CHE656

Process Analysis and Modeling I

Modeling Chemical Processes Using MATLAB

Exercise Problems

14th Edition

Prepared by

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1. *System of Linear Algebraic Equations, I*

Use MATLAB to solve the following system of linear algebraic equations, correct to 4 decimal places:

$$
\begin{aligned}
x_1 + x_2 - x_3 + 2x_4 - x_6 - 6 &= 0\\
-2x_1 + x_3 + x_4 - x_5 + 2x_6 - 7 &= 0\\
4x_2 + 3x_3 + 2x_4 + x_5 + x_6 + 4 &= 0\\
x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 - 8 &= 0\\
-x_1 + x_2 + x_3 - x_4 - x_5 - x_6 + 22 &= 0\\
2x_2 + 2x_3 + x_5 + 10 &= 0\\
x_1 + 2x_3 + x_4 + x_5 + x_7 &= 0
\end{aligned}
$$

2. *System of Linear Algebraic Equations, II*

Use MATLAB to solve the following system of linear algebraic equations, correct to 4 decimal places:

$$
\begin{aligned}
x_1 + 3x_2 + 2x_3 - x_5 + 4x_6 &= -2\\
2x_1 - 2x_2 + 4x_3 + x_4 + x_5 &= 1\\
-3x_1 - 2x_2 + 4x_3 + 5x_4 + 2x_5 - x_6 &= 0\\
-x_2 + 2x_4 + 6x_5 + 4x_6 &= 3\\
-2x_1 + 3x_4 + 4x_5 + 5x_6 &= -6\\
6x_1 - 2x_2 - x_3 - 3x_4 + 4x_5 + 2x_6 &= 5
\end{aligned}
$$

3. *System of Nonlinear Algebraic Equations*

Use MATLAB to solve the following system of nonlinear algebraic equations:

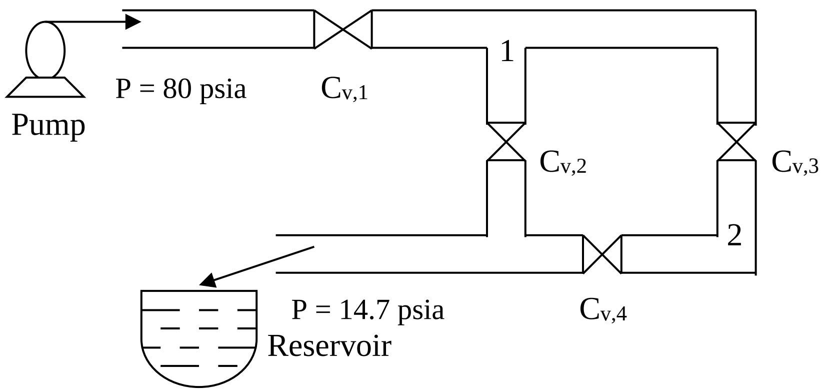
$$
\begin{aligned}
\exp(-x_1) + x_1 x_2 &= 4\\
x_1^2 - 2x_2 - \ln(x_3) &= 0\\
\sin(x_1 x_3) - 0.5\tan(x_2 x_3) + x_1 x_2 x_3 &= 20
\end{aligned}
$$

4. *Pressures in a Pipeline Network*

Consider the following interconnected liquid pipeline network which contains 4 valves with the following valve coefficients. Calculate the pressure at each location/node indicated in the network.

$C_{v,1} = 0.5$ ft^3/(psia)$^{1/2}$-hr $C_{v,2} = 0.4$ ft^3/(psia)$^{1/2}$-hr

$C_{v,3} = 0.3$ ft^3/(psia)$^{1/2}$-hr $C_{v,4} = 0.2$ ft^3/(psia)$^{1/2}$-hr

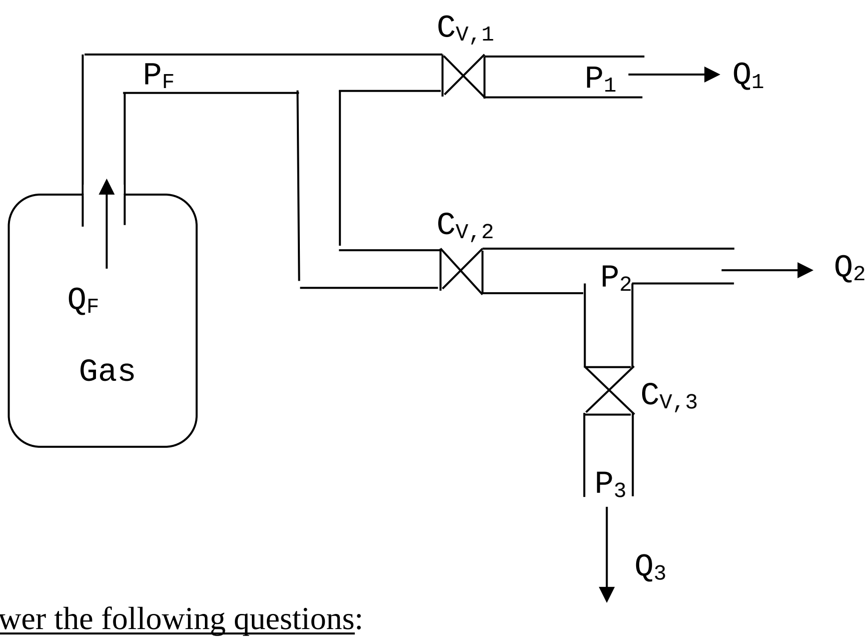


5. *Solving for Pressures in a Gas Pipeline Network*

A storage vessel contains a gas that is to be distributed via a network of pipeline as shown. You are to use MATLAB to solve for the following unknowns in the system: P_F, Q_1, Q_2, and Q_3. On the other hand, the known parameters in the system are:

Q_F = 50 ft^3/min	P_1 = 20 psia	P_2 = 30 psia	P_3 = 15 psia
$C_{V,1}$ = 2.0 ft^3/(psia)-min	$C_{V,2}$ = 1.5 ft^3/(psia)-min		$C_{V,3}$ = 1.0 ft^3/(psia)-min

Assume that the gas behaves ideally but is compressible, there is no pressure drop around any bend in the pipeline, and the system is isothermal.



Answer the following questions:

P_F = ____________ psia Q_1 = ____________ ft^3/min

Q_2 = ____________ ft^3/min Q_3 = ____________ ft^3/min

6. *Simple Calculations and Array Manipulations in MATLAB*

Consider the following arrays:

$$\mathbf{A} = \begin{pmatrix} 1 & 3 & 5 \\ 10 & 5 & 30 \\ 6 & 10 & 4 \\ 3 & \pi & 8 \end{pmatrix} \qquad \mathbf{B} = \log_{10}(\mathbf{A}) \qquad \mathbf{C} = \begin{pmatrix} 2 & 4 & 4 & 8 \\ 8 & 12 & 24 & 7 \\ 0 & -1 & 5 & 6 \end{pmatrix}$$

Write MATLAB expressions in an M-file (script file) to do the following (use "format short" in all calculations unless otherwise told):

(a) Determine the sum of the second column of **B**.
(b) Select the first 3 columns and the first 3 rows of **A** and **B** and add their determinants .
(c) Determine the square root of the product (a scalar) between the last row of **C** and the second column of **A**.
(d) Determine the sum of the second row of **A** divided element-by-element by the third column of **C**.
(e) Evaluate the hyperbolic secant of $(0.01 * \mathbf{A} * \mathbf{C})$.
(f) Evaluate the following function: $\tan^{-1}(0.1 * \mathbf{B} * \mathbf{C})$ in 6 decimal places.

7. *Inverse and Determinant of 2×2 and 3×3 Matrices*

Use MATLAB to write a program that can determine the inverse and determinants of any 2×2 and 3×3 matrices, which can then be used to solve a system of linear algebraic equations in 2 or 3 unknowns.

Recall that the formulae for calculating the determinant of 2×2 and 3×3 matrices are as follows:

If $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ then $\det(A) = a_{11}a_{22} - a_{12}a_{21}$ $\qquad A^{-1} = \dfrac{1}{\det(A)}\begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$

If $A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$ then

$$\det(A) = a_{11}(a_{33}a_{22} - a_{32}a_{23}) - a_{21}(a_{33}a_{12} - a_{32}a_{13}) + a_{31}(a_{23}a_{12} - a_{22}a_{13})$$

and

$$A^{-1} = \frac{1}{\det(A)}\begin{bmatrix} a_{33}a_{22} - a_{32}a_{23} & a_{32}a_{13} - a_{33}a_{12} & a_{23}a_{12} - a_{22}a_{13} \\ a_{31}a_{23} - a_{33}a_{21} & a_{33}a_{11} - a_{31}a_{13} & a_{21}a_{13} - a_{23}a_{11} \\ a_{32}a_{21} - a_{31}a_{22} & a_{31}a_{12} - a_{32}a_{11} & a_{22}a_{11} - a_{21}a_{12} \end{bmatrix}$$

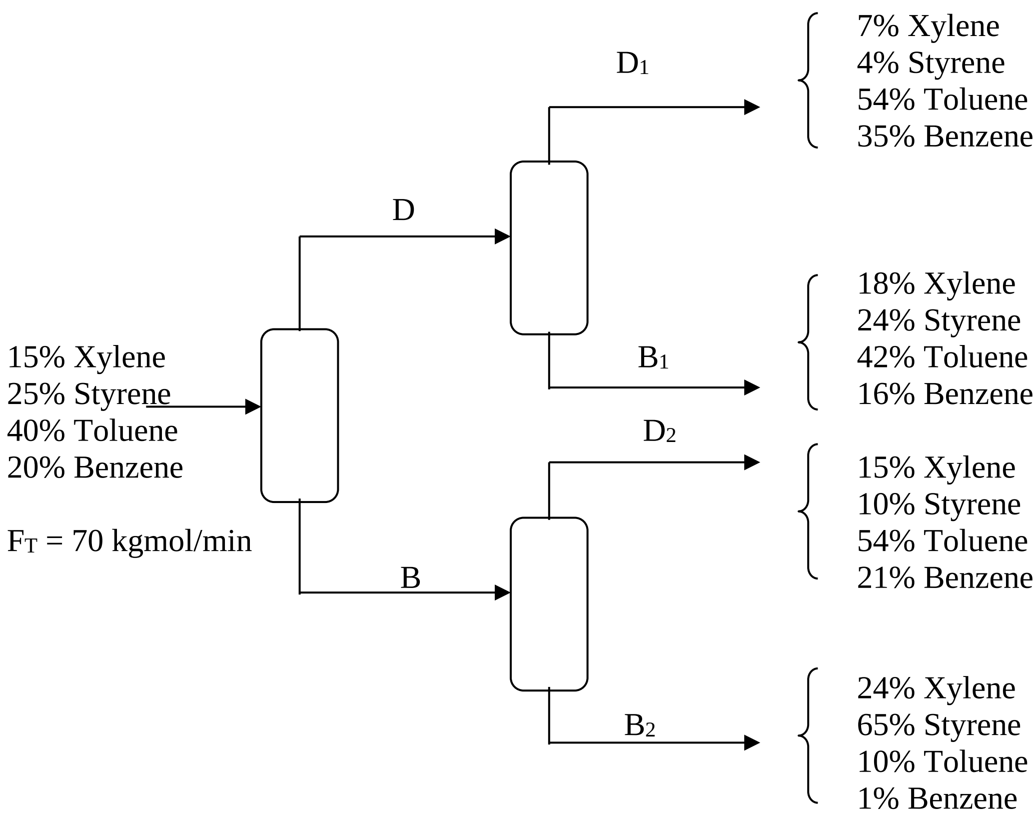
Use the above formulae to solve the following two systems of linear algebraic equations:

$(a)\quad 2x_1 - 3x_2 = 6 \qquad -x_1 + 2x_2 = -1$

$(b)\quad x_1 + 2x_2 - 6x_3 = -2 \quad -5x_1 + 3x_2 + x_3 = 0 \quad 4x_1 - x_2 - 2x_3 = 3$

8. *Steady-State Material Balances on a Separation Train*

Paraxylene, styrene, toluene, and benzene are to be separated with an array of distillation columns shown in the figure below.



Formulate the problem as a system of simultaneous linear equations and solve it using MATLAB.

9. *Using MATLAB to Solve the Peng-Robinson Equation of State*

The Peng-Robinson equation of state contains 2 empirical parameters *a* and *b*, and its conventional form is given by:

$$P = \frac{RT}{V_m - b} - \frac{a}{V_m^2 + 2bV_m - b^2}$$

where

$$a = 0.45724\left(\frac{\alpha R^2 T_C^2}{P_C}\right)$$

$$b = 0.07780\left(\frac{RT_C}{P_C}\right)$$

$$\alpha = [1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_r^{0.5})]^2$$

$$T_r = \frac{T}{T_C}$$

$$\omega = -1.0 - \log_{10}\left[\frac{P^{VAP}(T_r = 0.7)}{P_C}\right]$$

The variables are defined by:

P	=	pressure in MPa
V_m	=	molar volume in cm^3/gmole
T	=	temperature in K
R	=	gas constant (8.314 cm^3-MPa/gmole-K)
T_C	=	the critical temperature (150.86 K for argon)
P_C	=	the critical pressure (4.898 MPa for argon)
P^{VAP}	=	vapor pressure (0.4946 MPa at $T_r = 0.7$ for argon)

Alternatively, this equation of state can be expressed in polynomial forms as given below:

$$A = \frac{aP}{R^2T^2}$$

$$B = \frac{bP}{RT}$$

$$Z^3 + (B-1)Z^2 + (A - 2B - 3B^2)Z + (-AB + B^2 + B^3) = 0$$

$$where\ \ Z = \frac{PV_m}{RT},\ \ the\ \ compressibility\ \ factor$$

Use MATLAB to compute the molar volume of argon using both the conventional form and the polynomial form at T = 105.6 K and P = 0.498 MPa. The two solutions should be the same. Because the two equation forms are both cubic in molar volume, you should obtain 3 different answers in volume. Briefly describe the physical meaning or significance of each answer.

10. *Using MATLAB to Component Fugacity Coefficients of Argon Gas*

The fugacity coefficient is defined by $\phi = f / P$, where f is the fugacity of the component with units of pressure and P is the pressure. The fugacity coefficients of pure substances can be calculated from a number of equations of state, such as van der Waals and Peng-Robinson which are summarized by Walas (1985).

