Choosing the Right Kind of Reactor

Chapter 10

- The important lessons learned in the first nine chapters of this book should guide us right away, or with a very minimum of calculations, to the optimum reactor system.
- Previously we have come up with six general rules.
- Let us present them and then practice using them.

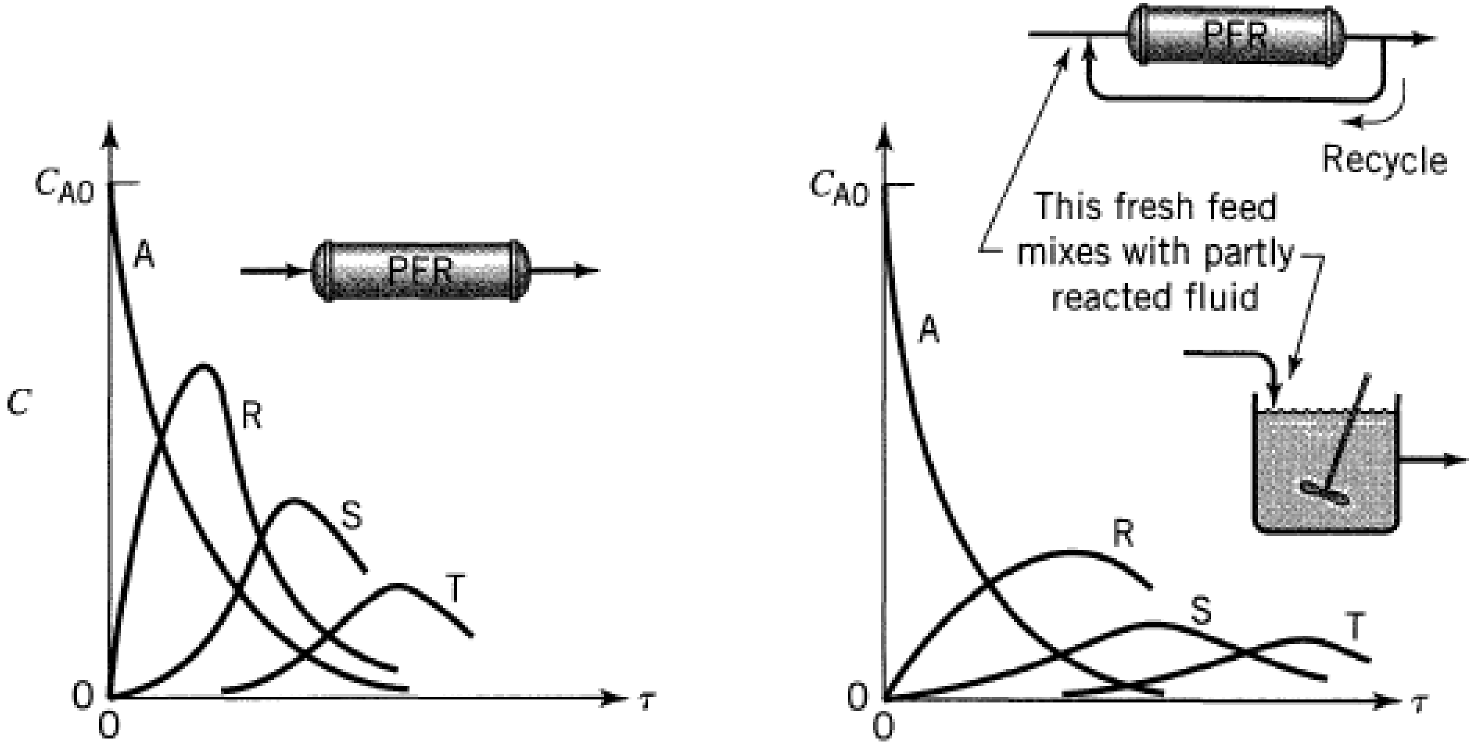
Rule 1. For Single Reactions

- To minimize the reactor volume, keep the concentration as high as possible for a reactant whose order is $n > 0$.
- For components where $n < 0$ keep the concentration low.

Rule 2. For Reactions in Series

$$A \rightarrow R \rightarrow S \rightarrow \cdots Y \rightarrow Z$$

- Consider reactions in series, as shown:
- To maximize any intermediate, do not mix fluids that have different concentrations of the active ingredients-reactant or intermediates.



