment. Assuming steady state conditions,

$$X_3^* = T_{12}(T_{23} + T_{24}T_{43})X_1^* \tag{23}$$

which could be referred to as a situation with parallel pathways (O'Brien, 1979; Miller and Buchanen, 1979).

In both examples, the steady state concentration in each compartment could be replaced by the exposure commitment, if the pulse of given pollutant is used. In the next section, the dynamic behaviour of the compartmental system of example 2 will be considered.

The following is an example in which a loop is present in the compartmental system. In this example, it is necessary to take into consideration that some of the pollutant is recycled through compartment 5.

It is found that

$$X_4^* = T_{12} \frac{T_{23}}{1 - T_{23}T_{35}T_{52}} T_{34}X_1^* \tag{24}$$

$$= \frac{T_{14}}{1 - T_{23}T_{35}T_{52}} X_1^*$$

This relation is established by noting

$$X_3^* = T_{23}X_2^* \tag{25}$$

$$X_2^* = T_{12}X_1^* + T_{35}T_{52}X_3^*$$

which gives

$$X_3^* = T_{23}T_{12}X_1^* + T_{23}T_{35}T_{52}X_3^* \tag{26}$$

and the relation is easily found. Thus, it is possible to derive relations between the steady state concentration or exposure commitment and the transfer coefficients, for a given compartment system under consideration.

The time-integrated approach proves useful in cases where the interest lies not in the dynamics of the system, but rather in overall intake or loading to the compartments in the system. The exposure commitment, the transfer coefficients, and the intake commitments to each compartment prove to be key parameters, and these can often be estimated in cases where data are too scarce to allow estimation of the parameters in a more detailed dynamic model. In cases of steady state, the concentration in each compartment can be used to estimate the transfer coefficient between compartments, even in rather complex systems where recycling occurs.

In some instances, however, it is impossible to ignore the dynamic behaviour of a system. This is the case if the system is unaffected by the total input of a pollutant, but what matters is whether or not the concentration in a specified compartment reaches levels beyond a certain critical level. In this case, the requirement is to identify not the total loading to a compartment (which could be $+\infty$ without harm) but the peak value.

## 2 TIME-DEPENDENT COMPARTMENT MODELS

The idea of using compartment models to describe the dynamics of "matter" through a series of "black boxes" is not new. The first examples of utilising this approach dates back to the 1920's (Hevesey, 1923).

Around 1960, this approach began to develop very quickly, aided by the evolution of computers. Standard textbooks on compartment models include those by Atkins (1969) and by Jacquez (1972). Numerous textbooks developed the theory for employing compartment models to model the dynamic behaviour of pollutants in ecosystems (Butler, 1978; Neely, 1980;

Dickson *et al.*, 1982) or to describe the biogeochemical cycles in an ecosystem (Hutzinger, 1985).

Consider in a general *n*-compartment system, where for each pair of compartments $(i, j)$, $i \neq j$, following possible flows can be estimated. The basic equation for the transfer between the compartments is given as

$$\frac{dx_i}{dt} = \sum_{\substack{j=0 \\ j \neq i}}^{n} F_{ji}(t) - \sum_{\substack{j=0 \\ j \neq i}}^{n} F_{ij}(t) \qquad (27)$$

This basic mass balance equation provides an introduction to the deterministic compartment models. It says that when the initial concentration of each compartment is given, everything about the dynamic behaviour of the system in the future is known.

The simplest possible model is obtained by assuming that the input from the exterior is constant with time, and that the flow between each compartment is linear and donor controlled:

$$F_{ij}(t) = \quad F_{0j} \qquad \text{if } i = 0 \qquad (28)$$
$$= k_{ij}x_i(t) \quad \text{if } i \neq 0$$

which gives the following equations:

$$\frac{dx_j}{dt} = F_{0j} + \sum_{i=1}^{n} k_{ij}x_i(t) - (\sum_{i=0}^{n} k_{ij})x_j(t) \qquad (29)$$

This equation can be made more compact by utilising a matrix notation:

$$\frac{dx}{dt} = Ax + B \qquad (30)$$

where

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \qquad \frac{dx}{dt} = \begin{bmatrix} dx_1/dt \\ dx_2/dt \\ dx_3/dt \\ \cdot \\ \cdot \\ \cdot \\ dx_n/dt \end{bmatrix} \qquad B = \begin{bmatrix} F_{01} \\ F_{02} \\ F_{03} \\ \cdot \\ \cdot \\ \cdot \\ F_{on} \end{bmatrix} \qquad (31)$$

and $A$ is a matrix with elements $a_{ij} = k_{ji}$ outside the diagonal end:

$$a_{ij} = - \sum_{j=0}^{n} k_{ij} \qquad (32)$$

It is has been proved in Jacquez (1972) that under these conditions, a steady state exists, and is given by

$$X^* = -A^{-1}B \qquad (33)$$

In the case of zero input into the compartments (e.g., when the system under consideration consists of a pulse to one or more compartments at time $t = 0$, and the effect of this pulse on the other compartments is studied), then it is simple to give the dynamic behaviour until steady state is achieved. If it is assumed that $A$ has distinct eigenvalues $(\lambda_1, \lambda_2,...., \lambda_n)$ with corresponding eigenvectors $(e_{-1}, e_{-2},....,e_{-n})$, the solution is provided by

$$x(t) = \sum_{i=1}^{n} c_i\, e_i\, e^{\lambda_i t} \qquad (34)$$

where $c_i$ is determined by the initial conditions.

