CDS-130/004 SPRING 2016: HOMEWORK 10 (version 1)
ASSIGNED 20 APRIL 2016, DUE 27 APRIL 2016 AT THE END OF CLASS

MATLAB PROGRAMMING EXERCISE

THESE ARE MATLAB PROGRAMMING EXERCISE: YOU MUST SUBMIT A HARDCOPY PROGRAM LISTING, AND A HARD COPY OF THE PROGRAM'S CONSOLE OUTPUT AND/OR PLOT (AS SCREENSHOTS) TO RECEIVE CREDIT FOR THESE EXERCISES. ABSOLUTELY NO HANDWRITTEN PROGRAMS OR PROGRAM OUTPUT WILL BE ACCEPTED.

EXERCISE 1 (6 pts) "Petrochemical Processing"

Diethanolamine (**DEA**) is extensively used in the gas processing industry for removing acid gases such as carbon dioxide and hydrogen sulfide from light hydrocarbons. DEA's popularity is based on several factors: energy savings compared with certain other solvents; high affinity for acid gases; fair resistance to degradation. Degradation is defined as the irreversible transformation of DEA into undesirable compounds. The principal degradation compounds were found to be 3-(hydroxyethyl)-2-oxazolidone (**HEOD**), N,N,N-tris(hydroxyethyl)-ethylenediamine (**THEED**), and N,N-bis(hydroxyethyl)piperazine (**BHEP**).[1]

In this problem we will investigate a simplified chemical kinetic mechanism for degradation of DEA dissolved in water, using the compartment model framework introduced in our presentation entitled, "Introduction to Modeling III: Systems of Population Equations and Compartment Models."

Consider the following compartment model for the degradation of DEA:
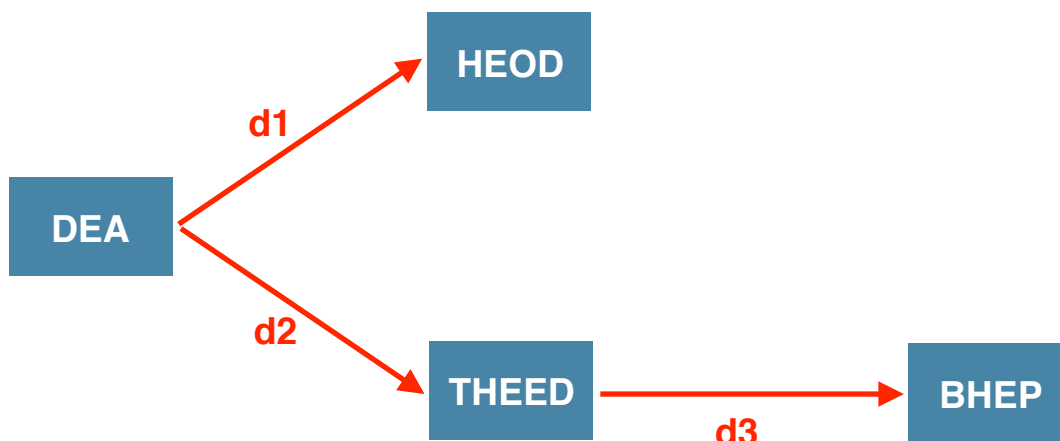
DEA dissociates (degrades) into HEOD at a rate of 0.0167% per minute, as indicated by the d1 pathway in the compartment diagram. DEA also dissociates into THEED at a rate of 0.025% per minute, as indicated by the d2 pathway. Finally, THEED degrades into BHEP at a rate of 0.0633% per minute, as indicated by the d3 pathway. If the initial solution mass fraction of DEA is 0.65, and the initial solution mass fractions of HEOD, THEED and BHEP all equal 0.0, then what are the solution mass fractions of DEA, HEOD, THEED and BHEP at the end of 33 hours? At the end of 100 hours? Prepare a plot of the variation over time of the solution mass fractions of DEA, HEOD, THEED and BHEP, from 1 minute (i.e., initial concentration at the end of the first minute) to 7,200 minutes.

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[1] Kennard, M.L. and Meisen, A., "Mechanisms and Kinetics of Diethanolamine Degradation", Industrial & Engineering Chemistry Fundamentals, l985, 24, 129-140.

NOTE:
DEA "dies twice" per minute, since it simultaneously dissociates into two different products. The overall "death rate" for DEA is therefore the sum of its two, individual dissociation rates. HOWEVER, both HEOD and THEED receive immigrants from DEA AT RATES CORRESPONDING TO THE RATE (d1 OR d2) THAT POINTS INTO THEIR RESPECTIVE COMPARTMENTS!

EXERCISE 2 (6 pts.): "Enthalpy Change"

INTRODUCTION: INDUSTRIAL GAS HEATING

Using Numerical Integration to Calculate the Increase in Energy Content of a Stream of Flowing Nitrogen Gas

A standard problem faced by process engineers is to calculate the increase in energy content of a flowing gas that is subject to **continuous heating**. Typically, a processing unit called a **tube heater** is involved:
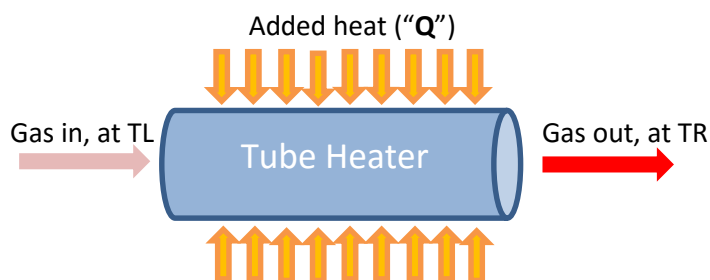
The continuous heating of industrial gases in tube heaters is one of the so-called unit operations of chemical process engineering; many tube heaters bundled together constitute a piece of process equipment called a **heat exchanger.** Heat exchangers work by transferring energy from hot fluids (liquids and gases) to colder fluids, thus heating the colder fluid—typically just prior to using it in the chemical process. This heating of cold fluids prior to use is called **preheating** and is often necessary for the efficient operation of downstream chemical reactors that transform reactant streams into product streams.

