ESS 312 - Transport models controlled by coupled differential equations

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(*For the simple 2-box model discussed in class,
these are the equations we want to solve.  v₁ and v₂ are the amounts of material in
  each reservoir.  v₁,₀ and v₂,₀ are the initial amounts at t = 0.  k₁₂ is the
  exchange coefficient for transport from reservoir 1 to reservoir 2; k₂₁ is the
 coefficient for transport from 2 to 1. We want solutions for v₁(t) and v₂(t),
i.e. the amounts of material in each reservoir as a function of time.*)

DSolve[{v₁'[t] == -k₁₂ * v₁[t] + k₂₁ * v₂[t],
   v₂'[t] == k₁₂ * v₁[t] - k₂₁ * v₂[t],
  v₁[0] == v₁,₀,
  v₂[0] == v₂,₀}, {v₁[t], v₂[t]}, t]
```

Solutions for v_1 (t) and v_2 (t)

The solutions are :

$$v_1\,(t) \;=\; \frac{e^{(-k_{12}-k_{21})\,t}\;k_{12}\,v_{1,0}+k_{21}\,v_{1,0}+k_{21}\,v_{2,0}-e^{(-k_{12}-k_{21})\,t}\;k_{21}\,v_{2,0}}{k_{12}+k_{21}},$$

and ... $$v_2\,(t) \;=\; \frac{-k_{12}\,v_{1,0}+e^{(-k_{12}-k_{21})\,t}\;k_{12}\,v_{1,0}-k_{12}\,v_{2,0}-e^{(-k_{12}-k_{21})\,t}\;k_{21}\,v_{2,0}}{k_{12}+k_{21}}$$

which is a bit complicated. No need to see how we got to this,
or memorize it for the exam, etc.

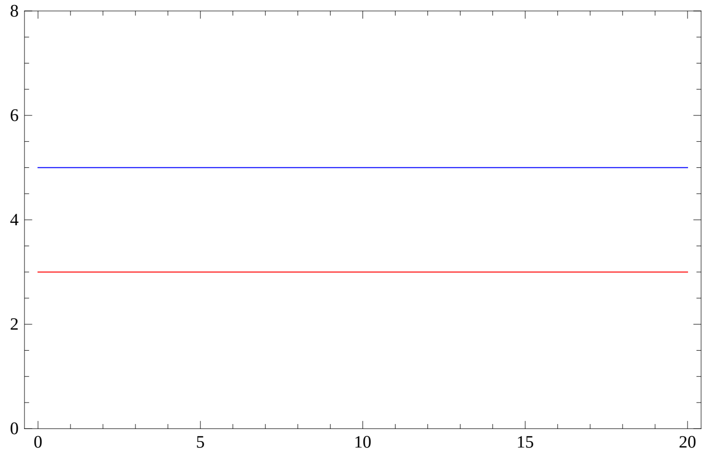
Instead, let's just look at the solutions graphically :

Starting from steady state ...

(*Let's set the total amount of exchangeable material $v_1 + v_2 = 8$,
with v1 at 5, and v2 at 3. To keep the system at steady state,
we need exchange coefficients that will make the
fluxes the same in both directions. To make this simple. choose
cofficients $k_{12} = 1/5\ yr^{-1}$ and $k_{21} = 1/3\ yr^{-1}$. With these values,
the system remains in steady state because the fluxes are the
same in both directions: $k_{12} \times v_{1,0} = 1$ and $k_{21} * v_{2,0} = 1$,
so the net fluxes back and forth balance and the amounts
remain at their initial (steady-state) values.*)

Plot[{v_1[t] /. {$k_{12} \to 0.2$, $k_{21} \to 0.333333$, $v_{1,0} \to 5$, $v_{2,0} \to 3$},
v_2[t] /. {$k_{12} \to 0.2$, $k_{21} \to 0.333333$, $v_{1,0} \to 5$, $v_{2,0} \to 3$}},
{t, 0, 20}, PlotRange → {0, 8}, Frame -> True, PlotStyle → {Blue, Red}]

Out[9]=

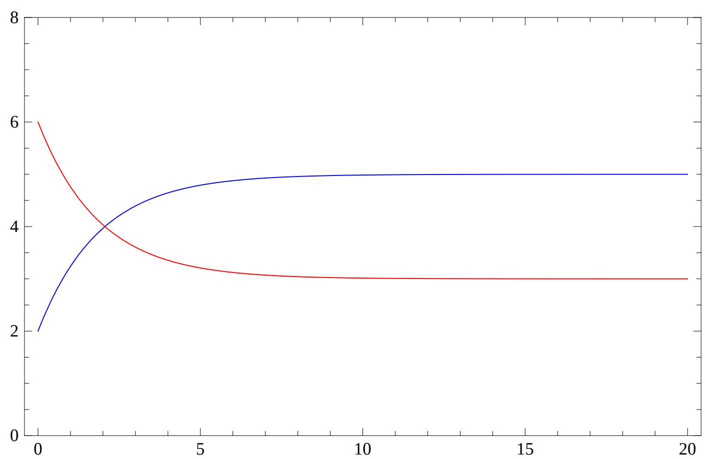


Starting from different initial conditions ...

In[10]:= (*Now start with different amounts in each reservoir: $v_{1,0} = 2$,
$v_{2,0} = 6$. The total amount of exchangeable
material remains the same ($v_1 + v_2 = 8$). Nonetheless,
both reservoirs end up at the same steady state values as in the previous run.*)

Plot[{v_1[t] /. {$k_{12} \to 0.2$, $k_{21} \to 0.333333$, $v_{1,0} \to 2$, $v_{2,0} \to 6$},
v_2[t] /. {$k_{12} \to 0.2$, $k_{21} \to 0.333333$, $v_{1,0} \to 2$, $v_{2,0} \to 6$}},
{t, 0, 20}, PlotRange → {0, 8}, Frame -> True, PlotStyle → {Blue, Red}]

Out[10]=



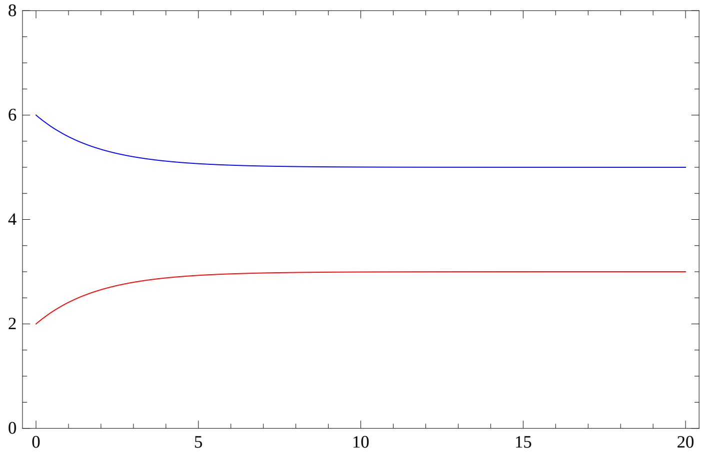
Why? In this case the initial fluxes are out
of balance : The initial flux from reservoir 1 to 2,

$\phi_{12} = k_{12} * v_{1,0} = 0.2 * 2 = 0.4$, whereas the flux ϕ_{21} from reservoir 2 to 1 $= k_{21} * v_{2,0} = 0.333 * 6 = 2$. This imbalance increases the amount of material in reservoir 1 and decreases the amount in reservoir 2. Eventually the amount in reservoir 1 reaches 5 and the amount in reservoir 2 drops to 3, at which point the fluxes come back into balance and the system remains in steady state.

In[11]:=
```
(*The same thing happens if we atart the other way around, with v1,0 = 6, v2,0 = 2.*)

