A First Course on Kinetics and Reaction Engineering

Class 23 on Unit 22

Where We're Going

- Part I - Chemical Reactions
- Part II - Chemical Reaction Kinetics
- Part III - Chemical Reaction Engineering
    - A. Ideal Reactors
    - B. Perfectly Mixed Batch Reactors
    - C. Continuous Flow Stirred Tank Reactors
        - 21. Reaction Engineering of CSTRs
        - 22. Analysis of Steady State CSTRs
        - 23. Analysis of Transient CSTRs
        - 24. Multiple Steady States in CSTRs
    - D. Plug Flow Reactors
    - E. Matching Reactors to Reactions
- Part IV - Non-Ideal Reactions and Reactors

Design Equations and Other Useful Relationships

- Mole Balance
  - $0 = \dot{n}_i^0 - \dot{n}_i + V \sum_{\substack{j=all\\reactions}} \nu_{i,j} r_j$
- Energy Balance on the Reacting Fluid
  - $0 = \sum_{\substack{i=all\\species}} \left(\dot{n}_i^0 \int_{T^0}^{T} \hat{C}_{pi}\, dT \right) + V \sum_{\substack{j=all\\reactions}} r_j \Delta H_j(T) - \dot{Q} + \dot{W}$
- Energy Balance on a Perfectly Mixed Heat Transfer Fluid
  - $0 = \dot{m}_{water} \tilde{C}_{p,e} \left(T_e^0 - T_e \right) - UA\left(T_e - T \right)$
- Other Relationships

$$P_i = \frac{\dot{n}_i}{\sum\limits_{k\,=\,\text{all species}} \dot{n}_k} P \qquad C_i = \frac{\dot{n}_i}{\dot{V}} \qquad \text{ideal gas: } \dot{V} = \frac{RT \left(\sum\limits_{k\,=\,\text{all species}} \dot{n}_k \right)}{P}$$

$$\text{constant density liquid: } \dot{V} = \dot{V}^0$$

- Sensible Heat Term

$$\sum_{\substack{i=all\\species}} \left(\dot{n}_i^0 \int_{T^0}^{T} \hat{C}_{pi}\, dT \right) \qquad \dot{V}^0 \int_{T^0}^{T} \rho_{soln} \tilde{C}_{p,soln}\, dT \qquad \dot{V}^0 \int_{T^0}^{T} \widehat{C}_{p,soln}\, dT$$

A General Approach to Solving Quanitative Reaction Engineering Problems

- Read through the problem statement and determine
  - the type of reactor being used
  - whether it operates transiently or at steady state
  - whether it is heated/cooled, isothermal or adiabatic
  - (if the reactor is a PFR) whether there is a significant pressure drop
- Read through the problem statement a second time
  - assign each quantity given in the problem statement to the appropriate variable symbol
  - if all of the given quantities are intensive, select a value for one extensive variable as the basis for your calculations
  - determine what quantities the problem asks for and assign appropriate variable symbols to them
- Write a mole balance equation for each reactant and product; expand all summations and continuous products, and eliminate all zero-valued and negligible terms
- Write an energy balance design equation (unless the reactor is isothermal and the problem does not ask any questions related to heat transfer); expand all summations and continuous products, and eliminate all zero-valued and negligible terms
  - if information about the heat transfer fluid, beyond its temperature, is provided, write an energy balance on the heat transfer fluid

