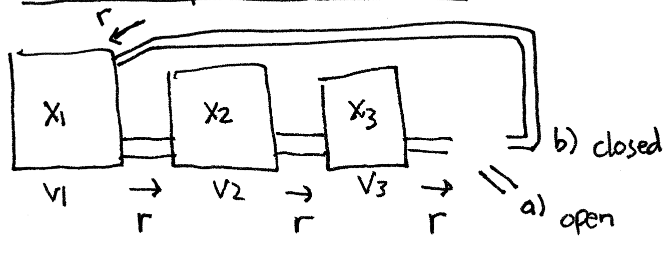
3 tank compartmental analysis



$$\left\{\begin{array}{lll} r = \text{rate of solution flow} & \text{gal/s} & \\ x_i = \text{amount of solute} & \text{lbs} & \text{(liquid volume)} \\ \dfrac{x_i}{V_i} = \text{concentration of solute} & \dfrac{\text{lbs}}{\text{gal}} & \\ \dfrac{x_i}{V_i} r = \dfrac{\text{amount of solute}}{\text{time unit}} & \dfrac{\text{lbs}}{\text{s}} & \end{array}\right.$$

$$\underset{\frac{\text{lbs}}{\text{s}}}{\frac{dx_1}{dt}} = \underset{\text{outflow}\ \frac{\text{lbs}}{\text{s}}}{\underset{\uparrow}{-}\frac{x_1}{V_1}r} \qquad \frac{dx_2}{dt} = \underset{\text{inflow}}{\underset{\uparrow}{+\frac{x_1}{V_1}r}} \underset{\text{outflow}}{\underset{\uparrow}{-\frac{x_2}{V_2}r}} \qquad \frac{dx_3}{dt} = \underset{\text{inflow}}{\underset{\uparrow}{+\frac{x_2}{V_2}r}} \underset{\text{outflow}}{\underset{\uparrow}{-\frac{x_3}{V_3}r}}$$

$$+\left\{\begin{array}{ll} 0 & \text{a) open} \\ \frac{x_3}{V_3}r & \text{b) closed}\end{array}\right\}$$ two options for model (in open case only solvent flows into tank 1)

$\boxed{\text{introduce } k_i = \frac{r}{V_i}}$

$$\frac{dx_1}{dt} = -k_1x_1 \quad \overset{\text{b):}}{[+k_3x_3]}$$
$$\frac{dx_2}{dt} = k_1x_1 - k_2x_2$$
$$\frac{dx_3}{dt} = k_2x_2 - k_3x_3$$

note: $x_1+x_2+x_3$ = total solute amount = constant (case b only)

initial conditions: $x_1(0)=x_0$, $x_2(0)=0$, $x_3(0)=0$ would correspond to starting with all solute in first tank

$$\frac{d\underline{x}}{dt} = \underline{A}\,\underline{x}$$

$$\underline{A} = \begin{bmatrix} -k_1 & 0 & [k_3] \\ k_1 & -k_2 & 0 \\ 0 & k_2 & -k_3 \end{bmatrix}$$

$A: \lambda_1, \lambda_2, \lambda_3$; $B = [E_1\ E_2\ E_3]$; $A_B = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}$

$$\left\{\begin{array}{l} \underline{x} = B\underline{y} \\ \underline{y} = B^{-1}\underline{x} \end{array}\right\} \frac{d\underline{y}}{dt} = A_B\underline{y} \qquad \begin{bmatrix} y_1' \\ y_2' \\ y_3' \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \qquad \begin{array}{ll} y_1' = \lambda_1 y_1 & y_1 = c_1e^{\lambda_1 t} \\ y_2' = \lambda_2 y_2 & y_2 = c_2e^{\lambda_2 t} \\ y_3' = \lambda_3 y_3 & y_3 = c_3e^{\lambda_3 t} \end{array}$$

$$\underline{x} = \underline{B}\begin{bmatrix} c_1e^{\lambda_1 t} \\ c_2e^{\lambda_2 t} \\ c_3e^{\lambda_3 t} \end{bmatrix} = \underbrace{c_1e^{\lambda_1 t}\underline{E_1}} + \underbrace{c_2e^{\lambda_2 t}\underline{E_2}} + \underbrace{c_3e^{\lambda_3 t}\underline{E_3}}$$

each mode has constant ratios of amounts which overall change in time.

