Reactor Design I: 1. Reactor Systems

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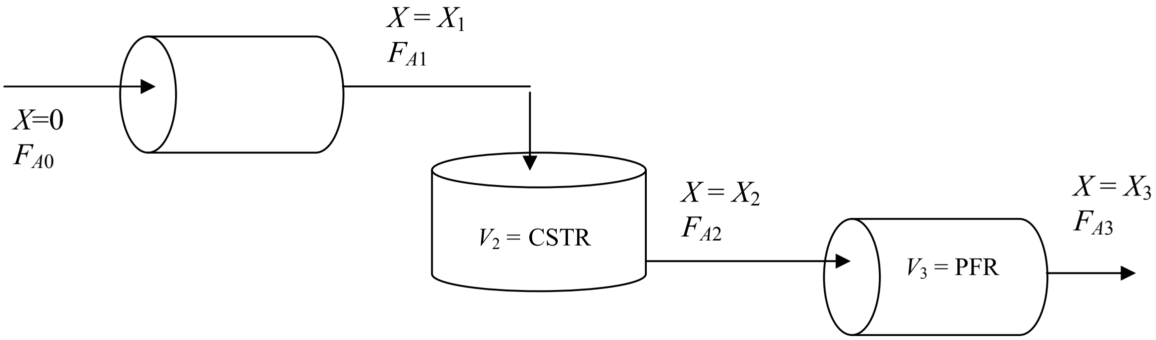
Where multiple reactors are used in a process, these may be connected in series or parallel. Here we consider the possible benefits, or otherwise, of these configurations.

1. Conversion in reactors in series.

On connecting reactors in series, the exit stream of one reactor becomes the feed stream to the next. In these systems it is common to define the conversion achieved in the series of reactors, rather than with respect to a single reactor. This approach is valid provided that no side streams are removed or additional feed streams added to the reactor train. Consider a reactor train of a PFR followed by a CSTR, followed by a PFR:



$$X_2 = \frac{\text{total moles A reacted up to point 2}}{\text{Moles A fed into first reactor (i.e. system)}}$$

Also,

$$F_{A,1} = F_{A0} - F_{A,0}X_1$$
$$F_{A,2} = F_{A0} - F_{A,0}X_2$$
$$F_{A,3} = F_{A0} - F_{A,0}X_3$$

For reactor 1:

$$V_1 = F_{A0}\int_0^{X_1}\frac{dX}{-r_A}$$

For reactor 2, CSTR balance gives:

$$V_2 = \frac{F_{A1} - F_{A2}}{-r_{A2}}$$

Substituting for F_{A1} and F_{A2}, we get:

$$V_2 = \frac{F_{A0}(X_2 - X_1)}{-r_{A2}}$$

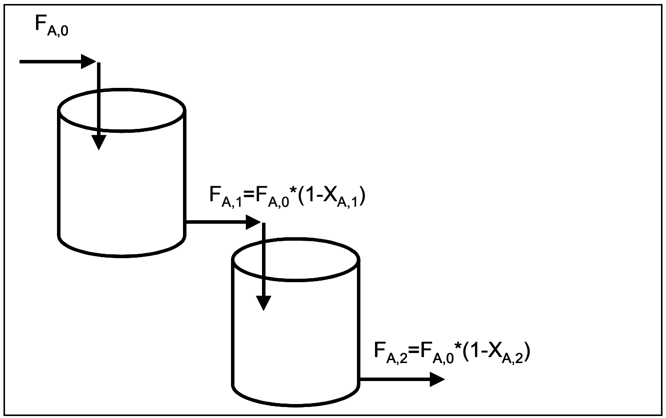
For reactor 3 (PFR):

$$V_3 = F_{A0}\int_{X_2}^{X_3}\frac{dX}{-r_A}$$

Conversion X_3 is then the conversion delivered by the reactor *system*, and it remains to be seen what configuration of reactors will enable us to enjoy a conversion of X_3. Would, for instance, putting the CSTR as the first unit in the train, improve the conversion? The answer is: it depends. Various case studies are presented here which demonstrate this issue.

Ex: what if 1CSTR, 1PFR available, curve is as given, which config is better?

