Process model formulation and solution, 3E4

Assignment 1

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Assignment objectives

- Some questions that will help you get comfortable modelling chemical engineering processes.

Recap of assignment rules

- Due: 27 September, in printed form, at class.
- They may be completed in groups of no more than **three** people; please put all group member names on the submission.

Question 1 [1]

Note: Distillation tray modelling.

The distillation column is a common unit operation in refineries, air-separation, and fine-chemical processes. The figure, taken from Wikipedia, shows a cross-section of two trays in a distillation column.

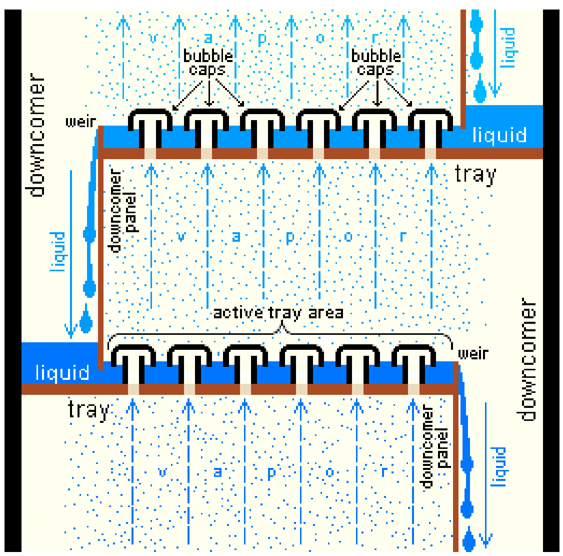


Figure 1: *Source*: http://en.wikipedia.org/wiki/File:Bubble_Cap_Trays.PNG

1. Redraw the figure, and add to it a boundary you would use to write the mass and energy balance equations for a single tray.
2. Which physical phenomena would you need to consider for an accurate model?
3. Which reasonable simplifying assumptions would you make to reduce the complexity of your model?

Question 2 [2]

Note: This question will slowly build up the equations and assumptions for solving a common chemical engineering problem: heat loss from a pipe.

Our final goal is to be able to predict the temperature profile, along the length of a tube. Such tubes could occur, for example, in a shell and tube heat exchanger, as shown in the figure below from the Wikipedia article.

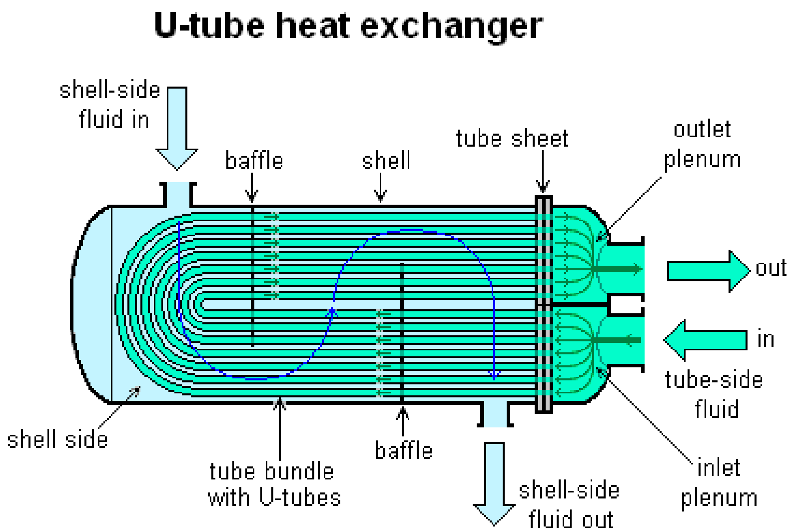
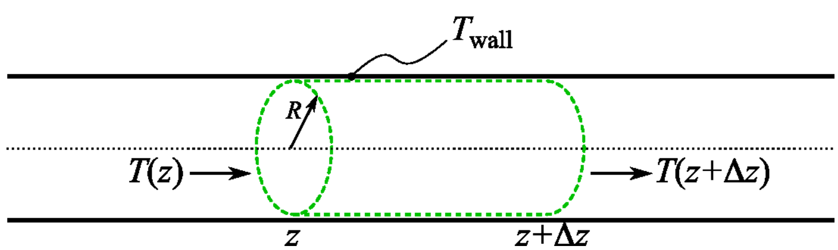


Figure 2: *Source*: http://en.wikipedia.org/wiki/Shell_and_tube_heat_exchanger

1. Write down all the possible controlling mechanisms you might consider for a high-accuracy model of this shell and tube heat exchanger.
2. Now let's start simple, and consider only the fluid flow in the pipe. What would the cross-sectional profile for the flow look like under (a) laminar flow and (b) turbulent flow?
3. Consider a short cross-sectional segment, of width Δz, where the temperature is $T(z)$ at the entry and $T(z+\Delta z)$ at the exit. The figure below contains the boundary region already drawn, in green.