- If the reactor is a PFR and there is a significant pressure drop, write a momentum balance; expand all summations and continuous products, and eliminate all zero-valued and negligible terms
- Identify the type of the design equations
  - if they are algebraic, identify the unknowns
    - the number of unknowns must equal the number of equations
  - if they are differential, identify the independent and dependent variables
    - if the number of dependent variables is greater than the number of equations, choose one dependent variable and express it and its derivatives in terms of the remaining dependent variables
- Determine what you will need to provide in order to solve the design equations numerically and show how to do so
  - For algebraic equations written in the form $0 = \underline{f}(\underline{x})$ you must provide a guess for x and code that evaluates $\underline{f}$ given $\underline{x}$
  - For initial value ordinary differential equations written in the form $\frac{d}{dx}\underline{y} = \underline{f}\left(x,\underline{y}\right)$ you must provide initial values of x and $\underline{y}$, a final value for either x or one element of $\underline{y}$, and code that evaluates $\underline{f}$ given x and $\underline{y}$
  - For boundary value differential equations (without a singularity) written in the form $\frac{d}{dx}\underline{y} = \underline{f}\left(x,\underline{y}\right)$ you must provide the lower and upper limits of x, boundary conditions that must be satisfied for each dependent variable and code that evaluates $\underline{f}$ given x and $\underline{y}$
- After the design equations have been solved numerically, yielding values for the unknowns (algebraic equations) or the independent and dependent variables (differential equations), use the results to calculate any other quantities or plots that the problem asked for

Questions?

Activity 22.1

In Example 20.2, the operation of a batch reactor was analyzed. Specifically, a coolant flow rate of 0.2 kg min^{-1} was selected to maximize the net rate of production of B (0.0153 mol min^{-1} including turnaround time) via reaction (1). Suppose that reactor is converted to a CSTR that operates with a space time equal to the total processing time of the two steps in the batch reactor operational protocol (63.8 min). That is, the feed to the CSTR has the same composition and temperature as the initial charge to the batch reactor (a 2 M solution of A at 23 °C), and the 20 °C cooling water flows into the jacket at a rate of 0.2 kg min^{-1}. What will the final steady state temperature and outlet molar flow rate of B equal?

The rate expression for reaction (1) is given in equation (2). The heat of reaction (1) may be taken to be constant and equal to -22,200 cal mol^{-1}. The heat capacity of the reacting solution is approximately constant and equal to 440 cal L^{-1} K^{-1}, and its density is constant. The reaction volume is 4 L, and the jacket volume is 0.5 L with a heat transfer area of 0.6 ft^2 and a heat transfer coefficient of 1.13 x 10^4 cal ft^{-2} h^{-1} K^{-1}. The cooling water may be taken to have a constant density of 1 g cm^{-3} and a constant heat capacity of 1 cal g^{-1} K^{-1}.

$$A \rightarrow B \qquad (1)$$

$$r_1 = \left(2.59 \times 10^9 \text{ min}^{-1}\right)\exp\left(\frac{-16500 \text{ cal mol}^{-1}}{RT}\right)C_A \qquad (2)$$

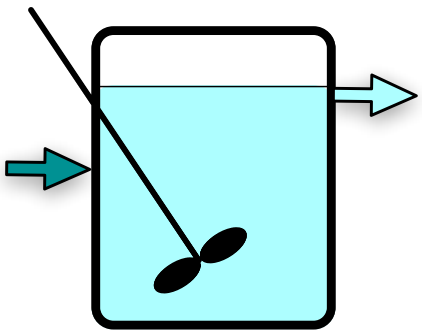
Read through the problem statement and determine the type of reactor being used, whether it operates transiently or at steady state, whether it is heated/cooled, isothermal or adiabatic and (if the reactor is a PFR) whether there is a significant pressure drop

Read through the problem statement a second time and (a) assign each quantity given in the problem statement to the appropriate variable symbol (b) if all of the given quantities are intensive, select a value for one extensive variable as the basis for your calculations and (c) determine what quantities the problem asks for and assign appropriate variable symbols to them

Write a mole balance equation for each reactant and product; expand all summations and continuous products, and eliminate all zero-valued and negligible terms

A → B; $r_1 = k_0 \cdot \exp(-E/RT) \cdot C_A$

$\dot{V}^0 = V/\tau$
$T^0 = 23\ °C$
$\dot{n}_A^0 = C_A^0 \cdot \dot{V}^0$
$\dot{n}_B^0 = 0$



