BT209

Bioreaction Engineering

11/01/2023

Course objective

- This course will provide an overview of chemical/biochemical kinetics and bioreactor design at basic to an inter mediate level. Coverage will be relatively broad.

- This course applies the concepts of reaction rate, stoichiometry and equilibrium to the analysis of chemical and biological reacting systems such as derivation of rate expressions from reaction mechanisms and equilibrium or steady state assumptions and design of chemical and biochemical reactors via synthesis of biochemical kinetics, and mass and energy balances.

- The goal is to provide students with the theoretical/analytical background to understand chemical/biochemical kinetics and bioreactor design and to tackle the sort of complex problems.

Applicability of Bioreaction Engineering

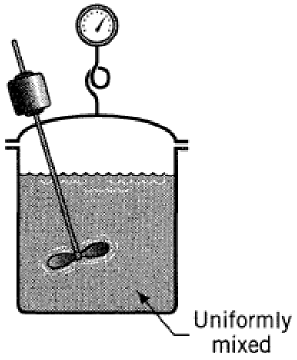
- Here we will talk about single or multiple enzyme/cell reaction

- *Example I: single enzyme*
- Converting cellulosic materials to simple sugar
- Any immobilized enzyme application
- Dairy industry lactose to glucose and galactose by beta-galatosidase

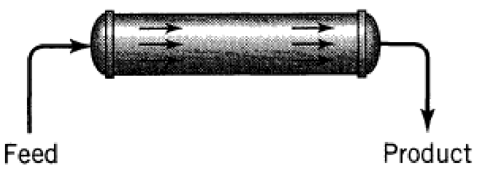
- *Example II: not single enzyme (combination of enzymes)*
- In reactor cell assume acting as enzyme and it converts substrate to desired product and undesired product

Reactor for Single reaction?

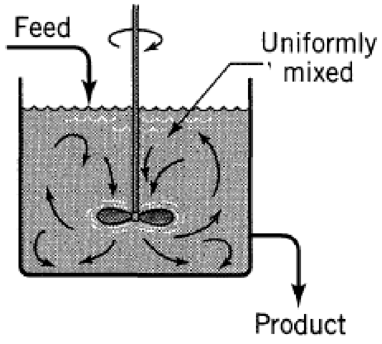
A→P



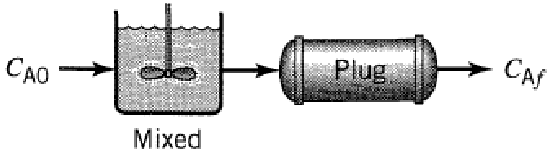
Batch

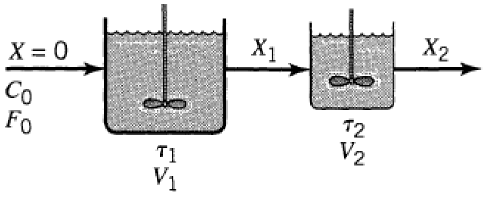


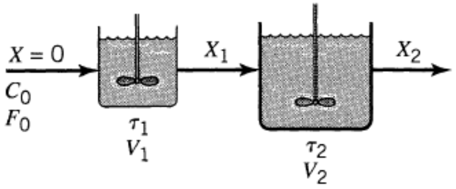
tubular



CSTR







Which reactor?

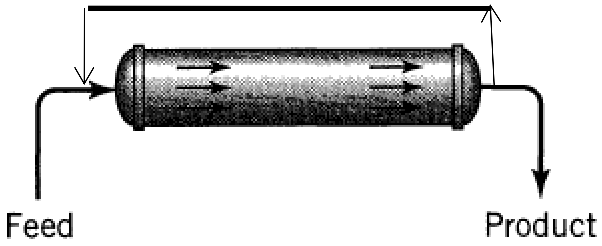
COST ????

