Reactor analysis

Mass balance analysis

(Reaction kinetics) + (Mass balance) = (Reactor analysis)

- **Applying mass balance**

1) Draw a simplified schematic of the system and identify the control volume (CV). Make assumptions if necessary.

2) Write a mass balance equation:

(rate of accumulation) = (rate of inflow) – (rate of outflow) + (rate of generation)

3) Solve or rearrange the equation to a useful form.

Mass balance analysis

- **Steady-state simplification**
  - In most applications in water/wastewater treatment, we are concerned with long-term operation → assume steady state
  - Steady-state: no accumulation in the CV (rate of accumulation = 0)

0

(rate of accumulation) = (rate of inflow) – (rate of outflow) + (rate of generation)

Some definitions

- **Hydraulic retention time**

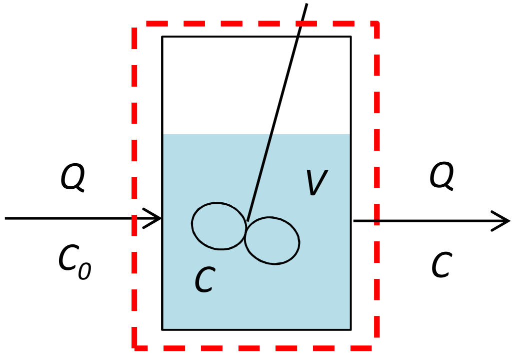
  $$\tau = V/Q$$

  τ = hydraulic retention time [T]; V = volume of the reactor [L^3]
  Q = flowrate [L^3/T]

- **Conservative tracers**: substances that do neither chemically transform nor partition from water; used to analyze the flow characteristics either in natural/engineered systems

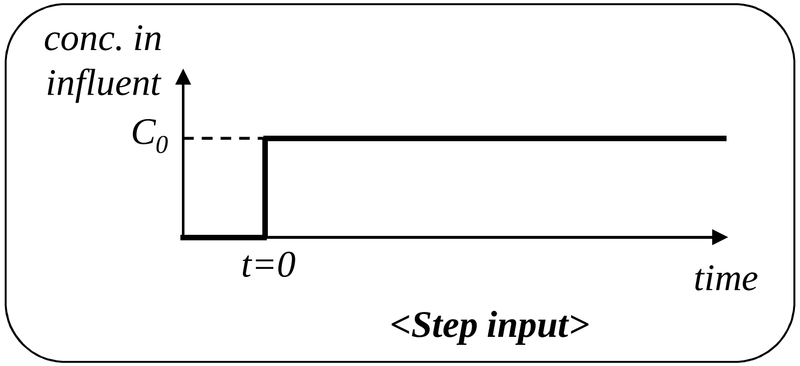
Ideal CSTR – tracer response

1) Draw schematic, identify CV



Assumptions:

- $C = 0$ at $t \leq 0$
- <u>Step input</u> of tracer: influent concentration of C_0 at $t \geq 0$
- Complete mixing in the reactor
- No reaction (conservative tracer)



2) Write mass balance eq.

(rate of accumulation)

= (rate of inflow) – (rate of outflow) + (rate of generation)

$$V\frac{dC}{dt} = QC_0 - QC$$

Ideal CSTR – tracer response

3) Solve the eq.

$$\frac{dC}{dt} = \frac{Q}{V}(C_0 - C) = \frac{C_0 - C}{\tau}$$

$$\int_0^C \frac{dC}{C_0 - C} = \frac{1}{\tau}\int_0^t dt$$

$$-ln(C_0 - C)\Big|_0^C = \frac{1}{\tau} \cdot t\Big|_0^t$$

$$-ln\frac{C_0 - C}{C_0} = \frac{t}{\tau}$$

Ideal CSTR – tracer response

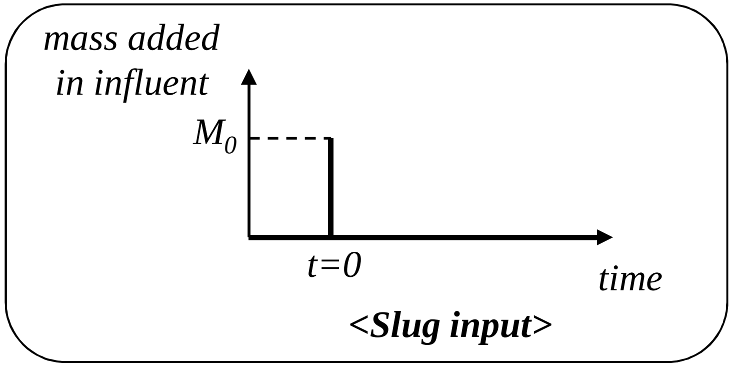
$$\boxed{C = C_0\left[1 - exp\left(-\frac{t}{\tau}\right)\right]}$$

