10.37 Chemical and Biological Reaction Engineering, Spring 2007
Prof. K. Dane Wittrup

Lecture 9: Reactor Size Comparisons for PFR and CSTR

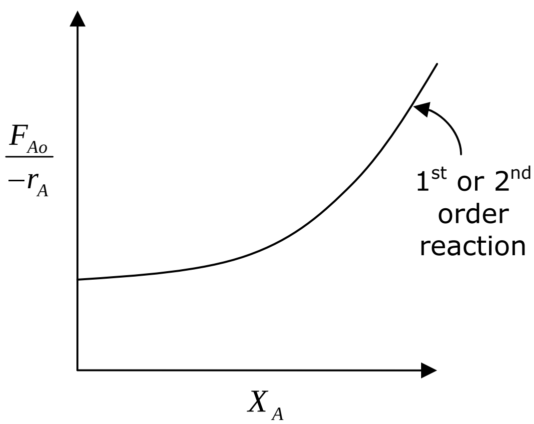
This lecture covers reactors in series and in parallel, and how the choice of reactor affects selectivity versus conversion.

PFR vs. CSTR: Size and Selectivity

Material balance:

CSTR	PFR
$\mathrm{V} = \dfrac{F_{Ao}}{-r_A} X_A$	$\mathrm{V} = \int_0^{X_A} \dfrac{F_{Ao}}{-r_A} dX_A$

"Levenspiel Plot"



- as X_A increases, C_A decreases
  $-r_A$ decreases, for 1st and 2nd order,
  so $\dfrac{F_{Ao}}{-r_A}$ increases

Figure 1. General Levenspiel Plot.

CSTR Volume | PFR Volume

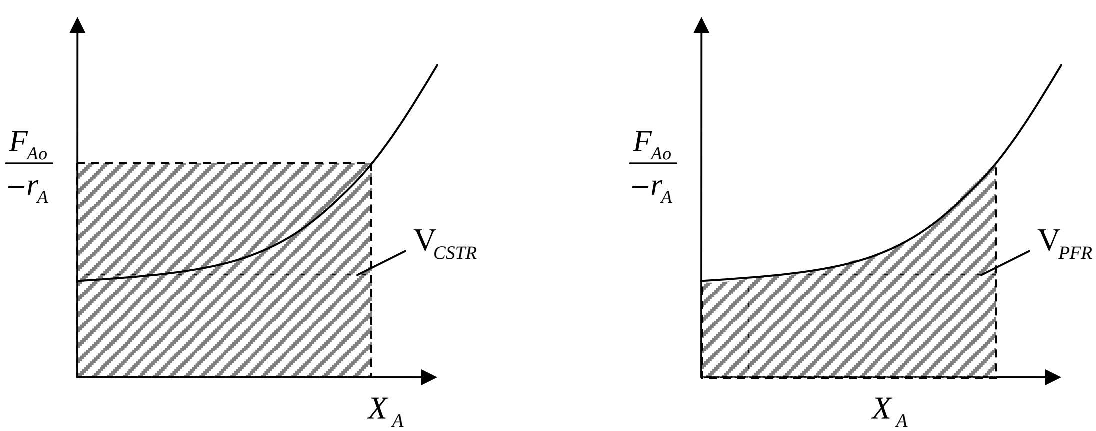


Figure 2. Levenspiel plots for a CSTR and a PFR for positive order reactions.

So PFR is always a smaller reactor for a given conversion when kinetics are positive order.

Non-monotonically positive order kinetics arise:

- Autocatalytic reactions (e.g. cell growth)
- Adiabatic or non-isothermal exothermic reactions
- Product inhibited reactions (some enzymes)

Series of Reactors

Example: 2 CSTRs

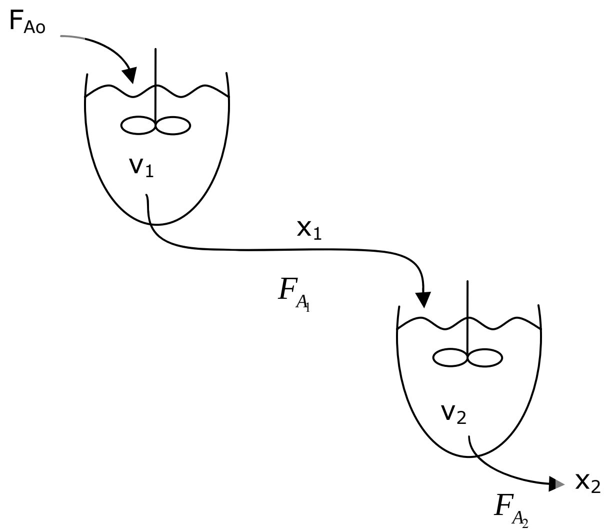


Figure 3. Schematic of two CSTRs in series.