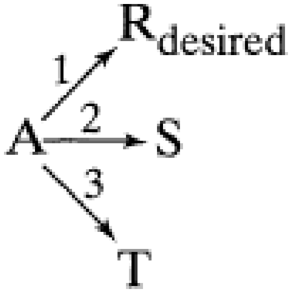
(a)

(b)

(a) Plug flow (no intermixing) gives the most of all the intermediates.
(b) Intermixing depresses the formation of all intermediates.

Rule 3. For Parallel Reactions

Consider the parallel reactions with reaction orders $\boldsymbol{n_i}$



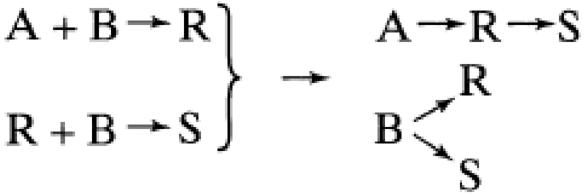
n_1 ··· low order
n_2 ··· intermediate
n_3 ··· high order

To get the best product distribution,

- low *C,* favors the reaction of lowest order
- high *C,* favors the reaction of highest order
- If the desired reaction is of intermediate order then some intermediate *C,* will give the best product distribution.
- For reactions all of the same order the product distribution is not affected by the concentration level.

Rule 4. Complex Reactions

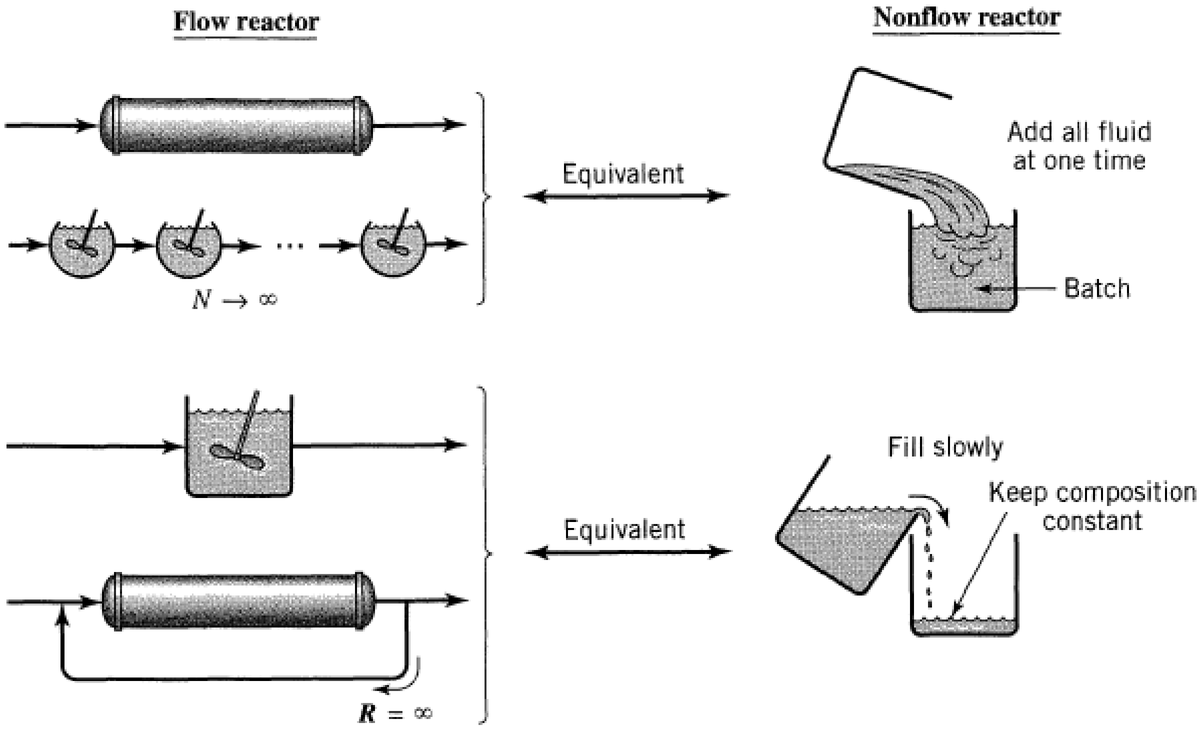
- These networks can be analyzed by breaking them down into their simple series and simple parallel components.
- For example, for the following elementary reactions,
- Where R is the desired product, the breakdown is as follows:



- This breakdown means that A and R should be in plug flow, without any recycle,
- While B can be introduced as you wish, at any concentration level,
- since it will not affect the product distribution.