CSTR solution for ***step input of conservative tracer***

cf) CSTR solution for slug input of conservative tracer:

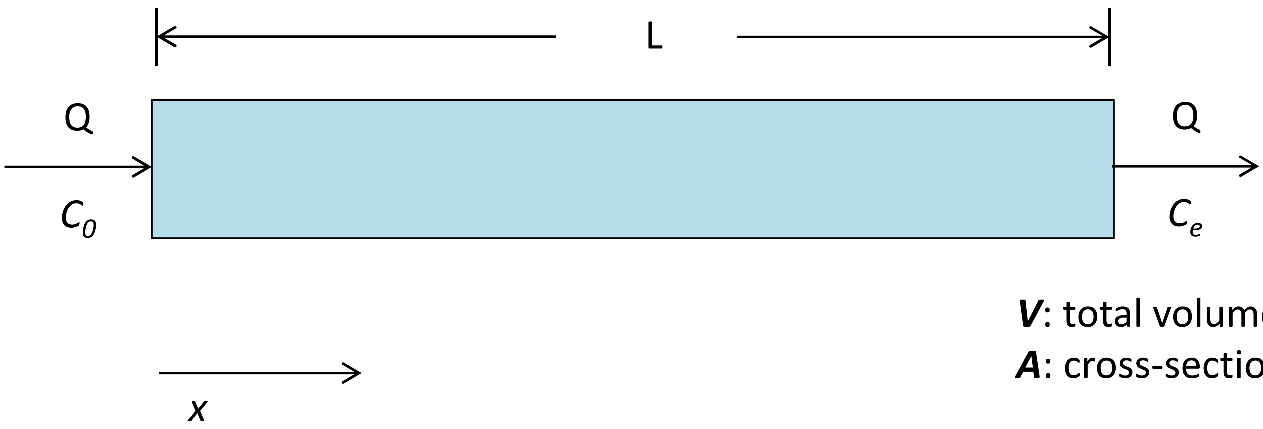
$$\frac{C}{C_0} = e^{-t/\tau}$$

C_0 = concentration at t=0 in CSTR due to slug input of tracer (C_0/V)



Ideal PFR - tracer response

1) Draw schematic, identify CV



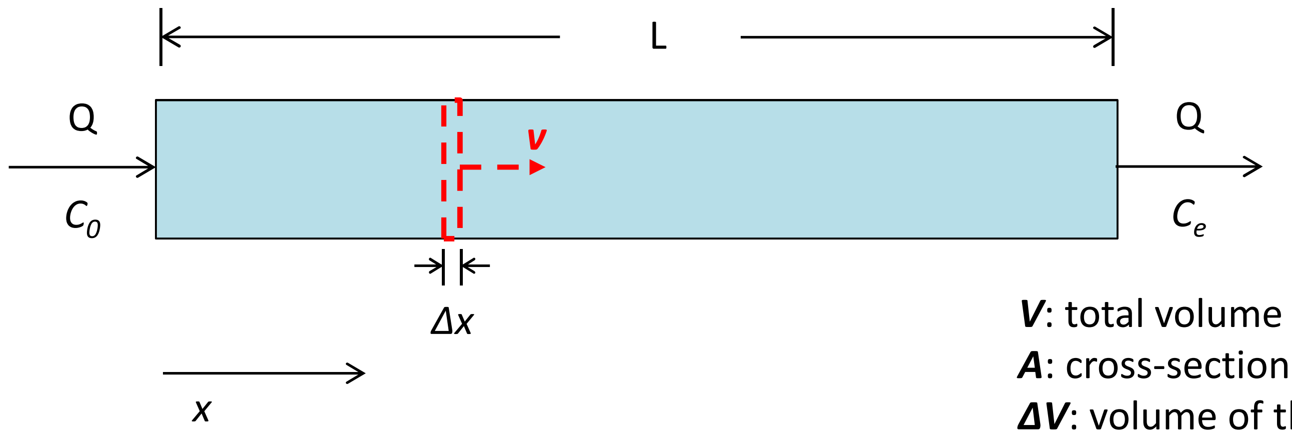
V: total volume of the reactor
A: cross-sectional area