2. CSTRs in series:



Mole balance for compound A over the 1st CSTR:

$$F_{A,0} - F_{A,1} + r_{A,1}\cdot V_1 = 0$$

Also $\quad F_{A,1} = F_{A,0} - F_{A,0}X_1$

So $\quad \dfrac{V_1}{F_{A,0}} = \dfrac{X_{A,1}}{-r_{A,1}}$

Mole balance for compound A over 2nd CSTR:

$$F_{A,1} - F_{A,2} + r_{A,2}\cdot V_2 = 0$$

Also

$$F_{A1} = F_{A0} - F_{A0}X_1$$
$$F_{A2} = F_{A0} - F_{A0}X$$

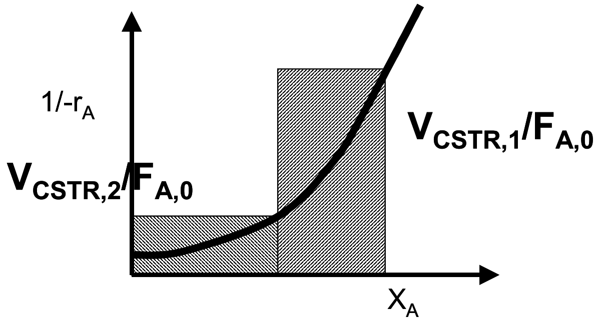
$$\frac{V_2}{F_{A,0}} = \frac{X_{A,2} - X_{A,1}}{-r_{A,2}}$$

The total reactor volume V is given by:

$$V = V_1 + V_2 = F_{A,0} \cdot \left(\frac{X_{A,1}}{-r_{A,1}} + \frac{X_{A,2} - X_{A,1}}{-r_{A,2}} \right) \neq F_{A,0} \cdot \frac{X_{A,2}}{-r_{A,2}}$$

Note: The rate of reaction in reactor 1 ($-r_{A,1}$) differs from the rate of reaction in reactor 2 ($-r_{A,2}$).

Considering the reactor sizes, note that in this case the combined reactor size is smaller than the volume of a single reactor to carry out the same reaction.



Example (Fogler)

Consider the isothermal gas-phase decomposition reaction:

$$A \rightarrow B + C$$

where the rate of reaction is given as:

$$-r_A = k \cdot C_{A,0} \cdot (1 - X_A)$$

In Table 1, the rate of reaction is given as a function of conversion, based on laboratory data collected at 422 K and a total pressure of 10 atm. The initial charge is an equimolar mix of reactant A and inerts. The volumetric feed rate to each reactor will be 6.0 dm^3 s^{-1}, correlating to 0.867 mol s^{-1}.

Table1: Raw data

X	0.0	0.1	0.2	0.3	0.4
-rA	0.0053	0.0052	0.0050	0.0045	0.0040

X	0.5	0.6	0.7	0.8	0.85
-rA	0.0033	0.0025	0.0018	0.00125	0.0010

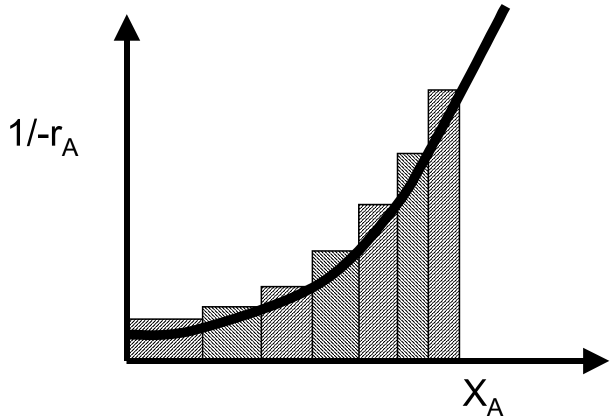
Here we use two CSTRs in series to attain an overall conversion of 80%. The conversion in the first reactor is 40%. Calculate the total reactor volume and construct a Levenspiel plot ($-1/r_A$ vs X) for these reactors.

n equally sized CSTRs in series:

