Introduction to Box Models

Box models are a simple class of models used to study the behavior of a system. In Earth Sciences, they are used to understand the exchange of mass (and chemical concentrations) between interconnected reservoirs such as lakes, oceans and the atmosphere. Matter is transferred between these reservoirs via rivers, currents, rainfall and evaporation. In addition to transportation, matter can also be added from sources such as emissions and chemical production. Matter can also be removed from a box through chemical loss and deposition. A simplifying assumption used in box models is that matter is instantaneously and perfectly mixed within a given reservoir.

Box models can be used to answer questions about how a system will respond dynamically (i.e., over time) to perturbations. In other words, how does a system of reservoirs respond in time to varying inputs and outputs? For example, how does the mass in a lake respond to changes in the input and output fluxes from rivers? Or how does the concentration of a toxic pollutant in rainwater runoff impact its concentration in a lake over time? Or how are the concentrations of chemical species in the atmosphere controlled by the rates of emissions, reactions, transport and deposition?

A Single Box

We will begin with a simple box model consisting of a single reservoir with mass M and input flux F_{in} and output flux F_{out}, as shown in Figure 1. The fluxes F_{in} and F_{out} have units of mass per unit time.

In this example, the reservoir could represent a lake with total water mass M and the fluxes are from a river flowing in (F_{in}) and a river flowing out (F_{out}).

We can use the principle of *conservation of mass*, which states that mass can neither be created nor destroyed (but it can be moved around), to write a simple differential equation:

$$\frac{dM}{dt} = F_{in} - F_{out}. \tag{1}$$

This equation says that the time rate of change of mass in the reservoir ($\frac{dM}{dt}$) is equal to the difference between the input and output fluxes. For example, if there is no outlet river

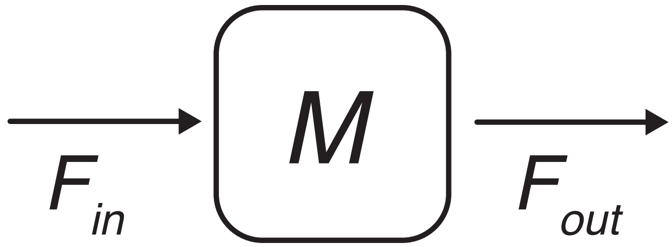

Figure 1: A simple box model consisting of a reservoir with mass M and input flux F_{in} and output flux F_{out}.

then $F_{out} = 0$ and the lake will mass will increase at a rate equal to the input of mass from the input river flux F_{in}. Conversely, if there is no input flux $F_{in} = 0$, the lake mass will decrease as fast as it is drained by F_{out}.

Let's further consider the lake-draining example where $F_{in} = 0$. We can integrate the equation to find

$$M(t) = c - F_{out}\, t, \tag{2}$$

where c is an unknown constant. To find the value of c we must introduce what is referred to as an *initial condition*. For our lake example, the initial condition is simply the initial mass of the lake M_0 at $t = 0$. Setting $t = 0$ in the above equation, we find

$$c = M_0, \tag{3}$$

and thus we have

$$M(t) = M_0 - F_{out}\, t, \tag{4}$$

where the above equation is applicable for times $0 \leq t \leq M_0/F_{out}$. You can see that the lake starts with an initial mass and after some time t its mass will be equal to $M_0 - F_{out}\, t$, up until the time when the lake will be completely empty.

A special case of equation 1 is when $F_{in} = F_{out}$. This is known as the *steady state* since

$$\frac{dM}{dt} = 0, \tag{5}$$

and the mass of the reservoir is no longer changing.

Now let's consider a more complicated case where the output drainage of the reservoir is proportional to the mass of water in the reservoir, so that $F_{out} = aM$, where a is some positive constant. This might be more intuitive by thinking about how a river draining a lake will flow faster when the water level of the lake is high (and its mass is larger), whereas during a period of drought the outlet river flows more slowly due to the lower water level in the lake; in other words the outlet river's flow rate is proportional to the mass in the river. For the example here we will assume that the inlet river flux is constant, so $F_{in} = b$, where b is some positive constant. Inserting these into equation 1 gives:

$$\frac{dM}{dt} = F_{in} - F_{out} = b - aM. \tag{6}$$

While we are interested in dynamic changes predicted by this equation, its insightful to first consider the steady state solution, which could be reached after a sufficiently long period of time so that $\frac{dM}{dt} = 0$. The state state solution is then

$$\frac{dM}{dt} = 0 = b - aM, \tag{7}$$

$$M = \frac{b}{a}. \tag{8}$$

Thus in the long term, the mass of water in the lake will be equal to the ratio b/a where b is the influx rate and a is the constant of proportionality for the outflux rate.