The van der Waals equation of state is given by:

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT$$

where

$$a = \frac{27}{64}\left(\frac{R^2 T_C^2}{P_C}\right)$$

$$b = \frac{RT_C}{8P_C}$$

$$\ln\phi = Z - 1 - \frac{a}{RTV} - \ln\left[Z\left(1 - \frac{b}{V}\right)\right]$$

The Peng-Robinson equation of state contains 2 empirical parameters a and b, and its conventional form is given by:

$$P = \frac{RT}{V - b} - \frac{a}{V^2 + 2bV - b^2}$$

where

$$a = 0.45724\left(\frac{\alpha R^2 T_C^2}{P_C}\right)$$

$$b = 0.07780\left(\frac{RT_C}{P_C}\right)$$

$$\alpha = [1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_r^{0.5})]^2$$

$$T_r = \frac{T}{T_C}$$

$$\omega = -1.0 - \log_{10}\left[\frac{P^{VAP}(T_r = 0.7)}{P_C}\right]$$

The variables are defined by:

P = pressure in MPa

V = molar volume in cm^3/gmole

T = temperature in K
R = gas constant (8.314 cm^3-MPa/gmole-K)
T_C = the critical temperature
P_C = the critical pressure
P^{VAP} = vapor pressure
ϕ = fugacity coefficient

Alternatively, the Peng-Robinson equation of state can be expressed in polynomial forms as given below:

$$A = \frac{aP}{R^2T^2}$$

$$B = \frac{bP}{RT}$$

$$Z^3 + (B-1)Z^2 + (A-2B-3B^2)Z + (-AB + B^2 + B^3) = 0$$

$$where\ \ Z = \frac{PV}{RT},\ \ the\ \ compressibility\ \ factor$$

$$\ln\phi = Z - 1 - \ln(Z-B) + \left(-\frac{A}{2\sqrt{2}B}\right)\ln\left[\frac{Z+2.414B}{Z-0.414B}\right]$$

Write a MATLAB script file to compute the following of argon gas at the temperature T = 100 K and the pressure P = 0.1 MPa:

(a) The molar volume of argon gas from van der Waals and Peng-Robinson equations
(b) The compressibility factor of argon gas from van der Waals and the two forms of Peng-Robinson equations
(c) The fugacity coefficients of argon gas from van der Waals and Peng-Robinson equation.

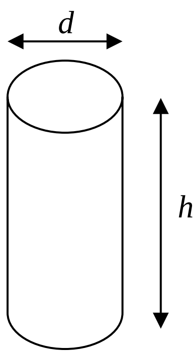
For argon, T_C = 150.86 K and P_C = 4.898 MPa. P^{VAP} = 0.4946 MPa at T_r = 0.7.

<u>Answers</u>:

	Gas Molar Volume (cm^3/gmole)	Z	ϕ
van der Waals			
Traditional Peng-Robinson			
Polynomial Peng-Robinson			

11. *Propane Cylinder*

A gas cylinder, whose exterior dimensions are a height of h = 1.35 m and a diameter of d = 0.25 m, is shown below. The cylinder contains m = 2.9 kg of propane at T = 120°C.



Suppose that readings from a pressure gauge attached to the cylinder indicate that the pressure of the propane is P = 30 bars (absolute). The objective is to determine the interior volume of the cylinder and from that the wall thickness.

Use the Redlich-Kwong equation of state which contains 2 empirical parameters a and b as follows:

$$P = \frac{RT}{\underline{V} - b} - \frac{a}{\underline{V}(\underline{V} + b)\sqrt{T}}$$

where for propane, a = 182.23 bar-m^6-K^5/kmol^2 and b = 0.06242 m^3/kmol

12. *Statistical Analyses Using Matrices in MATLAB*

You are to use MATLAB to carry out some statistical analyses on a set of data given in the table below.

Undergr. GPA	ChEPS GPA
3.58	3.97
3.33	3.71
3.28	3.57
3.27	3.54
3.15	3.61
3.33	3.75
2.97	3.72
3.09	3.42
3.22	4.00
2.89	3.66
3.05	3.89
2.90	3.28
3.10	3.71
3.01	3.64
3.31	3.64
3.45	3.64
3.22	3.64
3.19	3.61
3.14	3.78
3.16	3.64
3.45	3.85

The data consist of undergraduate GPAs of 21 students from ChEPS Class-11 and their ChEPS GPAs upon graduation. We like to find out if there is a strong correlation between these two set of data. You are asked to carry out a number of statistical analyses using MATLAB's matrix functionality. You must first create a 21×2 matrix that contain the data given in the table. From that matrix, do the following:

1. Compute the maximum, minimum, mean, and median of the students' undergraduate GPAs and ChEPS GPAs.
2. Compute the standard deviations of undergraduate GPAs and ChEPS GPAs using the following formula:

$$s = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(x_i - \mu)^2}$$

where N = total data size and μ = mean of the data. Do not use the built-in function in MATLAB to compute this number.

3. Compute the Pearson's correlation coefficient r, which indicates the correlation between undergraduate GPA and ChEPS GPA, as given by the formula below:

$$r = \frac{N\left(\sum xy\right) - \left(\sum x \sum y\right)}{\sqrt{\left[N\left(\sum x^2\right) - \left(\sum x\right)^2\right]\left[N\left(\sum y^2\right) - \left(\sum y\right)^2\right]}}$$

where x = undergraduate GPA and y = ChEPS GPA.

Please note that you are <u>not</u> allowed to use *for* loop or any control statements in your calculations. Use only vectors, matrices, and their manipulations. Finally, use *fprintf* to output your results that look like the table below. The spacing is not important as long as your table looks neat. Note that I want 2 decimal places for the maximum and the minimum and 3 decimal places for the mean, the median, and the standard deviation. For the correlation coefficient, I want an answer in 4 decimal places.

	Maximum	Minimum	Mean	Median	STDEV	
Underg GPA	x.xx	x.xx	x.xxx	x.xxx	x.xxx	
ChEPS GPA		x.xx	x.xx	x.xxx	x.xxx	x.xxx

Pearson correlation coefficient r = 0.xxxx

	Maximum	Minimum	Mean	Median	STDEV
Underg GPA	________	________	________	________	________
ChEPS GPA	________	________	________	________	________

Pearson’s correlation coefficient *r* = ____________

13. *Using MATLAB to Solve Simple ChE Problems, I*

Use MATLAB to determine the stoichiometric ratios of molecular species in the following reaction:

$$C_6H_{12}O_6 + \alpha NH_3 + \beta O_2 \rightarrow \gamma C_5H_9NO_2 + CO_2 + \delta H_2O$$

α = __________ β = __________ γ = __________ δ = __________

14. *Using MATLAB to Solve Simple ChE Problems, II*

It is proposed that a steel tank be used to store carbon dioxide at 300 K. The tank is 2.5 m^3 in volume, and the maximum pressure it can safely withstand is 100 atm. Using the Beattie-Bridgeman equation of state given below, determine the maximum number of moles of CO_2 that can be stored in the tank

$$P = \frac{RT}{V} + \frac{\beta}{V^2} + \frac{\gamma}{V^3} + \frac{\delta}{V^4}$$

where R = gas constant = 0.08206 L-atm/gmole-K

P, V, T = pressure in atm, molar volume in L/gmole, and temperature in K respectively

$$\beta = R\,T\,B_0 - A_0 - \frac{R\,c}{T^2}$$

$$\gamma = R\,T\,B_0\,b - A_0\,a - \frac{R\,c\,B_0}{T^2}$$

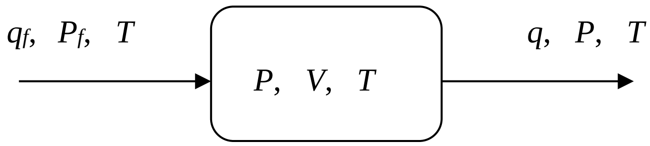
$$\delta = \frac{R\,T\,B_0\,b\,c}{T^2}$$

For CO_2, A_0 = 5.0065, a = 0.07132, B_0 = 0.10476, b = 0.07235, and $c = 66.0\times10^4$

Note that 1 m^3 = 1000 L and 1 kg-mole = 1000 gmoles

15. *Dynamics of a Gas Surge Drum*

Surge drums are often used as intermediate storage capacity for gas streams that are transferred between chemical process units. Consider a drum in the figure below, where q_f is inlet molar flowrate and q is the outlet molar flowrate.



(a) Let V, P, and T be the volume, the pressure, and the temperature of the drum, respectively. Write a model (one differential equation) to describe how the pressure in the tank varies with time. Assume ideal gas and isothermal operation.

(b) Solve for P analytically using the following data:

q_f = 2.0 + 0.1t kmol/min $\qquad$ q = 3.0 kmol/min
V = 50 m^3 $\qquad$ T = 300 K
R = 8314 m^3-Pa/kmol-°K

if the drum initially contains 10 kmol of methane. Assuming that the vessel was built to withstand a maximum pressure of 50 atm, how long can we run this operation before the inlet gas flow must be shut off?

(c) The ideal gas law is a poor assumption because of high pressure in the drum. Suppose the methane gas stream obeys the virial equation of state as follows:

$$\frac{PV}{RT} = 1 + \frac{B(T)}{\underline{V}} + \frac{C(T)}{\underline{V}^2} + \frac{D(T)}{\underline{V}^3} + ...$$

For simplicity, we will truncate all terms after the second virial coefficient $B(T)$. Repeat the calculations in Part (b). For methane, $B(T{=}300\text{ K})$ = 0.04394 m^3/kmol.

16. *Implementing a Matrix Processing Algorithm as a MATLAB Function*

Write a function in MATLAB that processes each element, one by one from left to right and from top to bottom, of a given $n \times m$ matrix called A entered into a main script file. The matrix contains both integers and real numbers (i.e. numbers with decimal places). The processing algorithm is as follows:

1. Separate the elements of A into two row vectors based on whether they are integer numbers or real numbers. But do not sort the numbers from smallest to largest or vice versa.
2. Combine the two vectors by alternatively taking elements from each vector, starting with the first element in each vector, but the first element in the combined vector must be an integer. When you run out of elements to take from either row vector, stop. As a result, your combined row vector will contain equal number of integer numbers and real numbers.
3. Display all elements in your combined row vector in one column as shown in the program output below

Your function must take n, m, and A as input and display the output on the computer screen as shown below. The matrix A is given as:

$$A = \begin{bmatrix} pi & 1.2340 & 10 & e^2 & 4 \\ 2 & 5.9824 & 6.1832 & 1.1111 & 8 \\ 12 & 5 & 9.9999 & 1 & 5.4321 \\ 7.2467 & 2.1414 & 15 & 3.3333 & 0.3245 \end{bmatrix}$$

The output should look as follows:

The combined column vector:
10
3.1416
4
1.2340
2
7.3891
8
5.9824
12
6.1832
5
1.1111
1
9.9999
15
5.4321

17. *Solving a 2nd-Order Boundary-Value ODE*

Consider the following 2nd-order boundary-value ODE over the domain t = [0, 3], where *a*, *b*, *c*, and *d* are constant coefficients in the equation.

$$a \frac{d^2y}{dt^2} + b \frac{dy}{dt} + c\,y = d\,y \sin(t) \qquad \text{s.t.} \quad y(0) = 1,\ y(3) = 2$$

(a) Determine the constant coefficients *a*, *b*, *c*, and *d* in the ODE as follows:

Given:

$$A = \begin{pmatrix} 10 & 3 & 4 & 8 & 12 \\ 20 & 7 & 1 & 14 & 9 \\ 3 & 2 & 5 & 6 & 15 \end{pmatrix} \qquad B = \begin{pmatrix} \ln(\pi) & -2 & \sinh(1) \\ -8 & 10 & 3 \\ 11 & e^{\sin(2)} & \log_{10}(\pi) \end{pmatrix}$$

The coefficient *a* is equal to the inner product between the first row of Matrix *B* and the third column of Matrix *A*.

The coefficient *b* is equal to the sum of a row vector obtained from multiplying element-by-element between the last row of Matrix B and the sub-matrix [7 1 14] extracted from Matrix A.

The coefficient *c* is equal to the largest eigenvalue of Matrix *B*.

The coefficient *d* is equal to *inverse hyperbolic cosecant* of the first element (row-1, column-1) in the *inverse* matrix of Matrix *B*.

Use FORMAT SHORT in all your calculations.

(b) Solve the above 2nd-order ODE using ***ode45***. Show answers in FORMAT SHORT.

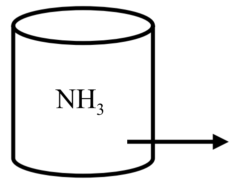
Answers:

(a) *a* = ______________; *b* = ______________; *c* = ______________; *d* = ______________

(b) $y'(0)$ = ______________ (accurate to 4 decimal places)

18. *Solving a Gas Leak Problem Using an Equation of State*

A storage vessel contains ammonia gas that is slowly leaking out. A pressure gauge shows that the tank is losing 0.1 atm every minute. We are to use a very old equation of state first proposed in 1899 called Dieterici equation of state to describe the *P*-*V*-*T* behavior of the ammonia gas inside the vessel.



Dieterici equation of state is given as follows:

$$P = \frac{RT}{\underline{V} - b} \exp\left(-\frac{a}{RT\underline{V}}\right)$$

where $a = \frac{4R^2 T_C^2}{P_C\, e^2}$ $b = \frac{RT_C}{P_C\, e^2}$ $T_C = 405.5$ K and $P_C = 111.3$ atm for NH_3

$R = 0.08206$ atm-L/gmole-K

The temperature inside the storage vessel, whose volume is 100 L, is held constant at 320 K. The initial pressure of the vessel (before the leakage starts) is 50.0 atm. Use MATLAB to solve the following problems. You must carry out all calculations inside MATLAB without using a calculator to determine any intermediate or final results.

(a) First, determine the initial number of moles of NH_3 inside the vessel, i.e. at t = 0 minute.

(b) Solve for the number of moles left in the vessel at t = 100 min, t = 300 min, and t = 460 min using the *solve* function.

(c) Derive a 1st-order ODE, *dn*/*dt*, i.e. $\frac{dn}{dt} = F(n, t)$, where n is the number of moles of NH_3 inside the vessel at any given time t. Then use MATLAB to solve for the rate of mole leakage at t = 100 min, t = 300 min, and t = 460 min.

(d) Finally, use *ode45* in MATLAB to solve the ODE in Part (c) which also gives the number of moles left in the vessel at any given time. Note answers from Part (b) and Part (d) should be the same.