Mole balance for compound A over the nth CSTR:

$$F_{A,n-1} - F_{A,n} + r_{A,n} \cdot V = 0$$

$$\frac{V}{F_{A,0}} = \frac{X_{A,n} - X_{A,n-1}}{-r_{A,n}}$$

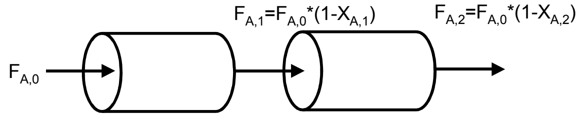


Note:

1) The rate of reaction in reactor differs in each reactor
2) The areas for all CSTRs shown (V/F$_{A,0}$) are identical
3) n CSTRs approach PFR behaviour, if n→ ∞

PFRs in series:

Consider 2 PFRs in series:



Mole balance for compound A over the 1st PFR:

$$\frac{V_1}{F_{A,0}} = \int_{X_A=0}^{X_A=X_{A,1}} \frac{dX_A}{-r_A}$$

Mole balance for compound A over 2nd PFR:

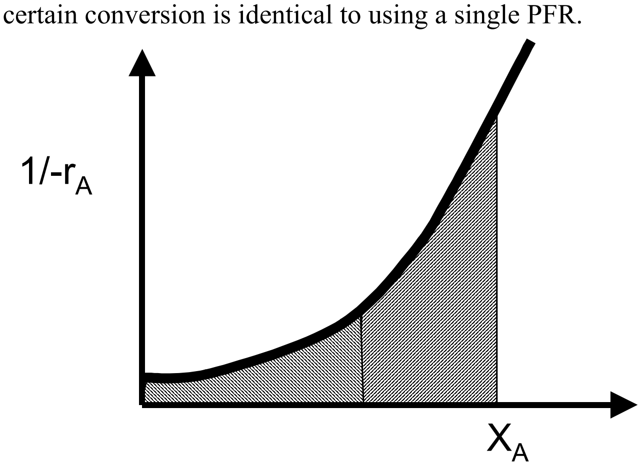
$$\frac{V_2}{F_{A,0}} = \int_{X_A=X_{A,1}}^{X_A=X_{A,2}} \frac{dX_A}{-r_A}$$

The total reactor volume V is given by:

$$V = V_1 + V_2 = F_{A,0} \cdot \left(\int_{X_A=X_{A,0}}^{X_A=X_{A,1}} \frac{dX_A}{-r_A} + \int_{X_A=X_{A,1}}^{X_A=X_{A,2}} \frac{dX_A}{-r_A} \right)$$

$$V = F_{A,0} \cdot \int_{X_A=X_{A,0}}^{X_A=X_{A,2}} \frac{dX_A}{-r_A}$$

Note:There is no gain with respect to reactor volume on putting two PFRs in series The size needed to obtain a certain conversion is identical to using a single PFR.



Let's Reflect on These Results

Why do you think reactors in series can add up to one big reactor for the plug flow case, whereas the results are different when we use CSTRs?

Consider the type of flow inherent in the PFR. By definition, the fluid flows in plugs, i.e. discrete and separate entities. As such, a reaction rate at one particular point will change the concentration at only that point. The rate is therefore localised, and does not depend on the spatial position of that plug.

In the CSTR, however, the fluid is, by definition, perfectly mixed, and so the rate depends on the concentration in that reactor, which, itself, depends on the contributions of all the reacting fluid elements in the space.

By changing the reactor volume, we are changing the size of the reaction space, and hence the amount of contribution from the various fluid elements to the overall rate.

The higher up the curve we go, the greater is 1/ra, and so the lower is the rate. In physical terms, higher conversion means lower reactant concentration and hence we expect the lower reaction rate.

In the case of the PFR, we see this low rate only at the end of the reactor, whereas for the CSTR, we MUST have this low rate through the reactor. In other words, since we require a specific concentration in the exit, we must have this same concentration throughout the reactor, which means the rate must be low throughout the reactor.

So PFR is always better from this point of view, but CSTR has practical advantages.

