

# Reactor analysis II

# Some definitions

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- **Hydraulic retention time**

$$\tau = V/Q$$

*$\tau$  = hydraulic retention time [T];  $V$  = volume of the reactor [L<sup>3</sup>]*

*$Q$  = flowrate [L<sup>3</sup>/T]*

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

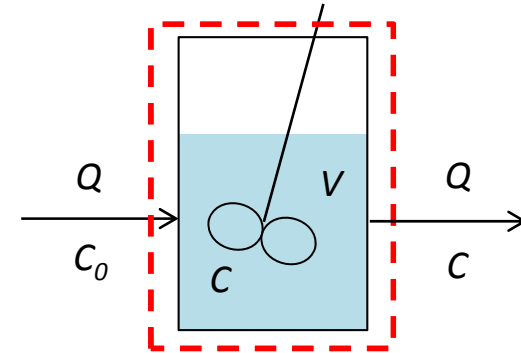
# Ideal CSTR – tracer response

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## i) Draw schematic, identify CV

Assumptions:

- $C = 0$  at  $t = 0$
- Step input of tracer: at  $t \geq 0$  in the influent with a concentration of  $C_0$
- Complete mixing in the reactor
- No reaction (conservative tracer)



## ii) Write mass balance eq.

*(rate of accumulation)*

$$= (\text{rate of inflow}) - (\text{rate of outflow}) + (\text{rate of generation})$$

## iii) Solve the eq.

# Ideal CSTR – tracer response

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**Solution (step input):**

$$\frac{C}{C_0} = 1 - e^{-t/\tau}$$

***cf) solution (slug input):***

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

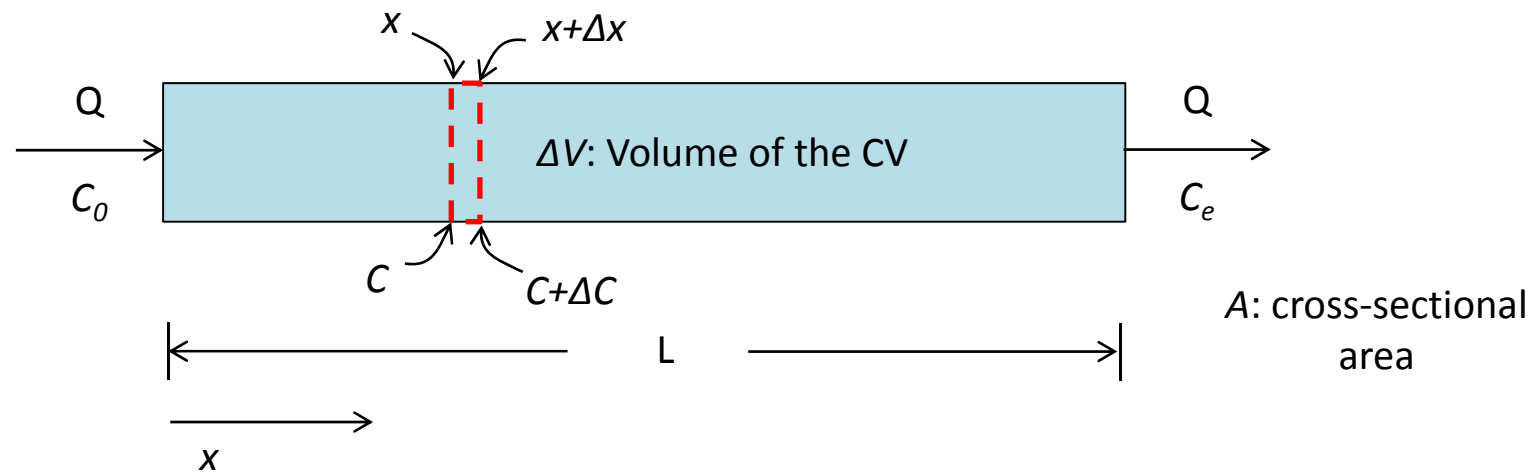
*$C_0$  = concentration at  $t=0$  due to slug input of tracer*

# Ideal PFR - tracer response

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Assume any type of tracer input in the influent, described as  $C_0=F(t)$

