Introduction to Reactor Design, 3K4

Assignment 2

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Assignment objectives:

- To refresh concepts from your math and chemistry pre-requisites

- Learn how to work with conversion to size a reactor

- To demonstrate that you understand material on design reactors, and know what rate laws and stoichiometric tables are used for.

Question 1 [4]

Make sure you can do these in a test/exam (i.e. without internet access). Let X be conversion; find:

1. $\displaystyle\int \frac{1}{(1-X)^2}\, dX =$

2. $\displaystyle\int_{X_1}^{X_2} \frac{1}{(1-X)^2}\, dX =$

3. And in general, what is: $\displaystyle\int \frac{a+x}{bx}\, dx =$

Solution

1. $\displaystyle\int \frac{1}{(1-X)^2}\, dX = \frac{1}{1-X} + C$

2. $\displaystyle\int_{X_1}^{X_2} \frac{1}{(1-X)^2}\, dX = \frac{1}{1-X_2} - \frac{1}{1-X_1}$, which can be simplified further, or left like this.

3. $\displaystyle\int \frac{a+x}{bx}\, dx = \frac{a\ln(x) + x}{b} + C$

Question 2 [10]

For the question we covered in the end of class last week (see last page of this tutorial), we showed the volume of a PFR required is the area under the curve. The volume required was $2.16\,\text{m}^3$ to obtain 80% conversion.

If we used 4 CSTRs in series:

1. What would be the size of each reactor if we wanted 20% conversion in each reactor?

2. What is the total volume of these 4 reactors?

3. How does this total CSTR volume compare with (a) the single CSTR volume and (b) the single PFR volume?

4. What is the reaction rate in each reactor?

Solution

1. Answering this question graphically, and using that the reactor volume is the area given by the formula $V_i = (X_{i,\text{out}} - X_{i,\text{in}}) \dfrac{F_{A0}}{-r_A}$, where $-r_A$ is the CSTR's operating point *on the curve*:

   (a) $V_1 = (0.2 - 0)(1.33) = 0.266 \, \text{m}^3$

   (b) $V_2 = (0.4 - 0.2)(2.05) = 0.41 \, \text{m}^3$

   (c) $V_3 = (0.6 - 0.4)(3.54) = 0.708 \, \text{m}^3$

   (d) $V_4 = (0.8 - 0.6)(8.0) = 1.60 \, \text{m}^3$

   It is interesting to note how the reactors are progressively larger, which makes sense, since each one operates at lower and lower concentration, so to obtain the same amount of conversion, 20%, requires a greater volume.

2. The total volume is $2.98 \, \text{m}^3$.

3. It is much smaller than the total CSTR volume of $V = (0.8 - 0.0)(8.0) = 6.4 \, \text{m}^3$, but just greater than the total PFR volume of $2.16 \, \text{m}^3$.

4. The rate values are actually given in the table. The key is to recognize that the entire CSTR operates at a single rate, given by the exit conditions

   (a) $-r_{A_1} = 0.30 \, \text{mol.m}^{-3}.\text{s}^{-1}$

   (b) $-r_{A_1} = 0.195 \, \text{mol.m}^{-3}.\text{s}^{-1}$

   (c) $-r_{A_1} = 0.113 \, \text{mol.m}^{-3}.\text{s}^{-1}$

   (d) $-r_{A_1} = 0.05 \, \text{mol.m}^{-3}.\text{s}^{-1}$

   Note the diminishing rates in each subsequent reactor, emphasizing the point made earlier for the need for larger reactors.

Question 3 [20]

The following reaction rate, $-r_A$ measured in units of $\left[\dfrac{\text{kmol}}{\text{hr.m}^3}\right]$ is observed at a particular conversion, X:

Reaction rate	Conversion
78	0.0
106	0.2
120	0.4
70	0.6

We showed in class that the area under this curve is related to volume of the plug flow reactor.

1. Start from the general mol balance and derive the equation that shows the area is equal to the plug flow reactor's volume; clearly state all assumptions used in your derivation.

2. Assuming these assumptions are all met, calculate the plug flow reactor's volume to achieve a 60% conversion given a feed rate of $15\,\text{mol.s}^{-1}$ to the reactor.

3. If there is zero conversion at the entry to the PFR and 60% at the exit; what is the conversion half-way along the reactor?

