Compartmental Analysis

June 14, 2016

Compartment models are often used to describe transport of material in systems.

- defining the **compartments**, and
- describing the flows of material between the compartments.

This approach in typically used to determining the time course of a substances (for example, drugs) that are administrated to an animal by a veterinarian or to a human by a physician. In this case the subject is called **pharmacokinetics**. In **epidemiology** the compartments may be *susceptible infected*, and *recovered* (SIR model). It can also be used to model the flow of energy in an ecosystems or the dynamics of chemical reactions.

The basic assumption of compartment models is that the density of the substance is uniformly distributed. For k compartments, the values

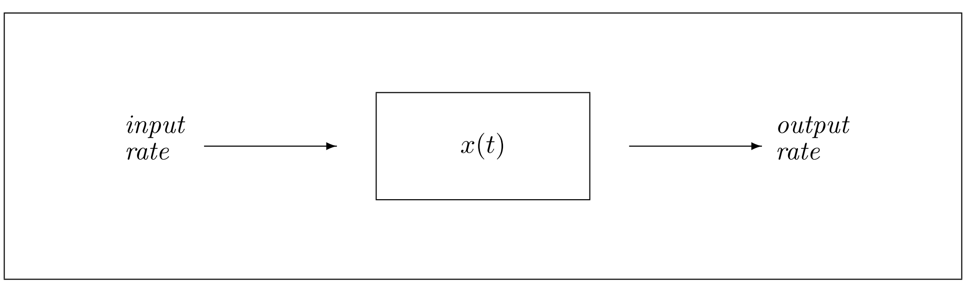
$$x_1(t), \ldots, x_k(t).$$

gives the amount of the substance at time t in compartment $1, \ldots k$. This gives a **system** of differential equations in which

$$\frac{dx_k}{dt}(t)$$

is a linear function of the amounts in each compartment.

In this section, we begin the study of compartmental analysis by looking at a single compartment.



Because the input and output rate are both linear,

$$\begin{aligned} \frac{dx}{dt} &= \text{input rate } - \text{output rate} \\ &= a + kx \end{aligned}$$

To solve,

$$\frac{dx}{dt} - kx = a$$

we use the integrating factor $\exp(kt)$,

$$\begin{aligned}
\frac{d}{dt}\left(xe^{-kt}\right) &= ae^{-kt} \\
x(t)e^{-kt} - x(0) &= \frac{a}{k}(1 - e^{-kt}) \\
x(t)e^{-kt} &= x(0) + \frac{a}{k}(1 - e^{-kt}) \\
x(t) &= (x(0) + \frac{a}{k})e^{kt} - \frac{a}{k}
\end{aligned}$$

Exercise 1. *If $k < 0$, what is the steady state (or limiting) value of x.*

Example 2. *A large tank holds 1000 L of pure water. A brine solution begins to flow at a constant rate of 6 L/min. The solution inside the tank is kept well stirred and is flowing out of the tank at a rate of 6 L/min. The concentration of salt in the brine entering the tank is 0.1 kg/L.*

Brine flows into the tank at a rate of 6 L/min. Since the concentration is 0.1 kg/L, we conclude that the input rate of salt into the tank is

$$6\frac{L}{min} \times 0.1\frac{kg}{L} = 0.6\frac{kg}{min}.$$

For the output rate of brine, note that we assume that the concentration of salt in the tank is uniform. That is, the concentration of salt in any part of the tank at time t is just $x(t)/1000$ Kg/L. Because the tank is kept at a constant 1000L, flow out of water 6 L/min equals flow in. Hence, the output rate of salt is

$$6\frac{L}{min} \times \frac{x(t)}{1000}\frac{L}{min} = \frac{3x(t)}{500}\frac{kg}{min}.$$

Thus,

$$a = 0.6\frac{kg}{min} \quad k = -\frac{3}{500}\frac{1}{min}.$$

and

$$x(t) = \frac{a}{k}e^{kt} - \frac{a}{k} = \frac{3/5}{3/500}(1 - \exp\left(-\frac{3}{500}t\right)) = 100(1 - \exp\left(-\frac{3}{500}t\right))$$

Here is the R code for a plot for the first 1000 minutes. The graph is Figure 1.

```
> t<-0:1000
> x<-100*(1-exp(-3*t/500))
> plot(t,x,type="l")
```

Exercise 3. *Referring to the example above.*

1. *What is the concentration of brine in 1 hour.?*
2. *What is the limiting amount of brine?*
3. *When does the brine reach half its maximum? 99% of maximum?*

