Reactors II

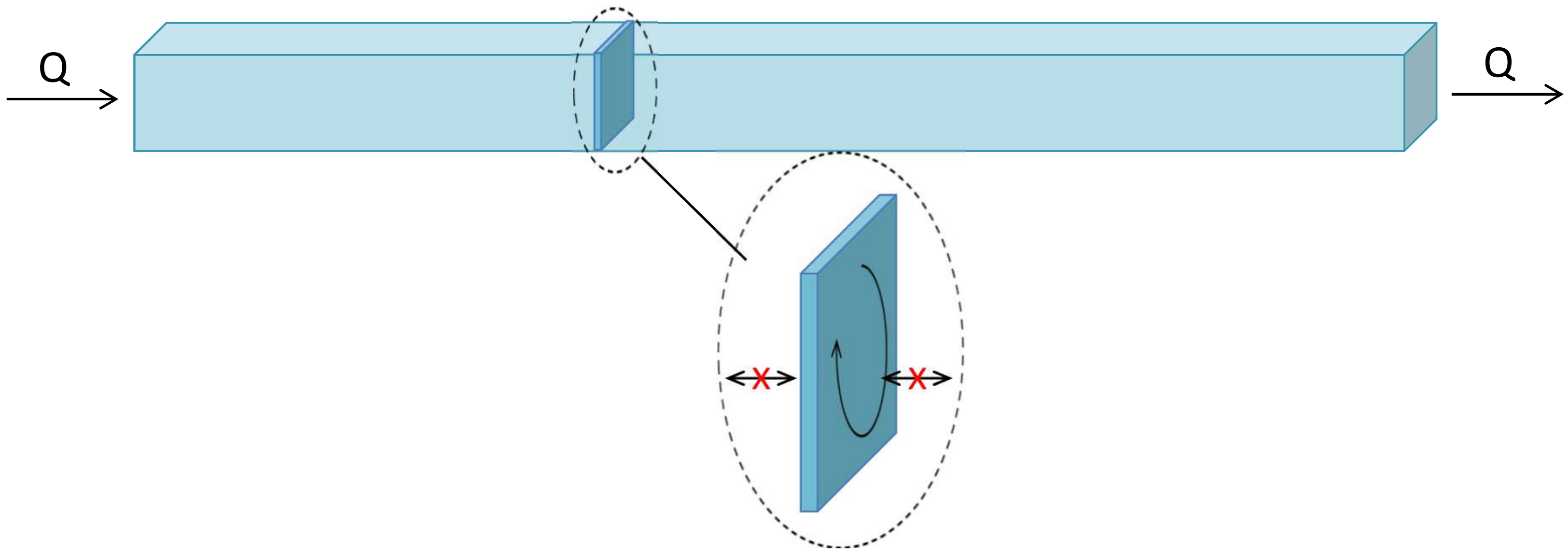
Today's class

- **Plug flow reactor**
  - Concept
  - PFR analysis for 1st order reaction
  - PFR analysis for Monod kinetics

- **Continuous-stirred tank reactor**
  - CSTR analysis for 1st order reaction
  - PFR vs. CSTR
  - CSTR analysis for Monod kinetics