4. What is the reaction rate at the entry of the reactor?

5. And at the midpoint?

6. And at the exit?

Solution

1. See the course slides, emphasizing that the assumptions are well mixed behaviour in the radial direction, with flow in the axial direction. Take limits as the slice thickness tends to zero to obtain:

$$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A}$$

   but the area under the curve must be related to an equation in terms of F_A, $-r_A$ and X. So recognize that $F_A(X) = F_{A0} - F_{A0}X$, so $dF_A = -F_{A0}dX$. The limits of the integral will also change accordingly, according to standard calculus rules, so:

$$V = \int_{0}^{X} \frac{dX}{-r_A}$$

   which now shows the area under the curve when plotting $\dfrac{F_{A0}}{-r_A}$ against X is equal to the PFR's volume.

2. The volume is the area under the plot of $\dfrac{F_{A0}}{-r_A}$ on the y-axis and X on the x-axis. Adjust units for $F_{A0} = 54\,\text{kmol.hr}^{-1}$ to be consistent with the rate data.

$\dfrac{F_{A0}}{-r_A}$	Conversion
0.692	0.0
0.509	0.2
0.45	0.4
0.77	0.6

Then using the 4-point Simpson's rule, the area under the curve, hence reactor volume, can be found as:

$$V = \int_{x_0}^{x_3=0.6} f(x)dx \approx \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right]$$

$$= \frac{3(0.2)}{8}\left[0.692 + 3(0.509) + 3(0.45) + 0.77 \right]$$

$$= 0.325\,\mathrm{m}^3$$

3. The conversion halfway along the reactor is the conversion value read when integrating half the area of the full reactor volume, i.e. at $0.16\,\mathrm{m}^3$. Note, the answer is not directly 30%, because conversion does not scale linearly with distance along the reactor!

   Visually the area that splits the region half-way is about at $X = 0.27$. Using curve fitting tools to the data you can estimate a slightly more accurate value, which is a good way of answering this question.

4. This is given directly as $78\,\mathrm{kmol.hr}^{-1}.\mathrm{m}^{-3}$.

5. Using a graphical technique, at the midpoint of the reactor, the conversion was found to be 0.27, but on the y-axis, the value of $\dfrac{F_{A0}}{-r_A}$ is 0.47, and so $-r_A = 115,\mathrm{kmol.hr}^{-1}.\mathrm{m}^{-3}$.

6. Finally, at the reactor exit, the rate has decreased again to $70\,\mathrm{kmol.hr}^{-1}.\mathrm{m}^{-3}$ (as given in the problem statement).

Question 4 [12]

A new drug is being prototyped in a batch reactor; as is becoming common-place now, this drug is grown *inside* a cell as a by-product of the regular cellular processes. So far, experiments have shown the rate of consumption of the starting material, an animal-derived cell A, is the only concentration in the rate expression.

$$-r_A = \frac{5.5C_A}{20 + C_A}$$

where $-r_A$ has units of $\left[\dfrac{\mathrm{mol}}{\mathrm{day.m}^3}\right]$

1. Why is a batch reactor suitable for this type of testing?

2. 30 mols of cellular material are added to a batch reactor of $0.5\,\text{m}^3$; the liquid food source is added at the same time to the reactor, in excess. Calculate the amount of cellular material remaining in the tank after 10 days.

3. How many days are required to convert 80% of the starting cellular material.

4. Show a plot of the concentration in the tank over time until there is almost 100% conversion.

Note: in tutorial 1 you solved a similar problem, but for a CSTR and PFR.

Solution

1. Batch reactors can be well-controlled and are suitable for developing products on a small scale, especially products of high value and small quantities, such as this one. The fact that batch reactors can be operated under multiple conditions (not just a single point like a CSTR), makes them very suitable for this sort of operation.

2. There are $C_{A0} = 60\,\text{mols.m}^{-3}$ added to the reactor. Assuming

   - well-mixed environment

   - constant liquid volume, then

   from the general mol balance we have that:

   $$\frac{dN_A}{dt} = r_A V$$

   but substituting in that $d(C_A V) = V\,dC_A = dN_A$, we get

   $$\frac{dC_A}{dt} = r_A = -\frac{5.5 C_A}{20 + C_A}$$

   which can be integrated (see question 1, part 3 of the tutorial):

   $$\int_0^{t_f} dt = t_f = -\int_{C_{A0}}^{C_A} \frac{20 + C_A}{5.5 C_A} = \frac{C_{A0} - C_A + 20\ln(C_{A0}) - 20\ln(C_A)}{5.5}$$

   Setting $t_f = 10\,\text{days}$ and using the bisection method (or any similar tool from 3E4), you can show $C_A \approx 23.6\,\text{mol.m}^{-3}$

3. At a conversion of 80% we have $C_A = 12.0\,\text{mol.m}^{-3}$, which would require 14.6 days, using the above equation.

