Homework 16

Ch En 263 – Numerical Tools
Due date: 28 May 2020

Instructions

- For the handwritten problems, submitted a single pdf file on Learning Suite with the name "LastName_FirstName_HW16.pdf".
- For the problems in Excel, submit a workbook named "LastName_FirstName_HW16.xlsx" where each worksheet tab is named "Problem_1", "Problem_2", etc.
- For the problems in Python, submit a separate file for each problem named "LastName_FirstName_HW16_ProblemXX.py" where XX is the problem number.
- **Please report how long it took you to complete the assignment (in hours) in the "Notes" section on Learning Suite.**

Problems

1. The enthalpy of gaseous CO_2 is given by

$$h(T) = h(298.15) + \int_{298.15}^{T} c_p(T)dT.$$

The units of h are J/mol. The heat capacity (J/mol K) is given by

$$c_p(T) = R_g(a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4),$$

where $R_g = 8.314$ J/(mol K), and $a_1 = 2.275724$, $a_2 = 0.009922$, $a_3 = -1.04091 \times 10^{-5}$, $a_4 = 6.86669 \times 10^{-9}$, $a_5 = -2.11728 \times 10^{-12}$. Also, $h(298.15) = -393549.1$ J/mol.

Use `scipy.optimize.root` to find the temperature where $h(T) = -362828$ J/mol.

Hints: This will be easiest if you first analytically evaluate the integral. Also, a choice of the form of $T = f(T)$ where large powers of T are in the denominator is more likely to converge than a form where large powers of T are in the numerator.

2. We have a parallel pipe network with three pipes. We want to find the flow rates Q_i through each pipe. The flow rates are written in terms of the friction factors f_i for each pipe, which gives six equations,

$$Q_0 + Q_1 + Q_2 = Q_{tot} \tag{1}$$

$$\frac{f_0 L_0 \rho}{2D_0}\left(\frac{4Q_0}{\pi D_0^2}\right)^2 = \frac{f_1 L_1 \rho}{2D_1}\left(\frac{4Q_1}{\pi D_1^2}\right)^2 \tag{2}$$

$$\frac{f_0 L_0 \rho}{2D_0}\left(\frac{4Q_0}{\pi D_0^2}\right)^2 = \frac{f_2 L_2 \rho}{2D_2}\left(\frac{4Q_2}{\pi D_2^2}\right)^2 \tag{3}$$

$$\frac{1}{\sqrt{f_0}} = -2\log_{10}\left(\frac{\epsilon_0}{3.7D_0} + \frac{2.51\mu\pi D_0}{4\rho Q_0\sqrt{f_0}}\right) \tag{4}$$

$$\frac{1}{\sqrt{f_1}} = -2\log_{10}\left(\frac{\epsilon_1}{3.7D_1} + \frac{2.51\mu\pi D_1}{4\rho Q_1\sqrt{f_1}}\right) \tag{5}$$

$$\frac{1}{\sqrt{f_2}} = -2\log_{10}\left(\frac{\epsilon_2}{3.7D_2} + \frac{2.51\mu\pi D_2}{4\rho Q_2\sqrt{f_2}}\right) \tag{6}$$

and six unknowns, Q_0, Q_1, Q_2, f_0, f_1, f_2. The following quantities are given (in SI units):

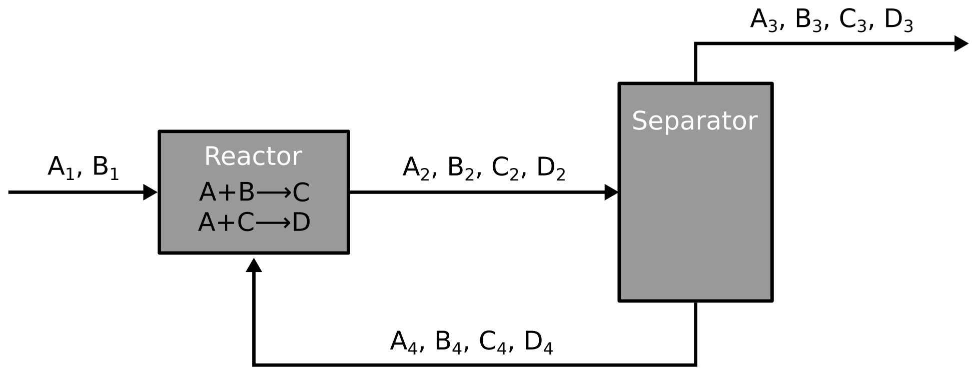
$Q_{tot} = 0.01333$ m^3/s	$\mu = 1.002 \times 10^{-3}$ kg/(m·s)	$\rho = 998$ kg/m^3
$L_0 = 100$ m	$L_1 = 150$ m	$L_2 = 80$ m
$D_0 = 0.05$ m	$D_1 = 0.045$ m	$D_2 = 0.04$ m
$\epsilon_0 = 0.00024$ m	$\epsilon_1 = 0.00012$ m	$\epsilon_2 = 0.0002$ m

