

IDEAL REACTORS

Definition: a reactor is a system (volume) with boundaries. Mass may enter and leave across boundary.

Characteristics:

System:

1. Closed or intermittent: no mass enters or leaves during reaction(s) are **batch or semi-batch reactors**
2. Open (control volume): mass enters/leaves during reaction(s) are **continuous flow reactors**

Mixing:

1. Completely mixed: mass is homogeneous throughout system
 - **Batch/semi-batch**
 - Continuous: **Continuous stirred tank reactor (CSTR)**
2. Completely segregated: mass does not mix, no dispersion with heterogeneous conditions
 - **Plug flow reactor (PFR)**

NON-IDEAL REACTORS

Definition: reactors do not meet ideal conditions of flow and mixing due to:

- **Dispersion** deviates from ideal plug flow conditions
- **Short-circuiting and dead spaces** deviate from ideal mixing and plug flow conditions
- **Filling and drawing** deviate from ideal batch conditions

MASS BALANCE

Mass Inflow + Mass generated = Mass outflow + Mass accumulated

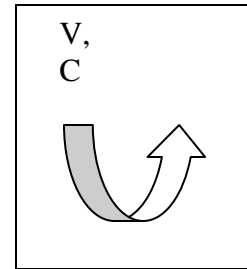
- Inflow and outflow terms are associated with mass crossing the system (reactor) boundary
- Generation term is associated with reactions (chemical or biological)
- Accumulation term is associated with the actual accumulation (or loss) of mass from the system resulting from combined effects of inflow, outflow and reaction.

APPLICATION OF MASS BALANCE

Ideal Batch Reactor, volume = V , reactant concentration = C

mass balance with inflow = out flow = 0

$$\frac{d(VC)}{dt} = Vr_c$$



for constant volume

$$V \frac{dC}{dt} = Vr_c$$

$$\frac{dC}{dt} = r_c$$

for a first-order reaction where C is consumed from an initial concentration of C_0 :

$$r_c = -kC$$

and

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

$$\int_{C_0}^C \frac{dC}{C} = -k \int_0^t dt$$

$$C = C_0 \exp(-kt)$$

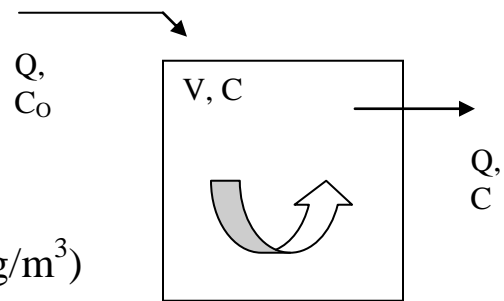
Ideal Continuous Stirred Tank Reactor (CSTR)

Q = fluid flowrate (m^3/d)

V = volume (m^3)

C_0 = influent concentration of C (g/m^3)

C = reactor and effluent concentration of C (g/m^3)



Steady-flow of water conditions: $Q_{\text{in}} = Q_{\text{out}} = Q$ and $\frac{dV}{dt} = 0$

$$QC_0 + Vr_C = QC + V \frac{dC}{dt}$$

$\div Q$

$$C_0 - C + \frac{V}{Q} r_C = \frac{V}{Q} \frac{dC}{dt}$$

Quantity $\frac{V}{Q}$ is defined as the hydraulic residence time (HRT) denoted with the symbol, τ .

For a conservative tracer, $r_C = 0$

Restate mass balance:

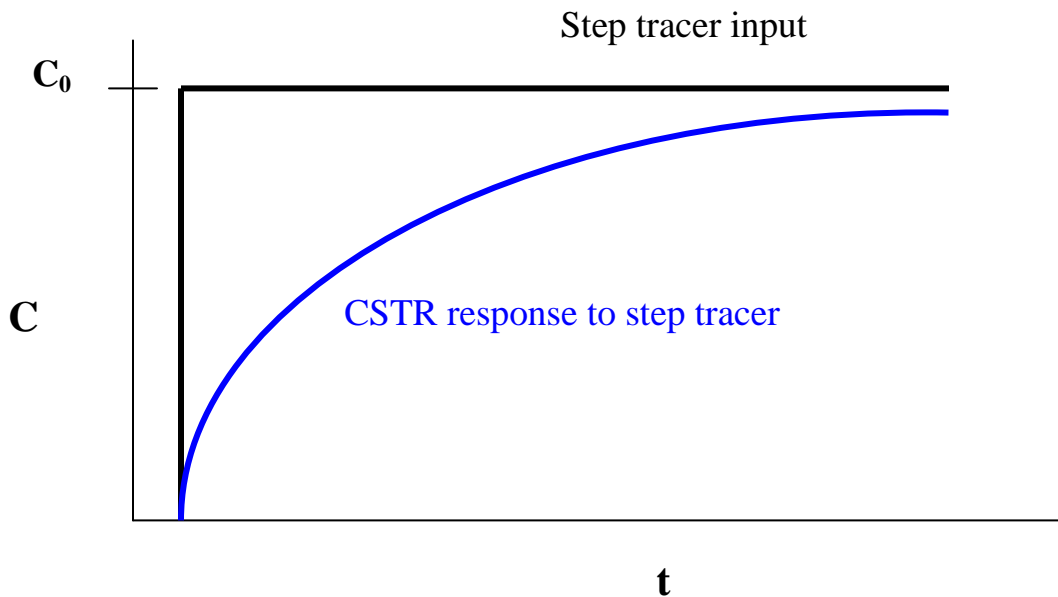
$$C_0 - C = \tau \frac{dC}{dt}$$

Integrate for CSTR with a step input of tracer, C_0 beginning at $t = 0$

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

$$\ln\left(\frac{C_0 - C}{C_0}\right) = -\frac{t}{\tau}$$

$$C = C_0(1 - \exp(-t/\tau))$$



Note asymptote, as $t \rightarrow \infty$, $C \rightarrow C_0$, which is equivalent to $dC/dt \rightarrow 0$, which defines the steady state condition (accumulation = 0)

Example:

Calculate time to reach 95% of the steady-state condition in a CSTR:

$$C/C_0 = 0.95 = (1 - \exp(-t/\tau))$$

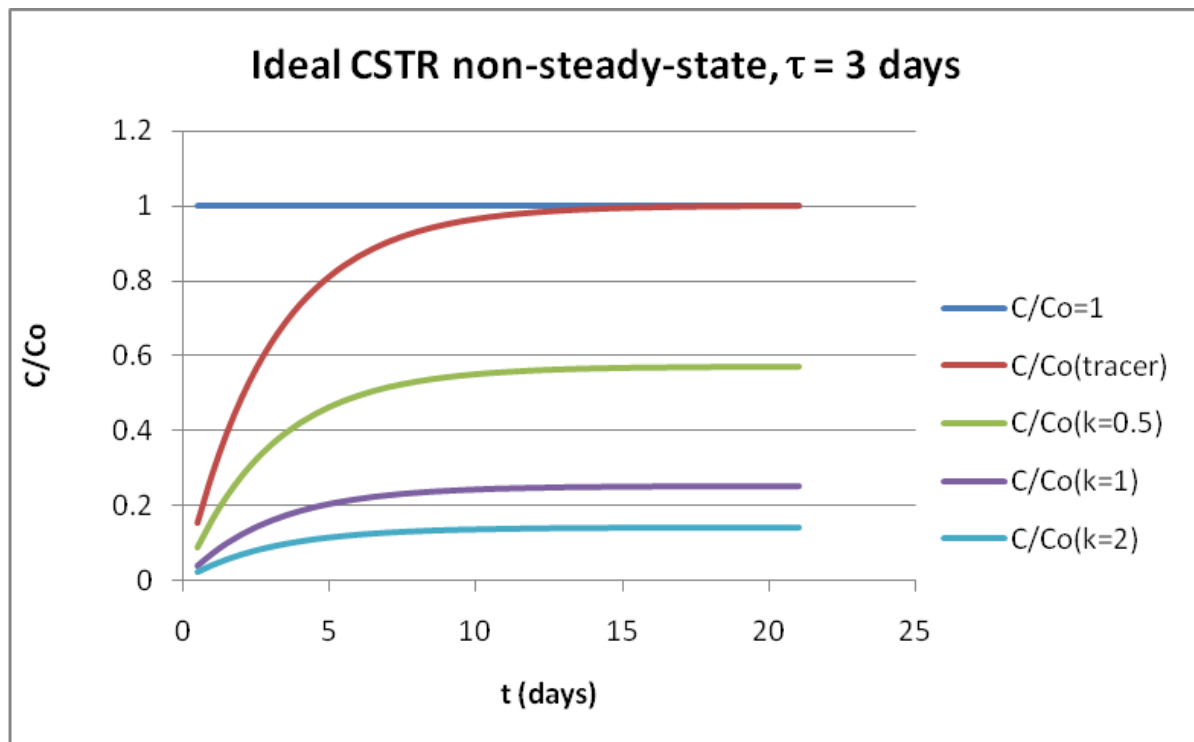
$$\exp(-t/\tau) = 1 - 0.95$$

$$-t/\tau = \ln(0.05) = -3$$

$$t_{95\%} = 3\tau$$

This is characteristic of CSTR flow, and also can be shown to be true in a CSTR with a reaction.

$$C = \frac{C_0}{(1 + k\tau)} \left(1 - \exp\left(-\frac{t}{\tau}\right)\right)$$



CSTR with first order reaction and steady-state conditions:

$$C_0 - C + \tau(-kC) = 0$$

$$C_0 - C(1 + k\tau) = 0$$

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