

Introduction to Reactor Design, 3K4

Assignment/Tutorial 1

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Assignment objectives: math refresher; chemistry refresher; review mol balances

- Always state assumptions in this assignment, midterms and exams.
- Never use an equation by just writing it down; state its origin and all simplifying assumptions. *For example:* using the general mol balance in a batch reactor, under the assumption of a well-mixed and constant volume system, we have: $\frac{dN_j}{dt} = r_j V$

Question 1 [10]

1. $\int \frac{1}{x} dx =$
2. $\int \frac{1}{x^2} dx =$
3. $\int \frac{1}{ax+b} dx =$
4. $\int \frac{1}{\sqrt{x}} dx =$
5. When do we require an integration constant; and when do we not require it?

Solution

1. $\int \frac{1}{x} dx = \ln x + C$
2. $\int \frac{1}{x^2} dx = -\frac{1}{x} + C$
3. $\int \frac{1}{ax+b} dx = \frac{1}{a} \ln(ax+b) + C$
4. $\int \frac{1}{\sqrt{x}} dx = 2\sqrt{x} + C$
5. We require an integration constant when the limits of integration are unspecified (indefinite integrals); otherwise we don't require the constant, since the integral is uniquely defined.

Question 2 [10]

1. A vessel contains a gas of concentration 20 mol.m^{-3} . The gas is stored at 375°C . Assuming this is an ideal gas, what is the pressure in the vessel measured in kPa? What assumption are you making (apart from the ideal-gas law)?

2. A constant volume batch reactor operates at 14.7 psi and 1340°F. The reactor volume is 290 ft³. How many mols are in the system, assuming an ideal gas?

Solution

Assumptions: Pure species in tank, at constant volume and temperature.

1. $T = 648 \text{ K}$, so from the ideal gas law: $P = CRT = (20 \text{ mol.m}^{-3})(8.314 \text{ J.mol}^{-1}.\text{K}^{-1})(648 \text{ K}) = 107.7 \text{ kPa}$.
2. At $P = 14.7 \text{ psi} = 1 \text{ atm}$, with $V = 290 \text{ ft}^3 = 8.205 \text{ m}^3$ and $T = 1000 \text{ K}$, then $R = 8.205746 \times 10^{-5} \text{ m}^3.\text{atm.K}^{-1}.\text{mol}^{-1}$, giving $n = 100 \text{ mol}$.

Question 3 [10]

Milk is pasteurized if it is heated to 63°C for 30 min, but if it is heated to 74°C it only needs 15 seconds for the same result. Find the activation energy of this sterilization process.

Recall the activation energy for a chemical reaction is the E term, and the rate constant in is given by $k = k_0 e^{\frac{-E}{RT}}$.

Hint: assume pasteurization proceeds via first-order kinetics; what is the “reactant”?

Solution

To ask for the activation energy of a process means assuming an Arrhenius temperature dependency for the process. Here we are told that

- $t_1 = 1800$ seconds are required at temperature $T_1 = 336 \text{ K}$
- $t_2 = 15$ seconds are required at temperature $T_2 = 347 \text{ K}$

As told, assuming first order kinetics, $-r_A = k_A C_A = k_0 e^{\frac{-E}{RT}} C_A$.

For a batch system, making the regular assumption of constant volume and well-mixed (both are suitable for pasteurization):

$$t = \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A} = \int_{C_{A0}}^{C_A} \frac{dC_A}{-k_A C_A} = \frac{1}{k_A} \ln \left(\frac{C_A}{C_{A0}} \right)$$

So for the 2 systems we have that C_{A0} and C_A are the same, so we can write the ratio:

$$\frac{t_1}{t_2} = \frac{1800}{15} = 120 = \frac{k_{A,2}}{k_{A,1}} = \frac{k_0 e^{\frac{-E}{RT_2}}}{k_0 e^{\frac{-E}{RT_1}}}$$

Simplifying, recognizing that k_0 , and R are the same for both systems:

$$\begin{aligned} 120 &= \exp \left(-\frac{E}{RT_2} + \frac{E}{RT_1} \right) \\ \ln(120) &= -\frac{E}{R} \left(\frac{1}{347} - \frac{1}{336} \right) \\ -E &= \frac{\ln(120)(8.314)}{-9.43 \times 10^{-5}} \\ E &= 421885 \text{ J.mol}^{-1} \end{aligned}$$

Question 4 [13]

The fermentation of an active ingredient A is to be carried out in a reactor. The reaction kinetics are given by:

$$A \longrightarrow R$$
$$-r_A = \frac{0.1C_A}{1 + 0.5C_A} \left[\frac{\text{mol}}{\text{L.min}} \right]$$

1. Consider a batch reactor filled with 750 L of reactant at $C_{A,0} = 2 \text{ mol.L}^{-1}$. How long must the reactor be operated to achieve an exit concentration of A of 0.1 mol.L^{-1} ?

If the feed rate is continuously fed at 25 L.min^{-1} , with $C_{A,0} = 2 \text{ mol.L}^{-1}$. Determine the volume required for a

2. CSTR
3. PFR

to achieve an exit concentration of A of 0.1 mol.L^{-1} .

