Consider two CSTRs in series. A liquid phase reaction \( \text{A} \rightarrow \text{B} \) is conducted in these reactors under isothermal conditions. Pure \text{A} is given in the feed. For the following conditions, determine the optimum volume of the reactors, i.e. minimize the total volume of the reactor.

(i) For a first order reaction.
(ii) For a second order reaction, given that \( Q = 25 \text{lit-min}^{-1}, C_{\text{A-in}} = 0.04 \text{mol/lit}, \quad -r_A = kC_A^2, \quad k= 0.075 \text{lit/mol/min}, \quad x_{\text{out}} = 0.85 \)

Let \( V_1 \) be the volume of first reactor and \( V_2 \) be the volume of the second reactor. We need to minimize the total volume \( V_1 + V_2 \).

By varying \( V_1 \), we can vary the \( x_1 \). Then \( V_2 \) can be calculated since \( x_{\text{out}} \) (i.e. \( x_2 \)) is given.

For a first order reaction, with \( \text{e} \)

\[
F_{\text{A-in}} + V_1 r_A = F_{\text{A-out}}
\]

\[
F_{\text{A-in}} - V_1 k C_{\text{A-in}} (1-x_1) = F_{\text{A-in}} (1-x_1)
\]

Hence, \( V_1 = \frac{F_{\text{A-in}} x_1}{kC_{\text{A-in}} (1-x_1)} \)

Similarly,

\( V_2 = \frac{F_{\text{A-in}} (x_2-x_1)}{kC_{\text{A-in}} (1-x_2)} \)

Total volume = \( V_1 + V_2 \). \( V = \frac{F_{\text{A-in}} x_1}{kC_{\text{A-in}} (1-x_1)} + \frac{F_{\text{A-in}} (x_2-x_1)}{kC_{\text{A-in}} (1-x_2)} = \frac{F_{\text{A-in}}}{kC_{\text{A-in}}} \left[ \frac{x_1}{(1-x_1)} + \frac{(x_2-x_1)}{(1-x_2)} \right] \)

Differentiating this with respect to \( x_1 \) we get

\[
\frac{\partial V}{\partial x_1} = \frac{F_{\text{A-in}}}{kC_{\text{A-in}}} \left[ \frac{(1-x_1) + x_1}{(1-x_1)^2} - \frac{1}{(1-x_2)^2} \right] = \frac{F_{\text{A-in}}}{kC_{\text{A-in}}} \left[ \frac{1}{(1-x_1)^2} - \frac{1}{(1-x_2)^2} \right]
\]

Setting this to zero, we get \( (1-x_1)^2 = (1-x_2) \)

i.e. \( x_2 = 2x_1 - x_1^2 \)

Under these conditions,
\[
V_2 = \frac{F_{A\text{-in}} (x_2 - x_1)}{kC_{A\text{-in}} (1-x_2)} = \frac{2x_1 - x_1^2}{kC_{A\text{-in}} (1-x_1)} = \frac{F_{A\text{-in}} (x_1 - x_1^2)}{kC_{A\text{-in}} (1-x_1)^2} = \frac{F_{A\text{-in}} x_1}{kC_{A\text{-in}} (1-x_1)} = V_1
\]

Hence equal sized reactors are the best.

For second order reaction (or in general for any order) we have to use the values and find the solution. For example, \( Q = 25 \text{ lit-min}^{-1}, C_{A\text{-in}} = 0.04 \text{ mol/lit}, -r_A = kC_A^2, k= 0.075 \text{ lit/mol/min}, x_{out} = 0.85 \)

Using the same procedure we get

\[
V_1 = \frac{F_{A\text{-in}} x_1}{kC_{A\text{-in}}^2 (1-x_1)^2} \text{ and } V_2 = \frac{F_{A\text{-in}} (x_2 - x_1)}{kC_{A\text{-in}}^2 (1-x_2)^2}
\]

Therefore, \( V = \frac{F_{A\text{-in}} x_1}{kC_{A\text{-in}}^2 (1-x_1)^2} + \frac{F_{A\text{-in}} (x_2 - x_1)}{kC_{A\text{-in}}^2 (1-x_2)^2} = \frac{F_{A\text{-in}}}{kC_{A\text{-in}}^2} \left[ \frac{x_1}{(1-x_1)^2} + \frac{(x_2 - x_1)}{(1-x_2)^2} \right] \)

Differentiate wrt \( x_1 \) and set it to zero.

\[
\frac{\partial V}{\partial x_1} = \frac{F_{A\text{-in}}}{kC_{A\text{-in}}^2} \left[ \frac{(1-x_1)^2 + 2(1-x_1)x_1}{(1-x_1)^3} - \frac{1}{(1-x_2)^2} \right] = \frac{F_{A\text{-in}}}{kC_{A\text{-in}}^2} \left[ \frac{1 - x_1^2}{(1-x_1)^3} - \frac{1}{(1-x_2)^2} \right]
\]

\[
= \frac{F_{A\text{-in}}}{kC_{A\text{-in}}^2} \left[ \frac{1 + x_1}{(1-x_1)^3} - \frac{1}{(1-x_2)^2} \right] = 0
\]

I.e. \( (1-x_2)^2 = \frac{(1-x_1)^4}{1-x_1^2} \),

\( (1-x_2) = \frac{(1-x_1)^2}{\sqrt{1-x_1^2}} \)

\( x_2 = 1 - \frac{(1-x_1)^2}{\sqrt{1-x_1^2}} \)

For the given values, \( F_{A\text{-in}} = 1 \text{ mol/min}, V = 8333 \times \left[ \frac{x_1}{(1-x_1)^2} + 44.4 \times (0.85 - x_1) \right] \)

Taking the derivative and setting it to zero, we get

\[
\frac{(1-x_1)^2 + 2(1-x_1)x_1}{(1-x_1)^4} - 44.4 = 0
\]
Solving it, using numerical tools, we get

\[ X_1 = 0.665 \]

\[ V_1 = 49.4 \text{ kL} \text{ and } V_2 = 67 \text{ kL}. \text{ Total volume } = 117 \text{ kL}. \]

Instead, if we have used equal sized reactors, what would be the total volume to achieve the same conversion?

\[
V'_1 = \frac{F_{A_{\text{in}}} x_1}{kC_{A_{\text{in}}}^2 (1-x_1)^2} = V'_2 = \frac{F_{A_{\text{in}}} (x_2 - x_1)}{kC_{A_{\text{in}}}^2 (1-x_2)^2}
\]

Eliminating the common factors, we get

\[
\frac{x_1}{(1-x_1)^2} = \frac{(x_2 - x_1)}{(1-x_2)^2}.
\]

Rearranging this, we get \((1-x_2)^2 x_1 = (x_2 - x_1)(1-x_1)^2 \).

Substitute \(x_2 = 0.85\), we can solve this equation using numerical tools and get \(x_1 = 0.69\)

For this value of \(x_1\), \(V_1 = 60 \text{ lit} = V_2\).

Total volume = 120 lit. Although it is not ‘optimal’, it is only slightly larger than the optimal volume. Other factors such as availability and stock of spare parts will influence the choice of reactors and frequently a plant will use equal sized reactor even if it is not optimal from the point of view of total volume.