4. Plotting concentration against time over a reasonable time frame, where the vertical axis represents concentration in mol.m^{-3}, and the horizontal axis is time measured in days. The plot must show a logarithmic decline in the concentration.
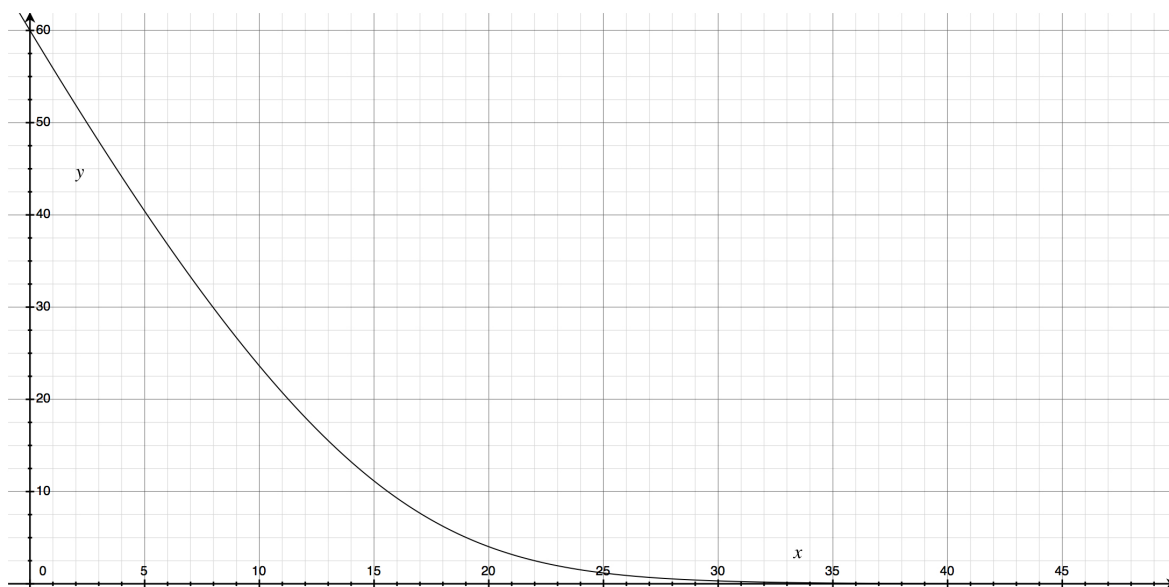
Question 5 [5]

For the elementary liquid-phase reaction, $A + B \rightleftharpoons C$ with $C_{A0} = C_{B0} = 2\,\text{mol.L}^{-1}$ and $K_C = 10\,\text{L.mol}^{-1}$

1. What is the equilibrium concentrations of all the species?

2. Does it matter in which reactor this occurs? Explain your answer.

3. What is the equilibrium conversion of A?

Solution

1. Using the notation that $\{A\}$ represents the equilibrium concentration of A, we have:

$$K_C = \frac{\{C\}}{\{A\}\{B\}}$$

which is one equation in 3 unknowns. Other equations are that $\{A\} = \{B\}$ and that the number of moles of A reacting, α will also be the number of moles of C formed. This leads to a single equation in one unknown:

$$K_C = 10 = \frac{\alpha}{(2 - \alpha)^2}$$

which solves for $\alpha = 1.6$.

The final concentrations at equilibrium are: $\{A\} = \{B\} = 0.4\,\text{mol.L}^{-1}$ and

$\{C\} = 1.6\,\text{mol.L}^{-1}$.

2. In general it DOES matter in which reactor type the reaction takes place. You can see that more clearly if we work in terms of conversion, X, then expressions for concentration in terms of conversion are different for flow reactors than for a constant volume batch reactor.

However, because this is a liquid phase system and the total volume does not change, this does not affect equilibrium conversion in this question.

3. The conversion of A at equilibrium, $X_{eq} = 80\%$

Question 6 [10]

Set up a stoichiometric table for the isothermal, isobaric gas-phase pyrolysis of ethane, and express the concentration of each species in the reaction as a function of conversion.