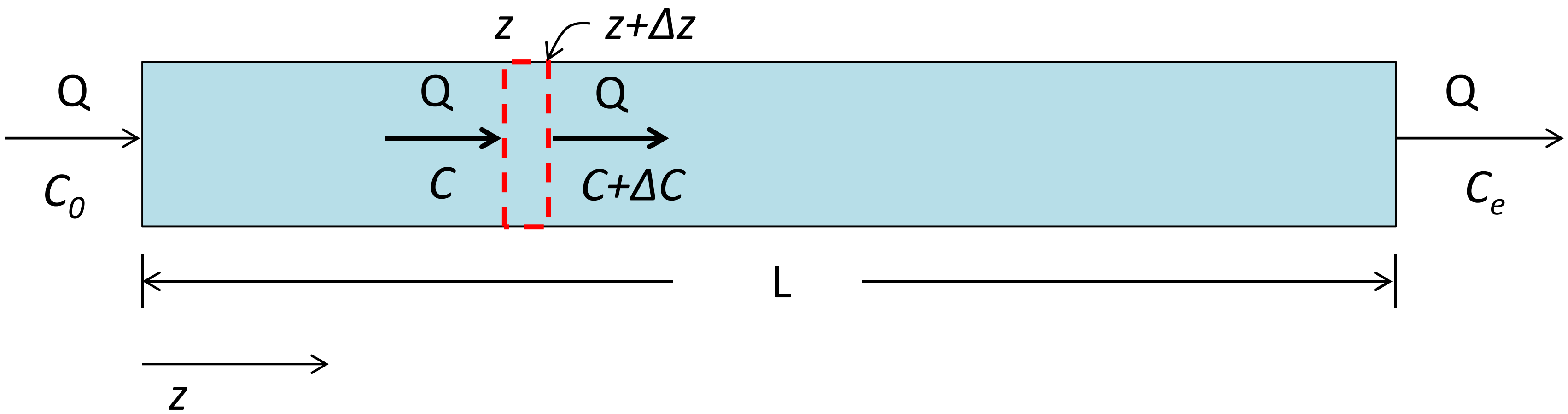
Plug flow reactor

- Plug flow assumption: no mixing in the direction of flow & completely mixed in the direction perpendicular to the flow
- Reactors get close to PFR as the length gets longer than the width and depth (e.g., rivers)



Reactor analysis: PFR, 1st order

1) Schematics, CV & assumption

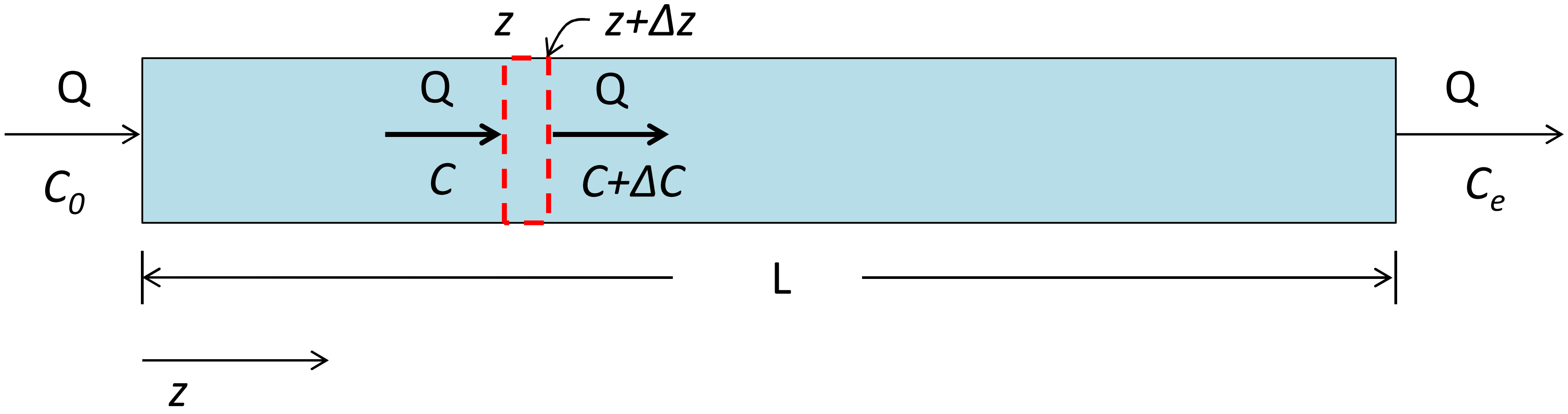


We may take CV as a thin plate perpendicular to the flow at *z=z* with a dimension of *Δz* in *z* dir.