$\dot{V} = \dot{V}^0$
$T =$
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$V = 4$ L
$V_{jacket} = 0.5$ L
$A = 0.6$ ft^2
$U = 1.13 \times 10^4$ cal ft^{-2} h^{-1} K^{-1}
$\dot{m}_{water} = 0.2$ kg min^{-1}
$T_e^0 = 20\ °C$; $T_e =$

Reactor Relationships

$$\tau = \frac{V}{\dot{V}^0}\ ;\ SV = \frac{1}{\tau};\ \frac{dn_i}{dt} = V\left(\sum_{\substack{j=\text{all}\\ \text{reactions}}} \nu_{i,j} r_j\right);\ \dot{Q} - \dot{W} = \left(\sum_{\substack{i=\text{all}\\ \text{species}}} n_i \hat{C}_{p,i}\right)\frac{dT}{dt} + V\left(\sum_{\substack{j=\text{all}\\ \text{reactions}}} r_j \Delta H_j\right) - V\frac{dP}{dt} - P\frac{dV}{dt};$$

$$\boxed{\dot{n}_i^0 + V \sum_{\substack{j=\text{all}\\ \text{reactions}}} \nu_{i,j} r_j = \dot{n}_i + \frac{d}{dt}\left(\frac{\dot{n}_i V}{\dot{V}}\right);}$$

$$\dot{Q} - \dot{W} = \sum_{\substack{i=\text{all}\\ \text{species}}} \left(\dot{n}_i^0 \int_{T^0}^{T} \hat{C}_{p-i}\, dT\right) + V \sum_{\substack{j=\text{all}\\ \text{reactions}}} \left(r_j \Delta H_j(T)\right) + V\left(\sum_{\substack{i=\text{all}\\ \text{species}}} \frac{\dot{n}_i \hat{C}_{p-i}}{\dot{V}}\right)\frac{dT}{dt} - P\frac{dV}{dt} - V\frac{dP}{dt};$$

$$\frac{\partial \dot{n}_i}{\partial z} = \frac{\pi D^2}{4}\left[\left(\sum_{\substack{j=all\\ reactions}} \nu_{i,j} r_j\right) - \frac{\partial}{\partial t}\left(\frac{\dot{n}_i}{\dot{V}}\right)\right];\ \frac{\partial P}{\partial z} = -\frac{G}{g_c}\left(\frac{4}{\pi D^2}\right)\frac{\partial \dot{V}}{\partial z} - \frac{2fG^2}{\rho D};$$

$$\frac{\partial P}{\partial z} = -\frac{1-\varepsilon}{\varepsilon^3}\frac{G^2}{\rho \Phi_s D_p g_c}\left[\frac{150(1-\varepsilon)\mu}{\Phi_s D_p G} + 1.75\right];$$

$$\pi D U (T_e - T) = \frac{\partial T}{\partial z}\left(\sum_{\substack{i=\text{all}\\ \text{species}}} \dot{n}_i \hat{C}_{p-i}\right) + \frac{\pi D^2}{4}\left(\sum_{\substack{j=\text{all}\\ \text{reactions}}} r_j \Delta H_j\right) + \frac{\pi D^2}{4}\left[\frac{\partial T}{\partial t}\left(\sum_{\substack{i=\text{all}\\ \text{species}}} \frac{\dot{n}_i \hat{C}_{p-i}}{\dot{V}}\right) - \frac{\partial P}{\partial t}\right];$$

$$\frac{dn_i}{dt} = \dot{n}_i + V \sum_{\substack{j=all\\ reactions}} \nu_{i,j} r_j\ ;\ \dot{Q} - \dot{W} = \sum_{\substack{i=all\\ species}} \dot{n}_i\left(\hat{h}_i - \hat{h}_{i,stream}\right) + \frac{dT}{dt}\sum_{\substack{i=all\\ species}} \left(n_i \hat{C}_{pi}\right) + V \sum_{\substack{j=all\\ reactions}} \left(r_j \Delta H_j\right) - \frac{dP}{dt}V - P\frac{dV}{dt};$$