$$\det(A-\lambda I) = \left\{\begin{array}{ll} -(\lambda+k_1)(\lambda+k_2)(\lambda+k_3) & \text{a)} \\ -\lambda[\lambda^2+(k_1+k_2+k_3)\lambda+(k_2k_3+k_3k_1+k_1k_2)] & \text{b)} \end{array}\right.$$

■ case a) 3 distinct real roots (if $k_1 \neq k_2 \neq k_3$), all negative → 3 decay modes, different rates

$$\text{soln: } \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = c_1e^{-k_1t}\begin{bmatrix} (k_1-k_2)(k_1-k_3)/(k_1k_2) \\ -(k_1-k_3)/k_2 \\ 1 \end{bmatrix} + c_2e^{-k_2t}\begin{bmatrix} 0 \\ -(k_2-k_3)/k_2 \\ 1 \end{bmatrix} + c_3e^{-k_3t}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$t \gg \max(k_1^{-1}, k_2^{-1}, k_3^{-1})$, $x_i(t) \sim 0$ compared to initial values.

■ case b) $\lambda = 0,\ \underbrace{-\frac{(k_1+k_2+k_3)}{2}}_{k} \pm \frac{1}{2}\sqrt{(k_1+k_2+k_3)^2 - 4(k_2k_3+k_1k_3+k_1k_2)}$

$= k_1^2+k_2^2+k_3^2 - 2(k_2k_3+k_1k_3+k_1k_2) = (k_1-k_2)^2+(k_2-k_3)^2+(k_3-k_1)^2 - k_1^2-k_2^2-k_3^2 < 0?$

sum of differences squared ~~always~~ usually smaller than sum of squares!

$-k \pm i\omega$ $\qquad \omega^2 = \frac{1}{4}[k_1^2+k_2^2+k_3^2 - (k_2-k_3)^2 - (k_1-k_3)^2 - (k_1-k_2)^2]$

damped oscillations → decay away → $Q = \omega/k_{avg} \leq 1/\sqrt{3}$ suggests only slight underdamping

$e^{0t} = 1$ constant soln → equilibrium solution approached as oscillations damp out. → $E_0 = \begin{bmatrix} k_2k_3 \\ k_1k_3 \\ k_1k_2 \end{bmatrix} \propto \begin{bmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \end{bmatrix}$

[one can write down the solutions as in case a) but they are much more complicated]

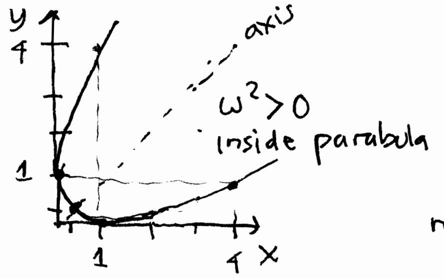
$\tau_i = 1/k_i$

3 tank compartmental analysis (2)

$$-\frac{\omega^2}{k^2} = \frac{k_1^2+k_2^2+k_3^2-2(k_2k_3+k_1k_3+k_1k_2)}{(k_1+k_2+k_3)^2}$$ homogeneous function

zero when $\frac{k_1^2+k_2^2+k_3^2-2(k_2k_3+k_1k_3+k_1k_2)}{k_3^2} = x^2+y^2+1-2(x+y+xy)=0$

$x=\frac{k_1}{k_3}>0,\ y=\frac{k_2}{k_3}>0.$



A C B

$x^2+y^2-2xy-2x-2y=0$

discr: $B^2-4AC = 4-4=0$

real eigenvalues only when near axes or near origin

$x=y \to \quad 2x^2+1-2(2x+x^2) = 1-4x \to x=\frac{1}{4} \to k_1=k_2=\frac{1}{4}k_3$

conclusion: for most of the parameter space for case b)
get complex eigenvalue pair and
damped oscillations