Answers: (Show all numbers in 4 decimal places)

The initial number of moles = _______________ gmoles

Time (min)	**Moles Left in Vessel *n* in Part (b)**	**Moles Left in Vessel *n* in Part (d)**	**Rate of Leakage (gmoles/min)**
100			
300			
460			

19. *The Shooting Method to Solve a Linear ODE*

Solve the following 2nd-order linear ODEs, which is a boundary-value problem, using MATLAB's *ode45* function with an increment in x of 0.05:

$$y'' - xy' + 3y = 11x$$

subject to: $y(1) = 1.5$
$y(2) = 15$

Make a plot of the equation $y(x)$, and compare your MATLAB solution with the exact solution of $y'(1) = 5.500000$ by reporting the relative % difference. Include 6 decimal places in reporting all your numbers.

20. *Solving a 3rd-Order Boundary-Value ODE Using the Shooting Method*

Consider the following 3rd-order ODE which is a boundary-value problem:

$$y''' + 2y'' - ty' + y = (2t+1)e^{-2t} - 4t^2 + 16 \qquad 0 \le t \le 1$$

$$s.t. \quad y(0) = 1, y(1) = 5.135335, y''(1) = 8.541341$$

The analytical solution to the above ODE is:

$$y(t) = ae^{-2t} + bt^2 + ct$$

Use *ode23* in MATLAB to solve for numerical solutions of the above ODE between $t = 0$ and $t = 1$ using a step interval of 0.1. Compare the MATLAB solutions with those from the analytical solutions in terms of % relative errors. You will need to solve for the coefficients a, b, and c in the analytical equation either by MATLAB or by hand (or both).

<u>Answers</u>: (Show 6 decimal places in the MATLAB solutions and write them down here)

Time	MATLAB $y(t)$	Exact $y(t)$	% Relative Error
$t = 0.0$		1.000000	
$t = 0.2$			
$t = 0.4$			
$t = 0.6$			
$t = 0.8$			
$t = 1.0$		5.135335	

21. *Solving a 2nd-Order Nonlinear ODE Boundary-Value Problem*

Consider the following 2nd-order ODE which is a boundary-value problem:

$$y'' + (y')^2 - y = 14t^2 - 7t + 4 \qquad 0 \le t \le 2, \quad s.t. \quad y(0) = 1, y(2) = 7$$

Use *ode45* in MATLAB to solve for numerical solutions of the above ODE between $t = 0$ and $t = 2$ using a step interval of 0.1. Start your shooting method with G1 = –2 and G2 = 2 which will result in G3 by linear interpolation. Because the ODE is nonlinear, G3 will not produce or match $y(2) = 7$. Use a WHILE loop to keep performing linear interpolation between G1 and the newly calculated G3 in the WHILE loop until the relative error between $y(2) = 7$ and the MATLAB answer from *ode*45 is less than or equal to 10^{-6}. Also, keep track of the number of iterations in the loop needed to produce the accuracy given above.

Answers: (Show 6 decimal places in the MATLAB solutions)

Number of iterations required = ___________

Time	$y(t)$	$y'(t)$
$t = 0.0$		
$t = 0.5$		
$t = 1.0$		
$t = 1.5$		
$t = 2.0$		

22. *Solving a 3rd-Order ODE Boundary-Value Problem*

Consider the following 3rd-order ODE which is a boundary-value problem

$$y''' = ty + (t^3 - 2t^2 - 5t - 3)e^t \qquad 0 \le t \le 1, \quad s.t. \quad y(0) = 0, y(1) = 0, y'(1) = -e^1$$

Use *ode45* in MATLAB to solve for numerical solutions of the above ODE between $t = 0$ and $t = 1$, showing a step size of 0.1.

The analytical (exact) solution of the above ODE is: $y(t) = t(a + bt)\exp(ct)$ where a, b, and c are constant coefficients. Also, use MATLAB and the numerical answers from *ode45* to determine the correct values of a, b, and c, without taking any derivatives of $y(t)$

Answers:

$y(t{=}0)$ = ______0______ $\quad$ $y'(t{=}0)$ = ______________ $\quad$ $y''(t{=}0)$ = ______________

$y(t{=}0.5)$ = ____________ $y'(t{=}0.5)$ = ____________ $y''(t{=}0.5)$ = ____________

$y(t{=}1)$ = ______0______ $y'(t{=}1)$ = ___–2.7183___ $y''(t{=}1)$ = ____________

The values of coefficients are: a = _____ b = _____ c = _____

23. *Solving a 3rd-Order ODE Boundary-Value Problem*

Consider the following 3rd-order ODE which is a boundary-value problem:

$$y''' - l^2 y' + a = 0 \qquad 0 \le t \le 1, \quad s.t. \quad y(0) = 0.0894, y(0.5) = 0, y'(0.5) = -0.2640$$

The analytical (exact) solution of the above ODE is:

$$y(t) = \frac{a}{l^3}\left[\left(\sinh\left(\frac{l}{2}\right) - \sinh(lt)\right) + l\left(t - \frac{1}{2}\right) + \tanh\left(\frac{l}{2}\right)\left(\cosh(lt) - \cosh\left(\frac{l}{2}\right)\right)\right]$$

Use *ode23* in MATLAB to solve for numerical solutions of the above ODE between t = 0 and t = 1, when l = 2 and a = −3, showing a step size of 0.1. Then compare the numerical solutions with the exact solutions by calculating the relative percentage deviation in 6 decimal places at t = 0, 0.2, 0.4, 0.6, 0.8, and 1.0. Note that the percentage deviations must be positive numbers.

Answers: (accurate to 6 decimal places)

$y(t{=}0)_{\text{MATLAB}}$ = __________ $y(t{=}0)_{\text{EXACT}}$ = __________ % Deviation = __________

$y(t{=}1)_{\text{MATLAB}}$ = __________ $y(t{=}1)_{\text{EXACT}}$ = __________ % Deviation = __________

24. *Solving a 2nd-Order Boundary-Value ODE Using the Shooting Method*

The diffusion and simultaneous first-order irreversible chemical reaction in a single phase containing only reactant A and product B results in a second-order ODE given by:

$$\frac{d^2 C_A}{dz^2} = \frac{k}{D_{AB}} C_A$$

where C_A is the concentration of reactant A (kmol/m^3), z is the distance variable (m), k is the homogeneous reaction rate constant (s^{-1}), and D_{AB} is the binary diffusion coefficient (m^3/s). A typical geometry for the above ODE is that of a one-dimensional layer that has its surface exposed to a known concentration and allows no diffusion across its bottom surface. Thus, the initial and boundary conditions are:

$$C_A(z = 0) = C_{A0} \quad \text{and} \quad \frac{dC_A}{dz}(z = L) = 0$$

where C_{A0} is the constant concentration at the surface ($z = 0$) and there is no transport across the bottom surface ($z = L$) so the derivative is zero. This differential equation has an analytical solution given by:

$$C_A = C_{A0} \frac{\cosh\left[L\left(\sqrt{\frac{k}{D_{AB}}}\right)\left(1 - \frac{z}{L}\right)\right]}{\cosh\left[L\left(\sqrt{\frac{k}{D_{AB}}}\right)\right]}$$

(a) Is the above ODE linear or nonlinear? Write a MATLAB program to implement the shooting method to solve the above ODE (use *ode23*), in which $C_{A0} = 0.2$ kmol/m^3, $k = 0.001$ s^{-1}, $D_{AB} = 1.2\text{x}10^{-9}$ m^2/s, and $L = 0.001$ m. Use "format short e".

(b) Compare the concentration profiles over the thickness as predicted by the numerical solution of (a) with the analytical solution by reporting the relative percentage differences accurate to 6 decimal places with an increment of $\Delta z = 10^{-4}$.

(c) Obtain a numerical solution for a second-order reaction that requires the C_A term on the right side of the ODE to become squared. The second-order rate constant is given by $k = 0.02$ m^3/(kmole-s). Use "format short e" and *ode23*. Is this new ODE linear or nonlinear?

25. *Solving a Nonlinear 3rd-Order ODE Boundary-Value Problem*

Consider the following *nonlinear* 3rd-order ODE which is a boundary-value problem:

$$4y(y''') - t^3 y' + \cos(y) = e^{2t}$$

with the following boundary conditions: $y(0) = 1.0$, $y(2) = 29.3373$, $y''(2) = 5.1807$. Use the shooting method and *ode45* in MATLAB to solve the above equation numerically from $t = 0$ to $t = 2$. Because the ODE is nonlinear, your answer will not be correct after 3 trials. Rather than guessing the answer repeatedly, you are to use the *while* loop in MATLAB to keep interpolating linearly between the two latest guesses until | answer – target | < 0.0001. Start your shooting method with the following two guesses: G1 = 10 and G2 = 20. After obtaining G3 from linear interpolation, your G1 becomes G2 and G2 becomes G3. Keep repeating the process until the tolerance of 0.0001 is achieved.

Answers: (accurate to 4 decimal places)

$y(0)$ = __1.0000__ $y'(0)$ = ________ $y''(0)$ = ________

$y(1)$ = ___________	$y'(1)$ = ___________	$y''(1)$ = ___________
$y(2)$ = 29.3373	$y'(2)$ = ___________	$y''(2)$ = 5.1807

26. *Isothermal Compression of Ethane*

Ethane is being compressed isothermally at 50 °C (323.15 Kelvin) to 1/100th (i.e. 1%) of its initial volume in a closed vessel. The initial pressure of the gas is 1.01325 bar.

We wish to calculate the work per gmole required in this compression. For a closed system in a reversible isothermal compression from V_1 to V_2, the work W done on the system can be calculated from:

$$\frac{\mathrm{d}W}{\mathrm{d}V} = -P$$

Use MATLAB to do the following:

(a) Calculate the work W using the ideal gas assumption.

(b) Calculate the work W using the Redlich-Kwong-Soave equation of state, which is given by:

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)}$$

where

$$b = 0.08664\frac{RT_c}{P_c}$$

$$a = 0.42748\frac{(RT_c)^2}{P_c}\left[1 + m\left(1-\sqrt{T_r}\right)\right]^2$$

$$T_r = \frac{T}{T_c}$$

and

$$m = 0.480 + 1.574\omega - 0.176\omega^2$$

P = pressure in bar

V	=	molar volume in L/gmole
T	=	temperature in K
R	=	gas constant (0.08315 bar-L/gmole-K)
T_C	=	critical temperature in K (305.556 K for ethane)
P_C	=	critical pressure in atm (48.2989 bar for ethane)
ω	=	Pitzer acentric factor (0.1064 for ethane)

Answers:

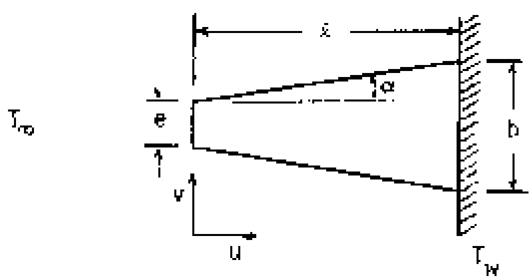
(a) Work (ideal gas) = ____________________ bar-L/gmole

(b) Work (RKS gas) = ____________________ bar-L/gmole

27. *Heat Transfer in a Tapered Fin*

Consider a tapered fin of trapezoidal profile:

$$v(g) = \frac{e}{2} + (\ell - u)\left(\frac{b}{2} - \frac{e}{2}\right) / \ell$$



The governing equation for the temperature distribution in the fin is the dimensionless second-order differential equation

$$\frac{d^2y}{dx^2} = \frac{2(N_4)\,y/\cos\alpha + (N_3 - N_2)\,dy/dx}{N_2 + (N_3 - N_2)(1 - x)} - N_1$$

where y = dimensionless temperature = $(T - T_\infty) / (T_w + T_\infty)$
x = dimensionless distance = u / ℓ

$$N_1 = q\,\ell^2 / k(T_w - T_\infty)$$

where q is the uniform rate of internal heat generation per unit volume (via nuclear fission, electrical dissipation, chemical reaction, etc.) and k is the thermal conductivity.

$N_2 = e / \ell$ $\qquad$ $N_3 = b / \ell$ $\qquad$ $N_4 = \bar{h}\ \ell / k$

where $\bar{h}$ is the average convective heat transfer coefficient.

Based upon the known physical conditions for a fin, it is possible to solve for the one dimensional temperature distribution inside the fin if we know the boundary conditions. For this problem, the fin has adiabatic ends, i.e. $T = T_\infty$ at $u = 0$ and $T = T_w$ at $u = l$.

The physical conditions of the fin are given as follows:

e = 30 cm	b = 60 cm	l = 300 cm
k = 60 J/sec-cm-°C	q = 0.016 J/cm^3-sec	$\bar{h}$ = 0.01 J/cm^2-sec-°C
T_∞ = 20°C	T_w = 100°C	

Use *ode45* in MATLAB to solve the above ODE numerically and answer the following questions. Use *format short* to show all your calculations. Also in your output, plot *y* and *y*′ versus *x*. Label your *x*-axis and *y*-axis properly and include a legend in your graph as well.

<u>Answers</u>: (accurate to 4 decimal places)

y′(0) = ________________ $\qquad$ T(u=150 cm) = ________________ °C

28. *Maclaruin Series Expansion*

A Maclaurin series is a Taylor series expansion of a function about 0, and are named after the Scottish mathematician Maclaurin. If enough terms are carried, the Maclaurin series can approximate any mathematical function to the desired accuracy. The Maclaurin formula for the sine function and the square root are as follows:

$$\sin x = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots \quad \text{for all } x$$

$$\sqrt{1+x} = \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{(1-2n)(n!)^2(4^n)} x^n = 1 + \tfrac{1}{2}x - \tfrac{1}{8}x^2 + \tfrac{1}{16}x^3 - \tfrac{5}{128}x^4 + \ldots \quad \text{for } |x| < 1$$

Write a MATLAB program to compute the value of the following two functions at the given point using the given Maclaurin formulae:

$$\frac{\sin(x)}{x} \quad at \;\; x = 2, \;\; where \;\; x \;\; is \;\; in \;\; radians$$

$$x\sqrt{1+x} \quad at \;\; x = 0.5$$

Both values should be computed accurate to 14 decimal places which is the accuracy of *format lo*ng in MATLAB when compared with the exact solution. This means using the following convergence criterion:

$$\left| Exact \;\; Solution - Maclaurin \;\; Solution \right| \leq 10^{-14}$$

Also, in your MATLAB program, report the total number of terms needed in the series expansion in order to achieve the desired accuracy.