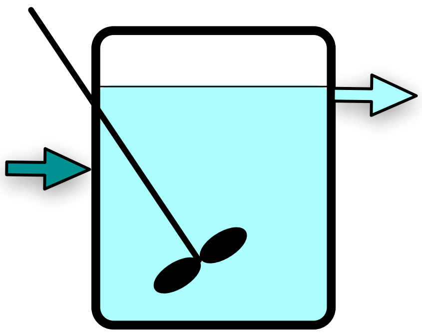
$$-D_{ax}\frac{d^2 C_i}{dz^2} + \frac{d}{dz}(u_s C_i) = \sum_{\substack{j=all\\ reactions}} \nu_{i,j} r_j\ ; D_{er}\left(\frac{\partial^2 C_i}{\partial r^2} + \frac{1}{r}\frac{\partial C_i}{\partial r}\right) - \frac{\partial}{\partial z}(u_s C_i) = \sum_{\substack{j=all\\ reactions}} \nu_{i,j} r_j\ ;$$

$$\lambda_{er}\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) - u_s \rho_{fluid} \tilde{C}_{p,fluid}\frac{\partial T}{\partial z} = \sum_{\substack{j=all\\ reactions}} r_j \Delta H$$

Write an energy balance design equation (unless the reactor is isothermal and the problem does not ask any questions related to heat transfer); expand all summations and continuous products, and eliminate all zero-valued and negligible terms

$A \rightarrow B$; $r_1 = k_0 \cdot \exp(-E/RT) \cdot C_A$

$\dot{V}^0 = V/\tau$
$T^0 = 23$ °C
$\dot{n}_A^0 = C_A^0 \cdot \dot{V}^0$
$\dot{n}_B^0 = 0$



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$V = 4$ L
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$A = 0.6$ ft^2
$U = 1.13 \times 10^4$ cal ft^{-2} h^{-1} K^{-1}
$\dot{m}_{water} = 0.2$ kg min^{-1}
$T_e^0 = 20$ °C; $T_e =$

- Mole balances
    - $0 = f_1\left(\dot{n}_A, \dot{n}_B, T, T_e\right) = \dot{n}_A^0 - \dot{n}_A - Vr_1$
    - $0 = f_2\left(\dot{n}_A, \dot{n}_B, T, T_e\right) = \dot{n}_B^0 - \dot{n}_B + Vr_1$

Reactor Relationships

$$\tau = \frac{V}{\dot{V}^0};\ SV = \frac{1}{\tau};\ \frac{dn_i}{dt} = V\left(\sum_{\substack{j=\text{all}\\ \text{reactions}}} \nu_{i,j} r_j\right);\ \dot{Q} - \dot{W} = \left(\sum_{\substack{i=\text{all}\\ \text{species}}} n_i \hat{C}_{p,i}\right)\frac{dT}{dt} + V\left(\sum_{\substack{j=\text{all}\\ \text{reactions}}} r_j \Delta H_j\right) - V\frac{dP}{dt} - P\frac{dV}{dt};$$

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If information about the heat transfer fluid, beyond its temperature, is provided, write an energy balance on the heat transfer fluid

A → B; $r_1 = k_0 \cdot \exp(-E/RT) \cdot C_A$

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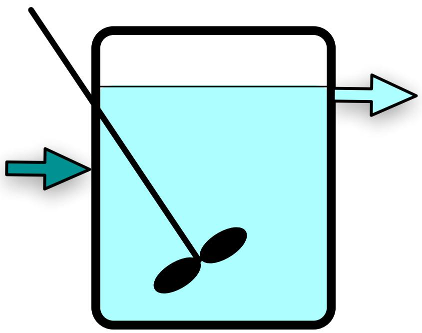