Kinetics known

Less volume,

Conversion,

Heat effect

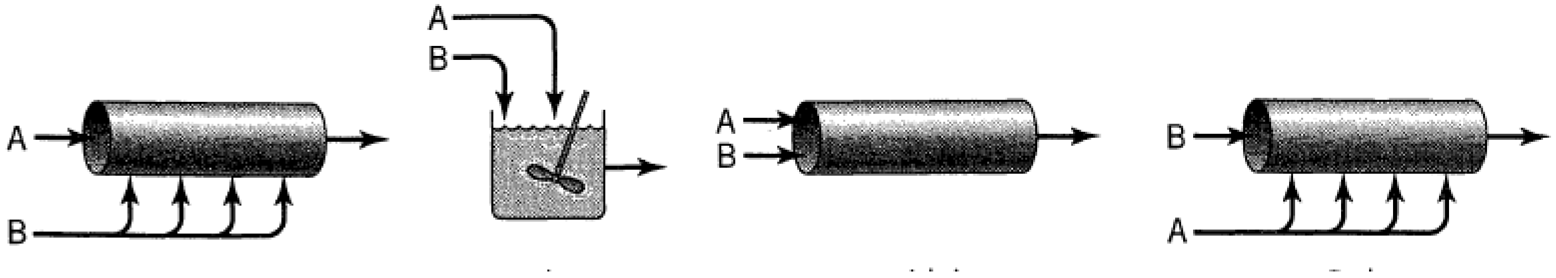


Recycle tubular

For Multiple reaction?

$$A + B \begin{cases} \nearrow R + T, & r_R = 50C_A \ \dfrac{\text{mol}}{\text{m}^3 \cdot \text{hr}} \\ \searrow S + U, & r_S = 100C_B \ \dfrac{\text{mol}}{\text{m}^3 \cdot \text{hr}} \end{cases}$$

R: desired product



Which reactor?

Course content

Kinetics of bioreaction:

- Bioreaction stoichiometry,
- Lumped stoichiometry in complex systems such as enzymatic bioconversions and cell growth,
- Homogeneous/Heterogeneous bioreaction,
- Molecularity, Order, Rate of bioreaction,
- Elementary and non-elementary bioreaction,
- Single reactions and reaction networks, Bioreaction network,
- Reactive intermediates and steady state approximation in bioreaction mechanisms,
- Rate-limiting step.

Rate of bioreaction parameters:

- Conversion,
- Determine the kinetic parameters for reversible and irreversible bioreactions,
- Shifting order bioreaction,
- Temperature effect on rate of bioreaction, Arrhenius equation.

Cont..

Ideal bioreactors:

- Introduction of bioreactor design: concept of ideal Batch, Fed batch/semi batch
- Ideal steady state continuous bioreactors: Continuous stirred tank state bioreactor (CSTR) and plug flow bioreactor (PFR).

Design for Single bioreactions:

- Size comparison of bioreactors: single bioreactors for single reaction,
- Series and parallel combination of multiple bioreactors for single reaction,
- Recycle bioreactor,
- Autocatalytic reaction such as biomass growth.

Design for Multiple bioreactions:

- Multiple bioreaction: series and parallel bioreaction,
- Design for parallel bioreactions, product distribution, yields, selectivity and bioreactor size,
- Design for series reaction and successive reactions of shifting orders in different reactors, Combination of irreversible series and parallel bioreaction.

Cont..

Heterogeneous bioreaction:

- Heterogeneous reaction in bioprocessing,
- Immobilization of cell and enzyme, concentration gradient and reaction rates in immobilized cell and enzyme,
- Internal mass transfer and bioreaction,
- Thiele modulus and effectiveness factor,
- External mass transfer.

Non-Ideal bioreactor mixing patterns:

- Basics of non-ideal flow, E, the age distribution of fluid,
- Residence time distribution (RTD), prediction of conversion,
- Reactor modeling with RTD, Segregation model, Tanks in series model, Dispersion model.

Text/ Reference books

Text Books

1. O. Levenspiel, Chemical Reaction Engineering, 3rd Ed., John Wiley & Sons, Inc. 1999.

2. Doran, Bioprocess Engineering Principles, 2nd Edition, Academic Press, 2014

References

1. H. S. Fogler, Elements of Chemical Reaction ,BT 209 Bio-reaction Engineering, Engineering, Prentice Hall, 2nd Ed., New Jersey, 1992.

2. J. Smith, "Chemical Engineering Kinetics", 3rd edition. McGraw-Hill, (1990).

3. Bailey, J. E., and D. F. Ollis. Biochemical Engineering Fundamentals. 2nd ed. New York, McGraw-Hill, 1986.

Grade

- ***Grade Weighting***
  - Quiz (2) 2 x 10 =20
    - Quiz-1 (pre-midsem)/ February
    - Quiz-2 (post midsem) April
  - Tutorial (3, 2 marks each), 3 x 2= 6
  - Assignment -1 5
  - Attendance 4
  - Mid Semester Exam 30
  - End Semester Exam 35

Total 100

Classification

- Based on number and type of phase
  - Homogeneous :

    reaction is takes place in one phase alone

  - Heterogeneous:

    it requires the presence of at least two phases to proceed.

