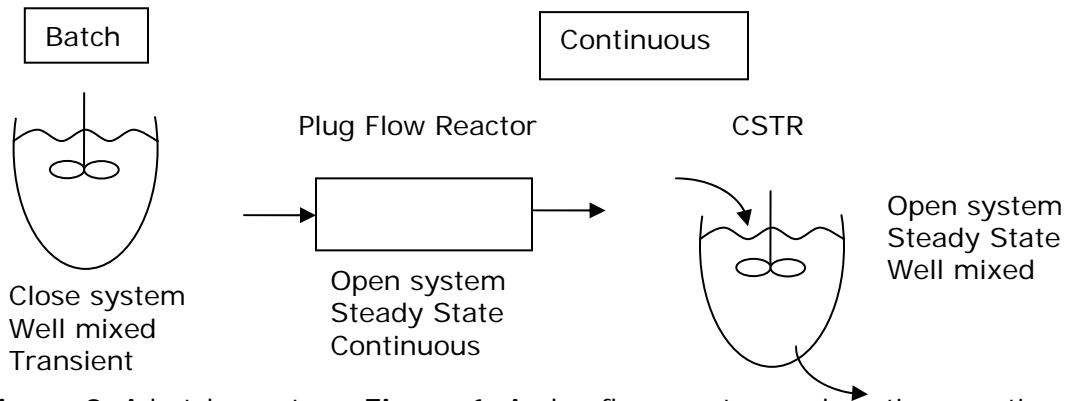


**Lecture 5: Continuous Stirred Tank Reactors (CSTRs)**

This lecture covers: Reactions in a perfectly stirred tank. Steady State CSTR.

**Continuous Stirred Tank Reactors (CSTRs)**



**Figure 2.** A batch reactor. **Figure 1.** A plug flow reactor, and continuous stirred tank reactor.

**Mole Balance on Component A**

In-Out+Production=Accumulation

$$F_{Ao} - F_A + r_A V = 0 \text{ (steady state)}$$

$$V = \frac{F_{Ao} - F_A}{-r_A} \quad F_A = F_{Ao} - X_A F_{Ao}$$

In terms of conversion,  $X_A$ ?

What volume do you need for a certain amount of conversion?

$$V = \frac{F_{Ao} X_A}{-r_A}$$

where  $r_A$  is evaluated at the reactor concentration. This is the same as the exit concentration because the system is well mixed.

For a liquid phase with constant P:

$$F_{Ao} = C_{Ao} v_0 \text{ (} v_0 = \text{volumetric flow rate)}$$

$$F_A = C_A v_0$$

$$\frac{V}{v_0} = \frac{C_{Ao} X_A}{-r_A}$$

$$\tau = \frac{V}{v_0} \leftarrow \text{average time a volume element of fluid stays in the reactor}$$

$$\tau = \frac{C_{A0} X_A}{-r_A}$$

## Consider: 1<sup>st</sup> Order Reaction Kinetics

$$-r_A = kC_A \quad \text{concentration or conversion?}$$

→ convert rate law from  $C_A$  to  $X_A$

$$C_A = C_{A0} (1 - X_A)$$

$$-r_A = kC_{A0} (1 - X_A)$$

$$\tau = \frac{C_{A0} X_A}{kC_{A0} (1 - X_A)} = \frac{X_A}{k(1 - X_A)} \quad \left. \vphantom{\tau} \right\} \text{ reactor size in terms of conversion and rate constant}$$

→ rearrange to find how much conversion for a given reactor size

$$X_A = \frac{\tau k}{1 + \tau k}$$

$\tau \equiv$  average reactor residence time

$$\frac{1}{k} \equiv \text{average time until reaction for a given molecule}$$

We can now define a "Damköhler number"

$$Da = \frac{\text{reaction rate}}{\text{flow}} = \frac{-r_{A0} V}{F_{A0}}, \quad r_{A0} \text{ is the reaction rate law at the feed conditions}$$

For a liquid at constant pressure with 1<sup>st</sup> order kinetics:

$$Da = k\tau$$

$$\Rightarrow X_A = \frac{Da}{1 + Da}$$

therefore:

As  $Da \uparrow$ ,  $X_A \rightarrow 1$

As  $Da \downarrow$ ,  $X_A \rightarrow 0$  (molecule probably leaves before it can react)