Assumptions:

- $C = 0$ at $t \leq 0$ for any x
- Step input of tracer: influent concentration (C for $x = 0$) of C_0 at $t > 0$
- No mixing in the direction of flow and complete mixing in the direction perpendicular to the flow
- No reaction (conservative tracer)

Ideal PFR - tracer response

1) Draw schematic, identify CV



V: total volume of the reactor
A: cross-sectional area
ΔV: volume of the CV

CV selection:

- A thin plate moving at the same speed as the flow velocity
- The plate is thin enough (Δt → dt) such that the concentration is homogeneous within the plate

Then: $v = \frac{Q}{A}$; Length of time the CV stays in the reactor

$$= \frac{L}{v} = \frac{L \times A}{v \times A} = \frac{V}{Q} = \boldsymbol{\tau}$$

Ideal PFR - tracer response

2) Write mass balance eq.

(rate of accumulation)

= (rate of inflow) – (rate of outflow) + (rate of generation)

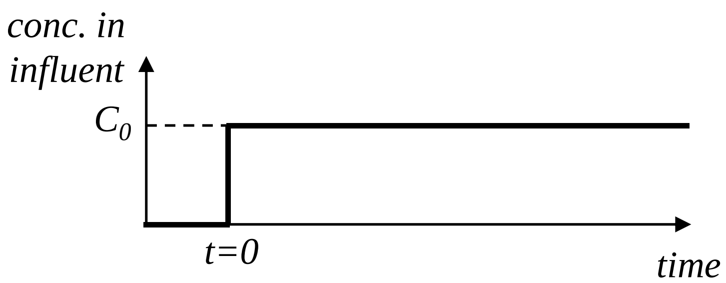
$$\Delta \boldsymbol{V} \frac{\boldsymbol{dC}}{\boldsymbol{dt}} = \mathbf{0} - \mathbf{0} + \mathbf{0}$$

$$\frac{dC}{dt} = 0$$ *No change in concentration while the CV travels through the reactor*

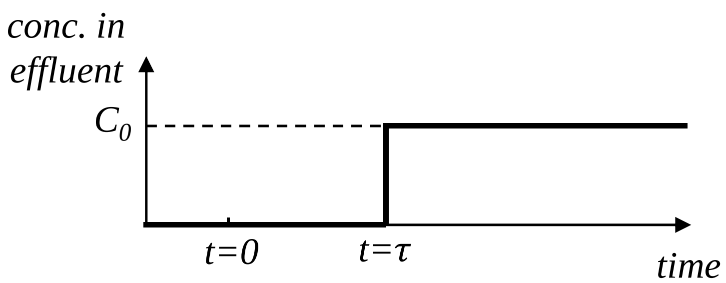
Ideal PFR - tracer response

3) Solve the eq. (appreciate the result in this case!)

- The CV experiences no change in concentration while it moves along the ideal PFR
- The CV stays in the PFR for a time of $\boldsymbol{\tau}$
- So, for the following step input condition in the influent



we get effluent concentration as:



Ideal PFR - tracer response generalization

For any $C_0 = C(x=0,t) = F(t)$:

$$C_e = C(x=L,t) = F(t-\tau)$$

For a PFR, the inflow concentration profile of a tracer is observed exactly the same in the outflow with a time shift of τ

Non-ideal flow in CSTR & PFR

- In practice, the flow in CSTR and PFR is seldom ideal – there are some extent of deviations from the ideal cases