Tube heaters and heat exchangers therefore lie at the heart of modern chemical processing. Understanding how they operate is essential to optimizing their performance. And optimizing the performance of tube heaters and heat exchangers is critically important for energy security: For example, as of 2002, the petroleum and coal processing industries together accounted for 20% of all energy consumed by the entire U.S. industrial manufacturing infrastructure.[2]

THERMODYNAMIC ANALYSIS OF THE TUBE HEATER:

One unit (mol) of gas enters the left side of the tube heater at a **temperature TL** (in °C), and exits the tube heater on the right at a **higher temperature TR** (in °C). Heat ("**Q**", measured in joules) is added continuously to the gas through the walls of the tube heater as the gas flows through it from left to right. The added heat is responsible for the observed temperature increase of the gas between inlet and outlet.

If we assume that the tube heater is operating at constant pressure, that there is no heat transfer resistance from either the tube heater walls (thin wall approximation) or from the gas in the tube (perfect mixing approximation), then thermodynamics tells us that the increase in energy content of one unit (mol)of the gas is equal to its change in enthalpy, ΔH, as the gas flows between the left side

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[2] http://energy.gov/sites/prod/files/2013/11/f4/bandwidth.pdf

of the tube heater and the right side of the tube heater. The change in enthalpy of the gas between the left and right sides of the tube heater is given as:

$$\Delta H = \int_{TL}^{TR} C_p dT \qquad \text{(equation 1)}$$

where

$$C_p = a_0 + a_1 T + a_2 T^2 + a_3 T^3 \qquad \text{(equation 2)}$$

And thus:

$$\Delta H = \int_{TL}^{TR} \left(a_0 + a_1 T + a_2 T^2 + a_3 T^3 \right) dT \qquad \text{(equation 3)}$$

PROBLEM STATEMENT:

The goal, then, is to calculate the change in enthalpy, ΔH , by computing the integral in (equation 3) between the temperature on the left (**TL**) and the temperature on the right (**TR**). Doing so will give us the enthalpy change (and thus increase in energy content) for the one unit (mol) of gas as it flows across the tube heater from left to right. What we need are values for the parameters a_0, a_1, a_2 and a_3. These vary for each gas. For example, the values for one unit of nitrogen gas (N_2) are:

$a_0 = 29.0$ (in joules/°C)
$a_1 = 0.2199 \times 10^{-2}$ (in joules/°C^2)
$a_2 = 0.5723 \times 10^{-5}$ (in joules/°C^3)
$a_3 = -2.871 \times 10^{-9}$ (in joules/°C^4)

When substituting these values into equation 3, we can compute the enthalpy change of one unit of N_2 as its temperature is raised from **TL** to **TR** as a result of passage through the tube heater. To obtain the enthalpy change, we compute the value of the integral in equation 3. And to compute the equation 3 integral, we need values for a_0, a_1, a_2, a_3, **TL** and **TR**. When computed, the value of the equation 3 integral will have units of energy (joules).

Use numerical integration to compute the change in enthalpy of one unit of N_2 gas entering a tube heater at a temperature of 20°C and exiting the tube heater at a temperature of 100 °C. Use values for parameters a_0, a_1, a_2 and a_3 shown above, in the Introduction, and use 500 trapezoid panels for the integration. (see **Introduction to Numerical Integration**)

Note that the integral (equation 3) can be solved analytically in this case since the integrand is a polynomial function of T. But analytic solutions are the exceptions, not the rule, and numerical integration is typically used to solve integration problems when analytic solutions are not available.

Exercises 3 and 4 are based on the above analysis and the numerical integration code in Exercise 2.

HEAT CAPACITY PARAMETERS FOR ETHYLENE AND METHANE:

	Ethylene (C_4H_4)	Methane (CH_4)
a_0	40.75	34.31
a_1	11.47×10^{-2}	5.469×10^{-2}
a_2	-6.891×10^{-5}	0.3661×10^{-5}
a_3	17.66×10^{-9}	-11.00×10^{-9}

EXERCISE 3 (6 pts.): "Enthalpy Change of Ethylene and Methane"

Use numerical integration to compute the difference between the change in enthalpy of one unit (mol) of ethylene gas and one unit (mol) of methane, both entering a tube heater at a temperature of 15°C and exiting the tube heater at a temperature of 175°C. Use the heat capacity parameters a_0, a_1, a_2 and a_3 for ethylene and methane shown in the above table, and use 175 trapezoid panels for the numerical integration of area between the curves.

EXERCISE 4 (6 pts.): "Molar Flow Rate of Methane"
Many units (mols) of methane gas flow through a tube heater in one second, entering the heater on the left at a temperature of 25°C and exiting the heater on the right at a temperature of 1075 C. If the total amount of energy transferred by the heater to the methane is equal to 13,495,112 joules, how many units (mols) of methane flowed through the tube heater during that one second? Use the heat capacity parameters a_0, a_1, a_2 and a_3 for methane shown in the above table, and use 450 trapezoid panels for the numerical integration (HINT: How many joules are transferred to just one unit of methane traveling from left to right?)