Numerical Examples: Sequencing Reactors

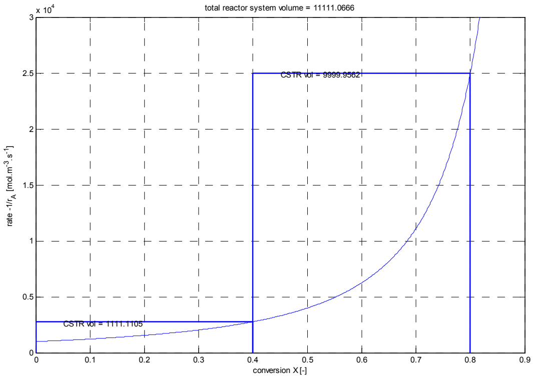
Example: Compare required volumes achieved for two reactors with 40% conversion after the first and 80% overall for the following combinations:

CSTR, CSTR;
CSTR, PFR;
PFR, CSTR;
PFR, PFR.

Reaction kinetics: second order, rate constant = 1x10^{-3} s-1.mol-1.m3, C_{A0} = 1 mol.m^{-3}.

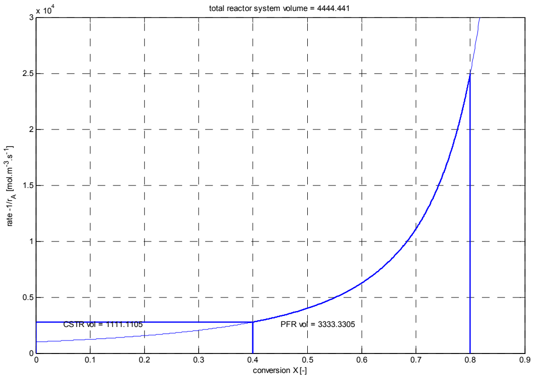
***Solutions*:**

a) CSTR, CSTR:



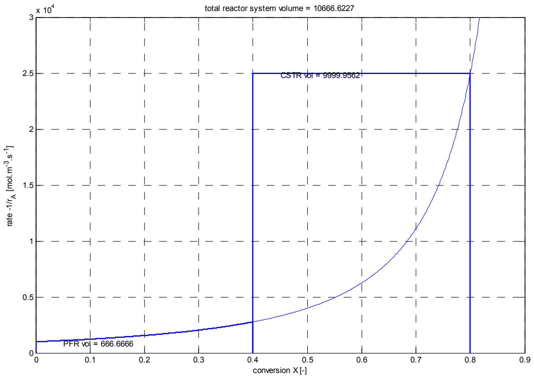
Vtot = 11111

CSTR, PFR:



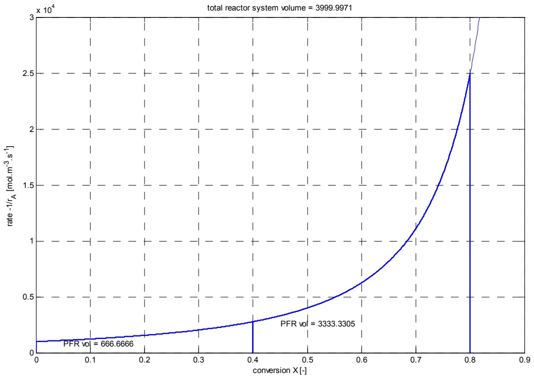
Vtot = 4444

PFR, CSTR:



Vtot = 10666

PFR, PFR:



Vtot = 4000.

Clearly, if reactor volume is the only consideration, PFRs are better. If we must combine PFRs with CSTRs, then smaller volumes can be achieved by using CSTRs where the 1/r vs X curve is has a small gradient and PFRs where it is steep.

Some general rules for ordering reactors

For a reaction whose rate concentration curve raises monotonically (any nth order reaction, $n > 0$, see module 3), the reactors should be connected in series. They should be ordered to keep the reactant concentration as high as possible if the curve is concave ($n > 1$), and as low as possible if the curve is convex ($n < 1$). For the former, the preferred order is PFR, small CSTR, large CSTR.