<u>Answers</u>:

Maclaurin series solution for the sine function = ______________________________

Number of terms required = ___________

Maclaurin series solution for the square root function = _______________________

Number of terms required = ___________

29. *pH of Natural Rain Water*

CO_2 is a trace yet important constituent of the atmosphere that keeps the earth warm enough for life in their current forms. The concentration of CO_2 before the industrial revolution has been relatively constant over a long period. CO_2 is slightly water soluble, which makes the natural rain in a clean atmosphere slightly acidic due to the dissolution of CO_2 into the cloud droplets. The partitioning of CO_2 into a droplet can be described by the following equilibrium relations:

$$CO_{2(g)} \rightleftarrows H_2CO_{3(aq)}$$

$$H_2CO_{3(aq)} \rightleftarrows H^+ + HCO_3^-$$

$$HCO_3^- \rightleftarrows H^+ + CO_3^{2-}$$

$$H_2O \rightleftarrows H^+ + OH^-$$

The concentration of hydrogen ion (H^+) in the water determines its acidity. A higher concentration of H^+ means higher acidity. The acidity of a rain or cloud droplet is usually quantified by the pH of the droplet, which is related with the concentration of H^+ ($[H^+]$) using the following equation: $pH = -\log_{10}[H^+]$. Thus, lower pH means higher acidity.

Based on the above equilibrium relationships and the principle of charge balance in an aqueous solution, the $[H^+]$ in the CO_2/H_2O system (and thus the pH) can be determined using the following equation:

$$\frac{K_w}{[H^+]} + \frac{K_{a1,CO_2} K_{H,CO_2} p_{CO_2}}{[H^+]} + \frac{2K_{a1,CO_2} K_{a2,CO_2} K_{H,CO_2} p_{CO_2}}{[H^+]^2} - [H^+] = 0 \qquad (1)$$

where pCO_2 is the partial pressure of CO_2 in the atmosphere (in units of atm); $K_{H,CO2}$, $K_{a1,CO2}$, $K_{a2,CO2}$ are Henry's law constant (in units of M/atm), and first and second acid dissociation constants for CO_2, respectively, and K_w is the water dissociation constant (which varies with temperature). For a given value of the partial pressure of CO_2, the concentration of H+ and thus the pH can be determined.

(a) Given that $K_w = 1.8\times10^{-14}$ (when $T = 30°C$) $K_{H,CO2} = 10^{-1.46}$, $K_{a1,CO2} = 10^{-6.3}$, $K_{a2,CO2} = 10^{-10.3}$, and pCO2 = 280 ppm (atm), use function *solve* in MATLAB to determine the pH of natural rain water. Use *format short* in all your calculations.

(b) Verify the answer in Part (a) by using the function *roots* in MATLAB.

(c) Equation (1) which is nonlinear can be solved using a root-finding algorithm. One such method discussed in class is *Newton-Raphson* whose iterative formula for one variable is given by:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \qquad k = 1, \;\; 2, \;\; 3, \;\; \ldots$$

Write a MATLAB program to generate a plot of CO_2 partial pressure (ppm) vs. pH of natural rain water using Newton-Raphson. Provide a title and label your *x*-axis and *y*-axis properly. The pH should be calculated at CO_2 partial pressures between the range of 280 ppm and 420 ppm using an increment of 20 ppm (use a FOR loop). At pCO_2 = 280 ppm, use an initial guess of $[H^+] = 5.0\times10^{-6}$ to solve Equation (1). For subsequent pCO_2's, use the answer from the previous increment as the initial guess, e.g. use the $[H^+]$ solution from the case where pCO_2 = 280 ppm as a starting point for the case where pCO_2 = 300 ppm. You may rearrange Equation (1), $f([H^+]) = 0$, into another form in order to help determine $f'([H^+])$ more easily. The termination criterion for Newton-Raphson is when the absolute relative percent error of the pH (not $[H^+]$) between two successive iterations is less than 10^{-4}.

<u>Answers</u>: pH (pCO_2 = 280 ppm) = ____________

pH (pCO_2 = 360 ppm) = _________ pH (pCO_2 = 420 ppm) = ____________

30. *Producing a Palindromic Number by Reverse-Then-Add Algorithm*

A palindromic number or numeral palindrome is a number that remains the same when its digits are reversed. Examples of numeral palindrome are 22, 16461, and 23232 (notice the symmetry in the numbers). An algorithm called reverse-then-add is known to produce a palindromic number. The algorithm is very simple to state:

Given a positive integer of two digits or more, reverse the digits and add this new number to the original number. Repeat the operation until a palindromic number is obtained.

For example, let's start with a positive integer 19. The reverse-then-add algorithm gives the following sequence of numbers: 19, 91, 110, 11, and 121, the last of which is a palindromic number. Interestingly, this algorithm does not produce palindromes for a few known integers, such as 196, 295, 394, 493, 592, 689, 691, 788, 790, 879, and 887, the smallest of which is 196. As a result, the reverse-then-add algorithm is sometimes known as the 196-algorithm.

On the other hand, some small integers are known to produce very large palindromes. An example is the integer 89 which eventually produces the palindrome 8813200023188.

Write a MATLAB code that implements the 196-algorithm, given a positive integer with two digits or more (no error checking is required except that if the given integer is already palindromic, then your script file should print out this message and exit the program). To implement the algorithm, you will need to know how to reverse an integer. The following compact formula is known to produce the reverse of an integer number *x*:

$$x10^{\lfloor \log_{10} x \rfloor} - 99 \sum_{k=1}^{\lfloor \log_{10} x \rfloor} \left\lfloor x10^{-k} \right\rfloor 10^{\lfloor \log_{10} x \rfloor - k}$$

where $\lfloor \log_{10} x \rfloor$ is the floor of $\log_{10}(x)$ For example, $\lfloor 10.2 \rfloor = 10$ and $\lfloor 10.8 \rfloor = 10$ as well

You must implement this reverse formula as a function in MATLAB. For example, if you call your function *reverse*, then *reverse*(12345) will produce 54321. In your output, store and show the sequence of numbers generated by the 196-algorithm as an $n \times 2$ matrix. For example, given the integer 5208, your MATLAB output should look as follows:

```
5208        8025

13233       33231

46464       46464
```

Test your MATLAB program with the following integers: 18, 551, and 8534.

<u>Answer the following questions</u>:

Starting Integer	Palindrome
18	
551	
8534	

31. *Programming with MATLAB (Classification of Numbers)*

In this problem, you are given a list of positive integers that we like to classify as either prime number, square number, semi-square number, or neither (i.e. the number does not belong to any of the 3 classes). You are to write a MATLAB to do the classification. Here are the definitions of each class of number:

1. *Prime number* – a positive integer larger than 1 that is not divisible by any integer except 1 and the number itself. Examples of prime numbers are 3, 11, 23, and 29.

2. *Square number* – a positive integer *n* which is the sum of the square of consecutive positive integers starting at 1. For example, 140 is a "square" number because $140 = 1^2 + 2^2 + 3^2 + 4^2 + 5^2 + 6^2 + 7^2$.

3. *Semi-square number* – a positive integer *n* which is the sum of the square of consecutive positive *odd* or *even* integers starting at 1 or 2, respectively. For example, 84 is a semi-square number because $84 = 1^2 + 3^2 + 5^2 + 7^2$. So is 120 because $120 = 2^2 + 4^2 + 6^2 + 8^2$.

Note that a given positive integer will only belong to one of the four number classes. Finally, you need to know the 4 simple rules of finding a prime number as follows:

(i) Rule 1: Check if the number is even. If it is, it is not a prime number because it is divisible by 2 (Note that 2 is the exception and is a prime number).
(ii) Rule 2: Check if the number is divisible by 3 or 5. If it is, it is not a prime number.
(iii) Rule 3: Find the square root of the number. If the square root results in an integer, the number is not a prime number.
(iv) Rule 4: Divide the number by all the prime numbers less than the square root (but can skip 2, 3, and 5). If the number is not divisible by any of the prime number less than the square root, the number is a prime. Otherwise, it is a composite. You will also need the following prime numbers up to 100 in Rule (iv):

[7 11 13 17 19 23 29 31 37 41 43 47 53 59 61 67 71 73 79 83 89 97]

You will test your program on a total of 10 positive integers with the following values which you should put into a vector:

[455, 647, 650, 731, 991, 969, 652, 819, 560, 863]

The output from MATLAB should show which class or classes a given number belongs to.

<u>Answers</u>:

Prime numbers are: ________________________________

Square numbers are: ________________________________

Semi-square numbers are: ________________________________

Neither are: ________________________________

32. *Implementing a Matrix Processing Algorithm as a MATLAB Function*

Write a function in MATLAB that processes each element, one by one from left to right and from top to bottom, of a given $n \times m$ matrix called **A**, which is to be entered into a main script file. The matrix contains different types of numbers, namely negative numbers (both integer and real), positive integer numbers, positive real numbers, and complex numbers (with both real and imaginary parts). The processing algorithm is as follows:

1. If an element is negative, check to see if the number is an integer. If the number is a negative integer, reverse the sign so that it becomes positive. If the number is a negative real number, take the square root of the number to obtain a complex number.
2. If an element is a positive integer, square the number.
3. If an element is a positive real number, create two numbers from it. One number is the integer part and the second number is the decimal part. For example, if the element has a value of 3.1415, then the first number obtained is an integer 3 while the second number is a real number 0.1415.
4. If an element is a complex number, take the imaginary part of the complex number and make it a real number.

Now write a MATLAB function that takes n, m, and **A** as input. The output from the function which is to be passed back to the script file must contain all the processed numbers sorted by 3 columns. The first column contains all numbers that are integers (can be positive, negative, or zero). The second column contains all numbers that are real (i.e. with decimal places). The third column contains all complex numbers. Note that you <u>need not</u> sort numbers in each column in ascending/descending order. Instead, the numbers in each column appear in the order in which the elements in the matrix **A** is processed. Because the number of elements in each column may not be equal, we will use zeroes as fillers to ensure that each column has the same length of p. Thus, your output from the MATLAB function will be a $p \times 3$ matrix **M**.

Note that you every number in the matrix should be displayed using Format Short (i.e. with 4 decimal places), regardless of whether the number is real, integer, or complex, in the script file.

$$A = \begin{bmatrix} pi & -1.2340 & 3 & -e^2 & -8 & 2.5+1.2i \\ \sqrt{-20} & 5.8934 & -6.1008 & 1.1111 & 8 & -15 \\ 5 & \sqrt[3]{12} & -15.15 & 1 & 5.4321 & -10.25 \\ \sqrt[3]{-30.5} & 0.65^{-2} & -15 & \sqrt[4]{81} & 1.3245 & -3.3333 \end{bmatrix}$$

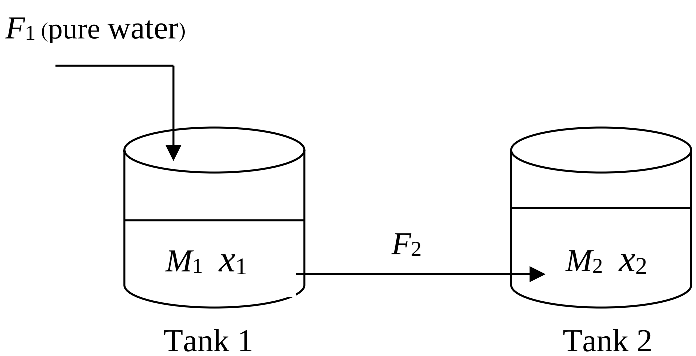
The output matrix **M** should look as follows:

The output matrix M:

```
   3.0000             0.1416             0 + 1.1109i
   9.0000             1.2000             0 + 2.7183i
   8.0000             4.4721             0 + 2.4700i
   5.0000             0.8934             0 + 3.8923i
   1.0000             0.1111             0 + 3.2016i
  64.0000             0.2894             0 + 1.7676i
  15.0000             0.4321             0 + 1.8257i
  25.0000             0.3669             0
   2.0000             0.3245             0
   1.0000                  0             0
   5.0000                  0             0
   2.0000                  0             0
  15.0000                  0             0
   9.0000                  0             0
   1.0000                  0             0
```

33. *Mass Balance in a Two-Tank System*

Consider the following two vessels connected in series. We will model this system over a total time domain of 20 minutes. Initially (at $t = 0$), Tank 1 is filled with 20 kg of brine solution with 60 mass% salt, while Tank 2 is filled with 20 kg of pure water. For the first 10 minutes, pure water with a flow rate of $F_1 = 1 + t$ (in kg/min) is added to Tank 1 (assuming the added salt dissolves instantly), while F_2 is kept to zero. We define M_1 and M_2 as the total mass and define x_1 and x_2 as the mass fraction of salt, all respectively in Tank 1 and Tank 2.



(a) Derive an analytical expression of x_1 as a function of time t, for $0 \le t \le 10$ min. Note that you must integrate your derived ODE by hand and show intermediate results using known techniques, such as separation of variables, substitution, integrating factors, etc. Do not use tables of integrals or online help or points will be deducted.

<u>Answers</u>: M_1 (t = 10 min) = __________ kg x_1 (t = 10 min) = ____________

(b) Between $10 \le t \le 20$ min, F_1 is shut off (i.e. its flow rate is kept to zero now) and F_2 is turned on and set equal to 1 kg/min. Derive an analytical expression of x_2 as a function of time t, for $10 \le t \le 20$ min. Note that the initial time in your integration must be set to 10 min, not 0 min. Again, you must integrate your derived ODE by hand and show all intermediate results.

<u>Answers</u>: M_2 (t = 20 min) = __________ kg x_2 (t = 20 min) = ____________

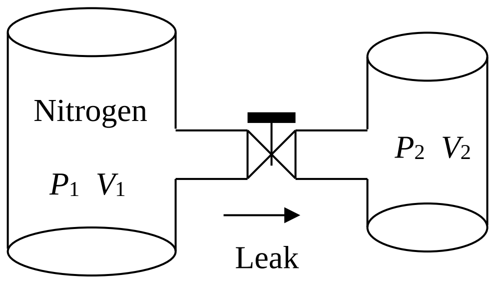
34. *A Two-Tank System*

A large tank is connected to a smaller tank by means of a valve, which remains closed at all times. The large tank contains nitrogen (assume it is an ideal gas) at 700 kPa, while the small tank is evacuated (vacuum). The valve between the two tanks starts to leak and the rate of gas leakage is proportional to the pressure difference between the two tanks, as given by

$$Leak\ \ Flow = C_V \sqrt{P_{AVG}(P_1 - P_2)}$$

where P_{AVG} = average absolute pressure across the valve = $(P_1 + P_2)/2$

Valve constant $C_V = 3.6\times10^{-4}$ kmol/kPa-hour.
Tank volumes are 30 m^3 and 15 m^3.
Assume constant temperature of 293.15 K in both tanks.
Universal gas constant = 8.31439 kPa-m^3/kmol-K.