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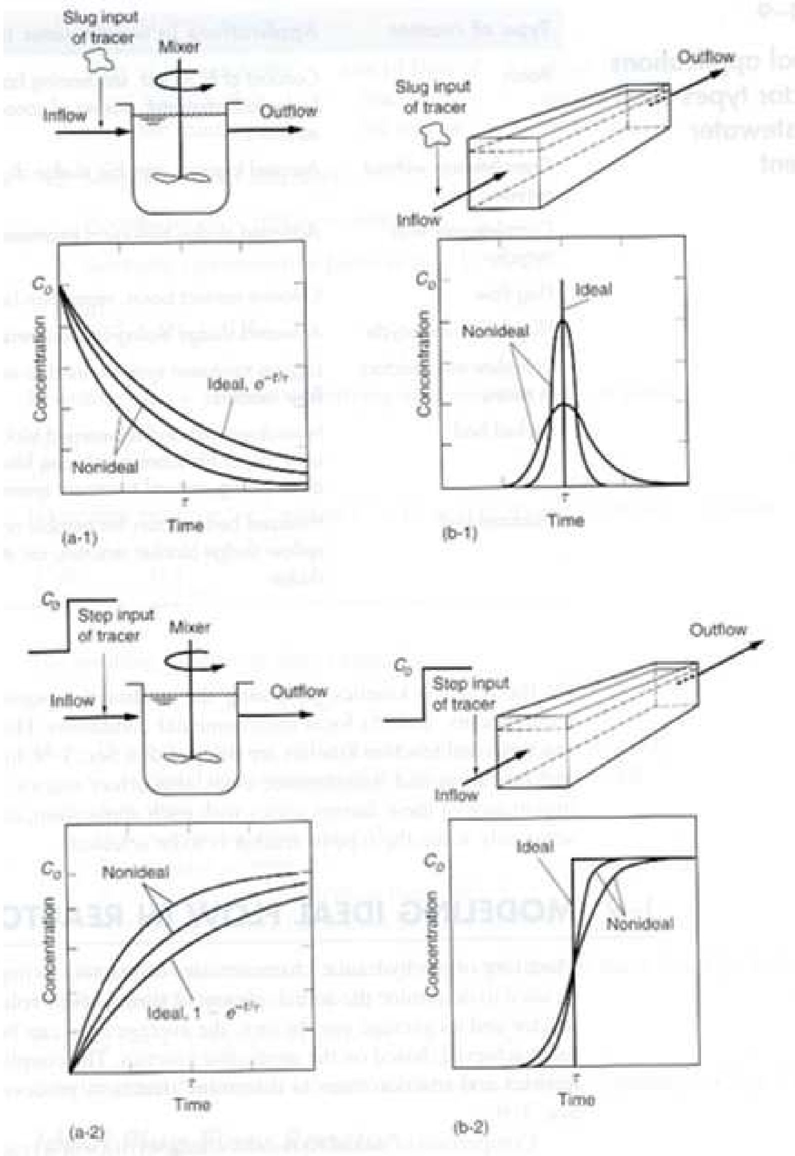


Non-ideal flow in CSTR & PFR

- Factors leading to non-ideal flow (short-circuiting)
  - **Temperature differences**: temperature difference developed within a reactor → density currents occur → water does not flow at a full depth
  - **Wind-driven circulation patterns**: wind creates a circulation cell which acts as a dead space
  - **Inadequate mixing**: insufficient mixing of some portions of the reactor
  - **Poor design**: dead zones developed at the inlet and the outlet of the reactor
  - **Axial dispersion in PFRs**: mechanical dispersion and molecular diffusion in the direction of the flow

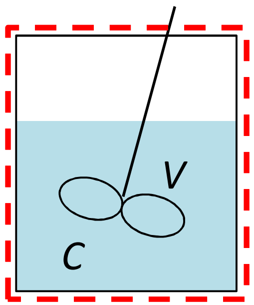
Reactor analysis – including reactions

- Now, let's deal with a non-tracer compound, which undergoes reactions when staying in a reactor
- Incorporate the reaction rate expression into the mass balance equation!
- Batch reactor with first-order reaction

1) Draw schematic, identify CV

- Assume homogeneous mixing
- C_0 at $t = 0$
- 1st order reaction:

$$\left.\frac{dC}{dt}\right|_{reaction} = -kC$$



Batch reactor analysis, 1st order reaction

2) Write mass balance eq.

