

Chemical Reaction Engineering Notes

M. P. Dudukovic

1. EFFECT OF MIXING ON REACTOR PERFORMANCE FOR HOMOGENEOUS SYSTEMS - INTRODUCTION

In dealing with homogeneous reaction systems we have seen that basically all problems encountered can be classified into two broad categories:

- I. Reactor design is required for a given reaction system, and "a priori" prediction of reactor performance is therefore needed.
- II. Assessment of performance of existing reactors is asked for, and suggestions for improvement are solicited.

So far in dealing with these problems we have assumed two limits in mixing pattern (realizing that mixing and flow patterns affect reactor performance). For systems with continuous flow at steady state they are:

- CSTR - perfectly mixed (on molecular level) tank
- PFR - plug flow reactor (no mixing in direction of flow, piston like flow)

For a single reaction at isothermal conditions, reactor performance is measured by conversion of the limiting reactant and we know that for each of the ideal reactors it is a function of kinetics, feed concentrations and thermodynamic limitations i.e

$$x_A = f \left(Da, \frac{C_{B_o}}{C_{A_o}}, K \right) \quad (1)$$

where

$$Da - \text{Damkohler Number} = \frac{\text{characteristic process time}}{\text{characteristic reaction time}} = \frac{\tau_P}{\tau_R}$$

$$\frac{C_{B_o}}{C_{A_o}} - \text{reactant ratio in the feed}$$

K - equilibrium constant

For an n-th order irreversible reaction with constant density, a mass balance on the limiting reactant A readily yields an explicit relationship for the Damkohler number as a function of conversion, which, for each of the two ideal flow patterns, takes the following form:

$$Da_n = \frac{x_A}{(1 - x_A)^n} ; \quad (CSTR) \quad (2a)$$

$$Da_n = \frac{1}{1-n} \left[1 - (1-x_A)^{1-n} \right] ; n \neq 1$$

$$Da_1 = \ln \left(\frac{1}{1-x_A} \right) ; n = 1$$

(PFR) (2b)

where

$$Da_n = kC_{Ao}^{n-1} \bar{t}$$

For example, for a first order irreversible reaction the ideal reactors design equations become:

$$\text{In a CSTR: } Da_1 = \frac{x_A}{1-x_A}, \quad x_A = \frac{Da_1}{1+Da_1} \quad (3a)$$

$$\text{In a PFR: } Da_1 = \ln \left(\frac{1}{1-x_A} \right), \quad x_A = 1 - e^{-Da_1}. \quad (3b)$$

Implicitly, in deriving the above expressions, we have assumed that the feed can be intimately premixed, down to molecular level, without reaction (i.e the mixing time in generating a homogeneous feed is extremely short compared to characteristic reaction time and no reaction occurs during that time).

Thus, we realize that besides the characteristic reaction and process time we have to worry about characteristic mixing time (or mixing intensity which is proportional to its reciprocal) and about the scale of mixing. Then

$$\text{Reactor Performance} = f(\text{kinetics, flow pattern, mixing intensity and scale}) \quad (4)$$

We can intuitively recognize that the reaction system and its performance are characterized by four parameters (in a simplistic approach):

$$\tau_p = \frac{V}{Q} \quad - \text{ characteristic process time}$$

$$\tau_R = \frac{1}{kC_{ao}^{n-1}} \quad - \text{ characteristic reaction time}$$

$$\tau_m \quad - \text{ characteristic mixing time}$$

$$\ell_m \quad - \text{ characteristic mixing scale}$$

When $\tau_R \gg \tau_m$, and ℓ_m is small, ideal reactor concepts are useful but even then extremely high conversion cannot be predicted accurately in real reactors unless we have more information on the flow pattern and on the distribution of times that various elements of the fluid reside in the vessel. The concept of Residence Time Distribution (RTD), to be introduced next, is useful here.

When $\tau_m \gg \tau_R$ reactor performance completely depends on the scale of mixing ℓ_m and mixing intensity ($1/\tau_m$). If we can describe mixing in the vessel we can describe reaction progress as well. There is another way of looking at the concepts of scale and intensity of mixing by describing the degree of segregation of the fluid and the nature of exchange, or mixing, of all fluid elements that entered together with their environment comprised of all other fluid elements. The former approach is useful in very fast reactions, the outcome of which is completely determined by the turbulent field. The second approach is useful for those reactions the rate of which is comparable or slower to the rate of mixing. Then one can say that

$$\text{Reactor Performance} = \left(\begin{array}{l} \text{kinetics, flow pattern, state of aggregation} \\ \text{of the fluid and earliness of mixing} \end{array} \right) \quad (5)$$

We can now consider the description of the mixing process by two levels: macromixing and micromixing.

- **Macromixing** is a global description of mixing yielding the information on how long various elements of the incoming flow spend in the process vessel.
- **Micromixing** is a more detailed description of mixing on a microscopic level providing the information on the scale of aggregation of the fluid and earliness or lateness of mixing, i.e on the environment that the individual fluid elements experience in the vessel.