1. Set up the table for a *flow reactor* at 6 atm and 1110K for the reaction: $C_2H_6 \longrightarrow C_2H_4 + H_2$

Solution

Species	Flow into reactor	Change	Leaving reactor	Leaving concentration
C_2H_6 = A	F_{A0}	$-F_{A0}X$	$F_{A0}(1 - X)$	$C_A = C_{A0} \left(\dfrac{1 - X}{1 + \epsilon X} \right)$
C_2H_4 = B	F_{B0}	$F_{A0}X$	$F_{A0}(\theta_B + X)$	$C_B = C_{A0} \left(\dfrac{\theta_B + X}{1 + \epsilon X} \right)$
H_2 = C	F_{C0}	$F_{A0}X$	$F_{A0}(\theta_C + X)$	$C_C = C_{A0} \left(\dfrac{\theta_C + X}{1 + \epsilon X} \right)$

The unknowns in the concentration expression are:

- $\delta = 1 + 1 - 1 = 1$

- $\epsilon = \delta y_{A0} = y_{A0}$

- $\theta_B = \dfrac{F_{B0}}{F_{A0}}$

- $\theta_C = \dfrac{F_{C0}}{F_{A0}}$

- $C_{A0} = \dfrac{y_{A0}P}{RT} = \dfrac{y_{A0}607950}{(8.314)(1110)} = 65.88 y_{A0}$

Since we aren't provided with the molar flows of the species, nor the incoming mol fraction, the above is the best we can do to express the concentrations in terms of conversion.

Question 7 [10]

For the system considered in class previously (see last page of this tutorial's PDF) we have designed a single CSTR to achieve a conversion of 80%. I will teaching in you the 4N4 course how to estimate the capital cost of the CSTR vessel. For now, please use this formula to estimate the capital cost in dollars, in 2011 prices:

$$\text{Cost} = 2800 \cdot \left(\frac{V}{100} \right)^{0.53} \cdot 4 \cdot \left(\frac{1490}{300} \right)$$

where V is the CSTR tank volume, in US gallons (these reason for the formula structure will become clear in the 4N4 course).

1. Estimate the price of a single CSTR to obtain 80% conversion.

2. Estimate the price of two equally-sized CSTR's to obtain 80% conversion. Also write down the reaction rate in each tank, and the conversion leaving each tank.

3. Would it be more economically viable to purchase 3 equally-sizes CSTR's, ordered in series, than to buy a single large CSTR? Show your calculations and explain.

Solution

1. A since CSTR has volume of $6.4\,\text{m}^3 = 1690.7\,\text{US}$ gallons, to obtain an 80% conversion (derived in class and in an earlier tutorial).

   Using the formula provided, this reactor would cost approximately $2800 \cdot \left(\frac{1690}{100}\right)^{0.53} \cdot 4 \cdot \left(\frac{1490}{300}\right) \approx \$248,900$

2. Two CSTR's, of the same volume that give a total conversion of 80% are found by estimating the areas so that the 2 rectangles add up to give 80% conversion, but both rectangles have the same area.

   This can be found for reactor 1 going from $X = 0$ to $X \approx 0.57$, operating at a point of about $3.4 = \dfrac{F_A}{-r_A}$ on the y-axis ($-r_A \approx 0.117\,\text{mol.L}^{-1}.\text{s}^{-1}$). The area under this curve is $(0.57 - 0)(3.4) = 1.94\,\text{m}^3$.

   Reactor 2 operates at 80% conversion, so its volume is $(0.80 - .57)(8.0) = 1.84\,\text{m}^3$. With a bit more refinement we can get the two volumes to agree more closely, but this is good enough for a graphical solution.

   The cost of these reactors are about the same, at $2800 \cdot \left(\frac{500}{100}\right)^{0.53} \cdot 4 \cdot \left(\frac{1490}{300}\right) \approx \$130,500$, giving a total cost that's double that, at **\$261,000**.

3. Two reactors are already more expensive than a single reactor. The general rule of thumb for first order reactions, as described in class, is that the total cost will come down for multiple reactors, but eventually the costs will increase. Here we see already that two reactors are just marginally more costly than a single reactor. So without doing any calculations, for sure, 3 reactors will be more expensive than two.

   If you do the calculations, make sure you pick three reactors of *equal volume*. Suppliers of these reactors make them in standard sizes; you cannot ask the supplier, for example, to make a CSTR of unusual volume, such as 184 L. Furthermore, if you really did need an unusual volume, you would purchase a large reactor, and simply operate it at the desired volume (for liquid-phase reactions).

Table 2-2. Processed Data

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A \left(\dfrac{\text{mol}}{\text{m}^3 \cdot \text{s}} \right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A) \left(\dfrac{\text{m}^3 \cdot \text{s}}{\text{mol}} \right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$(F_{A0}/-r_A)(\text{m}^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0