(a) Derive an analytical expression of dn_1/dt as a function of n_1, where n_1 is the number of moles of nitrogen in the large tank. This ODE of yours should contain only n_1 as the unknown variable. Use MATLAB to solve for n_1 (use *ode45* and "format short"), and run the model up until t = 25 hours.

Answer: n_1 (t = 25 hours) = _______________ kmoles

(b) As a good chemical engineer, you always look for ways to simplify your engineering calculations. In this particular problem, it is possible to derive an analytical solution when t is small, i.e. when $P_2 << P_1$. Derive an analytical expression for n_1 as a function of time t. Calculate n_1 after 2 hours and 4 hours, and compare these solutions with those from Part (a) by reporting the absolute % relative errors (assuming the MATLAB solutions are exact and show 4 decimal places).

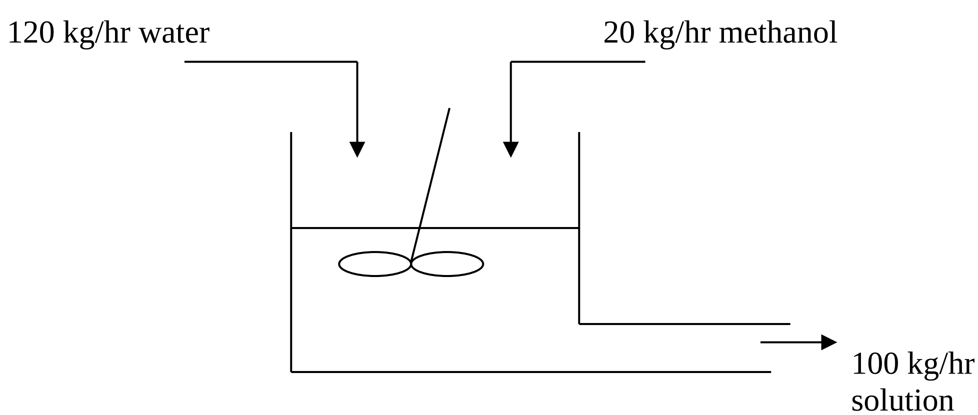
Answers:

n_1 (t = 2 hours) = _____________ kmoles % relative error = ___________

n_1 (t = 4 hours) = _____________ kmoles % relative error = ___________

35. *Mixing Tank with 2 Feeds*

Consider the following mixing tank problem. Water is flowing into a well-stirred tank at 120 kg/hr and methanol is being added at 20 kg/hr. The resulting solution is leaving the tank at 100 kg/hr. There is 100 kg of fresh water in the tank at the start of the operation. We are interested in determining the mass fraction of methanol in the outlet as a function of time t.



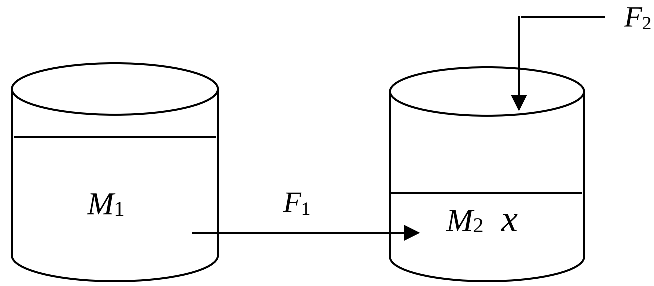
(a) Derive an analytical expression for solving the mass fraction of methanol as a function of time t. An analytical solution is possible for this particular system.

(b) Use MATLAB to solve for the mass fraction of methanol in the outlet after 1 hour, and compare the number to the exact solution in Part (a). Also, what is the methanol mass fraction in the outlet at steady state?

(c) Of course, steady-state condition probably cannot be achieved in this system because the inflow rate is greater than the outflow rate, and sooner or later, the tank will fill and overflow. Assuming that the density of the solution in the tank is always constant at 1000 kg/m^3 and the volume of the tank is 1.0 m^3, compute the time it takes for the tank to overflow.

36. ***Mass Balance in a Two-Tank System***

Consider the following two vessels connected in series which are initially filled with some liquid. Initially (at $t = 0$), Tank 1 is filled with 100 kg of pure water, while Tank 2 is filled with 10 kg of methanol-water solution with a mass concentration (fraction) of 80% alcohol. We define M_1 and M_2 as the total mass in Tank 1 and Tank 2 respectively, and x as the mass fraction of methanol in Tank 2.



(a) In this part, we will first model the system over the time domain $0 \leq t \leq 10$ min. The mass flow rate F_1 is set equal to t (in kg/min), i.e. F_1 increases linearly as a function of time, while a pure water stream F_2 is set equal to 5 kg/min. Derive an analytical expression of x as a function of time t, for $0 \leq t \leq 10$ min. Note that you must integrate your derived ODE by hand and show intermediate results using known techniques, such as separation of variables, substitution, integrating factors, etc. Do not use tables of integrals or online help or points will be deducted.

<u>Answers</u>: M_2 (t = 10 min) = __________ kg x (t = 10 min) = ____________

(b) Between $10 \leq t \leq t_1$ min where t_1 is the time at which Tank 1 becomes empty, F_1 and F_2 continue to flow at the same rate, but the stream F_2 now contains 20 mass% methanol instead of being pure water. Derive an analytical expression of x as a function of time t, for $10 \leq t \leq t_1$ min. Note that the initial time in your integration must be set to 10 min, not 0 min. Again, you must integrate your derived ODE by hand and show all intermediate results.

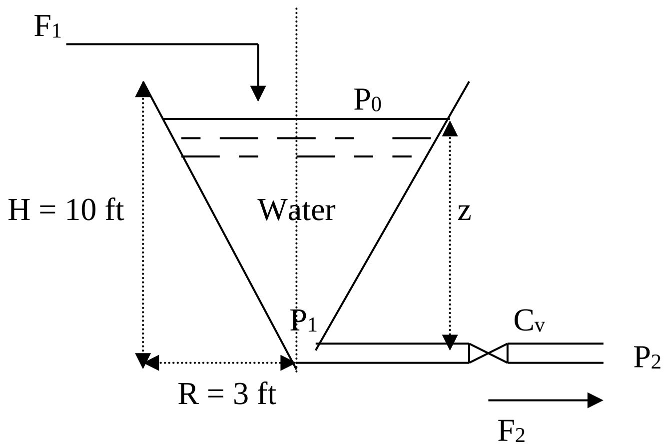
<u>Answers</u>: M_2 ($t = t_1$ min) = __________ kg x ($t = t_1$ min) = ____________

(c) Finally, over the time domain $t_1 \leq t \leq 20$ min, F_2 continues to flow at the same rate of 5 kg/min, but now contains pure methanol. Derive an analytical expression of x as a function of time t, for $t_1 \le t \le 20$ min. Again, you must integrate your derived ODE by hand and show all intermediate results, and the initial time in your integration must be set to t_1.

Answers: M_2 (t = 20 min) = __________ kg x (t = 20 min) = ____________

37. *Continuous Cone-Shaped Open Vessel*

Consider a conical open vessel as shown in the following figure. The vessel has a radius R at the top and a height H. Water flows into the vessel at a rate of F_1 and it flows out through a valve at a rate of F_2. The following data are given:



P_0 = P_2 = 14.7 psia
C_v = characteristic valve constant = 3.0 ft^3/psia$^{1/2}$-min
ϕ = water mass density = 62.4 lbm/ft^3
z_0 = initial liquid height = z(t = 0) = 5 ft

F_1 is not constant but is controlled such that it varies with the liquid height according to:

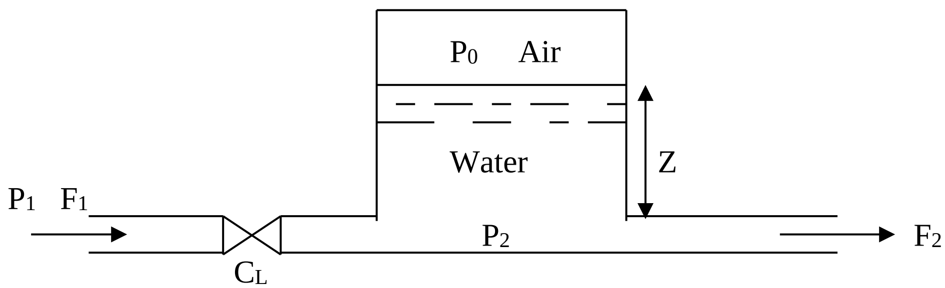
$$F_1 = 2z^{1/2} \quad \text{ft}^3\text{/min}$$

Solve for z analytically as a function of time.

Hint: Volume of a cone $V = \int_0^z A(z)dz$
where A(z) = cone cross-sectional area and is a function of z

38. *Adiabatic Expansion/Compression in an Enclosed Vessel*

Consider the following system in which air is trapped inside an enclosed vessel while water flows into the vessel at a rate of F_1 and flows out at a rate of F_2.



Initially, the air is at 25°C and 1.01325×10^5 Pa (Pascal), and the liquid height is 5.0 meter. The following data are available:

Gravitational acceleration g = 9.80665 m/s^2
Air C_V (heat capacity at constant volume) = 2.0731×10^4 J/kmol°C

Vessel volume =10.0 m^3	Vessel cross-sectional area = 1.0 m^2
Water density = 1000 kg/m^3	Gas constant R = 8314 m^{3}Pa/kmol°K = 8314 J/kmol°K
Air MW = 29.0 kg/kmol	Valve constant C_L = 0.001 m^3/Pa$^{1/2}$min
Outlet flow rate F_2 = 0.1 m^3/min	Source pressure P_1 = 3.0×10^5 Pa

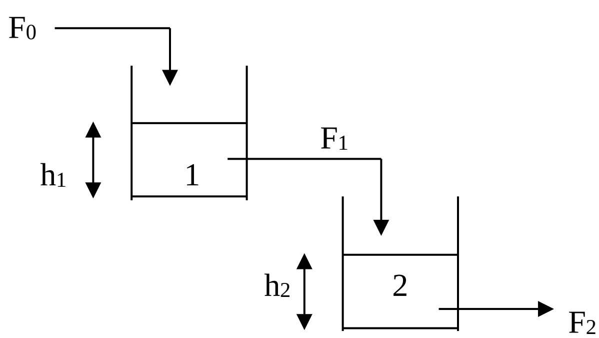
(a) Assuming adiabatic expansion/compression due to the rise/fall of the liquid height, write down all the system-describing equations. Be sure to define all your variables which are unknown. Use the data given and simplify each equation as much as possible.

(b) Derive an ordinary differential equation that relates the liquid height as a function of time. Your final equation must contain Z as the only dependent variable.

(c) Solve the ODE in Part (b) using MATLAB and plot the liquid height Z as a function of time.

39. *Two Open Continuous Flow Tanks in Series*

Consider two tanks in series as shown where the flow out of the first tank enters the second tank. Our objective is to develop a model to describe how the height of liquid in tank 2 changes with time, given the input flowrate $F_0(t)$. Assume that the flow out of each tank is a linear function of the height of liquid in the tank (i.e. $F_1 = \beta_1 h_1$ and $F_2 = \beta_2 h_2$) and each tank has a constant cross-sectional area.



(a) Develop a system of equations to describe the liquid height of the two tanks as a function of time, assuming constant liquid density. Be sure to define all your variables.

(b)Solve for h_1 and h_2 analytically if

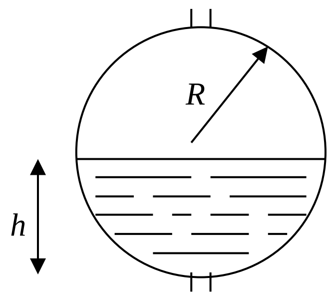
$A_1 = 10$ ft^2 $A_2 = 20$ ft^2 $F_0 = 2$ ft^3/hr
$\beta_1 = \beta_2 = 1$ ft^2/hr where A_i is the cross-sectional area of tank i

and tank 1 initially has a liquid height of 1 ft of while tank 2 is empty. Plot the two liquid height profiles as a function of time from 0 hr to 5 hr.

(c) Suppose F_0 is no longer constant but equals to $2t + 1$ ft^3/hr. Use MATLAB to solve for the liquid heights in both tanks. Plot both profiles as a function time up to 5 hr.

40. *Liquid Height in a Spherical Tank*

The following figure shows a spherical tank for storing water. The tank is filled through a hole in the top and drained through a hole in the bottom. If the tank's radius is *R*, one can



use integration to show that the volume of water in the tank as a function of its height *h* is given by:

$$V(h) = \pi R h^2 - \frac{\pi h^3}{3}$$

Studies in fluid mechanics have identified the relation between the volume flow through the bottom hole and the liquid height as:

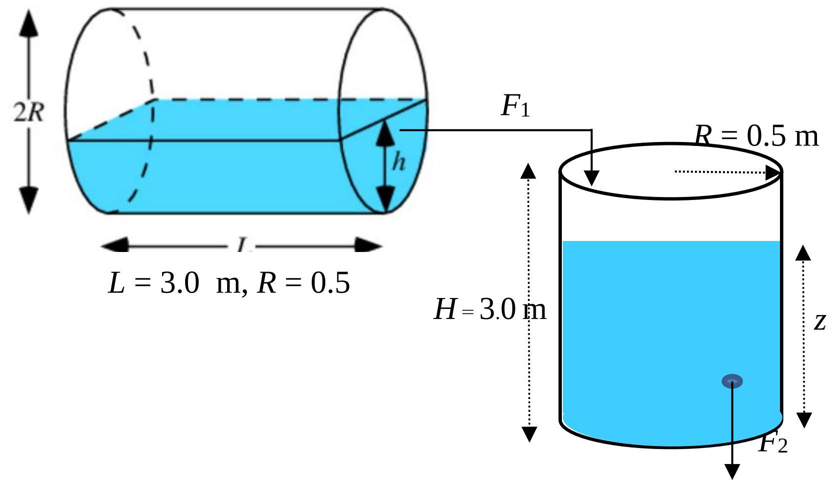
$$F = C_d A \sqrt{2gh}$$

where *A* is the area of the hole, *g* is the acceleration due to gravity (32.2 ft/sec^2), and C_d is an experimentally determined value that depends partly on the type of fluid (for water, C_d = 0.6).