(rate of accumulation)

= (rate of inflow) – (rate of outflow) + (rate of generation)

$$V\frac{dC}{dt} = 0 - 0 + V \cdot \left.\frac{dC}{dt}\right|_{reaction}$$

$$\frac{dC}{dt} = -kC$$

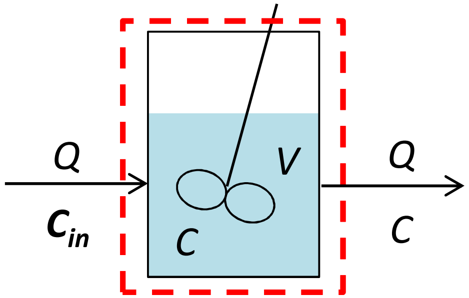
3) Solve the eq.

$$\boxed{C/C_0 = e^{-kt}}$$

CSTR analysis, 1st order reaction

1) Draw schematic, identify CV

- $C = C_0$ at $t = 0$



2) Write mass balance eq.

(rate of accumulation)

= (rate of inflow) – (rate of outflow) + (rate of generation)

$$\boldsymbol{V\frac{dC}{dt} = QC_{in} - QC + V \cdot \left.\frac{dC}{dt}\right|_{reaction}}$$

$$V\frac{dC}{dt} = QC_{in} - QC + V(-kC)$$

$$\frac{dC}{dt} = \frac{1}{\tau}C_{in} - \left(\frac{1}{\tau} + k\right)C$$

CSTR analysis, 1st order reaction

3) Solve the eq.

$$\frac{dC}{dt} = \frac{1}{\tau}C_{in} - \left(\frac{1}{\tau} + k\right)C$$

let $\beta = \frac{1}{\tau} + k$

$$C' + \beta C = \frac{1}{\tau}C_{in}$$

multiply both sides by an integrating factor, $e^{\beta t}$

$$e^{\beta t}(C' + \beta C) = \frac{1}{\tau}C_{in}e^{\beta t}$$

$$\left(Ce^{\beta t}\right)' = \frac{1}{\tau}C_{in}e^{\beta t}$$

$$Ce^{\beta t} = \frac{C_{in}}{\tau}\int e^{\beta t}dt = \frac{C_{in}}{\tau\beta}e^{\beta t} + K \qquad (K = constant)$$

$$C = \frac{C_{in}}{\tau\beta} + Ke^{-\beta t}$$

CSTR analysis, 1st order reaction

3) Solve the eq. (cont'd)

use the initial condition, $C = C_0$ at $t = 0$

$$K = C_0 - \frac{C_{in}}{\tau\beta}$$

Solution:

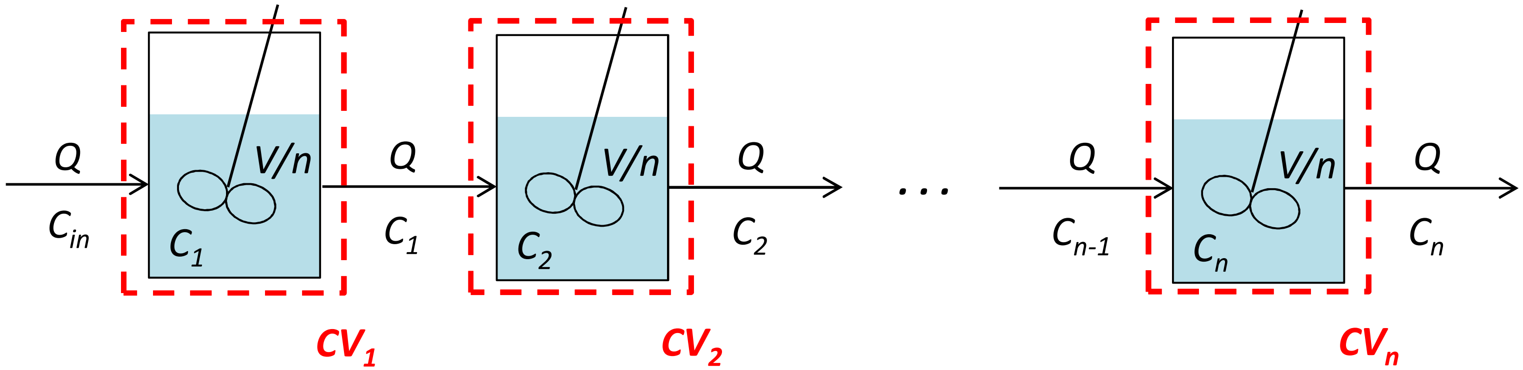
$$\boxed{\boldsymbol{C = C_0 e^{-(k+1/\tau)t} + \frac{C_{in}}{1+k\tau}\left(1 - e^{-(k+1/\tau)t}\right)}}$$