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- Mole balances
  - $0 = f_1\left(\dot{n}_A, \dot{n}_B, T, T_e\right) = \dot{n}_A^0 - \dot{n}_A - Vr_1$
  - $0 = f_2\left(\dot{n}_A, \dot{n}_B, T, T_e\right) = \dot{n}_B^0 - \dot{n}_B + Vr_1$
- Energy balance on reaction volume
  - $0 = f_3\left(\dot{n}_A, \dot{n}_B, T, T_e\right)$

$$= \dot{V}^0 \hat{C}_p \left(T - T^0\right) + Vr_1 \Delta H_1\left(T\right) - UA\left(T_e - T\right)$$

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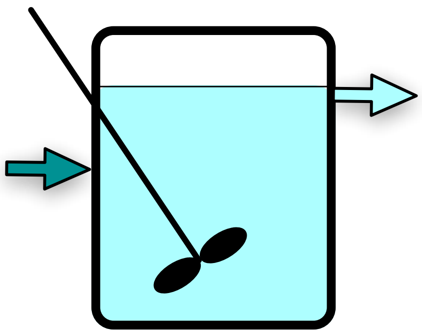

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- Energy balance on reaction volume
  - $0 = f_3(\dot{n}_A, \dot{n}_B, T, T_e)$
    $= \dot{V}^0 \widehat{C}_p (T - T^0) + Vr_1 \Delta H_1(T) - UA(T_e - T)$
- Energy balance on cooling water
  - $0 = f_4(\dot{n}_A, \dot{n}_B, T, T_e)$
    $= \dot{m}_{water} \tilde{C}_{p,e} (T_e^0 - T_e) - UA(T_e - T)$

- If the reactor is a PFR and there is a significant pressure drop, write a momentum balance; expand all summations and continuous products, and eliminate all zero-valued and negligible terms
- Identify the type of the design equations
  - if they are algebraic, identify the unknowns
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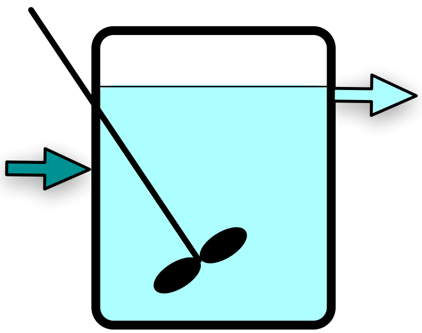

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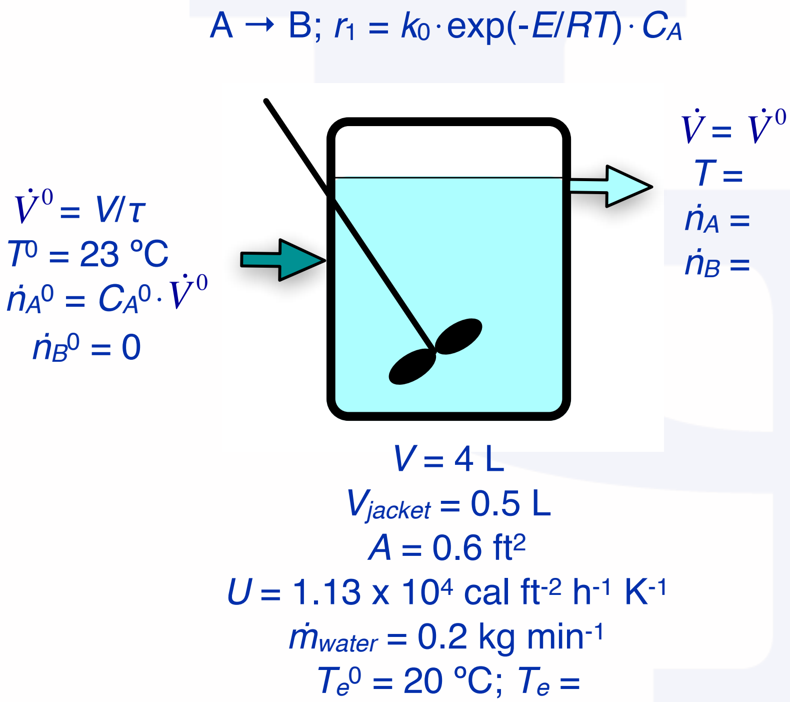
  - $0 = f_2(\dot{n}_A, \dot{n}_B, T, T_e) = \dot{n}_B^0 - \dot{n}_B + Vr_1$
- Energy balance on reaction volume
  - $0 = f_3(\dot{n}_A, \dot{n}_B, T, T_e)$
    $= \dot{V}^0 \widehat{C}_p (T - T^0) + Vr_1 \Delta H_1(T) - UA(T_e - T)$
- Energy balance on cooling water
  - $0 = f_4(\dot{n}_A, \dot{n}_B, T, T_e)$
    $= \dot{m}_{water} \tilde{C}_{p,e} (T_e^0 - T_e) - UA(T_e - T)$
- Four equations in 4 unknowns
  - To solve numerically, must evaluate functions, f_i, given $\dot{n}_A$, $\dot{n}_B$, T, T_e

