

BT209

Bioreaction Engineering

16/02/2023

Design for single reactions

- ❑ There are **many ways of processing a fluid**:
 - in a single batch or flow reactor,
 - In a chain of reactors possibly with interstage feed injection or heating,
 - in a reactor with recycle of the product stream using various feed ratios and conditions,

➤ Which scheme should we use?

Cont..

- ❑ Numerous factors may have to be considered in answering this question;
 - the reaction type,
 - planned scale of production,
 - cost of equipment and operations,
 - safety, stability and flexibility of operation,
 - equipment life expectancy,
 - length of time that the product is expected to be manufactured,
 - ease of convertibility of the equipment to modified operating conditions or to new and different processes.

- With the wide choice of systems available and with the many factors to be considered, no neat formula can be expected to give the optimum setup.

Experience, engineering judgment, and a sound knowledge of the characteristics of the various reactor systems are all needed in selecting a reasonably good design and, needless to say, the choice in analysis of cost of equipment (capital cost) and operations (running cost), will be dictated by the economics of the overall process.

Comparison of single reactors

Batch reactors:

Advantage:

- The batch reactor has the advantage of small instrumentation cost and
- flexibility of operation (may be shut down easily and quickly).

Disadvantage

- It has the disadvantage of high labor and handling cost,
 - often considerable shutdown time to empty, clean out, and refill,
 - and poorer quality control of the product.
- Batch reactor is well suited to produce small amounts of material and to produce many different products from one piece of equipment.
- ❑ On the other hand, for the chemical/Biochemical treatment of materials in large amounts the continuous process is nearly always found to be more economical.

Design for single reaction

- Regarding reactor sizes, a comparison for a given duty and for $\varepsilon = 0$ shows that **an element of fluid reacts for the same length of time in the batch and in the plug flow reactor.**
- Thus, the **same volume of these reactors is needed to do a given job.**
- Of course, **on a long-term production basis we must correct the size requirement estimate to account for the shutdown time between batches.**
- Still, it is easy to relate the performance capabilities of the batch reactor with the plug flow reactor.

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A} \quad \text{for } \varepsilon_A = 0$$

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} = - \frac{1}{C_{A0}} \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A} \quad \varepsilon_A = 0$$

Mixed versus (CSTR) and Plug flow reactors (PFR)

- For a given duty the ratio of sizes of mixed and plug flow reactors will **depend on the extent of reaction, the stoichiometry, and the form of the rate equation.**
- comparison for the large class of reactions approximated by the **simple n^{th} order rate law**

$$-r_A = -\frac{1}{V} \frac{dN_A}{dt} = kC_A^n$$

CSTR:
$$\tau_m = \left(\frac{C_{A0}V}{F_{A0}} \right)_m = \frac{C_{A0}X_A}{-r_A} = \frac{1}{kC_{A0}^{n-1}} \frac{X_A(1 + \varepsilon_A X_A)^n}{(1 - X_A)^n}$$

PFR:
$$\tau_p = \left(\frac{C_{A0}V}{F_{A0}} \right)_p = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = \frac{1}{kC_{A0}^{n-1}} \int_0^{X_A} \frac{(1 + \varepsilon_A X_A)^n dX_A}{(1 - X_A)^n}$$

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Dividing we find that

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left(\frac{C_{A0}^n V}{F_{A0}}\right)_m}{\left(\frac{C_{A0}^n V}{F_{A0}}\right)_p} = \frac{\left[X_A \left(\frac{1 + \varepsilon_A X_A}{1 - X_A}\right)^n\right]_m}{\left[\int_0^{X_A} \left(\frac{1 + \varepsilon_A X_A}{1 - X_A}\right)^n dX_A\right]_p}$$