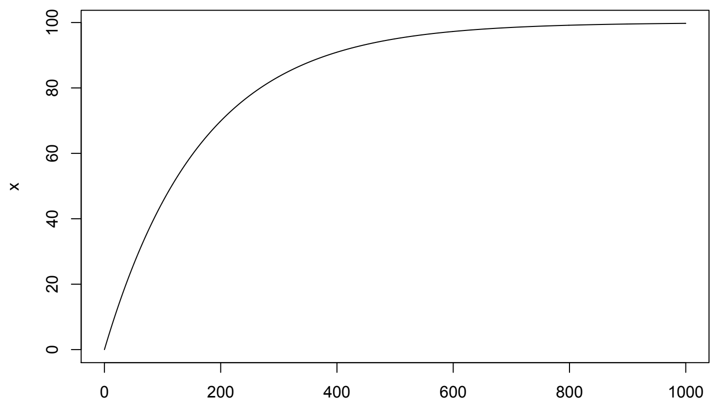


Figure 1: Amount of brine x in kilograms as a function of time t in minutes.

Exercise 4. *A typical adult has about 5 liters of blood. One cancer patient will receive a two-hour infusion that at 10 mg of a chemotherapy drug. The drug persist in the body, breaking down at a rate that is 2% of the substance per hour. The chemo is broken down by the kidneys and liver and excreted in the urine, stool, or sweat.*

For the first two hours

- *The input is 5 mg/hr.*
- *The output is $x(t)/20$.*

Thus the differential equation for the amount of chemotherapy drug is

$$
\begin{aligned}
\frac{dx}{dt} &= 5 - \frac{1}{20}x \\
\frac{dx}{dt} + \frac{1}{20}x &= 5 \\
e^{t/20}\frac{dx}{dt} + \frac{1}{20}e^{t/20}x &= 5e^{t/20} \\
\frac{dx}{dt}(e^{t/20}x) &= 5e^{t/20} \\
e^{t/20}x(t) &= 100(e^{t/20} - 1) \quad \textit{(We use the fact that } x(0) = 0.\textit{)} \\
x(t) &= 100(1 - e^{-t/20})
\end{aligned}
$$

At the end of the infusion

$$x(2) = 100(1 - e^{1/10}) = 9.516258$$

Subsequently,

- *The input is 0*

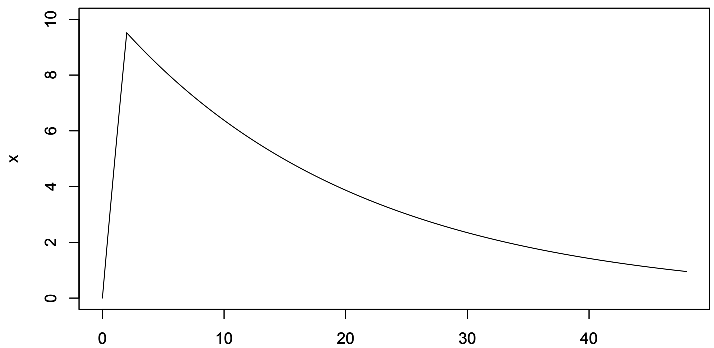


Figure 2: Amount of a chemotherapy drug x in milligrams as a function of time t in hours.

- *The output is $x(t)/20$.*

Thus the differential equation for the amount of chemotherapy drug in this time frame is

$$\begin{aligned}
\frac{dx}{dt} &= -\frac{1}{20}x \\
\frac{dx}{dt} + \frac{1}{20}x &= 0 \\
e^{t/20}\frac{dx}{dt} + \frac{1}{20}e^{t/20}x &= 0 \\
\frac{dx}{dt}(e^{t/20}x) &= 0 \\
e^{t/20}x(t) - e^{1/10}x(2) &= 0 \\
x(t) &= x(2)e^{-(t-2)/20}, \quad t > 1
\end{aligned}$$

Here are R commands for the plot of the amount of a chemotherapy drug for the first 2 days.

```
> t<-seq(0,2,0.1)
> x<-100*(1- exp(-t/20))
> x2<-100*(1- exp(-2/20))
> x2
[1] 9.516258
> t<-seq(2,48,0.1)
> x<-x2*exp(-(t-2)/20)
> par(new=TRUE)
> plot(t,x,xlim=c(0,48),ylim=c(0,10),type="l")
```