Suppose the initial height of water is 8 ft and the tank has a radius of 5 ft with a 1-inch diameter hole in the bottom. Use MATLAB to determine how long it will take for the tank to empty (i.e. drain completely), to the nearest second (i.e. no decimal places).

41. ***Dynamics of Liquid Height in Two Vessels in Series***

A horizontal cylindrical vessel and a vertical cylindrical vessel with the given dimensions are connected in series as shown.



Water flows out of the horizontal cylindrical vessel with F_1 = 1.0 m^3/min which then flows into the second vessel. There is a small spherical hole (radius = 2 cm or 0.02 m) at the bottom in the second vessel which drains the water based on gravity at a volumetric flow rate of:

$$F_2 = C_d A \sqrt{2gz}$$

where A is the area of the hole, g (9.81 m/s^2 or 35316 m/min^2) is the acceleration due to gravity, and C_d is an experimentally determined value that depends partly on the type of fluid (for water, C_d = 0.6).

The following very complicated formula has been derived for the volume of a horizontal cylindrical vessel which is partially filled as a function of L, R and h.

$$V(L, R, h) = L\left[R^2 \cos^{-1}\left(\frac{R-h}{R}\right) - (R-h)\sqrt{2Rh - h^2}\right]$$

(a) At t = 0, the horizontal cylindrical vessel is three-quarter full. Calculate the height above the bottom of the horizontal cylindrical vessel at t = 0.

h when the horizontal cylindrical vessel is three-quarter full = ______________ meter

(b) Derive an ODE that expresses h as a function of time in the horizontal cylindrical vessel. You must simplify the ODE as much as possible. Solve the ODE by *ode45* and plot the dynamics of the liquid height h and determine the time it takes for the vessel to become completely empty. You will need the following formula:

$$\frac{d(\cos^{-1} x)}{dx} = -\frac{1}{\sqrt{1-x^2}}$$

t when the cylindrical vessel is empty = _______________ minutes

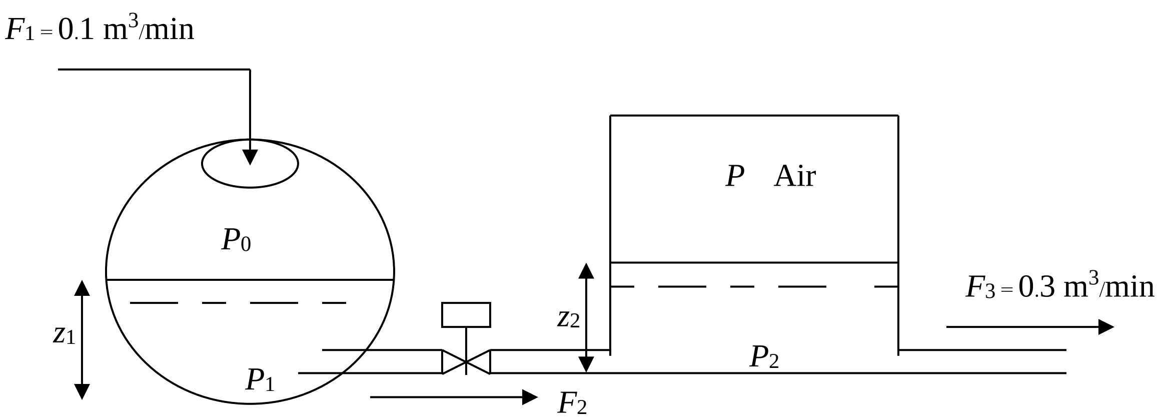
(Hint: You could use simple volume calculations to verify your MATLAB answer.)

(c) Derive an analytical solution for the liquid height z in the vertical cylindrical vessel as a function of time, given that at $t = 0$, the vertical vessel is one-half full.

z at $t = 1$ minute = _______________ meters

42. *Modeling Liquid Heights in a Two-Vessel System*

An open spherical vessel is connected to a closed rectangular tank through an open valve as shown in the figure below. Water flows continuously into the spherical vessel at a volumetric flow rate of F_1 with some of the water in the sphere also flowing into the rectangular tank at a rate of F_2. Water then flows out of the rectangular tank at a flow rate of F_3, and the temperature inside the tank is always maintained at 298.15 K. We wish to study the dynamics of the liquid heights in the two vessels using MATLAB.



The following data are known about the system:

$C_V = 1\times10^{-5}$ m^3/Pa$^{1/2}$-min (characteristic valve constant)
Cross-sectional area of rectangular tank = 3 m^2
Height of rectangular tank = 10 m
Initially at $t = 0$, $z_1 = 3$ m, $z_2 = 2$ m, $P = 1.01325\times10^5$ Pascal
Gravitational acceleration g = 9.80665 m/s^2

$P_0 = 1.01325\times10^5$ Pascal
Radius of sphere $R = 2$ m
ϕ (water) = 1000 kg/m^3

Universal gas constant R = 8314 m^3-Pa/kmol-K = 8314 J/kmol-K
Liquid volume inside a sphere as a function of liquid height z is given by:

$$V = \pi R z^2 - \frac{\pi z^3}{3}$$

Use MATLAB's *ode*45 to determine whether the liquid heights in the two vessels will ever be equal, i.e. $z_1 = z_2$. If so, report the time (accurate to one decimal place) at which this happens and the height.. If z_1 is never equal to z_2, determine when the two liquid heights are at the closest. Run your model for 20 minutes, which should be sufficient to answer the questions.

Answer the following questions:

Are the two liquid heights ever equal? ☐ Yes ☐ No

If yes, $z_1 = z_2$ = ____________ meters

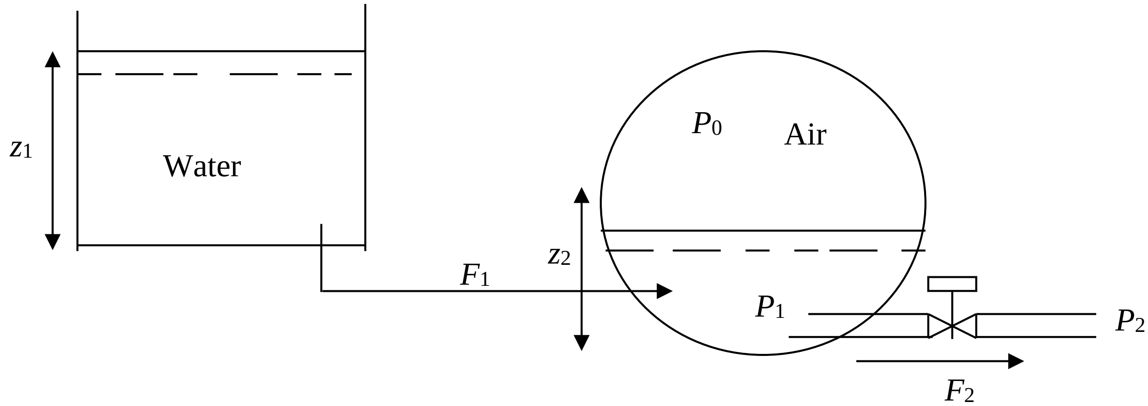
Time at which the two liquid heights are equal or at the closest = _____________ minutes

43. *Modeling Liquid Heights in a Two-Vessel System*

An open rectangular vessel is connected to a well-insulated (i.e. adiabatic) and closed spherical vessel shown in the figure below. Water from the rectangular vessel is drained through a hole (radius = 4 cm) at its bottom into the spherical vessel at a volumetric flow rate of:

$$F_1 = C_d A \sqrt{2 g z_1}$$

where A is the area of the hole, g is the acceleration due to gravity, and C_d is an experimentally determined value that depends partly on the type of fluid (for water, C_d = 0.6). Water then flows out of the spherical vessel at a flow rate of F_2. We wish to study the dynamics of the liquid heights in the two vessels using MATLAB.



The following data are known about the system:

$C_{valve} = 1\times10^{-3}$ m^3/Pa$^{1/2}$-min (characteristic valve constant)
Cross-sectional area of the rectangular vessel = 4 m^2
Radius of sphere R = 2 m $P_2 = 1.01325\times10^5$ Pascal ϕ (water) = 1000 kg/m^3
C_V (air heat capacity at constant volume) = 20850 J/kmol-K

Initially at t = 0, z_1 = 6 m, z_2 = 2 m, $P_0 = 1.01325\times10^5$ Pascal, T_G = 303.15 K
Gravitational acceleration g = 9.80665 m/s^2 = 35303.94 m/min^2

Universal gas constant R = 8314 m^3-Pa/kmol-K = 8314 J/kmol-K
Conversion factors: 1 Pascal = 1 N/m^2 = 1 kg/m-s^2, 1 N = kg-m/s^2, 1 J = kg-m^2/s^2
Liquid volume inside a sphere as a function of liquid height z is given by:

$$V = \pi R z^2 - \frac{\pi z^3}{3}$$

Derive an ODE for z_2 as a function of time (without z_1 in the ODE) and use MATLAB's *ode*45 to simulate its dynamics until either the rectangular vessel dries up or the spherical vessel is full. You must simplify your final ODE as much as possible before using it in MATLAB. Note that *ode45* may result in solutions with imaginary parts. You can ignore them as long as the values are small which come from inherent problems in numerical integrations. **Hint:** Be very careful with your units and their conversions.

Answer the following questions:

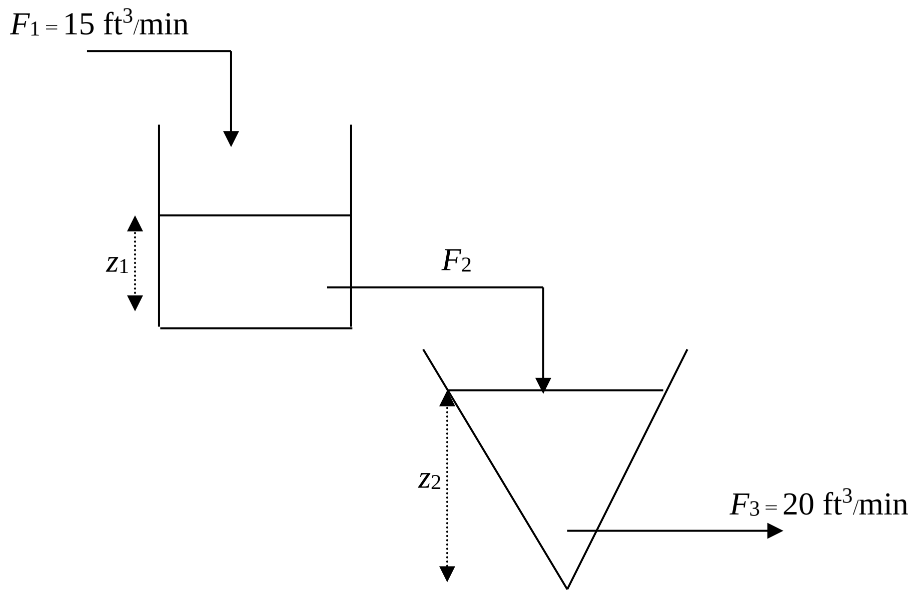
Time at which the rectangular vessel dries up or the spherical vessel is full (whichever is smaller) = ____________ minutes

44. *Modeling Liquid Heights in a Two-Vessel System*

Consider two tanks in series as shown where the water flow out of the first tank enters the second tank. The first tank is a cubic vessel with a width of 10 ft, a length of 10 ft, and a height of 10 ft, whereas the second tank is a cone-shaped vessel with a radius of 5 ft at the top and a height of 20 ft. The first tank is filled with water at a volumetric flow rate F_1 and is drained through a hole (radius = 1 inch) at the bottom. Studies in fluid mechanics have identified the relation between the volume flow through the bottom hole and the liquid height as:

$$F_2 = C_d A \sqrt{2 g z_1}$$

where A is the area of the hole, g is the acceleration due to gravity (32.2 ft/sec^2), and C_d is an experimentally determined value that depends partly on the type of fluid (for water, C_d = 0.6). Initially at t = 0, the cubic tank is filled with 2 ft of water and the cone-shaped tank is filled with 15 ft of water.



(a) Derive an analytical expression of liquid height z_1 of the cubic tank as a function of time. Does z_1 ever reach the steady-state, and if so, what is this value? Based on your analytical answer, also comment on whether z_1 reaches a maximum, reaches a minimum, overflows, or goes to zero and the time for that to happen. In your derivation, you are not allowed to use tables of integrals to perform the integration. Instead, use substitution and be careful with your unit conversions.

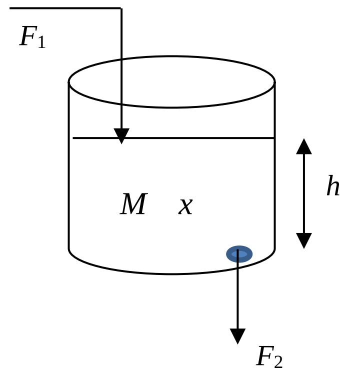
(b) Derive an ODE that describes the liquid height z_2 in the second tank. Together with the ODE for z_1 in Part (a), use MATLAB (*ode*45) to solve for z_2 as a function of time and plot both z_1 and z_2 as a function of time. Run the simulation for 20 minutes.

Answer the following questions:

z_1 (t = 10 minutes) = ____________ ft $\qquad$ z_2 (t = 10 minutes) = ____________ ft

45. *Mass Balance in a Flow Tank*

Consider a rectangular flow tank (width = 1 m and length = 2 m). The vessel is initially filled with pure water to a height of 3 m. After that, a brine solution with 10 mass% salt enters the tank at a mass flow rate F_1 = 2.0 kg/sec. There is a small circular hole (radius = 2 cm) at the bottom of the tank which is used to drain the solution as shown in the figure below.



(a) Derive analytically an expression of x, the mass fraction of salt in the vessel, as a function of time if the hole drains the solution at a constant rate of F_2 = 1.0 kg/sec.

(b) In reality, studies in fluid mechanics have identified the relation between the volume flow through the bottom hole and the liquid height as:

$$Q = C_d A\sqrt{2gh}$$

where A is the area of the hole, g is the acceleration due to gravity (9.81 m/sec^2), and C_d is an experimentally determined value that depends partly on the type of fluid (for water, C_d = 0.6). Solve the same problem again by deriving an analytical expression of M, the amount of liquid (in kg), as a function of time.

