CHN-302: Engineering Analysis and Process Modeling

Assignment1

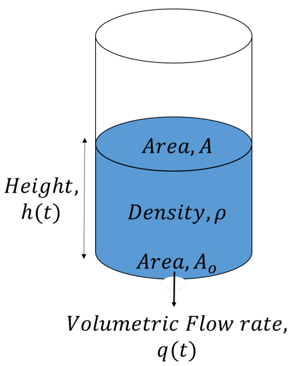
Weightage: 7% **Deadline: Jan 24, 2018, Midnight**

Instructions:

1. *Assignments need to be submitted individually, instances of plagiarism (copying assignment from others or allowing others to copy your assignment will be* ***strongly*** *peanlized.*
2. *Scans/photographs of handwritten assignments should be merged in a single pdf file and emailed to ch401.iitr@gmail.com (**Not** to any other email ID of instructor)*
3. *Hard copies of assignments or typed copies of assignments should not be submitted*
4. *All questions are of equal weightage*

1. An IITR Chemical Engineer boards the Jan Shatabdi Express from Roorkee to New Delhi. To kill boredom, he/she starts writing the material and energy balance equations for the train. Imagining you are that Chemical Engineer I am talking about,
   a. Write the appropriate material and energy balance equations, by first identifying the relevant system/subsystem, followed by the choice of appropriate variables and equations, with some reasonable assumptions. By performing a degree of freedom analysis, make a suitable choice of unknown variables.
   b. Compartments on the train resemble, to some extent, the tanks-in-series model used in reactor design. Write the general material and energy balance equations for the tanks-in-series model. When do we use the tanks-in-series model?
   c. Discuss the similarities and differences between the models of part (a) and part (b).

2. Consider the following physical situation of a tank filled with liquid draining by gravity through an orifice. Without using the Bernoulli equation or the Navier-Stokes equation, answer the following questions.



a) Draw expected profile of $h(t)$ versus t, just based on physical intuition, without doing any derivation. Justify your choice.

b) Define appropriate control volume and write mass balance.

c) Derive the expression of $h(t)$ for the following cases and plot $h(t)$ versus t. Which of these cases is the most accurate and why?

   i. $q = constant$
   ii. $q(t) \propto h(t)$
   iii. $q(t) \propto (h(t))^n$ for $n > 1$
   iv. $q(t) \propto (h(t))^n$ for $n < 1$

What happens when we put $n = 1$ in the expression derived in iii? Do we recover the result of ii? If not, why?

d) Consider the following experimental data from an experiment. Three sets of experiments are performed on an 100 ml cylinder draining by gravity.

	t [s]		
h(t) [cm]	Expt. 1	Expt. 2	Expt. 3
8	0	0	0
7	11	8	9
6	20	16	18
5	29	25	26
4	40	36	36
3	51	48	48
2	66	62	63
1	87	82	83
0	135	129	130

   i. Fit the expressions for $h(t)$ derived in part (c) to the experimental data using least square or other suitable method. Write the expression for the fitting equation and error values. Obtain the values of constants in the expressions derived in (c).

e) What can be the possible sources of disagreement in the three sets of experimental data?

f) Obtain an expression for $h(t)$ using dimensional analysis. This should involve the use of Buckingham-π theorem to find the number of dimensionless variables and then writing a dimensionless variables as function of other dimensionless variable(s). Note that only the characterizing dependent variables should be considered in the dimensional analysis.
   i. Without using viscosity
   ii. Using viscosity

   Does the results agree with what have been found in earlier parts of the question? If not, why?

g) Other models in c) are also valid for certain range of parameters (time scales). Derive appropriate time scale.
   Finally, you can compare the results with what you will get by the application of Bernoulli equation.