$$V_1 = \frac{F_{Ao}}{-r_{A_1}} X_1$$

2nd reactor:

In + Out + Prod = ~~Acc~~ → 0

$F_{A_1} - F_{A_2} + r_{A_2} V_2 =$ Steady state

$$F_{A_2} = F_{A_0} - X_2 F_{A_0} \quad \rightarrow \quad V_2 = \frac{F_{A_0}}{-r_{A_2}}(X_2 - X_1)$$

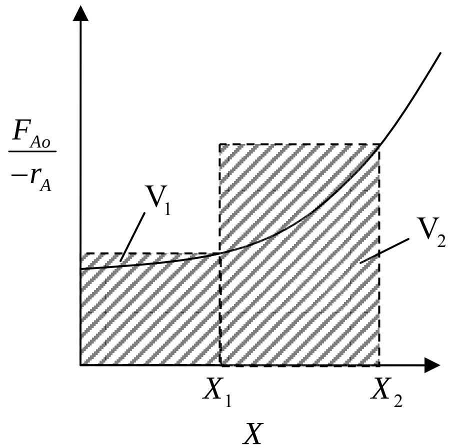


Figure 4. Reactor volumes for 2 CSTRs in series.

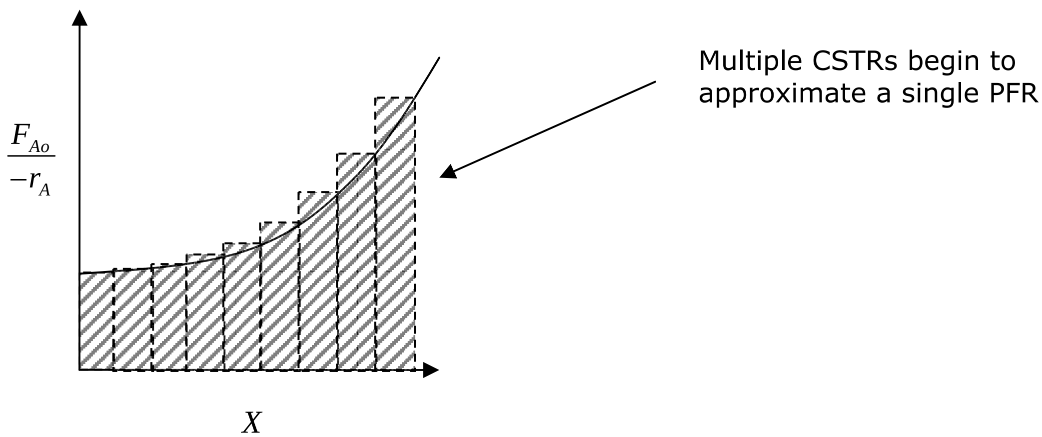


Figure 5. Reactor volumes for multiple CSTRs in series.