**i) Draw schematic, identify CV**



**ii) Write mass balance eq.**

**iii) Solve the eq.**

# Ideal PFR - tracer response

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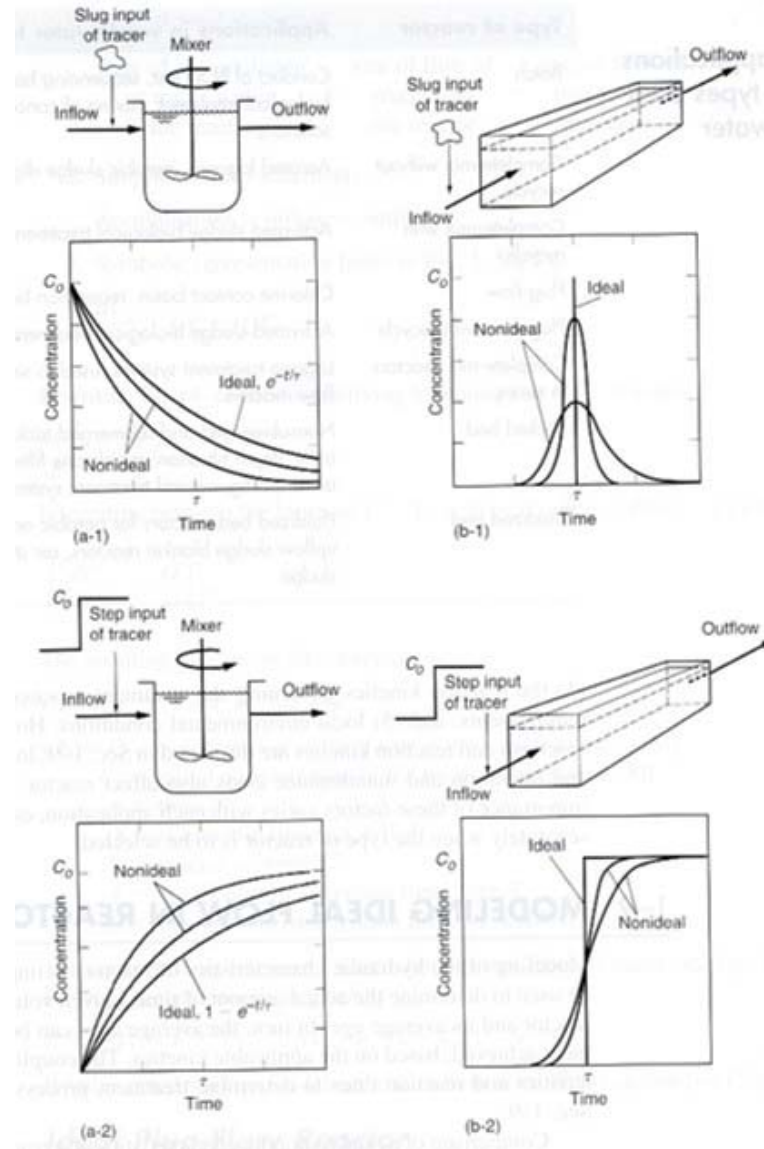
For any  $C_0 = C(x = 0, t) = F(t)$ :

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

*For a PFR, the inflow concentration profile of a tracer is observed exactly the same in the outflow with a time shift of  $\tau$*

# 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



# Non-ideal flow in CSTR & PFR

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- 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

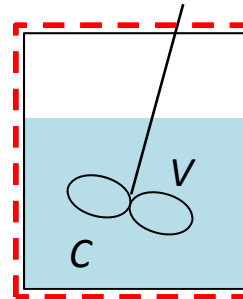


# Reactor analysis - treatment processes

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- Incorporate the reaction rate expression into the mass balance equation!
- Batch reactor with first-order reaction

i) Draw schematic, identify CV



ii) Write mass balance eq.

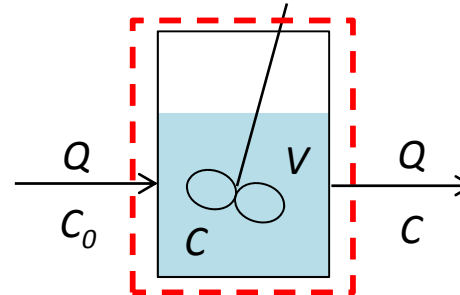
iii) Solve the eq.

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

# CSTR, 1<sup>st</sup> order reaction

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i) Draw schematic, identify CV



ii) Write mass balance eq.

iii) Solve the eq.