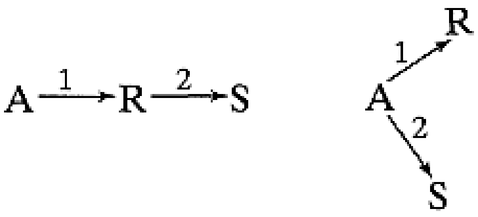
Rule 5. Continuous versus Non-continuous Operations

- Any product distribution that can be obtained in continuous steady-state flow operations can be gotten in a non-flow operation and vice versa.



Correspondence between the residence time distribution of steady Flow and either non-flow, batch or semibatch systems.

Rule 6. Effect of Temperature on Product Distribution



with

$$k_1 = k_{10} e^{-\mathbf{E}_1/\mathbf{R}T}$$

$$k_2 = k_{20} e^{-\mathbf{E}_2/\mathbf{R}T}$$

A high temperature favors the reaction with larger E, while a low temperature favors the reaction with smaller E.

Optimum Operation of Reactors

In reactor operations the word "optimum" can have different meanings. Let us look at two definitions which are particularly useful.

Feed a stream containing reactant A to a reactor and let R, S, T, . . . be formed, with R being the desired product. Then by optimum

1. We could mean maximizing the overall fractional yield of R, or

$$\Phi\left(\frac{R}{A}\right) = \left(\frac{\text{moles R formed}}{\text{moles of A consumed}}\right)_{\max}$$

2. we could mean running the reactor system so that the production of R is maximized, or

$$(\text{Prod R})_{max} = \left(\frac{\text{moles of R formed}}{\text{moles of A fed to the system}}\right)_{\max}$$

For reactions in series we calculate the maximum production rate of R directly.
However, for reactions in parallel we find it useful to first evaluate the instantaneous fractional yield of R, or and then proceed to find the optimum

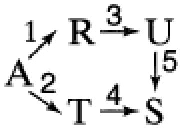
$$\varphi\left(\frac{R}{A}\right) = \left(\frac{\text{moles R formed}}{\text{moles A consumed}}\right)$$

If unused reactant can be separated from the exit stream, reconcentrated to feed conditions and then recycled, then

$$(\text{Prod R})_{\max} = \Phi(R/A)_{\text{opt}}$$

TEMPERATURE PROGRESSION FOR MULTIPLE REACTIONS

Consider the following scheme of elementary reactions:



$$\begin{cases} \mathbf{E}_1 = 79 \text{ kJ/mol} \\ \mathbf{E}_2 = 113 \text{ kJ/mol} \\ \mathbf{E}_3 = 126 \text{ kJ/mol} \\ \mathbf{E}_4 = 151 \text{ kJ/mol} \\ \mathbf{E}_5 = 0 \end{cases}$$

What temperature progression would you recommend if the desired product is:

(a) R, **(b)** S, **(c)** T, **(d)** U

(a) Intermediate R is Desired We want step 1 fast compared to step 2, and we want step 1 fast compared to step 3.

(b) Since **El** < **E2** and **El** < **E3**

use a low temperature and plug flow

(b) ***Final Product* S *is Desired.*** Here speed is all that matters.

So use a high temperature and plug flow.

(c) ***Intermediate* T *is Desired.*** We want step 2 fast compared to step 1, and we want step 2 fast compared to step 4.

Since $\mathbf{E}_2 > \mathbf{E}_1$ and $\mathbf{E}_2 < \mathbf{E}_4$ use a falling temperature and plug flow

(d) ***Intermediate* U *is Desired.*** We want step 1 fast compared to step 2, and step 3 fast compared to step 5.

Since $\mathbf{E}_1 < \mathbf{E}_2$ and $\mathbf{E}_3 > \mathbf{E}_5$ use a rising temperature and plug flow