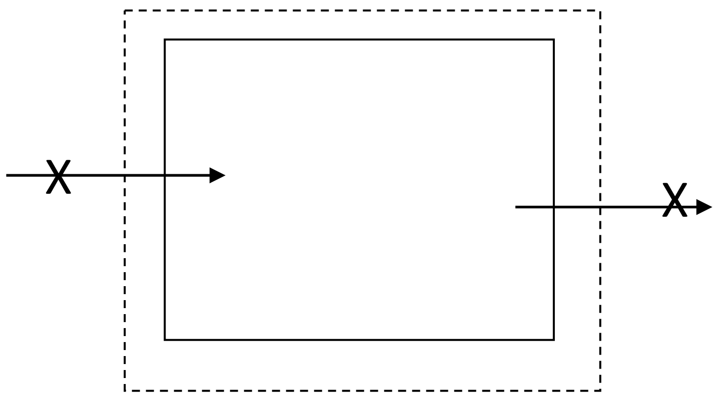
Sample Problem: Batch Reactor with Reaction

Problem:
Perchloroethylene[1] (PCE, C_2Cl_4) is known to degrade anaerobically to form trichloroethylene (TCE, C_2HCl_3). TCE anaerobically degrades to dichloroethane (DCE, $C_2H_2Cl_2$). The degradation reactions are first order with respect to the parent compound. The corresponding half-lives of PCE, TCE, and DCE are 10 years, 4 years and 6 years, respectively. A municipal landfill contains an initial concentration of PCE (10 $\mu g/g_{waste}$) in one of its cells with no initial TCE or DCE.

(a) Determine the concentration of PCE in the cell in 20 years.
(b) Sketch the concentration of PCE, TCE, and DCE as a function of time.

Solution:



PCE ➔ TCE ➔ DCE

Assume:
Batch reactor … therefore, no flow in or out
No generation mechanism for PCE

U.SS. Mass Balance for PCE:

$$In + Generation - Out - Consumption = Accumulation$$

With assumptions…

$$Consumption = Accumulation$$

$$-kVC_{PCE} = V\frac{dC_{PCE}}{dt}$$

[1] C_2Cl_4, a widely used liquid solvent, is found in many groundwater contaminated sites. It is referred to as a DNAPL (a dense, non-aqueous phase liquid; density greater than water).

$$\int_{Co}^{C} \frac{dC_{PCE}}{C_{PCE}} = -\int_{0}^{t} k\, dt$$

$$C_{PCE} = (C_{PCE})_o \exp(-kt)$$

$$k_{PCE} = \frac{0.693}{\tau_{1/2}} = \frac{0.693}{10y} = 0.0693\, y^{-1}$$

$$C_{PCE} = 10\, \mu g/g \exp(-0.0693\, y^{-1} * 20\, y)$$

$$C_{PCE} = 2.5\, \mu g/g$$

The concentration of PCE in the landfill cell in 20 years will be 2.5 $\mu g/g_{waste}$
(makes sense … twenty years is two half-lives so the concentration should be 1/4th the initial concentration)

b…

Sketch could be developed by logic…

- PCE will decline exponentially (as indicated in part a)

- TCE will start at zero (as given), it will increase as a result of PCE degradation, eventually it plateaus as the generation rate from PCE declines (as PCE is declining) and the consumption rate of TCE is increasing with the increased TCE levels, then the TCE will begin to decline as there is little PCE left to generate TCE and the TCE present is slowly being consumed. Eventually TCE will asymptotically approach zero.

- DCE will behave quite similar to TCE except the increase will occur later needing to wait for the TCE concentration to grow. The final drop in DCE will occur after the TCE drops off. DCE will eventually work its way to zero (asymptotically).

  (sketch challenges … where would the lines on the sketch cross?, where does the concentration peak?)

A non-sketch approach …

Setup 3 coupled differential equations that can be readily solved using Simulink.

Equation 1:

$$\frac{dC_{PCE}}{dt} = -k_{PCE}\, C_{PCE}$$

Equation 2: (Mass Balance for TCE)

$$\frac{dC_{TCE}}{dt} = +k_{PCE}C_{PCE} - k_{TCE}C_{TCE}$$

Equation 3: (Mass Balance for DCE)

$$\frac{dC_{DCE}}{dt} = +k_{TCE}C_{TCE} - k_{DCE}C_{DCE}$$

These equations should be solved with the concentrations in moles/g as the reaction has 1 mole of PCE becoming 1 mole of TCE and then 1 mole of DCE; A Matlab/Simulink model of this system is posted to permit you to play with the dynamics of the system. One resulting response is provided below. You are encouraged to use the posted model to explore response as a function of different half-lives.