For a liquid at constant pressure with 2<sup>nd</sup> order kinetics:

$$-r_A = kC_A^2$$

$$= kC_{A0}^2 (1 - X_A)^2$$

$$\tau = \frac{C_{A0} X_A}{-r_A} = \frac{C_{A0} X_A}{kC_{A0}^2 (1 - X_A)^2} = \frac{X_A}{kC_{A0} (1 - X_A)^2}$$

solving for conversion:

$$X_A = \frac{(1 + 2\tau k C_{A0}) - \sqrt{1 + 4\tau k C_{A0}}}{2\tau k C_{A0}}$$

$$Da = \frac{kC_{Ao} V}{C_{Ao} v_o} = \tau k C_{Ao}$$

Thus, conversion can be put in terms of Da.

$$X_A = \frac{(1+2Da) - \sqrt{1+4Da}}{2Da}$$

How long does it take for a CSTR to reach steady state?

In-Out+Production=Accumulation

$$F_{Ao} - F_A + r_A V = \frac{dN_A}{dt}$$

For a liquid at constant density this is:

$$C_{Ao} - C_A + r_A \tau = \tau \frac{dC_A}{dt}$$

→non-dimensionalize

$$\hat{C}_A = \frac{C_A}{C_{Ao}} \quad \hat{t} = \frac{t}{\tau}$$

$$C_{Ao} - C_{Ao} \hat{C}_A - k C_{Ao} \hat{C}_A \tau = \frac{\cancel{C_{Ao}}}{\cancel{t}} \frac{d\hat{C}_A}{d\hat{t}}$$

$$\frac{d\hat{C}_A}{d\hat{t}} + \left(1 + \frac{Da}{k\tau}\right) \hat{C}_A = 1$$

$$\frac{d\hat{C}_A}{d\hat{t}} + (1 + Da) \hat{C}_A = 1$$

with initial conditions:

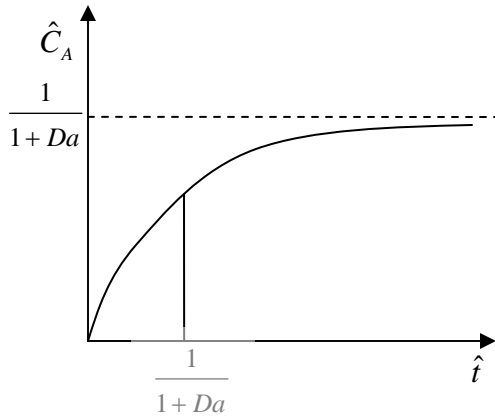
$$\hat{C}_A = 0, \hat{t} = 0$$

we have the solution:

$$\hat{C}_A = \frac{1}{1+Da} \left(1 - e^{-(1+Da)\hat{t}}\right)$$

In nondimensional terms, it exponentially approaches a new steady state with a

characteristic time  $\frac{\tau}{1+Da}$ .



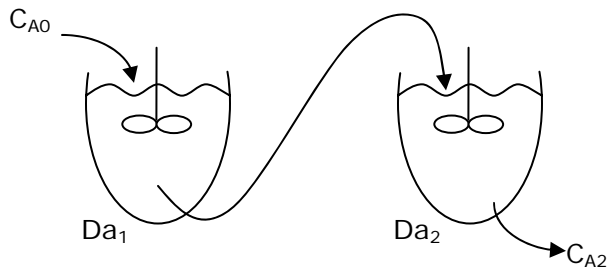
**Figure 3.** Approach to steady state in a continuous stirred tank reactor (CSTR).

The time at which  $\frac{1}{2}$  of the steady state concentration of  $C_A$  is achieved is the half

time:  $\frac{\ln(2)}{1+Da} \tau$

### CSTRs in Series

(Liquid and at constant pressure)



**Figure 4.** Two tanks in series. The output of the first tank is the input of the second tank.

1<sup>st</sup> order reaction kinetics

$$C_{A1} = \frac{C_{A0}}{1+Da_1}$$

For the second reactor  $\rightarrow$  iterate

$$C_{A2} = \frac{C_{A0}}{(1+Da_1)(1+Da_2)}$$

If the CSTRs are identical,

$$C_{An} = \frac{C_{A0}}{(1+Da)^n}$$

$\rightarrow$  many CSTRs in series looks like a plug flow reactor.