** Steady-state solution for CSTR, 1st order reaction

let $t \rightarrow \infty$:

$$\boxed{\boldsymbol{C = \frac{C_{in}}{1+k\tau}}}$$

CSTR in series, 1st order reaction



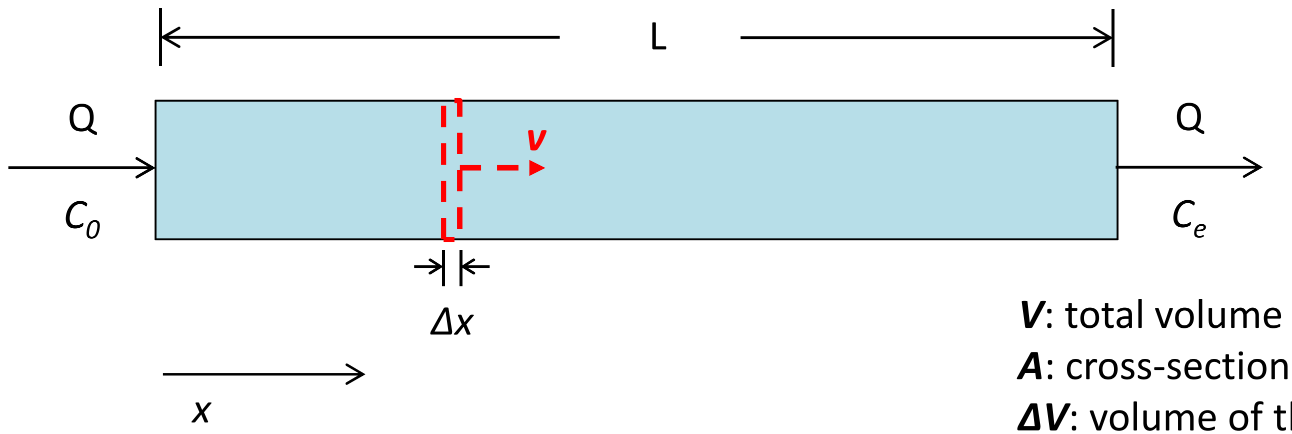
Steady-state solution:

$$\boxed{C_n/C_{in} = \frac{1}{(1+kV/nQ)^n} = \frac{1}{(1+k\tau/n)^n}}$$

V = sum of all reactor volumes

τ = hydraulic retention time in the entire system

PFR, 1st order reaction



V: total volume of the reactor
A: cross-sectional area
ΔV: volume of the CV

(rate of accumulation)

= (rate of inflow) – (rate of outflow) + (rate of generation)

$$\Delta V \frac{dC}{dt} = 0 - 0 + \Delta V \left.\frac{dC}{dt}\right|_{reaction}$$

$$\frac{dC}{dt} = \left.\frac{dC}{dt}\right|_{reaction} = -kC$$

PFR, 1st order reaction

A PFR solution should be obtained by replacing "t" in the batch reactor solution by "τ" ($= V/Q$):

batch reactor solution, 1st order reaction:

$$C/C_0 = e^{-kt}$$

PFR solution, 1st order reaction:

$$\boxed{\boldsymbol{C/C_0 = e^{-k\tau}}}$$

Comparison of reactor performances

Q: Compare the performance of i) a CSTR, ii) CSTRs in series, and iii) a PFR having the same hydraulic retention time of 0.2 days when the first-order reaction rate coefficient, k, is 10 day^{-1}. Assume steady state.