    It is immaterial whether the reaction takes place in one, two,or more phases; at an interface; or whether the reactants and products are distributed among the phases or are all contained within the single phase.

At least two phases are necessary for the reaction to proceed as it does

Single/multiple

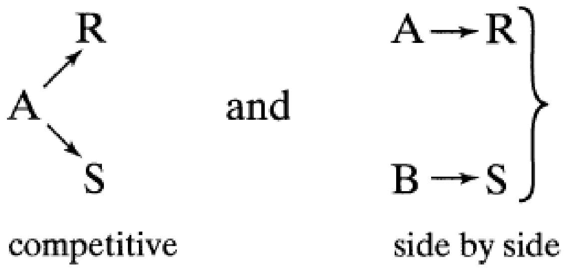
- Single reaction:
  - Single stoichiometric and single rate equation are sufficient to represent the progress of the reaction

$$A+B \rightarrow C+D$$

- Multiple reaction:
  - More than one stoichiometric equation to represent the observe change/more than one kinetic expression is needed to follow the changing composItion of all the reaction components

Series $A \rightarrow R \rightarrow S$

Parallel (Two types).



Complicated

$A+B \rightarrow R$

$R+B \rightarrow S$

in parallel w.r.t. B

but in series w.r.t. A , R and S

Rate of reaction/rate equation

- Stoichiometry: aA+Bb→cC+dD

- Rate of reaction, $-r_A = \frac{1}{V}\frac{dN_A}{dt} = \frac{\text{amount of A disappearing}}{(\text{fluid volume})(\text{time})}, \left[\frac{\text{mole}}{m^3.s}\right]$

$$-r_B = \frac{1}{V}\frac{dN_B}{dt}$$

$$\boxed{\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d}}$$

- $-r_A$, $-r_B$, (- for reactant)
- r_C, r_D (+ for product)

$$-r_A^{'} = \frac{1}{S}\frac{dN_A}{dt} \qquad \left[\frac{\text{mole}}{(\text{time}).(\text{interfacial surface area})}\right]$$

(For gas-liquid
gas-solid
liquid-solid)

$$r_A^{''} = \frac{1}{W}\frac{dN_A}{dt} \qquad \left[\frac{\text{mole}}{(\text{time}).(\text{catalyst mass})}\right]$$

$$r_A^{'''} = \frac{1}{V_S}\frac{dN_A}{dt} \qquad \left[\frac{\text{mole}}{(\text{time}).(\text{solid volume})}\right]$$

$$\boxed{Vr_j = Wr_j^{'} = Sr_j^{''} = V_S r_j^{'''}}$$

Elementary/non elementary

- Elementary
  - Rate equation corresponds to a stoichiometry equation

aA+Bb→cC+dD

$$-r_A = k_1 C_A{}^a C_B{}^b$$

- Non-elementary
  - There is no direct correspondence between stoichimetry and rate

Example: $H_2+Br_2 \rightarrow 2HBr$

$$-r_{HBr} = \frac{k_1 [H_2][Br_2]^{\frac{1}{2}}}{k_2 + \frac{[HBr]}{[Br_2]}}$$

aA+Bb→cC+dD

$$-r_A = k_1 C_A{}^{\frac{1}{2}} C_B{}^{\frac{1}{3}}$$

Molecularity and order

- Rate expresion

$$-r_A = k_1 C_A^{n_1} C_B^{n_2}$$

- Overall order of the reaction (n) = n_1+n_2

  n_1 order with respect to A

  n_2 order with respect to B

  n^{th} order overall

- order refers to the empirically found rate expression, it can have a fractional value and need not be an integer

Molecularity:

- number of molecules involved in the elementary reaction
- integer

Fractional Conversion

Reaction: aA+Bb→cC+dD

- Conversion, $X_j = \dfrac{N_{j0} - N_j}{N_{j0}}$

N_{j0} : initial mole of j^{th} reactant

N_j : mole of j^{th} reactant

$$N_A = N_{A0}(1 - X_A)$$

$$N_B = N_{B0}(1 - X_B)$$