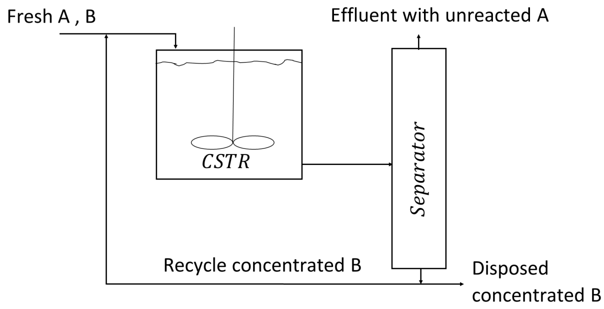
3. Consider the following reaction going on in the system shown on the right.

$$A + \beta B \rightarrow \gamma B + other\ products$$

with $\gamma > \beta$.

Assume the rate law: $r = kC_A C_B$.

Find concentration of B in the bottom stream of separator given the feed concentration of A, volume of CSTR, volumetric flow rate in/out of CSTR and recycle fraction.



4. Consider the following elementary reaction taking place in a CSTR

$$A \rightarrow products$$

Derive the expression for the transient (unsteady state) behavior of CSTR. When will steady state be achieved? Identify two time scales in the problem. Discuss their significance.

5. An elementary chemical reaction $A + B \xrightarrow{k} C$ involving light-sensitive reactants is occurring in a CSTR made of transparent material, which allows the manipulation of reaction rate constant k by periodic exposures to UV light. One exposure cycle consists of the UV-light turned on for a time period τ_{on} followed by UV-light turned off for a time period τ_{off} and this cycle is repeated continuously. $k = k_{on}$ when UV light is turned on for the time duration τ_{on} and $k = k_{off}$ when UV light is turned off for the time duration τ_{off}. Obtain the expression for the conversion of the reactor as a function of time and other relevant variables.

6. Consider a liquid phase polymerization process taking place in a CSTR under steady state conditions, involving the following simultaneous set of reactions:

$$A_1 + A_1 \xrightarrow{k_1} A_2$$
$$A_2 + A_1 \xrightarrow{k_2} A_3$$
$$\dots$$
$$A_{m-1} + A_1 \xrightarrow{k_{m-1}} A_m$$

Here, A_m is the longest polymer chain produced by the reaction. Reaction rate constants are given by the relation $k_i = k/i$ for $i = 1,2, \dots, m-1$, k being a constant. The reactor feed contains pure A_1 with a concentration (moles/volume) C_{A1}^0 and volumetric flow rate v. The reactor output contains concentrations C_{Ai} of component A_i ($i = 1,2, \dots, m$). Assume all the reactions follow elementary rate laws.

a. Draw a schematic of the system indicating relevant variables.
b. Write the mole balance equations for components A_i ($i = 1,2, \dots, m$) and the overall mass balance equation for the system in terms of concentrations of components A_i.
c. Write the equations derived in b) in a dimensionless form by defining dimensionless concentrations as
$$\hat{C}_{Ai} = \frac{C_{Ai}}{C_{A1}^0}$$
The dimensionless equations would contain one other dimensionless variable (say η). Discuss the physical significance of this dimensionless variable (η).
d. Derive the expression for dimensionless concentrations $\hat{C}_{Ai}$ ($i = 2, \dots, m$) in terms of $\hat{C}_{A1}$ for the following two cases. How can we estimate $\hat{C}_{A1}$ for these two cases?
   i. $\eta \ll 1$
   ii. $\eta \gg 1$

Which of the two cases in (d) give rise to higher values of m (corresponding to longest polymer chain)? How can we estimate m?

7. Consider a gas-phase, elementary chemical reaction A+B→AB following second order kinetics. Assume for simplicity that A and B are spherical molecules, with initial concentrations c_{Ao} and c_{Bo}, respectively. Define appropriate time scale and length scale for studying this system. Now imagine that the reaction is taking place in a cylindrical vessel of diameter D and length L. Find lower bounds on D and L in terms of the length scale you have defined. Draw the expected profiles of the concentrations of A, B, and AB, against the dimensionless time (actual time divided by the time scale) for a slow and a fast reaction.