Let $\Delta V = volume\ of\ the\ CV = A\Delta z$

$$u_z = flow\ velocity = \frac{Q}{A}$$

A = cross sectional area (L^2)



2) Set mass balance

$$\frac{dM}{dt} = \Delta V \frac{dC}{dt} = QC - Q(C + \Delta C) + (-kC\Delta V)$$

If $Q \neq f(t)$ & $C_0 \neq f(t)$, $\;C(z) \neq f(t)$.

So, we impose the steady-state assumption to the CV:

$$0 = QC - Q(C + \Delta C) + (-kC\Delta V)$$

$$0 = -Q\Delta C - kC\Delta V$$

3) Rearrange/solve

$$0 = -Q\Delta C - kC\Delta V$$

$$\frac{\Delta C}{\Delta V} = -\frac{kC}{Q}$$

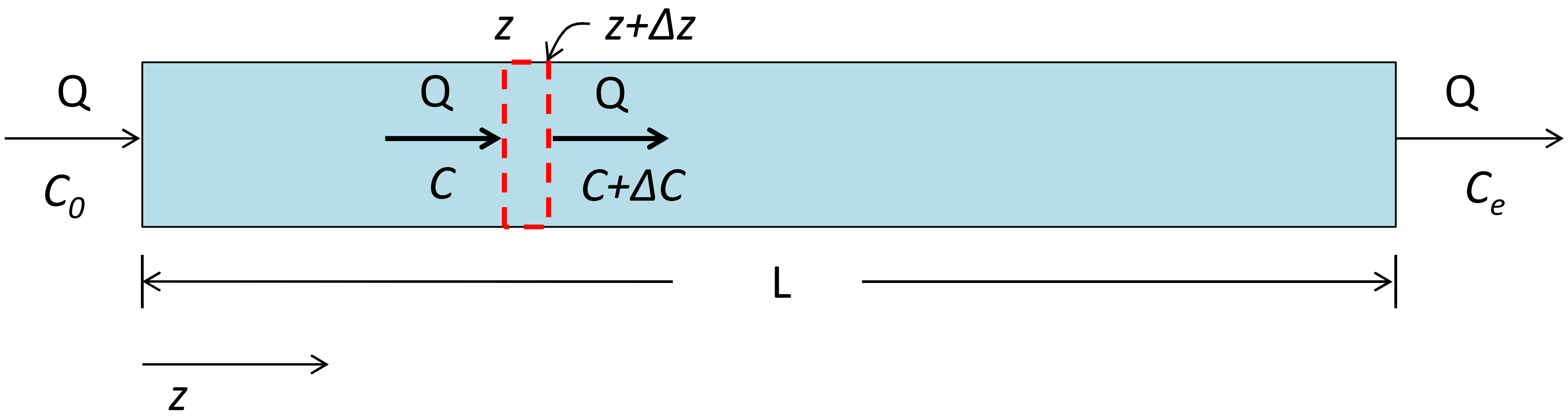
using $\Delta V \ = \ A\Delta z$ & $Q = Au_z$:

$$\frac{\Delta C}{\Delta z} = -\frac{kC}{u_z}$$

let $\Delta z \to 0$

$$\frac{dC}{dz} = -\frac{kC}{u_z}$$

$$\frac{dC}{C} = -\frac{k}{u_z}dz$$



$$\int_{C_0}^{C_e} \frac{dC}{C} = -\frac{k}{u_z}\int_0^L dz$$

$$ln(C_e/C_0) = -k\frac{L}{u_z}$$

$$\boxed{C_e/C_0 = e^{-k\theta}}$$

Same form as the batch reactor (why??)

where, $\theta \equiv \frac{V}{Q} = \frac{A \cdot L}{A \cdot u_z} = \frac{L}{u_z}$

θ = hydraulic retention time, HRT [T]

V = reactor volume [L^3]

What the PFR assumption implies

distance=0
time=0
$C=C_0$

distance=z
time=t
$C=C_0e^{-kt}$
$=C_0e^{-kz/u}$

distance=L
time=Θ
$C=C_0e^{-k\Theta}$
$=C_0e^{-kL/u}$

- We model plug flow reactor as a movement of a "plug"
- The plug has a cross sectional area same as the reactor dimension and an infinitesimal dimension in z-dir (a thin plate)
- Complete mixing within the plug → batch reactor moving in the direction of flow