Comparison of reactor performances

i) CSTR

$$\frac{C}{C_0} = \frac{1}{1 + k\tau} = \frac{1}{1 + (10\ day^{-1})(0.2\ day)} = 0.333$$ ⇨ 66.7% removal

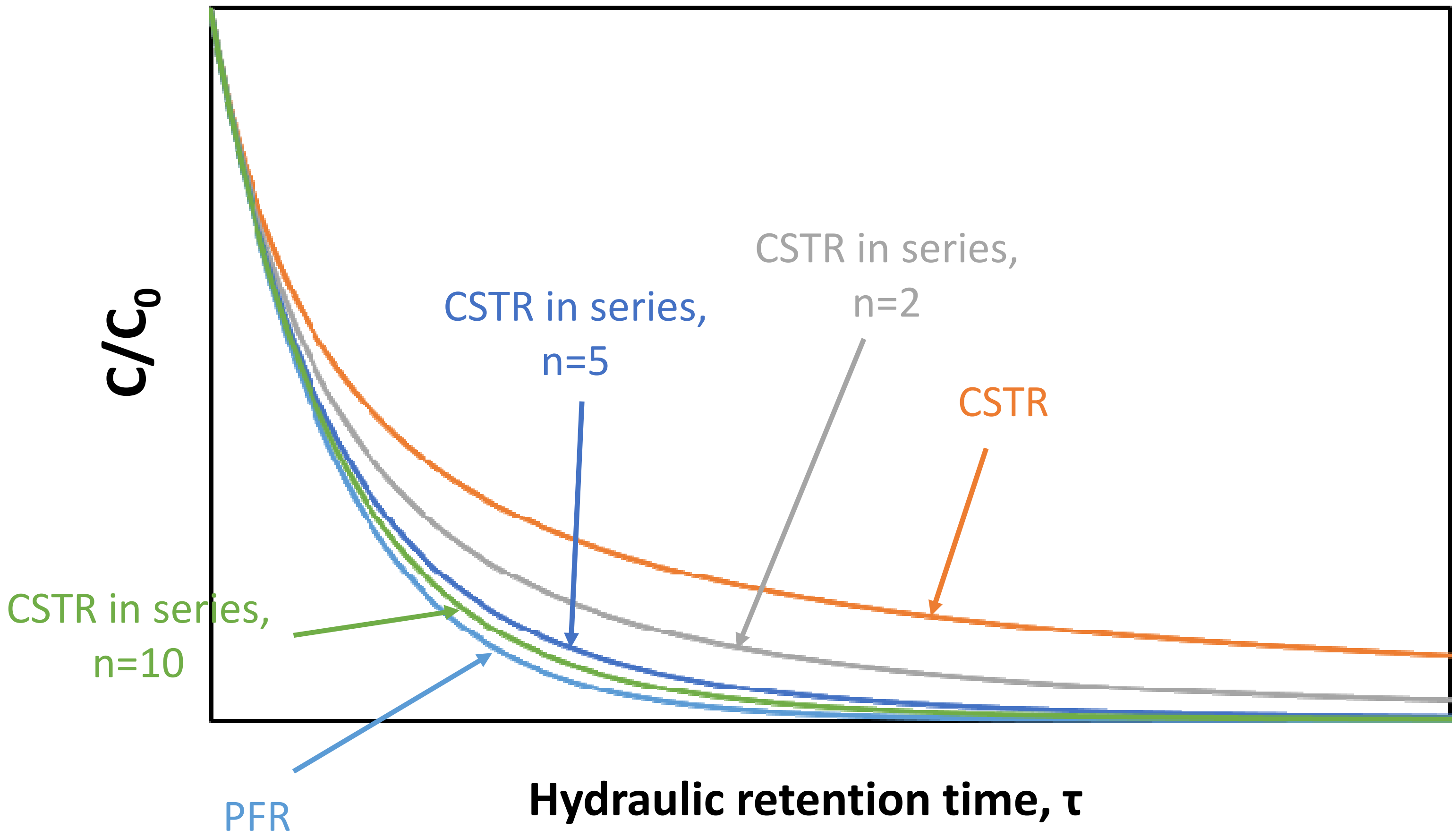
ii) 3 CSTRs in series

$$\frac{C}{C_0} = \frac{1}{(1 + k\tau/3)^3} = \frac{1}{\{1 + (10\ day^{-1})(0.2\ day)/3\}^3} = 0.216$$ ⇨ 78.4% removal

iii) PFR

$$\frac{C}{C_0} = e^{-k\tau} = e^{-(10\ day^{-1})(0.2\ day)} = 0.135$$ ⇨ 86.5% removal

Steady-state CSTR vs. PFR



References

#1) Metcalf & Eddy, Aecom (2014) Wastewater Engineering: Treatment and Resource Recovery, 5th ed. McGraw-Hill, p. 16.