   (a) Which specific assumption do you have to invoke so that the temperature in the radial direction is constant?

   (b) Assuming this assumption is true, write down the average temperature within the segment, and define it as $\overline{T}(z)$.

   (c) What is the surface area of the pipe in this segment?

   (d) Finally, using Newton's law of cooling, write down the rate of energy loss, Q, to the outside environment, where the wall temperature is defined as T_{wall}. What are the units of the heat transfer coefficient, and the units of Q?

4. Now perform an energy balance over this segment.
   - Heat in =
   - Heat out =
   - Heat generated =
   - Overall heat balance, assuming steady-state:
5. Lastly, divide this steady-state equation by Δz and take limits so that $\Delta z \rightarrow 0$. This allows you to reach our goal and write an equation that predicts the temperature profile along the length of a tube.

   Recall from calculus that:

$$\lim_{\Delta z \rightarrow 0} \frac{T(z+\Delta z) - T}{\Delta z} = \frac{dT}{dz}$$

Question 3 [1.5]

Consider a CSTR where an irreversible, first-order endothermic reaction of the form $A \xrightarrow{k} B$ takes place. Let C_A denote the concentration of the species A in the reactor, T_R and T_{in} denote the temperatures of the reactor and of the inlet stream, respectively, Q, is the heat added to/removed from the reactor, C_{A0} is the concentration of A in the inlet stream, V is the volume of the reactor, $k_0, E, \Delta H$ are the pre-exponential constant, the activation energy, and the enthalpy of the reaction and C_p and ρ are the heat capacity and fluid density in the reactor.

Develop a model that describes the evolution of the concentration and temperature in the reactor, using a systematic modelling approach that also outlines all assumptions made.

Question 4 [1.5]

The simplest example of biological wastewater treatment involves removing a single nutrient, N, from a liquid waste stream and converting it to (solid) biomass, B. This process is used, for example, by pop manufacturers to treat liquid waste from their processes, where N would be sugar (e.g. fructose). The microorganisms absorb N from the wastewater and use it to grow more and more biomass.

1. Draw a simple CSTR where this liquid stream enters, containing N_{in} [mg/L] and the stream leaving the reactor contains both liquid and solid fractions. The solids in the outlet stream can be separated, and the remaining liquid would contain much less N, allowing the company to discharge that liquid to municipal wastewater treatment systems.

   Draw the boundaries you will consider on your diagram as well.
2. Write an overall mass balance, where the flows, q, are expressed in units of litres per day, typically being in the order of megalitres per day.
3. Write a dynamic mass balance for N and B, where their units are expressed in mg/L. Assume there is no biomass in the inlet stream. The reaction rate for converting $\mathsf{N} \longrightarrow \mathsf{B}$ is given by r_B in units of mg/(L.day).
4. Write the two equations for the steady-state values of N and B if $r_B = \mu_{\text{max}} \frac{\mathsf{N}}{\mathsf{K}+\mathsf{N}} \mathsf{B}$, where K [mg/L] and μ_{max} [1/day] are constants from the Monod rate expression. Note that $r_N = -\frac{1}{Y_B} r_B$, where Y_B is the yield of B from N.
5. Are these equations solvable by hand if you are given the constants such as N_{in}, K, μ_{max}, *etc* in your equations?

Question 5 [2]

Note: To review and practice material related to number systems and round-off errors.

1. Convert the following binary numbers to base-10:
   - 01010111
   - 1110.0001
2. Convert the following hexadecimal numbers to base-10:
   - 9A8B7C6D
   - DEADB0EF
3. In either MATLAB or Python: write a short function that returns the smallest positive number used on your computer. In other words your computer will be unable to reliably distinguish between zero and a quantity smaller than this number.
4. How does your value (above) compare to what MATLAB or Python reports?
   - **MATLAB**:

     ```
     >> help eps  % read what this command does
     >> eps
     ```

   - **Python**:

     ```
     >>> np.finfo(np.double).eps
     ```

END