Reactor analysis: PFR, Monod

Recall the batch reactor solution applying Monod kinetics:

$$t = \frac{1}{\hat{q}}\left\{\left(\frac{K}{X_a{}^0 + YS^0} + \frac{1}{Y}\right) ln\left(X_a{}^0 + YS^0 - YS\right) - \left(\frac{K}{X_a{}^0 + YS^0}\right) ln\frac{SX_a{}^0}{S^0} - \frac{1}{Y} lnX_a{}^0\right\}$$

[5.11]

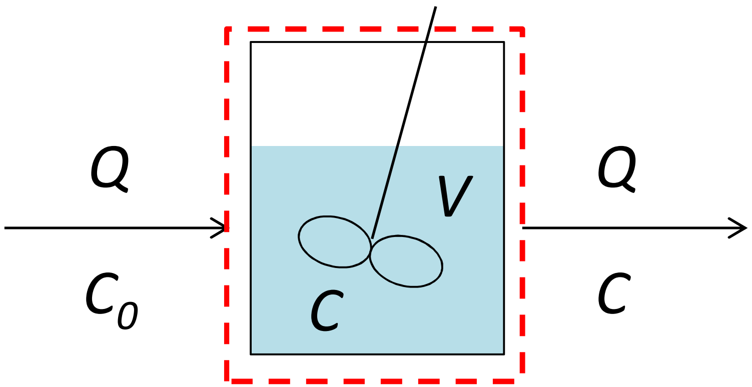
With no doubt, we obtain the PFR solution as:

$$\theta = \frac{1}{\hat{q}}\left\{\left(\frac{K}{X_a{}^0 + YS^0} + \frac{1}{Y}\right) ln\left(X_a{}^0 + YS^0 - YS^e\right) - \left(\frac{K}{X_a{}^0 + YS^0}\right) ln\frac{S^eX_a{}^0}{S^0} - \frac{1}{Y} lnX_a{}^0\right\}$$

[5.27]