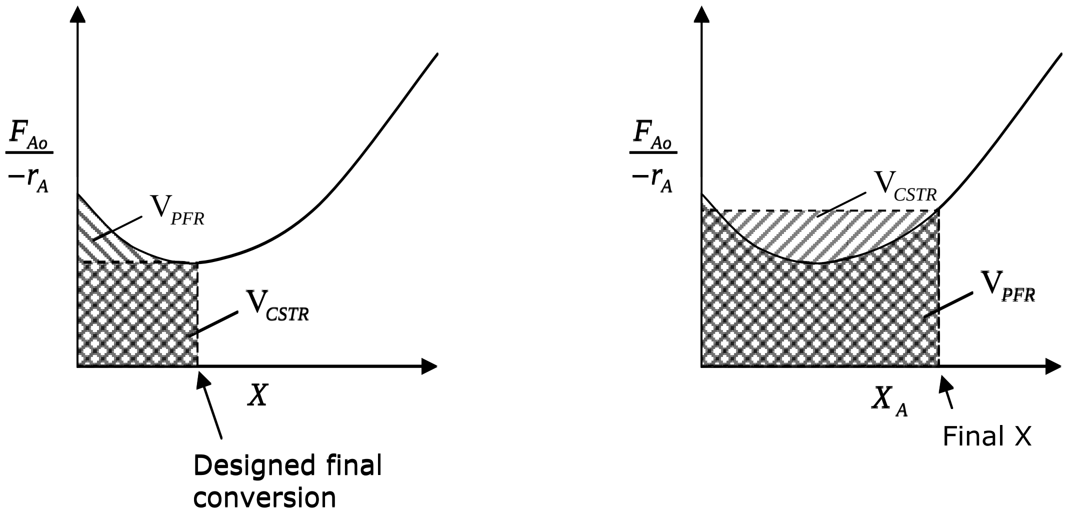


Figure 6. Levenspiel plots comparing CSTR and PFR volumes for changing kinetics. Left: The CSTR has the smaller volume. Right: The PFR eventually has the smaller volume.

Choice of PFR vs CSTR depends on conversion. Choose the reactor that has the smallest volume →reduce cost.

Reactors:

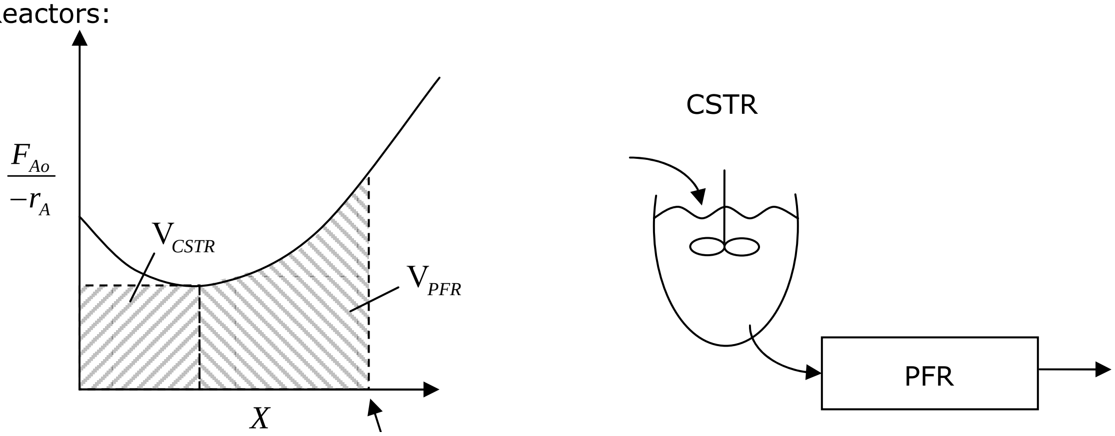


Figure 7. To achieve the desired conversion with smaller reactor volumes, use a combination. In this case, use a CSTR then a PFR. By doing so, the reactor volume is less than the area underneath the curve.

For competing parallel reactions, selectivity for desired product can dominate the choice.

<u>Example</u> $A \rightarrow D$ $\quad r_D = k_d C_A^{\alpha_1}$ $\quad$ D = Desired, U = Undesired

$A \rightarrow U$ $\quad r_U = k_u C_A^{\alpha_2}$

Define “selectivity” $S_{D/U} = \frac{r_D}{r_U} = \frac{k_d}{k_u} C_A^{(\alpha_1 - \alpha_2)}$

If $\alpha_1 > \alpha_2$, as C_A increases, $S_{D/U}$ increases

-Favors PFR because C_A starts at C_{Ao} then drops whereas CSTR concentrations are always at lower C_A.

If $\alpha_1 < \alpha_2$, as C_A increases, $S_{D/U}$ decreases

-CSTR favored

If $\alpha_1 = \alpha_2$ then $S_{D/U} = \frac{k_d}{k_u}$, no dependence on C_A

-Therefore no CSTR/PFR preference.

Define a fractional yield

$$\phi = \frac{dC_D}{-dC_A} = \frac{k_d C_A^{\alpha_1}}{k_d C_A^{\alpha_1} + k_u C_A^{\alpha_2}}$$

Overall fractional yield $\Phi = \frac{\text{All } D \text{ produced}}{\text{All } A \text{ consumed}}$

For a CSTR: $\Phi = \phi\big|_{\text{Exit } C_A}$

$\Delta C_A = C_{A_0} - C_{A_f}$

For a PFR: $\Phi = \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{At}} \phi \, dC_A$

If $\alpha_1 = \alpha_2$

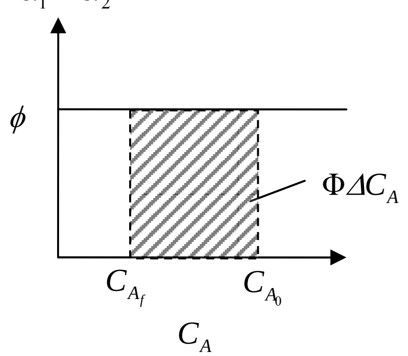


Figure 8. Fractional yield versus concentration. Selectivity does not depend on C_A.