Now let's return to the dynamic situation predicted by equation 6, which is a relatively simple ordinary differential equation (ODE). In this course you will learn how to numerically solve this equation (and much more complicated systems of these equations) using Julia. Once you learn how to do this in Julia, it becomes quite easy to solve increasingly complicated ODE's using a computer. However, while the numerical solution on a computer is great for its practicality and application to complicated scenarios, it lacks the insights that can be gained by the symbolic, or mathematical, solution to the ODE. In our example above, the ODE is simple enough that we can solve it using classical integration techniques.

We begin the analytical solution by rewriting equation 6 as:

$$\frac{dM}{b - aM} = dt. \tag{9}$$

Integrating both sides of this equation will yield the answer, but the denominator on the left hand side makes it more complicated. We ease this situation by using the substitution $y = b - aM$ which has the differential form $dy = -a\,dM$. Inserting these substitutions and applying the integration gives

$$\int \frac{dy}{y} = -a \int dt = -at + c \tag{10}$$

where c is a constant. The left hand side integral is equivalent to $\ln(y)$, thus we have

$$\int \frac{dy}{y} = \ln(y) = -at + c \tag{11}$$

$$e^{\ln(y)} = y = e^{-at+c} = C\,e^{-at}. \tag{12}$$

Substituting for y and rearranging gives

$$M(t) = \frac{b}{a} - \frac{C}{a}e^{-at}. \tag{13}$$

To get the value of the constant C, we substitute the initial value $M(t=0) = M_0$, giving

$$C = b - aM_0. \tag{14}$$

The resulting equation governing the time evolution of the mass of the lake is then

$$M(t) = \frac{b}{a} - \frac{b - aM_0}{a}e^{-at}. \tag{15}$$

This can be rearranged into a more insightful form:

$$M(t) = \frac{b}{a}(1 - e^{-at}) + M_0e^{-at}. \tag{16}$$

Think about which terms in this equation dominate when $t = 0$. What about when t grows really large?

Residence Time

When a system is in steady state (i.e. it is no longer changing with time), we can define a *residence time* or *lifetime* of matter within a given reservoir. The residence time is a useful concept since it allows for comparisons between different reservoirs. The residence time τ is defined as:

$$\tau = \frac{M}{F_{in}} = \frac{M}{F_{out}} \tag{17}$$

In our single box model example above, the residence time can be found when the system has reached steady state at time $t = \infty$:

$$\tau = \frac{b/a}{b} = \frac{1}{a} \tag{18}$$

We can then rewrite equation 19 as:

$$M(t) = \frac{b}{a}(1 - e^{-\frac{t}{\tau}}) + M_0 e^{-\frac{t}{\tau}}. \tag{19}$$

Thus the residence time is related to the time scale of the decay in the exponential terms in this equation. When $t = \tau$, the exponential terms will be equal to $e^{-1} = 0.37$ and thus the second term on the right will have decayed to 37% of the initial mass M_0 while the first term represents an increase of mass where $1 - e^{-1} = 63\%$ of the final mass value.

Suppose we have a single box model representing the mass of water in the atmosphere and the system is in steady state. The total mass of atmospheric water is $M = 1.3 \times 10^{16}$ kg and the rate of precipitation over the entire surface of the Earth is $F_{out} = 1.0 \times 10^{15}$ kg/day, then the residence time of water in the atmosphere is $\tau = 13$ days.

Two Box Models

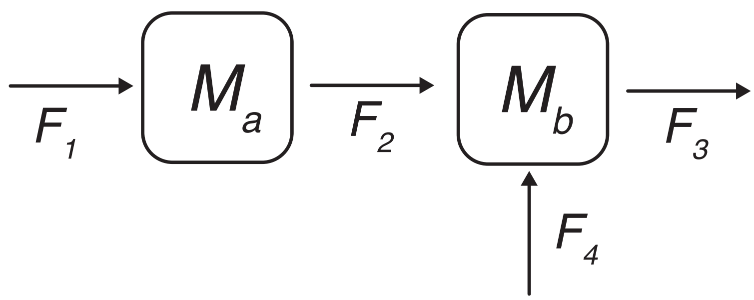

Figure 2: A simple box model consisting of two reservoirs with masses M_a and M_b and fluxes F_1 to F_4 that flow into or out of a given reservoir.

Now let's consider a box model with two reservoirs, as shown in Figure 2. This model could be representative of two lakes with connecting streams. F_1 is a stream flowing into lake M_a while F_2 is an outflow stream for M_a and an inflow stream for M_b. F_4 is another stream that flows into M_b.