4. Which of the CSTR or PFR require a smaller volume?

Solution

1. For a well-mixed batch reactor, the design equation is:

$$\frac{dC_A}{dt} = r_A$$
$$-\int_{C_{A0}}^{C_A} \frac{1 + 0.5C_A}{0.1C_A} dC_A = \int_{t=0}^t dt$$
$$-10 \ln \left(\frac{0.1}{2.0} \right) - 5.0 (0.1 - 2.0) = t$$
$$t = 29.95 + 9.5 = 39.45 \text{ minutes}$$

2. Using the design equation for CSTRs (assuming it to be well-mixed and operating at steady state, with a constant volumetric flow rate of 25 L.min^{-1}):

$$V = \frac{F_{A0} - F_A}{-r_A}$$
$$= \frac{50 - 2.5}{\frac{(0.1)(0.1)}{1 + (0.5)(0.1)}}$$
$$= 4987.5 \approx 5000 \text{ m}^3$$

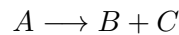
3. Use the mole balance equation for PFRs, making the usual assumption of steady state, and well-mixed in the radial direction, and using that $(q)(dC_A) = dF_A$, assuming constant volumetric flow

throughout the PFR:

$$\begin{aligned}\frac{dF_A}{dV} &= r_A \\ dV &= q \frac{dC_A}{r_A} \\ V &= q \int_{C_{A0}}^{C_A} -\frac{1.0 + 0.5C_A}{0.1C_A} dC_A \\ V &= -(25)(10) \ln \left(\frac{0.1}{2.0} \right) - (25)(5)(0.1 - 2.0) \\ V &= 986 \text{ L}\end{aligned}$$

Question 5 [7]

The gas phase reaction:



is carried out at 100°C in a 20 L constant-volume, sealed batch reactor, at atmospheric pressure. The reaction is second order: $-r_A = kC_A^2$ where $k = 2 \text{ L.mol}^{-1}.\text{min}^{-1}$.

One mole of pure A is initially placed in the reactor, which is well mixed (is this a reasonable assumption?). Determine:

1. the partial pressure due to A in the reactor
2. the concentration of A in the reactor after 5 minutes have elapsed
3. the partial pressure due to A in the reactor after 5 minutes have elapsed.

Solution

There was an error in the question, so as long as you attempted the question you got full grade. The problem was over-specified, so you get a partial pressure of A that exceeds atmospheric pressure.

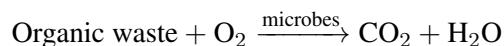
1. $p_A V = n_A RT$, or solving for $p_A = \frac{(1)(8.314)(373)}{20 \times 10^{-3}} = 155056 \text{ Pa}$.
2. After 5 minutes in a batch reactor that is assumed to be well-mixed:

$$\begin{aligned}\frac{dN_A}{dt} &= r_A V \\ \frac{dC_A}{dt} &= r_A \\ \int_{t=0}^t dt &= \int_{C_{A0}}^{C_A} \frac{dC_A}{-kC_A^2} \\ t &= \frac{1}{k_A} \left(\frac{1}{C_A} - \frac{1}{C_{A0}} \right) \\ C_A &= 0.033 \text{ mol.L}^{-1}\end{aligned}$$

3. The partial pressure due to A after 5 minutes have elapsed is $p_A = C_A RT = (33.0)(8.314)(373) = 102337 \text{ Pa}$

Question 6 [10]

Consider a municipal water treatment plant for a smallish community. Waste water at $32,000 \text{ m}^3 \cdot \text{day}^{-1}$, flows through the treatment plant with a mean residence time of 8 hours. Air is bubbled through the tanks, and microbes in the tank attack and break down the organic material:



A typical entering feed has a BOD (biological oxygen demand) of $200 \text{ (mg O}_2\text{).L}^{-1}$, the effluent has a negligible BOD. Find the average rate of reaction, or decrease in BOD, in the treatment tanks.

Solution

The rate of reaction is defined as $-r_{\text{O}_2} = \frac{\text{mol O}_2 \text{ used}}{(\text{day})(\text{m}^3)}$.

We can obtain an estimate of the tank volume from the residence time equation: $\tau = \frac{V}{q}$ or that $V = \frac{32000}{3} = 10667 \text{ m}^3$.

To obtain a value for the numerator, recognize that 1 mole of waste requires 1 mole of oxygen to remove its biological oxygen demand. We require 200 mg of oxygen though per litre of waste, or $\frac{0.2 \text{ g.L}^{-1}}{32 \text{ g.mol}^{-1}} \times 1000 \text{ L.m}^{-3} = 6.25 \text{ mol of oxygen required per m}^3 \text{ of waste}$. There will be $32000 \text{ m}^3 \cdot \text{day}^{-1}$ of waste water to treat, so this corresponds then to an average reaction rate of $\frac{6.25 \times 32000}{10667} = 18.75 \frac{\text{mol O}_2 \text{ used}}{(\text{day})(\text{m}^3)}$.

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