Assume the liquid density in the vessel is always constant at 1000 kg/m^3. Note that your analytical solution is an implicit function and that you must integrate your derived ODE by hand and show intermediate results using known techniques, such as separation of variables, substitution, integrating factors, etc. Do not use tables of integrals or online help or points will be deducted.

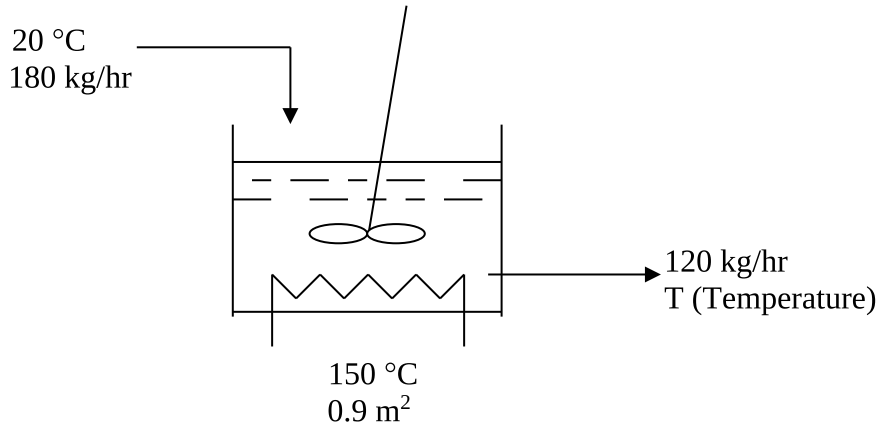
Answers: t (when h = 1.5 m) = ___________ sec; M at steady state = ___________ kg

(c) Derive an ODE expressing x, the mass fraction of salt in the vessel, as a function of time from Part (b). Then together with the ODE in Part (b), use MATLAB to solve for numerical solutions of x as a function of time. Hint: Plotting M and x as a function of time may tell you whether your final answers are correct.

Answers: M (t = 2000 sec) = _____________ kg; x (t = 2000 sec) = ____________

46. *Simultaneous Mass and Energy Balance*

Consider the following heating tank problem. A dilute solution at 20 °C is added to a well-stirred tank at the rate of 180 kg/hr. A heating coil having an area of 0.9 m^2 is located in the tank and contains steam condensing at 150 °C. The heated liquid leaves at 120 kg/hr and at the temperature of the solution in the tank. There is 500 kg of solution at 40 °C in the tank at the start of the operation. The overall heat-transfer coefficient is 342 kcal/hr-m^2-°C and the heat capacity of water is 1 kcal/kg-°C.



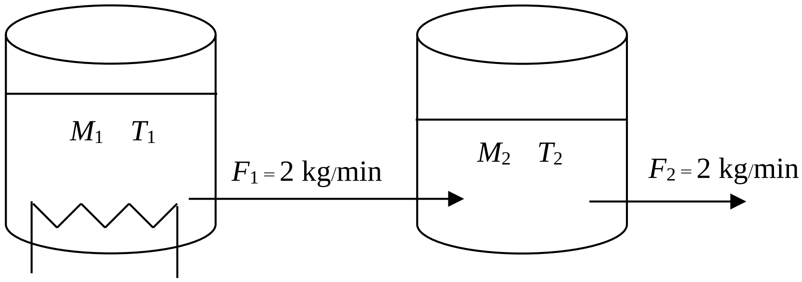
(a) Develop a system of mathematical equations to model this system. We are interested in determining the temperature of the solution in the tank at any given time.

(b) Solve for the temperature in the tank after 1 hour of heating. An analytical solution is possible for this particular system.

(c) Use MATLAB to solve for the temperature in the tank after 1 hour, and compare the answer with the exact solution in Part (b).

47. *Mass and Energy Balance of Two Vessels Connected in Series*

Consider two vessels connected in series, the first of which is heated as shown. Both vessels are initially filled with water, but some water in the first vessel flows into the second vessel at the rate of F_1 while some water leaves the second vessel at the rate of F_2. The first vessel is heated by steam inside a heating coil which is always submerged at the bottom of the first vessel (so the heat transfer area can be assumed to be constant).



The following symbols are defined for all parameters and variables in this system. Data are also given for all symbols considered as parameters.

M_1 = Mass of water inside the first vessel (in kg) = 200 kg at $t = 0$
M_2 = Mass of water inside the second vessel (in kg) = 100 kg at $t = 0$
T_1 = Temperature of water inside the first vessel (in °C) = 20 °C at $t = 0$
T_2 = Temperature of water inside the second vessel (in °C) = 40 °C at $t = 0$
F_1 = Outflow rate from the first vessel to the second vessel = 2.0 kg/min
F_2 = Outflow rate from the second vessel = 2.0 kg/min
T_S = Steam temperature in the first vessel = 100 °C
U = Overall heat transfer coefficient of the heating coil = 4.0 kcal/m^2-min-°C
A = Heat transfer area of the heating coil (in m^2) = 1.0 m^2
C_P = Heat capacity of water = 1.0 kcal/kg-°C
ϕ = Mass density of water = 1000 kg/m^3

(a) Derive an analytical expression of T_1 as a function of time. Answer the following question:

T_1 after 30 minutes = _______________ °C

(b) Derive an explicit analytical expression of T_2 as a function of time. Simplify your final equation as much as possible, and answer the following questions:

T_2 after 30 minutes = ______________ °C

T_2 when the first vessel becomes empty = ______________ °C

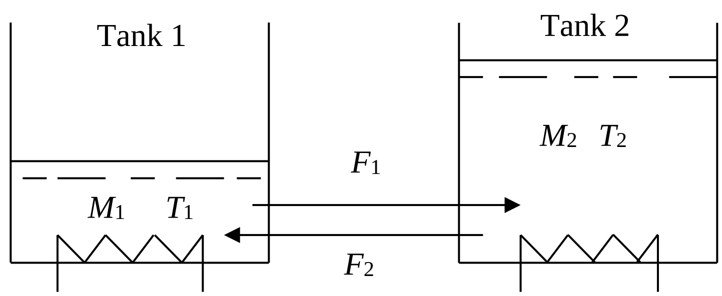
(c) Solve for T_1 and T_2 again, this time numerically using *ode45* in MATLAB, if the first vessel has a radius of 0.5 m and is heated via a jacketed steam chamber (T_S = 100 °C). The heat transfer area consists of the bottom and the surface area around the vessel. As a result, this heat transfer area cannot be treated as constant. Answer the following questions:

T_1 after 30 minutes = _______________ °C

T_2 after 30 minutes = _______________ °C

48. *Energy Balance in a Two-Tank System*

Consider the following two-tank system in which water in the first tank flows into the second one with a flow rate of F_1 = 2 kg/min and vice versa with a flow rate F_2 = 2 kg/min. Water in both vessels is being heated with a heating coil with the same constant heat transfer area of A = 0.5 m^2 and the same heat transfer coefficient of U = 4 kcal/m^2-min-°C. However, the temperature of the heating coil in Tank 1 (100 °C) is lower than that of the heating coil in Tank 2 (120 °C). We define M_1, T_1, M_2, and T_2 as the mass and the temperature of water in the first vessel and in the second vessel, respectively.



(a) Using the following data about the system, derive two ODEs that describe T_1 and T_2 as a function of time.

C_P (water) = 1.0 kcal/kg-°C

Initially at $t = 0$: $M_1 = 50$ kg of water, $T_1 = 20$ °C, $M_2 = 100$ kg of water, $T_2 = 10$°C

(b) Solve the two ODEs in Part (a) and derive an analytical expression for T_1 and T_2 as a function of time.

(c) What is the domain of this system, i.e. the maximum time the derived model is valid for? Also, determine the time at which the temperatures in Tank 1 and Tank 2 are equal.

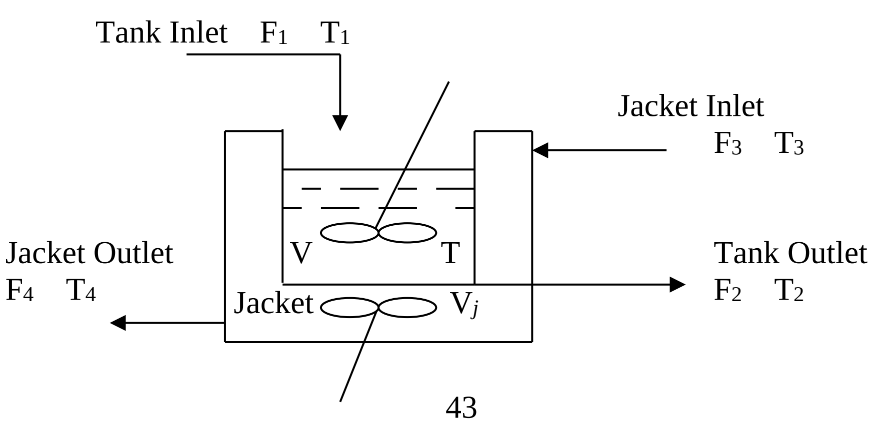
<u>Answer the following questions</u>:

Domain of this system = ____________ minutes

$T_1 = T_2 =$ ____________ °C when $t =$ ____________ minutes

49. *Mass and Energy Balance in a Stirred Tank Heater*

Consider the following stirred tank heater shown below, where the tank inlet stream is received from another process unit. A heat transfer fluid is circulated through a jacket to heat the fluid in the tank. Assume that no change of phase occurs in either the tank liquid or the jacket liquid. The following symbols are used: F_i = volumetric flowrate of stream *i*, and T_i = temperature of stream *i*.



Additional assumptions are:

1. The liquid levels in both the tank and the jacket are constant.
2. There is perfect mixing in both the tank and the jacket.
3. The rate of heat transfer from the jacket to the tank is governed by the equation $Q = UA(T_4 - T_2)$, where U is the overall heat transfer coefficient and A is the area of heat exchange.

(a) Write the dynamic modeling equations (ODEs) to find the tank and jacket temperatures. Do not use any numerical values – leave these equations in terms of the process parameters and variables. Be sure to define any new symbols you introduce into the equations.

(b) Assume that both the tank fluid and the jacket fluid are water. The steady-state values of this system variables and some parameters are:

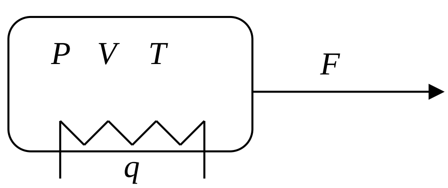
$F_1 = 1.0$ ft^3/min ρC_P (in tank) = ρC_P (in jacket) = 61.3 Btu/°F-ft^3
$T_1 = 50$ °F $T_2 = 125$ °F $V = 10$ ft^3
$T_3 = 200$ °F $T_4 = 150$ °F $V_j = 1$ ft^3

Solve for F_3 and UA (show units) at steady-state.

(c) If initially (t = 0), $T_2 = 50$ °F and $T_4 = 200$ °F, solve for T_2 and T_4 from the ODEs in Part (a) analytically as a function of time.

50. *Mass and Energy Balance in a Gas Surge Drum*

Consider a heated gas storage drum in which its gas is being drawn out at the rate of F (in kmol/min). Assume ideal gas behavior in the drum and that heat is being added to the tank at the rate of q.



(a) Derive the modeling equations (ODEs) that describe how the temperature T and pressure P inside the drum vary with time. Note that for a gas, the accumulation term on the left-hand side of the energy balance equation is

$$\frac{dH}{dt} - \frac{d(PV)}{dt} = \text{energy in} - \text{energy out}$$

where $\frac{dH}{dt} = \frac{d(\rho C_P VT)}{dt}$, ρ is the molar density of the gas, and C_P is assumed constant.

For liquids, the $d(PV)/dt$ term is considered negligible (incompressible fluid and constant volume). But this is not true for gas so we cannot ignore the PV derivative term in the energy balance. Your two ODEs must be in terms of the following symbols: P, V, T, R, C_p, F, and q. Hint: to obtain the right ODEs, you must be able to identify which symbols are constants and which are variables.

(b) Calculate the time at which the drum will become completely empty. Then solve the two ODEs in the Part (a) using MATLAB, running the model for 20 minutes (soon after which the drum will become empty). The data are:

V = 100 m^3

C_P (gas) = 125 kJ/kmol-K

q = 1.5x10^4 kJ/min

$P(t = 0)$ = 1 atm

R = 0.08205 m^3-atm/kmol-K
= 8.315 kJ/kmol-K

F = 0.2 kmol/min

$T(t = 0)$ = 298.15 K = 25 °C

Notice that the gas constant R is given in two different units. Both numbers must be used, depending on where in the ODEs which requires some dimensional analysis.

Answer the following questions:

While it is obvious that the temperature profile in the drum will rise continuously, the pressure profile may go through a maximum, depending on the draw-out rate. Of course, P inside the drum will eventually drop to zero, but it may rise for a brief moment because of the increasing temperature.

Time for the drum to become empty = ____________ minutes

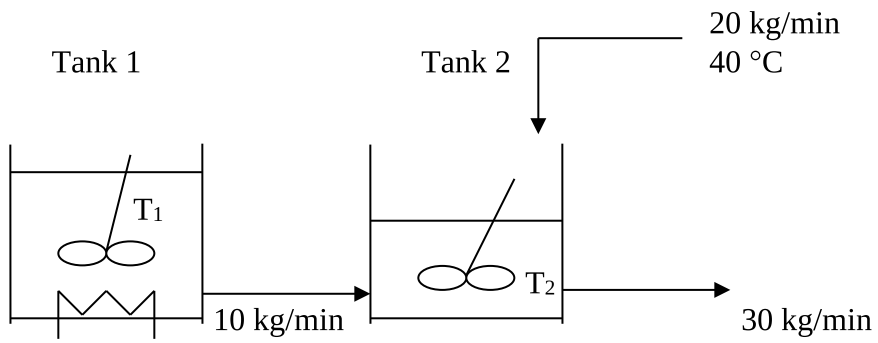
Does the pressure go through a maximum? Check one: Yes _____ No _____

If yes, P_{max} = ____________ atm at t = ____________ minutes

Time (min)	Pressure (atm)	Temp (Kelvin)
5		
10		
15		
20		

51. ***Mass and Energy Balance in a 2-Tank System***

Consider the following 2 tanks (both cylindrical vessels) in series used to store a liquid solution. Tank 1 is heated while Tank 2 is not. Liquid is drawn from Tank 1 into Tank 2 at the rate of 10 kg/min. At the same time, a feed (40 °C) enters Tank 2 at the rate of 20 kg/min, and an outflow of 30 kg/min leaves the vessel. Initially (at t = 0), Tank 1 is charged with 300 kg of the solution at a temperature of 20 °C, while Tank 2 is charged with 100 kg at a temperature of 30 °C.

