Chemical Reaction Engineering I

Reactor Design Workflow

by
Sureena Abdullah

Faculty of Chemical and Natural Resources Engineering
sureena@ump.edu.my

Design of Single CSTR

Consider a 1st order irreversible liquid phase reaction:

$$-r_A = kC_A$$ rate law

$$C_A = C_{A0}(1-X)$$ stoichiometry

$$V = \frac{F_{AO}X}{(-r_A)_{exit}} \quad \& \quad \tau = \frac{V}{v_0}$$

$$X = \frac{\tau k}{1+\tau k} = \frac{\mathrm{Da}}{1+\mathrm{Da}}$$ combine

$$C_A = \frac{C_{A0}}{1+\tau k}$$ combine

$Da = -r_{A0}V/F_{A0} = t_{mixing}/t_{rxn}$

- Da<<1: rapid mixing relative to reaction & less important. Da>>1: problematic mixing.
- τk is often referred to as Damköhler number for 1st order reaction
- Rule of thumbs
  If Da<0.1, then X<0.1
  If Da>10, then X>0.9

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Design of CSTRs in Series

Consider a 1st order irreversible liquid phase reaction, $-r_A = kC_A$

Find the outlet concentration of A in the 1st reactor. $C_{A1} = \frac{C_{A0}}{1+\tau_1 k_1}$

Find the outlet concentration of A in the 2nd reactor. $C_{A2} = \frac{C_{A1}}{1+\tau_2 k_2} = \frac{C_{A0}}{(1+\tau_1 k_1)(1+\tau_2 k_2)} = \frac{C_{A0}}{(1+\tau k)^2}$

If *n* equal-sized CSTRs connected in series $C_{An} = \frac{C_{A0}}{(1+\tau k)^n}$ Substitute C_{An} in terms of X $X = 1 - \frac{1}{(1+\tau k)^n}$

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Design of CSTRs in Parallel (1st Order Reaction)

Consider a 1st order irreversible liquid phase reaction, $-r_A = kC_A$

Step 1

For an individual reactor volume, $$V = \frac{F_{A0,i} - F_{A,i}}{-r_{Ai}}$$

Step 2

Substitution of

$F_{A0,i} = F_{A0}/n$

$F_{A,i} = C_{A,i} * v_0/n$

$$C_{A,i} = \frac{C_{A0}}{1 + nk\tau}$$

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Authors Information

Credit to the authors:
Assoc Prof Dr Maksudur Rahman Khan,
Madam Hamidah Abdullah