- Determine what you will need to provide in order to solve the design equations numerically and show how to do so
  - For algebraic equations written in the form $0 = \underline{f}(\underline{x})$ you must provide a guess for x and code that evaluates $\underline{f}$ given $\underline{x}$
  - For initial value ordinary differential equations written in the form $\frac{d}{dx}\underline{y} = \underline{f}\left(x,\underline{y}\right)$ you must provide initial values of x and $\underline{y}$, a final value for either x or one element of $\underline{y}$, and code that evaluates $\underline{f}$ given x and $\underline{y}$
  - For boundary value differential equations (without a singularity) written in the form $\frac{d}{dx}\underline{y} = \underline{f}\left(x,\underline{y}\right)$ you must provide the lower and upper limits of x, boundary conditions that must be satisfied for each dependent variable and code that evaluates $\underline{f}$ given x and $\underline{y}$

Solution



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- Energy balance on reaction volume
  - $0 = f_3(\dot{n}_A, \dot{n}_B, T, T_e)$
    $= \dot{V}^0 \widehat{C}_p (T - T^0) + Vr_1 \Delta H_1(T) - UA(T_e - T)$
- Energy balance on cooling water
  - $0 = f_4(\dot{n}_A, \dot{n}_B, T, T_e)$
    $= \dot{m}_{water} \tilde{C}_{p,e} (T_e^0 - T_e) - UA(T_e - T)$
- Four equations in 4 unknowns
  - To solve numerically, must evaluate functions, f_i, given $\dot{n}_A$, $\dot{n}_B$, T, T_e
    - Constants: $\dot{n}_A^0, \dot{n}_B^0, V, \dot{V}^0, \widehat{C}_p, T^0, \Delta H_1, U,$ $A, T_e^0, \dot{m}_{water}, \tilde{C}_{p,e}$
    - Other quantities: r_1, C_A
      - $r_1 = k_0 \exp\left(\frac{-E}{RT}\right) C_A; \quad C_A = \frac{\dot{n}_A}{\dot{V}}$

After the design equations have been solved numerically, yielding values for the unknowns (algebraic equations) or the independent and dependent variables (differential equations), use the results to calculate any other quantities or plots that the problem asked for

- The problem asked for the outlet temperature and the outlet molar flow rate of B
  - These are two of the four unknowns found by solving the design equations, so no additional calculations are needed

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- Part I - Chemical Reactions
- Part II - Chemical Reaction Kinetics
- Part III - Chemical Reaction Engineering
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  - B. Perfectly Mixed Batch Reactors
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