The time dependent mass balance equations for these lakes are:

$$\frac{dM_a}{dt} = F_1 - F_2 \tag{20}$$

$$\frac{dM_b}{dt} = F_2 + F_4 - F_3 \tag{21}$$

Suppose that the outflow from each lake is linearly proportional to the mass in each lake such that:

$$F_2 = k_2 M_a \quad (22)$$
$$F_3 = k_3 M_b \quad (23)$$

where k_2 and k_3 are the rate scaling factors. We can then write the mass balance equations as

$$\frac{dM_a}{dt} = F_1 - k_2 M_a \quad (24)$$
$$\frac{dM_b}{dt} = k_2 M_a + F_4 - k_3 M_b \quad (25)$$

Now we have a system of linear, coupled differential equations. The first equation only depends on M_a, whereas the coupling is due to the term $k_2 M_a$ in the second equation, which links it to the first equation. Obviously the mass in the first lake shouldn't depend on the second lake since water only flows downstream to the second lake. Whereas in the second lake the incoming flux F_2 depends entirely on the water flowing out from the first lake.

The steady state solution to these equations can be found by setting:

$$\frac{dM_a}{dt} = \frac{dM_b}{dt} = 0 \quad (26)$$

giving

$$M_a = \frac{F_1}{k_2} \quad (27)$$
$$M_b = \frac{F_1 + F_4}{k_3} \quad (28)$$

We will explore the time dependent behavior of this system as part of the homework assignment.

Multi-box Models

The time dependent mass balance equations for these lakes are:

$$\frac{dM_a}{dt} = F_1 + F_8 - F_2 - F_9 \quad (29)$$
$$\frac{dM_b}{dt} = F_2 - F_4 - F_3 \quad (30)$$
$$\frac{dM_c}{dt} = F_3 + F_9 - F_5 - F_6 \quad (31)$$
$$\frac{dM_d}{dt} = F_6 + F_7 - F_8 \quad (32)$$

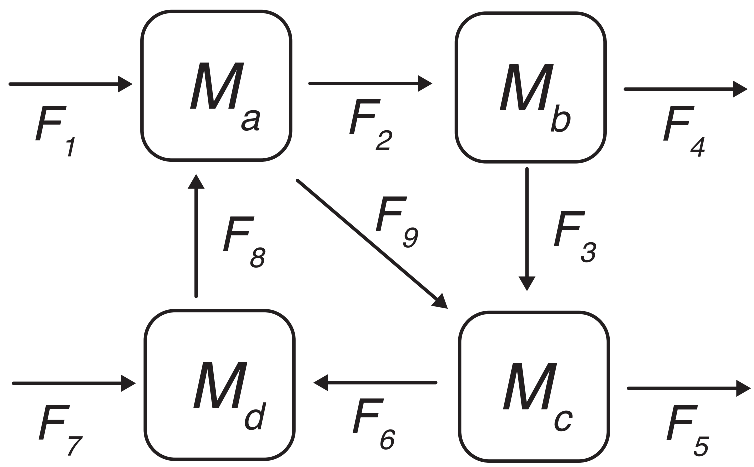

Figure 3: A more complicated box model consisting of four mass reservoirs. Here we have imposed the fluxes F_1 to F_9 that flow into or out of a given reservoir or connect two reservoirs, but other variants are possibles depending on the particular problem being modeled. These reservoirs could represent different parts of the oceans such as warm and cold surface water and intermediate and deep water regions, with fluxes possible between this components. Or the four regions could could represent parts of the atmosphere that vary in both latitude and altitude.

If we again assume the outflows are linearly proportional to the mass in each reservoir (i.e. $F_i = k_i M_j$), we can write this as the set of four coupled linear differential equations:

$$\frac{dM_a}{dt} = F_1 + k_8 M_d - (k_2 + k_9) M_a \quad (33)$$

$$\frac{dM_b}{dt} = k_2 M_a - (k_4 + k_3) M_b \quad (34)$$

$$\frac{dM_c}{dt} = k_3 M_b + k_9 M_a - (k_5 + k_6) M_c \quad (35)$$

$$\frac{dM_d}{dt} = k_6 M_c + F_7 - k_8 M_d \quad (36)$$

This coupled system of four equations looks pretty complicated compared to the one and two-box examples we considered. The steady state solution can be found by setting the time derivatives to zero and then using the four equations to solve for the four unknown masses. An analytical time-dependent solution is also possible but is tedious to formulate. Next week we will learn how to use a numerical ordinary differential equation solver in Julia to automatically compute the solution for at various times given initial values for the four masses and the coefficients for the fluxes.