If $\alpha_1 > \alpha_2$

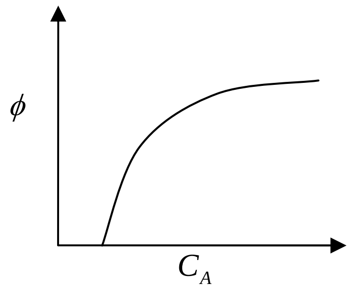


Figure 9. Fractional yield versus concentration when $\alpha_1 > \alpha_2$.

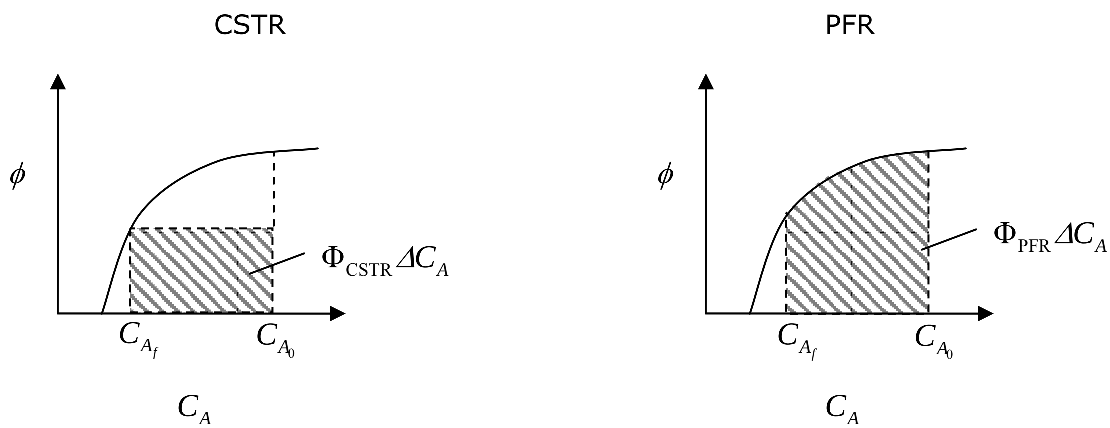


Figure 10. Comparison of overall fractional yield for a CSTR and a PFR when $\alpha_1 > \alpha_2$.

PFR is preferred because $\Phi_{PFR} > \Phi_{CSTR}$, therefore the yield of D per mol A consumed is higher.

If $\alpha_1 < \alpha_2$

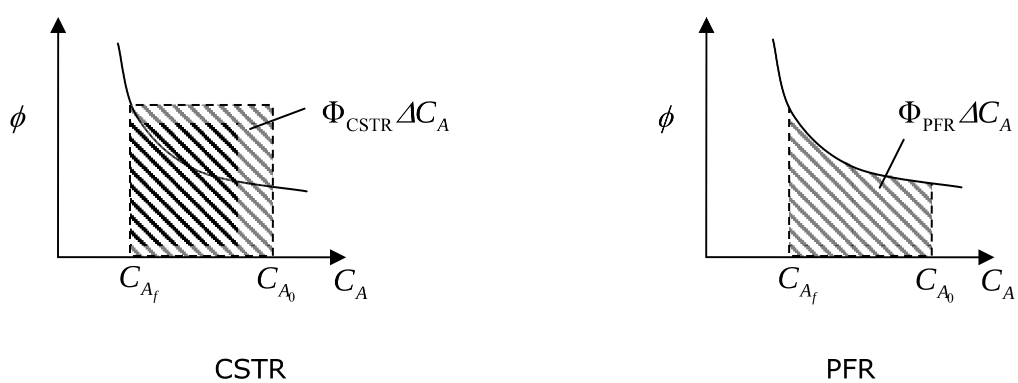


Figure 11. Comparsion of overall fractional yield for a CSTR and a PFR when $\alpha_1 > \alpha_2$.

$$\Phi_{PFR} < \Phi_{CSTR}$$