General solution:

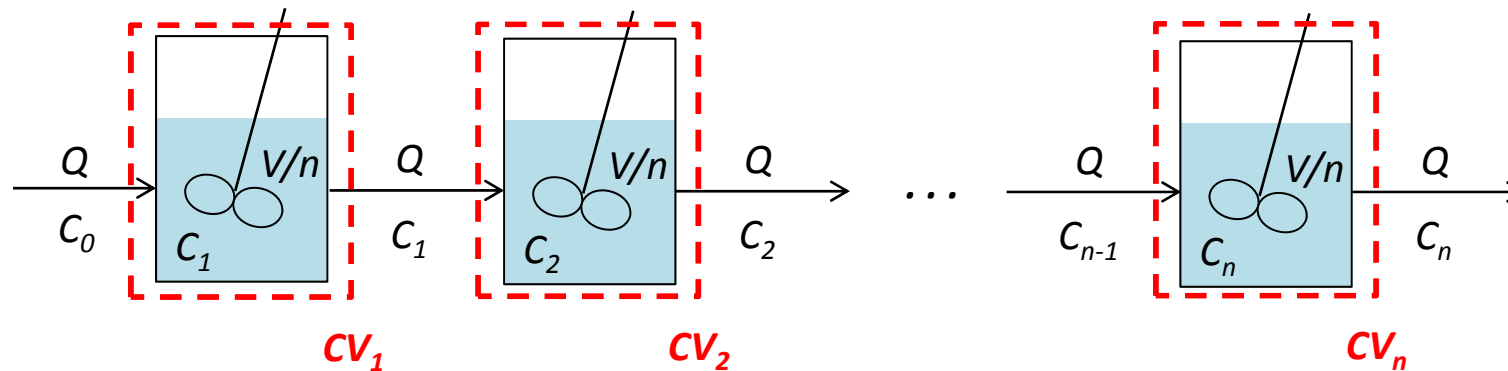
$$C/C_0 = \frac{1}{1 + k\tau} (1 - e^{-(k+1/\tau)t}) + e^{-(k+1/\tau)t}$$

Steady-state solution:

$$C/C_0 = \frac{1}{1 + k\tau}$$

# CSTR in series, 1<sup>st</sup> order reaction

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Steady-state solution:

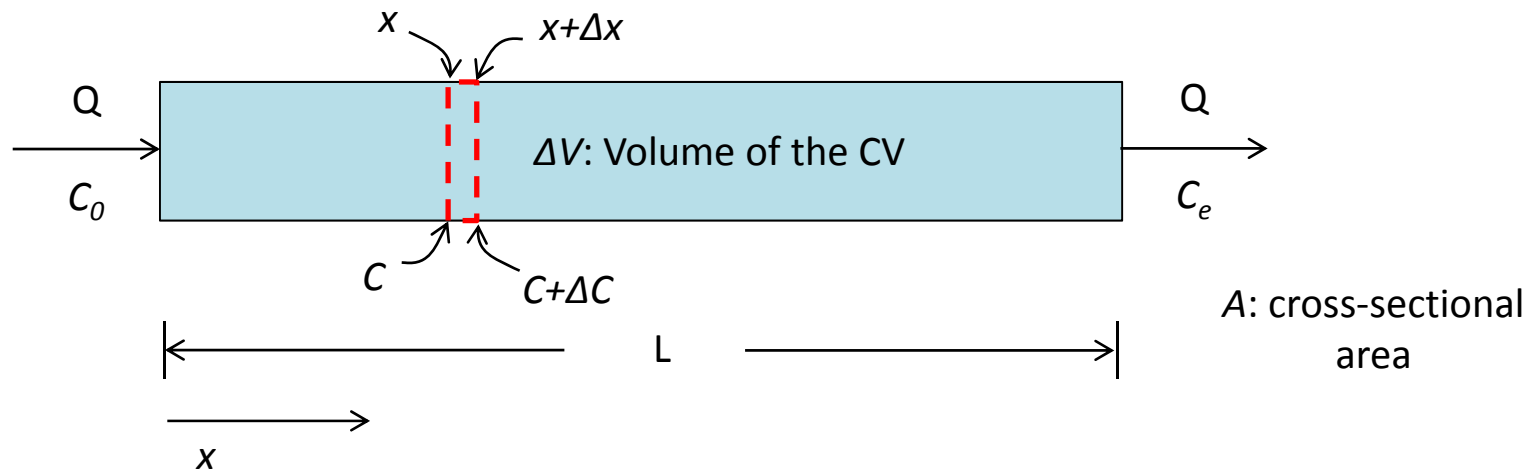
$$\begin{aligned} C_n/C_0 &= \frac{1}{(1 + kV/nQ)^n} \\ &= \frac{1}{(1 + k\tau/n)^n} \end{aligned}$$

$V$  = sum of all reactor volumes

$\tau$  = hydraulic retention time in the entire system

# PFR, 1<sup>st</sup> order reaction

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Steady-state solution:

$$\frac{C_e}{C_0} = e^{-k\tau}$$

- Equivalent to the batch reactor solution (why??)

# Treatment process modeling

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**Q:** Compare the performance of i) a CSTR, ii) three 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  $10 \text{ day}^{-1}$ . Assume steady state.

# CSTR vs. PFR

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