Plot[{v1[t] /. {k12 → 0.2, k21 → 0.333333, v1,0 → 6, v2,0 → 2},
      v2[t] /. {k12 → 0.2, k21 → 0.333333, v1,0 → 6, v2,0 → 2}},
 {t, 0, 20}, PlotRange → {0, 8}, Frame -> True, PlotStyle → {Blue, Red}]
```

Out[11]=



■ How fast does the system return to steady state, and why?

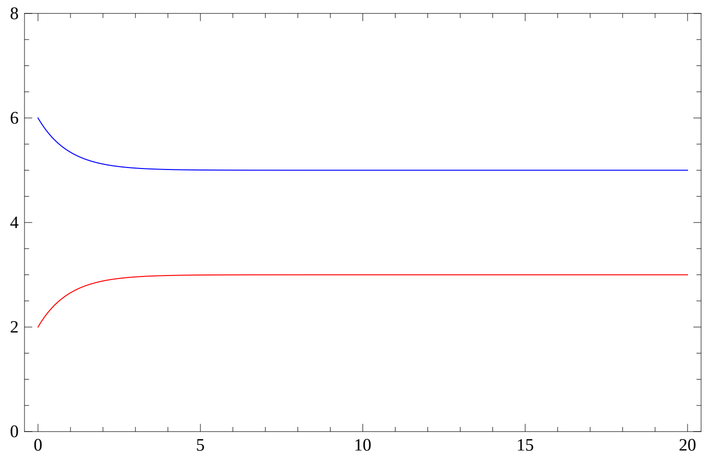
(*Look back at the solutions for $v_1(t)$ and $v_2(t)$, and notice that the time-dependent part of each equation is $e^{-(k_{12} + k_{21})\,t}$. This indicates that after any perturbation to v_1 and v_2, the system will return to steady-state exponentially with a "characteristic timescale" $\tau = 1/(k_{12} + k_{21})$. This is the time required to reduce the perturbation by a factor of 1/e (~0.368). In the 3 examples shown above the timescale is 1/(0.2 + 0.333) = 1.88 years.

By doubling both exchange coefficients we can preserve the same steady state distribution of material between the reservoirs, but the system will respond twice as fast to any imbalance in the fluxes. With k_{12} = 0.4 yr^{-1} and k_{21} = 0.667 yr^{-1}, we have τ = 1/(0.4 + 0.667) = 0.94 yr. In the example below, the return to steady state is twice as fast as in the last example above.*)

```
Plot[{v1[t] /. {k12 → 0.4, k21 → 0.666667, v1,0 → 6, v2,0 → 2},
      v2[t] /. {k12 → 0.4, k21 → 0.666667, v1,0 → 6, v2,0 → 2}},
 {t, 0, 20}, PlotRange → {0, 8}, Frame -> True, PlotStyle → {Blue, Red}]
```

■ Exchange material faster ...

Out[12]=



■ ... or slower

(*Halving the original exchange coefficients again preserves the same steady state distribution of material, but slows down the response time of the system.*)

```
Plot[{v1[t] /. {k12 → 0.1, k21 → 0.1666667, v1,0 → 6, v2,0 → 2},
      v2[t] /. {k12 → 0.1, k21 → 0.1666667, v1,0 → 6, v2,0 → 2}},
 {t, 0, 20}, PlotRange → {0, 8}, Frame -> True, PlotStyle → {Blue, Red}]
```

Out[13]=