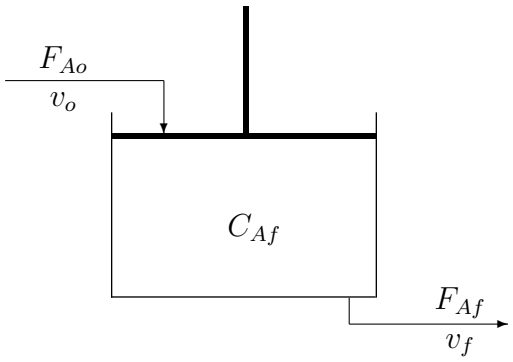
CP303 – Set #5 (July-October 2013)

Design of Ideal Continuous Stirred Tank Reactors (CSTRs)

operated at Steady State under Isothermal Conditions

(It is important to have this note set with you during all lecture classes.)

In a continuous stirred tank reactor (abreviated CSTR), reactants are fed to the reactor at the inlet and the products are removed from the reactor at the outlet. In an ideal continuous stirred tank reactor, the reacting mixture is assumed to be well mixed and therefore the properties of the reacting mixture are uniformly distributed through out the reactor. Also, it is assumed that in an ideal continuous stirred tank reactor, the properties of the exit stream are the same as the properties of the reacting mixture within the reactor.



Design equation for reactant A for the CSTR is obtained by writing the mass balance for reactant A over the entire volume of the reacting mixture V as follows:

mass of A entering the CSTR per unit time
= mass of A leaving the CSTR per unit time
+ mass of A accumulated within the CSTR per unit time
+ mass of A disappearing by the reaction within the CSTR per unit time

which becomes

$$F_{Ao}\,M_A = F_{Af}M_A + \frac{d}{dt}(C_{Af}\,M_A\,V) + (-r_A)\Big|_{at\,C_{Af}}\,M_A\,V \tag{5.1}$$

where F_{Ao} is the number of moles of A per unit time entering the CSTR, F_{Af} is the number of moles of A per unit time leaving the CSTR, M_A is the molar mass of A, C_{Af} is the molar concentration of A within the CSTR (which is assumed to be the same as the concentration of A at the exit) and $(-r_A)$ is the molar rate at which A is disappearing because of the progression of the reaction.

Removing M_A from (5.1) and rearranging it, we get the design equation for reactant A in an ideal CSTR operated at steady state as follows:

$$V_{CSTR} = \frac{F_{Ao} - F_{Af}}{(-r_A)\Big|_{at\,C_{Af}}} \tag{5.2}$$

Working out in terms of the concentration of A, C_A:

The respective concentrations of A at the inlet and at the exit of an ideal CSTR are defined as follows:

$$C_{Ao} \equiv \frac{\text{Molar flow rate of } A \text{ at the inlet}}{\text{Volumetric flow rate at the inlet}} = \frac{F_{Ao}}{v_o} \tag{5.3}$$

and

$$C_{Af} \equiv \frac{\text{Molar flow rate of } A \text{ at the exit}}{\text{Volumetric flow rate at the exit}} = \frac{F_{Af}}{v_f} \tag{5.4}$$

Substituting the above in (5.2), we get

$$V_{CSTR} = \frac{C_{Ao}v_o - C_{Af}v_f}{(-r_A)\Big|_{at\, C_{Af}}} \tag{5.5}$$

Working out in terms of the conversion of A, x_A:

The final conversion of A in a CSTR is defined by

$$x_{Af} \equiv \frac{F_{Ao} - F_{Af}}{F_{Ao}}\,, \tag{5.6}$$

using which (5.2) can be rewritten as follows:

$$V_{CSTR} = \frac{F_{Ao}x_{Af}}{(-r_A)\Big|_{at\, C_{Af}}} \tag{5.7}$$

Example 5.1: Consider the elementary liquid-phase reaction $A \longrightarrow products$ taking place in an ideal CSTR operated at steady state at constant temperature. Determine the space-time required for the concentration of A to become half of its inlet concentration.

Solution:

Since the given reaction is elementary, the reaction rate equation can be written as

$$r_A = -k\, C_A \tag{5.8}$$

where k, which is a function of temperature, remains constant since the reaction is said to take place at constant temperature.

Substituting r_A given by (5.8) in the design equation of an ideal CSTR operated at steady state, given by (5.2), we get

$$V = \frac{F_{Ao} - F_{Af}}{(k\, C_A)\Big|_{at\, C_{Af}}} = \frac{F_{Ao} - F_{Af}}{k\, C_{Af}} \tag{5.9}$$

Using $C_{Ao} = F_{Ao}/v_o$ and $C_{Af} = F_{Af}/v_f$ in (5.9), we get

$$V = \frac{C_{Ao}\, v_o - C_{Af}\, v_f}{k\, C_{Af}}$$

The given reaction is a liquid phase-reaction, and therefore it is acceptable to assume that the density of the reacting mixture remains a constant. At steady flow, the mass flow rate

of the reacting mixture remains a constant. Thus, the volumetric flow rate of the reacting mixture remains a constant, which helps to simplify the above equation to

$$V = \frac{v\,(C_{Ao} - C_{Af})}{k\,C_{Af}} \tag{5.10}$$

where $v = v_o = v_f$.