In the case of non-zero input to some of the compartments, it is also possible to find analytical solutions which give the dynamic behaviour until steady state is achieved, although the solution will look more complicated than the one given above (Jacquez, 1972; Gydesen, 1984).

The use of linear compartment models has developed considerably during the 1970s. A review of this type of model is given by O'Neill (1979). An obvious way to generalise the model, would be to let the coefficients in the linear model be time-dependent. This model could be used in situations where it is known that the flow into different compartments will show a time-dependent pattern, e.g., a fading input into a compartment after regulation of a chemical. Another possibility would be to make the model non-linear, such as,

$$\frac{dx_2}{dt} = F_{02} + K_{12}x_1^2 \qquad (35)$$

or perhaps a combination of these two approaches. The rule is when such generalisations are introduced, it is impossible to find the analytical solution provided by a linear compartment model. The equations have to be solved by use of numerical techniques. These aspects of compartment modeling are also covered by Jacquez (1972).

Another type of generalisation is to introduce some periodic functions for flow coefficients such as,

$$K_{ij}(t + \tau) = k_{ij}(t) \qquad\qquad t \geq 0 \qquad (36)$$

where $\tau$ can represent a day or a year when diurnal or yearly variations are studied. This equation represents seasonality in the model and is covered by Yakubovich and Sturzinskin (1975).

The possibility of introducing some kind of stochastic properties in the model also exist at three levels: (1) probabilistic transfer of the individual particles between the compartments; (2) randomly varying flow coefficients due to random variations in the environment; and (3) random variations in data due to measurement errors. Whether it is necessary to take one or more of these sources of random variability into account in a given situation has to be judged individually. Reviews of these models have been published by Matis and Wehrly (1979) and Purdue (1979).

Rather than producing generalisations of the model, the model can be simplified. The most obvious way to do this is to reduce the number of compartments. This is usually referred to as lumping or aggregation of compartments. Since every chosen model formulation consists of a compromise between a highly complex and the simplest model, lumping of compartments becomes central. Conditions for lumping compartments in the linear compartment model with constant coefficients has been addressed elsewhere. The more general problem of non-linear compartment models, and how to estimate the error introduced by lumping has been described by Cobelli *et al.* (1979) and Cole *et al.* (1983).

As an example of how the linear compartment analyses work in practice, let us reconsider a compartmental structure discussed in the preceding section. If it is assumed that a pollutant is released as a pulse to compartment 1, and that the level of the pollutant is zero at time zero in the other compartments, then we have the initial conditions:

$$x_i(0) = S_0 \qquad x_2(0) = x_3(0) = x_4(0) = 0 \tag{37}$$

Furthermore, if it is assumed that the compartmental system is governed by the linear donor controlled model, then the following set of equations prevails:

$$\frac{dx_1}{dt} = -k_{12}x_1 \tag{38}$$

$$\frac{dx_2}{dt} = k_{12}x_1 - k_{24}x_2 - k_{23}x_2$$

$$\frac{dx_3}{dt} = k_{23}x_2 + k_{43}x_4 - k_{30}x_3$$

$$\frac{dx_4}{dt} = k_{24}x_2 - k_{43}x_4$$

or in matrix notation:

$$\frac{dx}{dt} = \begin{bmatrix} -k_{12} & 0 & 0 & 0 \\ k_{12} & -(k_{23}+k_{24}) & 0 & 0 \\ 0 & k_{23} & -k_{30} & k_{43} \\ 0 & k_{24} & 0 & -k_{43} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \tag{39}$$

To study the dynamic behaviour until the system returns to its original state, the differential equations have to be solved. Usually the solution is found by noting that the eigenvalues for the matrix are given by

$$\gamma_1 = -k_{12} \qquad \gamma_2 = -(k_{23} = k_{24}) \qquad \gamma_3 = -K_{30} \qquad \gamma_4 = -K_{43} \tag{40}$$

The corresponding eigenvectors, $e_i$, are found by solving the equation

$$Ax - \gamma_i t \tag{41}$$

with respect to $x$ for each eigenvalue.
since all eigenvalues are less than zero, it is seen that

$$x(t) \rightarrow 0 \text{ for } t \rightarrow +\infty \tag{42}$$

which means that the level in each compartment returns to its original state after some time has elapsed.

This example shows that the dynamic approach makes it possible to describe how the compartmental system approaches a steady state. In the linear donor controlled case, it is even possible to provide an analytical solution. It is also clear that this description of the dynamic behaviour is obtained by employing more complicated mathematics than the simple methods used in the time-integrated approach.

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