Exercise 14

A second-order, homogeneous liquid-phase dimerization reaction has to be scaled up. The reactant (A) is diluted in an organic solvent. The reaction has so far been studied as a homogeneous organic system, but, being quite exothermic, it was proposed to run it as an emulsion in water (organic droplets dispersed in the aqueous phase), in order to better control the heat of reaction.

Data

$2A \xrightarrow{k} P$

Rate constant at reaction temperature: $k = 2 \cdot 10^{-3}\ m^3 mol^{-1} h^{-1}$

Initials concentration of A in organic phase: $c_{A0} = 1000\ mol\ m^{-3}$

Mean residence time in CSTR: $\tau_{CSTR} = 3h$

Batch reaction time: $t_{batch} = 3h$

Questions

Calculate the conversion attainable in the following reaction systems:

a. Homogeneous micro mixed system: batch reactor and ideal CSTR
b. Heterogeneous fully segregated system (emulsion): batch reactor and ideal CSTR

Solution

$$DaI = \frac{\tau}{t_r} = kc_{10}^{n-1}\tau = 6$$

a. Homogeneous micro mixed system: batch reactor and ideal CSTR

- Micro-mixed ideal CSTR: $DaI \cdot (1-X)^n - X = 0 \rightarrow X = 1 - \frac{\sqrt{1+4DaI}-1}{2Da} = \mathbf{66.7\%}$
- Micro-mixed batch: $X = 1 - [1 + (n-1)DaI]^{\frac{1}{1-n}} = \mathbf{85.7\%}$

c. Heterogeneous fully segregated system (emulsion): batch reactor and ideal CSTR

- Batch with full segregation: $X = 1 - [1 + (n-1)DaI]^{\frac{1}{1-n}} = \mathbf{85.7\%}$
- Ideal CSTR with full segregation: $\bar{X} = \int_0^{\infty} \left\{1 - [1 + (n-1)kc_{10}^{n-1}t]^{\frac{1}{1-n}}\right\} \frac{1}{\tau} e^{-\frac{t}{\tau}} dt = \mathbf{72.9\%}$ (by numerical integration)