The space-time for an ideal CSTR is defined as

$$\tau \equiv \frac{\text{Volume of the reactor}}{\text{Volumetric flow rate of the reacting mixture}} = \frac{V}{v} \tag{5.11}$$

where v is taken as a constant.

Using (5.11), we could rewrite (5.10) as

$$\tau = \frac{C_{Ao} - C_{Af}}{k\,C_{Af}} \tag{5.12}$$

Therefore, the space-time required to halve the initial concentration could be calculated as follows:

$$\tau = \frac{C_{Ao} - 0.5C_{Ao}}{k\,(0.5C_{Ao})} = \frac{1}{k} \tag{5.13}$$

Example 5.2: Determine the space-time taken to reach 90% conversion of A in the reaction considered in Example 5.1.

Solution:

Using $\tau = V/v$, $v\,C_{Af} = F_{Af}$ and $F_{Af} = F_{Ao}(1 - x_{Af})$ in (5.9) we get

$$\tau = \frac{x_{Af}}{k\,(1 - x_{Af})} \tag{5.14}$$

Since $x_{Af} = 0.9$, we get

$$\tau = \frac{0.9}{k\,(1 - 0.9)} = \frac{9}{k} \tag{5.15}$$

Example 5.3: Consider the gas-phase reaction $2\,A \longrightarrow B + 2\,C$, for which the rate equation is given by

$$r_A = -k\,C_A^2 \tag{5.16}$$

Conversion of A required is expected to be 90%. Determine the space-time required to carry out the above reaction in an ideal CSTR operated at steady state under constant temperature and constant pressure conditions.

Solution:

Substituting (r_A) given by (5.16) in the design equation of an ideal CSTR operated at steady state, given by (5.2), we get

$$V = \frac{F_{Ao} - F_{Af}}{(k\,C_A^2)|_{exit}} = \frac{F_{Ao} - F_{Af}}{k\,C_{Af}^2} \tag{5.17}$$

Since the problem is a gas-phase reaction, it is convenient to work it out in terms of conversion of A. In order to do that, we must first write the above equation in terms of F_{Ao} and F_{Af}, which is done as follows:

Using $C_{Af} = F_{Af}/v_f$ in (5.17), we get

$$V = \frac{F_{Ao} - F_{Af}}{k\, F_{Af}^2/v_f^2} \tag{5.18}$$

Using $F_{Af} = F_{Ao}\,(1 - x_{Af})$ in (5.18), we get

$$V = \frac{x_{Af}\, v_f^2}{k\, F_{Ao}\,(1 - x_{Af})^2} \tag{5.19}$$

Following the reasoning with the gas-phase reaction in an ideal PFR operated at steady state (see Set #4), we can say that volumetric flow rate at the exit, v_f, shall be written as

$$v_f = \frac{P_o}{P}\,\frac{T}{T_o}\,v_o\left(1 + \frac{F_{Ao}}{F_{To}}\,\frac{x_{Af}}{2}\right) . \tag{5.20}$$

Since the reactor is operated at constant pressure and constant temperature, (5.20) gives

$$v_f = v_o\left(1 + \frac{F_{Ao}}{F_{To}}\,\frac{x_{Af}}{2}\right) . \tag{5.21}$$

Substituting v_f of (5.21) in (5.19), we get

$$V = \frac{x_{Af}\, v_o}{k\, C_{Ao}}\;\frac{\left(1 + \frac{F_{Ao}}{F_{To}}\,\frac{x_{Af}}{2}\right)^2}{(1 - x_{Af})^2} \tag{5.22}$$

where C_{Ao} is the concentration of A at the entrance of the reactor given by (F_{Ao}/v_o).

Equation (5.22), therefore, gives the space-time of an ideal CSTR required to achieve 90% conversion of A as

$$\tau \equiv \frac{V}{v_o} = \frac{0.9}{k\, C_{Ao}}\;\left(\frac{1 + \frac{F_{Ao}}{F_{To}} \times 0.45}{0.1}\right)^2 \tag{5.23}$$

Let us suppose that only A is fed to the reactor. Then (5.23) reduces to

$$\tau = \frac{0.9}{k\, C_{Ao}}\;\left(\frac{1 + 0.45}{0.1}\right)^2 \tag{5.24}$$

For a general gas-phase reaction,

$$a\, A + b\, B + c\, C + \cdots \longrightarrow p\, P + q\, Q + s\, S + \cdots , \tag{5.25}$$

the volumetric flow rate v is related to x_A by

$$v = \frac{P_o}{P}\,\frac{T}{T_o}\,v_o\,(1 + \epsilon_A\, x_A) . \tag{5.26}$$

where

$$\epsilon = \frac{F_{Ao}}{F_{To}}\left[\frac{(p + q + s + \cdots) - (a + b + c + \cdots)}{a}\right] \tag{5.27}$$

and $F_{To} = (F_{Ao} + F_{Bo} + F_{Co} + \cdots) + (F_{Po} + F_{Qo} + F_{Ro} + \cdots) + F_{Io}$ is the total number of moles of the reacting mixture entering the reactor.