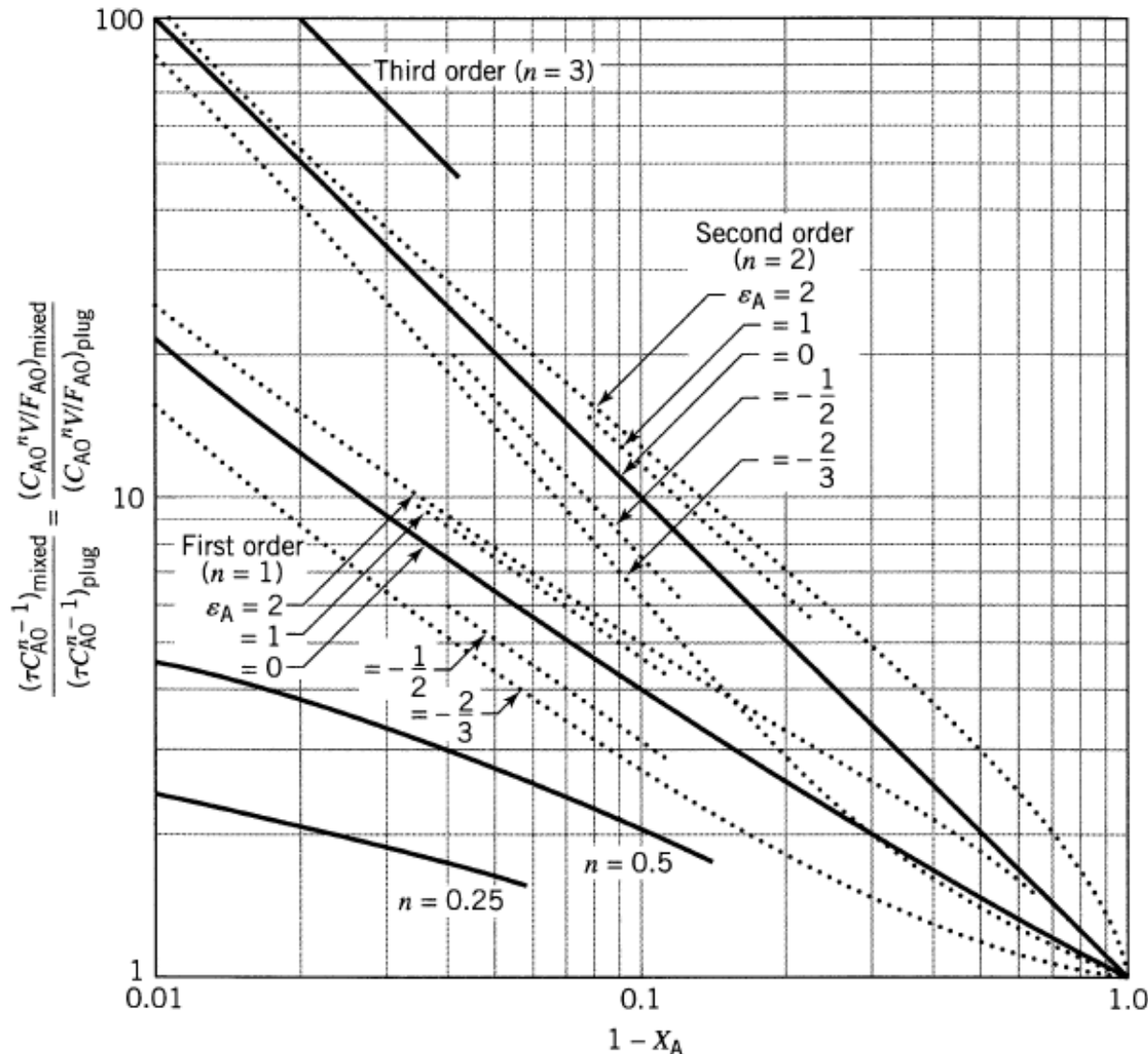
With constant density, or $\varepsilon = 0$, this expression integrates to

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left[\frac{X_A}{(1 - X_A)^n}\right]_m}{\left[\frac{(1 - X_A)^{1-n} - 1}{n - 1}\right]_p}, \quad n \neq 1$$

or

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left(\frac{X_A}{1 - X_A}\right)_m}{-\ln(1 - X_A)_p}, \quad n = 1$$

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- Fig provides a quick comparison of the performance of plug flow with mixed flow reactors.
- For identical feed composition C_{A0} and flow rate F_{A0} , the ordinate of this figure gives directly the volume ratio required for any specified conversion.
- For any particular duty and for all positive reaction orders the mixed reactor is always larger than the plug flow reactor. The ratio of volumes increases with reaction order.
- When conversion is small, the reactor performance is only slightly affected by flow type. The performance ratio increases very rapidly at high conversion;
- Density variation during reaction affects design;

The ordinate becomes the volume ratio V_m/V_p or space-time ratio τ_m/τ_p if the same quantities of identical feed are used.

Cont..

PFR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

CSTR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_{Af} - X_{Ai}}{(-r_A)_f}$$