Reactor analysis: CSTR, 1st order, steady state

1) Schematics, CV & assumption



2) Set mass balance

$$\cancel{\frac{dC}{dt}} = QC_0 - QC - kCV$$

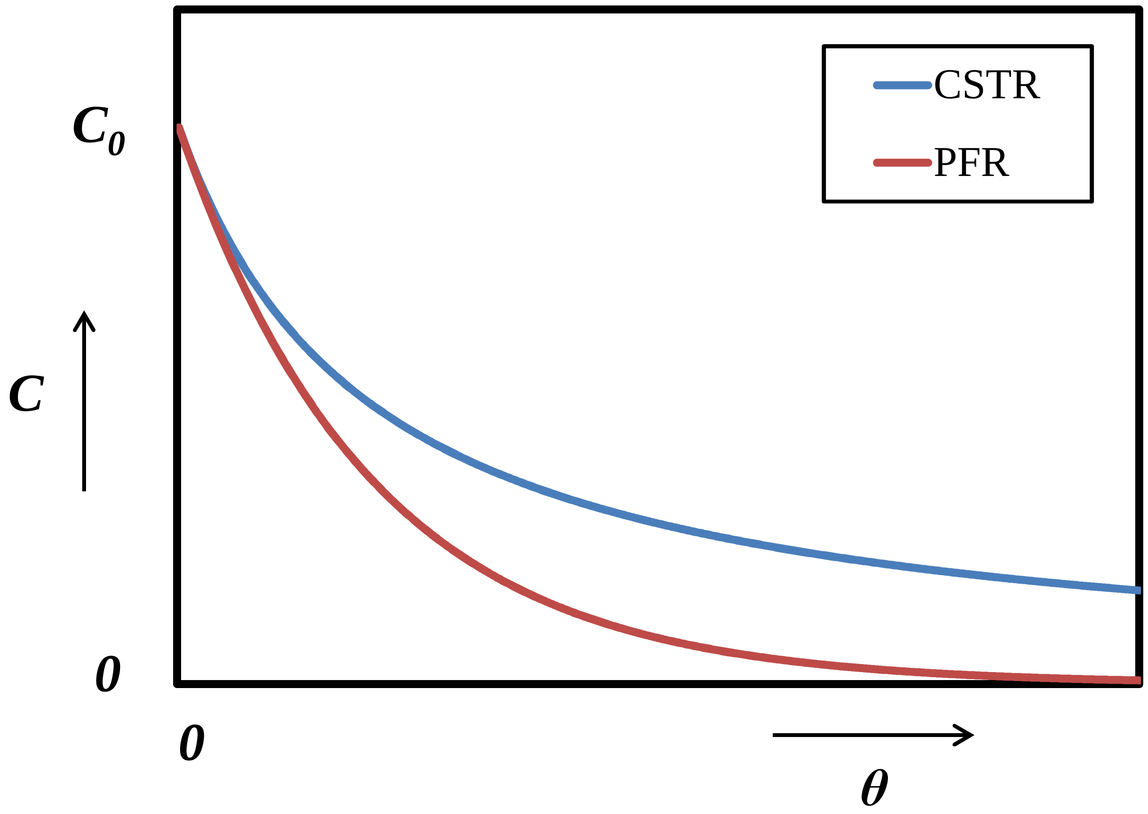
3) Rearrange/solve

$$0 = C_0 - C - kC\theta$$

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

where, $\theta \equiv \frac{V}{Q}$

PFR vs. CSTR



PFR shows better performance esp. at high HRTs

For 1st order reaction,

CSTR (s-s):

$$C = \frac{C_0}{1 + k\theta}$$

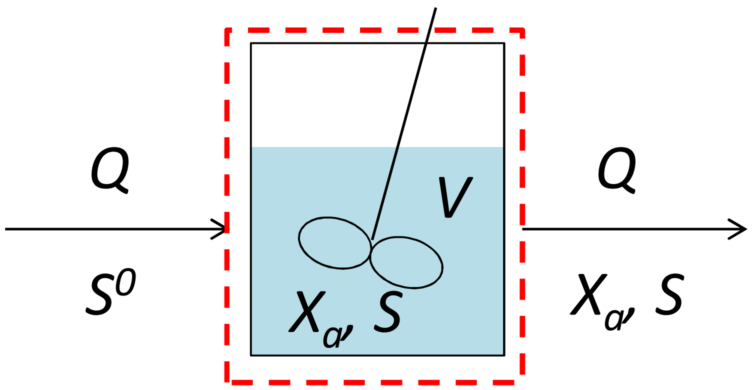
PFR:

$$C = C_0 e^{-k\theta}$$

Reactor analysis: CSTR, Monod, Steady-state

1) Schematics, CV & assumption

X_a = 0 in the influent
(negligible influent biomass)



2) Set mass balance

[substrate mass balance]

$$0 = QS^0 - QS + r_{ut}V$$

[active biomass mass balance]

$$0 = -QX_a + r_{net}V$$

3) Rearrange/solve

[substrate mass balance]

$$0 = QS^0 - QS + r_{ut}V$$

$$0 = Q(S^0 - S) - \frac{\hat{q}S}{K + S} X_a V$$

$$0 = (S^0 - S) - \frac{\hat{q}S}{K + S} X_a \theta$$

[active biomass mass balance]

$$0 = -QX_a + r_{net}V$$

$$0 = -QX_a + \left(Y \frac{\hat{q}S}{K + S} - b\right) X_a V$$

Analytical solution: CSTR, Monod, Steady-state

$$S = K\frac{1 + b\theta}{Y\hat{q}\theta - (1 + b\theta)}$$

-- surprisingly, not f(S^0)!

$$X_a = Y\frac{S^0 - S}{1 + b\theta}$$