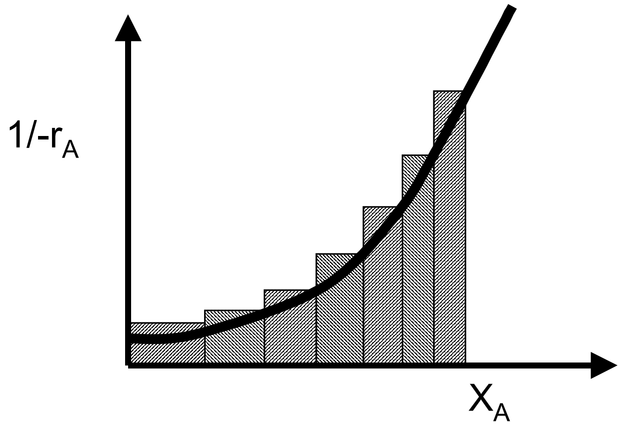
For reactions where the rate-concentration curve passes through a maximum or minimum, the preferred arrangement depends on the actual shape of the curve. No simple rules exist.

n equally sized CSTRs in series:

Mole balance for compound A over the nth CSTR:

$$F_{A,n-1} - F_{A,n} + r_{A,n} \cdot V = 0$$

$$\frac{V}{F_{A,0}} = \frac{X_{A,n} - X_{A,n-1}}{-r_{A,n}}$$



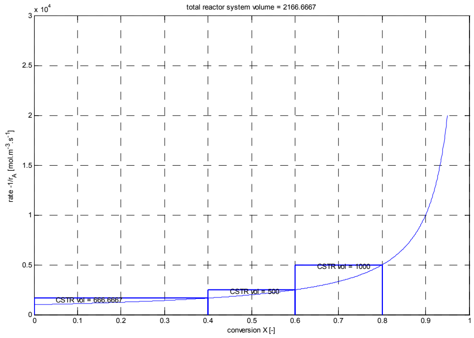
To note:

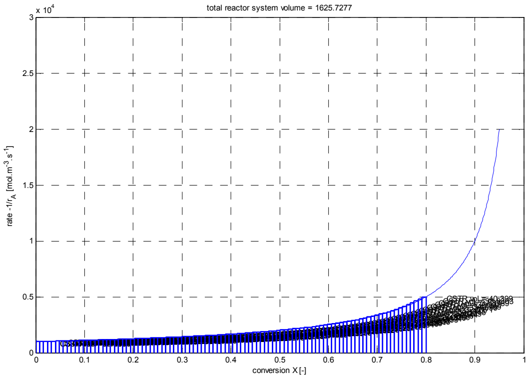
1) Rate of reaction in reactor differs in each reactor
2) Areas for all CSTR ($V/F_{A,0}$) are identical
3) n CSTRs approach PFR behaviour, if n→ ∞

<u>Example:</u> Chemistry as before, but let's look at one PFR, and then increasing numbers of CSTRs:

1PFR: V = 1609

3 CSTRs: V = 2167





100 CSTRs: V = 1626 (closer to PFR)

Reactors in parallel

There is never a good reason to put isothermally operating reactors in parallel, unless it is needed from a mechanical point of view.

Example

For a single CSTR of volume V: $\frac{V}{F_{A,0}} = \frac{X_A}{-r_A}$

By having two CSTRs in parallel we have to split the feed to the reactors. If e.g. the single CSTR is to be replaced by two equally sized CSTRs ($V_{½}$) operating in parallel, the feed to each of the reactor will be halved. Thus the mole balance for each reactor becomes:

$$\frac{V_{\frac{1}{2}}}{F'_{A,0}} = \frac{0.5 \cdot V}{0.5 \cdot F_{A,0}} = \frac{V}{F_{A,0}} = \frac{X_A}{-r_A}$$

The identical line of reasoning can be applied to PFRs in parallel.(tut1q1) In these reactors, one will choose to maintain optimum conditions in all reactors in parallel by maintaining τ or V/v_0 constant in each branch of the reactor network.

Definition of space time τ

the time needed to process one reactor volume of fluid based on entrance conditions

$\tau = \frac{V}{v_{inlet}}$ Also known as the *holding time* or the *mean residence time.*

Space velocity SV: the reciprocal of space time

$$SV = \frac{v_{inlet}}{V} = \frac{1}{\tau}$$

Note that although space time is always defined on inlet conditions, space velocity may be defined in terms of other conditions as well, hence it is not necessarily the inverse of space time.

(p57-58 in Scott Fogler)