LECTURE THREE: **Plug Flow Recycle Reactors design equation: Continuous Stirred Tank Reactors (CSTRs) -**Reactions in a perfectly stirred tank. Steady State CSTR.

Continuous Stirred Tank Reactors (CSTRs)

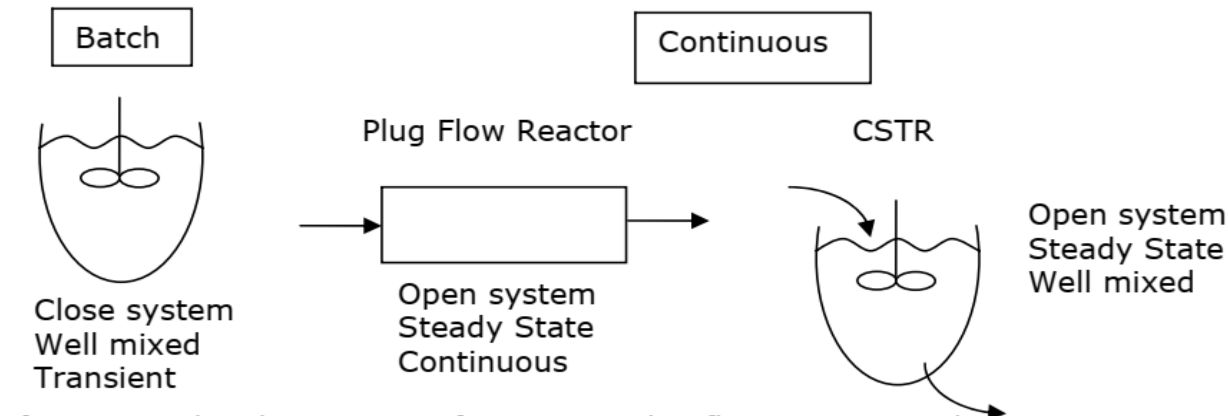


Figure 2. A batch reactor. **Figure 1.** A plug flow reactor, and continuous stirred tank reactor.

Mole Balance on Component A

In-Out+Production=Accumulation

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

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

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:

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

$F_A = C_A v_0$

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

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

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

Consider: 1st Order Reaction Kinetics

$-r_A = kC_A$ concentration or conversion?

→ convert rate law from C_A to X_A

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

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

$$\tau = \frac{C_{Ao}X_A}{kC_{Ao}(1 - X_A)} = \frac{X_A}{k(1 - X_A)}$$ } 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

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

We can now define a "Damköhler number"

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

For a liquid at constant pressure with 1st order kinetics:

$$Da = k\tau$$

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

therefore:

As Da↑, X_A→1

As Da↓, X_A→0 (molecule probably leaves before it can react)

For a liquid at constant pressure with 2nd order kinetics:

$$-r_A = kC_A^{\ 2}$$

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

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

solving for conversion:

$$X_A = \frac{(1 + 2\tau kC_{Ao}) - \sqrt{1 + 4\tau kC_{Ao}}}{2\tau kC_{Ao}}$$

$$Da = \frac{kC_{Ao}^{\cancel{2}}V}{\cancel{C_{Ao}}\,v_o} = \tau k C_{Ao}$$

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

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

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

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

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

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

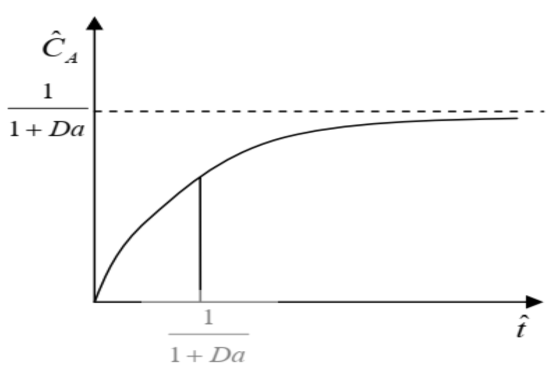


Figure 3. Approach to steady state in a continuous stirred tank reactor (CSTR).

The time at which ½ 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)

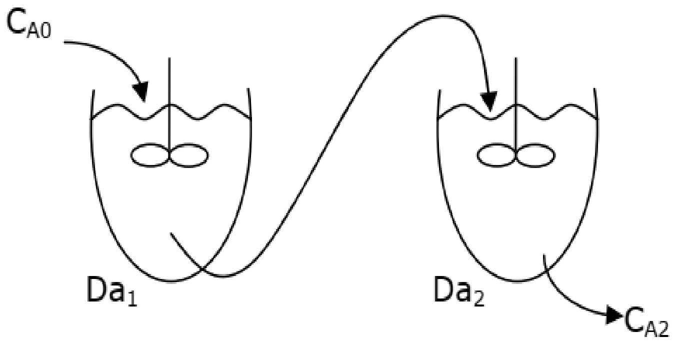


Figure 4. Two tanks in series. The output of the first tank is the input of the second tank.

1st order reaction kinetics

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

For the second reactor→ iterate

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

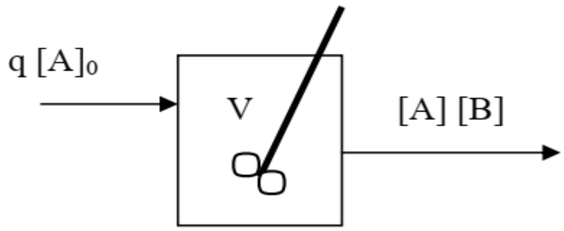
If the CSTRs are identical,

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

→ many CSTRs in series looks like a plug flow reactor.

Consider the unconstrained optimization of a CSTR with volume V.

$$A \rightarrow B$$
$$r = k[A]$$



The goal is to maximize F_B with respect to changes in the volumetric flow rate, q.

$$F_B = q[B]$$

Steady state material balances on species A and B give:

$$0 = F_{A0} - F_A - rV = q([A]_0 - [A]) - kV[A]$$
$$0 = F_{B0} - F_B + rV = -q[B] + kV[A]$$

Hence,

$$[B] = k[A](V/q)$$

and

$$F_B = rV = k[A]V\,;$$

thus production of B is maximized when [A] takes its maximum value, which is $[A]_0$.

Continuing with the material balances, we find:

$$[A] = \frac{[A]_0}{1 + (kV/q)} = \frac{[A]_0}{1 + k\tau}$$

When Da = kτ << 1, [A] goes to $[A]_0$.

$$F_B = rV = kV[A] = \frac{kV[A]_o}{1 + k\tau} = \frac{kV[A]_o}{1 + kV/q}$$

$$\lim_{q \to \infty} F_B = \lim_{q \to \infty}\left(\frac{kV[A]_o}{1 + kV/q}\right) = kV[A]_0$$

Unfortunately, in the limiting case of infinite flow rate, the concentration of B in the output solution is vanishingly small:

$$\lim_{q \to \infty}[B] = \lim_{q \to \infty}\big(k[A](V/q)\big) = \lim_{q \to \infty}\left(k\frac{[A]_0}{1 + (kV/q)}(V/q)\right) = 0\,.$$