Find the flow rates Q_0, Q_1 and Q_2. *Hint: It is a good idea to make your guesses consistent. That is, make sure your guesses for Q_0, Q_1, and Q_2 add up to the given Q_{tot}. Reasonable guesses for f_0, f_1, f_2 are 0.01.*

Notes on the physical interpretation of the equations (if you are interested):

- Eq. 1 says the total flow rate is the sum of the flow rates through each pipe.
- Eq. 2 says that the pressure drop through pipe 0 is the same as that through pipe 1, since pipes 0 and 1 are connected at their ends.
- Eq. 3 says that the pressure drop through pipe 1 is the same as that through pipe 2, since pipes 1 and 2 are connected at their ends.
- Eq. 4–6 relate the friction factor in each pipe to its flow rate and pipe properties.
- In the Eq. 2 and Eq 3, $4Q_i/(\pi D_i^2)$ is the velocity in the pipe. We substituted $v_i = 4Q_i/(\pi D_i^2)$ for convenience, but it makes the equations a bit harder to read. We could also define local terms like $v_0 = 4Q_0/(\pi D_0^2)$, and then use v_0 in the equations above instead of $4Q_0/(\pi D_0^2)$.
- In Eq. 4–6, $\mathrm{Re} = \dfrac{4\rho Q_i}{\mu \pi D_i}$. Again, we made the substitution for convenience.

3. The process shown in the figure below consists of two unit operations, a reactor and a separator.



The process takes in some flow rates A_1 and B_1 of species A and B. The reactor has a reaction

$$A + B \rightarrow C \text{ (Reaction 1)}$$

that produces an intermediate product C that then needs to be converted to the desired product D by a second reaction

$$A + C \rightarrow D \text{ (Reaction 2).}$$

The single-pass conversion of the reactor is 90% with a 30% selectivity for Reaction 2. The products of the reaction in stream '2" are fed to a separator, which produces the product stream "3" and a recycle stream "4." The specifications of the separator are a recycle of 65% of D and 85% of C. The flow B_2 is evenly split between the product and recycle streams, while 10% of A_2 is lost to the product stream. Steady state mass balances and the other specifications give the following equations:

Reactor Mass Bal.		Separator Mass Bal.	
$A_4 - A_2 - \xi_1 - \xi_2 = -A_1$	(3.1)	$A_2 - A_3 - A_4 = 0$	(3.5)
$B_4 - B_2 - \xi_1 = -B_1$	(3.2)	$B_2 - B_3 - B_4 = 0$	(3.6)
$C_4 - C_2 + \xi_1 - \xi_2 = 0$	(3.3)	$C_2 - C_3 - C_4 = 0$	(3.7)
$D_4 - D_2 + \xi_2 = 0$	(3.4)	$D_2 - D_3 - D_4 = 0$	(3.8)

Conversion/Selectivity		Separator Specs	
		$D_4 - 0.65D_2 = 0$	(3.11)
$\xi_1 + \xi_2 - 0.9A_4 = 0.9A_1$	(3.9)	$B_3 - B_4 = 0$	(3.12)
$0.3\xi_1 - 0.7\xi_2 = 0$	(3.10)	$0.1A_2 - A_3 = 0$	(3.13)
		$0.85C_2 - C_4 = 0$	(3.14)

where ξ_1 and ξ_2 are the extent of reaction for Reactions 1 and 2 respectively.

If $A_1 = 4$ mol/s and $B_1 = 3$ mol/s specify the inlet flow rates of A and B, what are the amounts of A, B, C, and D coming out of the separator at the end of the process?