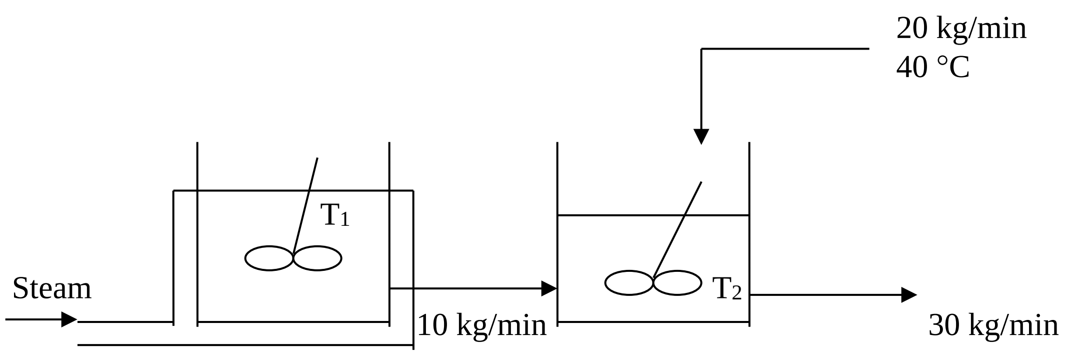


(a) Assuming that Tank 1 is being heated with a heating coil that remains submerged at all times (hence, the heat transfer area remains constant), derive an analytical expression for T_2, the temperature inside Tank 2 as a function of time. Also, compute T_2 at the time when Tank 1 is completely emptied. Use the following data:

C_P = liquid heat capacity = 2.0 kJ/kg-°C UA = 40 kJ/min-°C
T_S = heating coil temperature = 200 °C

Assume there is no phase change in either tank (i.e. no boiling occurs).

(b) Consider again a similar 2-tank system in which Tank 1 is jacketed and is heated with steam at 200 °C as shown in the figure below. In this case, the heat transfer area is no longer constant and will vary with the liquid volume inside Tank 1.

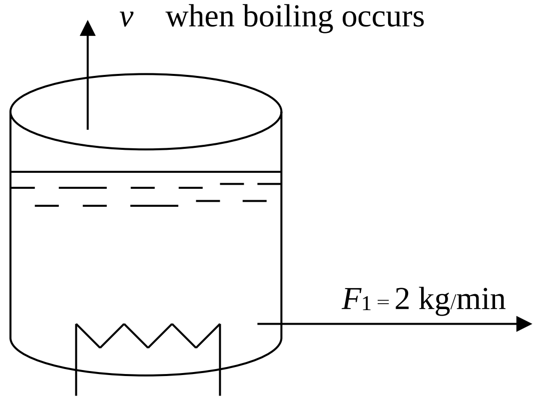


This liquid solution is known to boil at 150 °C. Determine the time it takes for the liquid in Tank 1 to boil off completely (including the time to heat the liquid to the boiling temperature). Use the following data:

C_P = liquid heat capacity = 2.0 kJ/kg-°C
U = overall heat transfer coefficient = 25 kJ/m^2-min-°C
T_S = steam temperature = 200 °C
ϕ = liquid mass density = 1200 kg/m^3
R = radius of both cylindrical vessels = 0.3 m
λ = heat of vaporization at 150 °C = 1500 kJ/kg
Use the initial conditions given in Part (a)

52. *Boiling of Ethanol in a Cylindrical Vessel*

Consider the following cylindrical vessel which is initially filled with 100 kg of ethanol at the temperature of 20 °C. The vessel is constantly being heated with a heating coil (assume constant heat transfer area) at T = 100 °C and UA = 10 kJ/min-°C. The heating goes on until ethanol starts to boil at its normal boiling point of 78.55 °C. While the heating is taking place and then later when boiling occurs as well, ethanol also flows out of the vessel at the rate of F_1. Use the following additional data about ethanol to calculate the time it takes for ethanol to completely disappear from the cylindrical vessel. Also, how much faster does the boiling help in emptying the vessel?



MW (molecular weight) = 46.07 λ (heat of vaporization) = 38600 kJ/kmol
C_P (heat capacity) = 78.28 kJ/kmol-°C

Hint: Watch the units and their conversions carefully in your calculations

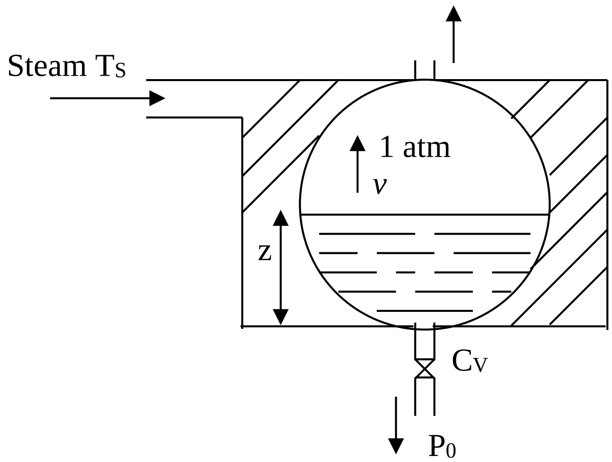
Answer the following question:

Time when ethanol disappears completely from the vessel = ____________ minutes

Time by which the boiling helps the vessel to empty faster = ____________ minute

53. *Boiling and Draining of Ethanol in a Spherical Vessel*

Consider the boiling of pure ethanol in a jacketed spherical vessel with a radius R = 1 meter, as shown in the diagram. The liquid is drained at the bottom of the vessel while some of it is boiled and escapes as vapor through the top of the vessel.



The following data are available:

$MW = 46.07$ $\lambda(T_B) = 3.858 \times 10^7$ J/kmol

$\rho = 16.575$ kmol/m^3 $C_P = 1.4682 \times 10^5$ J/kmol-°C

$$\log_{10} P^{vap} = 8.04494 - \frac{1554.30}{T + 222.65}$$ T in °C and P^{vap} in mmHg

$C_V = 4.5$ m^3-atm$^{-1/2}$/hr = valve constant

$T_S = 100$ °C $U = 2.0 \times 10^6$ J/hr-m^2-°C

$P_0 = 1$ atm $z_0 = z(t=0) = 1$ m

(a) Model this operation and use MATLAB to determine the time it takes for the vessel to completely empty, assuming that initially the liquid is at its boiling point. Note that the heat transfer area A_T is not constant.

(b) Repeat the calculations in Part (a), assuming that there is no draining of the liquid at the bottom (i.e. the liquid leaves the vessel only through boiling). Determine the solution analytically (an exact solution is possible in this case).

Useful conversion factors and formulae:

g = gravitational constant = 9.807 m/s^2

1 atm = 1.01325×10^5 N/m^2 1 N = 1 kg-m/s^2

The volume of liquid V(z) in a spherical vessel as a function of its height z is given by

$$V(z) = \pi R z^2 - \frac{\pi z^3}{3}$$

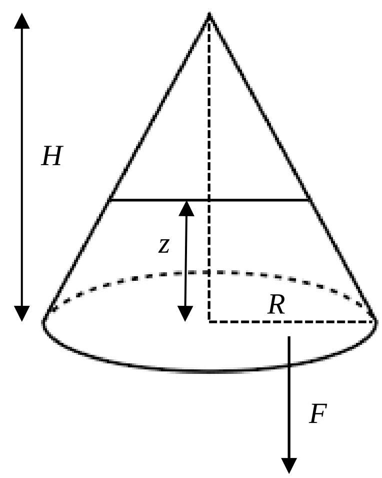
while the surface area S(z) is given by

$$S(z) = 4\pi R z - \pi z$$

$$\int \frac{x}{a+bx}dx = \frac{[a + bx - a\ln(a+bx)]}{b^2}$$

54. *Boiling and Heat/Mass Balance in an Open Inverted Cone-Shaped Vessel*

An inverted cone-shaped vessel (R = 0.5 m, H = 2.0 m) is initially filled with pure water at the height of 1.0 m as measured from the bottom of the vessel (see the figure). The liquid in the vessel flows out from bottom with a rate F = 0.01 m^3/min.



The following symbols are defined for all parameters and variables in this system. Data are also given for all symbols considered as parameters.

V	=	Water volume inside the vessel (m^3)
ϕ	=	Mass density of water = 1000 kg/m^3
z	=	Liquid height inside the vessel as measured from the bottom (in m)
F	=	Outflow rate from the vessel = 0.01 m^3/min
C_P	=	Heat capacity of water = 1.0 kcal/kg-°C

The volume of a cone = $\frac{1}{3}\pi R^2 H$

Note that you can use this formula to derive the volume of the inverted cone at any given liquid height z. Be very careful with this derivation because the cone is inverted; otherwise all your subsequent answers will be wrong.

(a) Derive an analytical expression for z as a function of time, and answer the following question:

t when the vessel becomes empty = _______________ minutes

(b) Now, suppose the cone-shaped vessel is being heated via steam through the circular area at the bottom of the vessel (hence, the overall heat transfer area can be assumed to be constant). With the additional data given below, derive an analytical expression for T as a function of time (valid up till the boiling-point temperature of water at 100 °C). Then taking into account the vaporization of water, calculate the total time it takes for the vessel to become empty without using MATLAB. Hint: note that this total time must be less than the time calculated in Part (a).

T = Temperature of water inside the vessel (in °C) = 20 °C at $t = 0$.
λ = Heat of vaporization of water = 539.4 kcal/kg at 100 °C
U = Overall heat transfer coefficient = 5.0 kcal/m^2-min-°C
T_S = Steam temperature = 150 °C
v = Vaporization or boiling rate of water from the vessel (in kg/min)

t when the temperature in the vessel reaches 100 °C = _______________ minutes

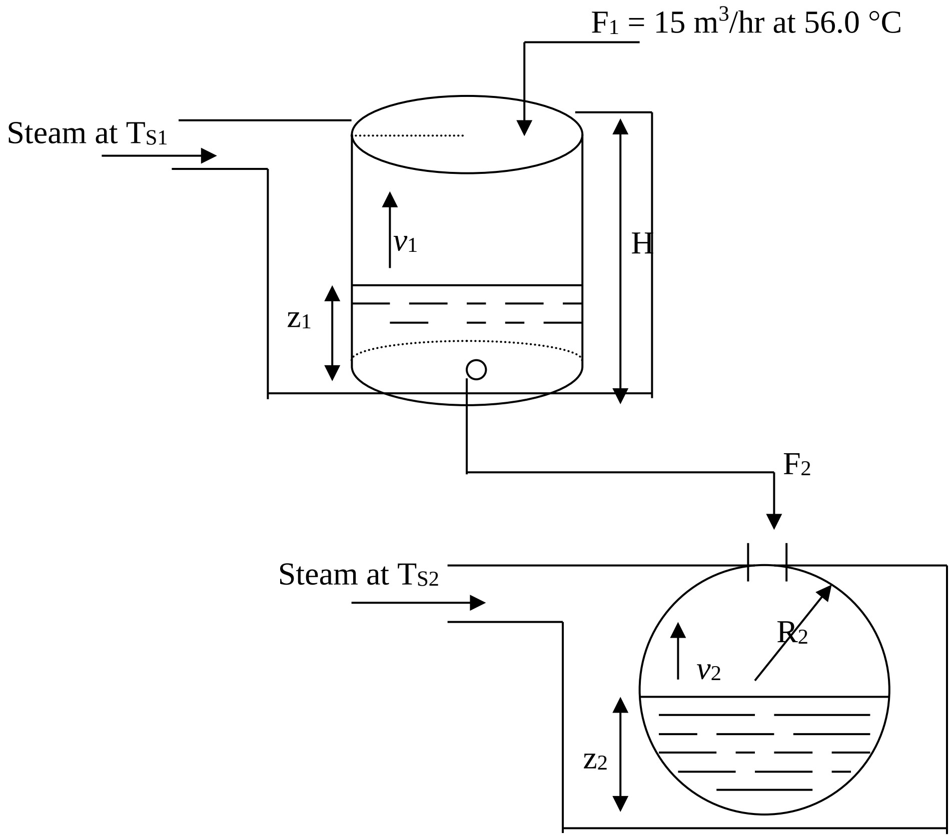
Total t when the vessel becomes empty = _______________ minutes

55. *Boiling of Acetone in a Cylindrical and a Spherical Vessels in Series*

Consider the boiling of pure acetone in a jacketed cylindrical vessel and a jacketed spherical vessel in series, as shown in the diagram. The cylinder has a radius of R_1 = 1.0 m and a height of H = 1.5 m, while the sphere has a radius of R_2 = 1.0 m. In addition to the liquid already in the vessel, pure acetone at its boiling point is added continuously at a rate F_1 = 15 m^3/hr. The cylinder also has a hole at the bottom, which allows acetone to flow out and into the sphere according to the relation

$$F_2 = C_d A(2gz_1)^{1/2} \qquad \text{(in m}^3\text{/hr)}$$

where A is the area of the hole, g is the acceleration due to gravity, and C_d is an experimentally determined value.



The following data are available:

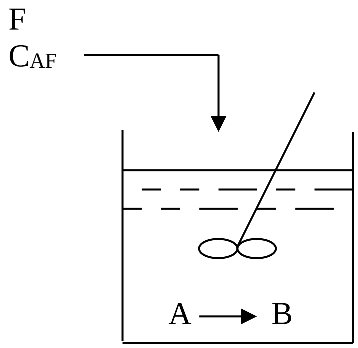
MW = 58.08	ρ = 13.62 kmol/m^3
$\lambda(T_B)$ = 3.02x10^7 J/kmol	T_B = 56.0 °C
C_P = 1.30735x10^5 J/kmol-°C	U = 3.0x10^6 J/hr-m^2-°C (for both vessels)
T_{S1} = 150 °C	T_{S2} = 100 °C
C_d = 0.5	g = gravitational constant = 1.271x10^8 m/hr^2
r = hole radius = 0.01 m	
$z_1(t=0)$ = 0.5 m	$z_2(t=0)$ = 1.5 m

(a) Model this operation and determine the time in hours (correct to 2 decimal places) at which the cylindrical vessel will either empty completely or overflow. Assume that the liquid in both vessels is already at its boiling point at t = 0.

(b) Determine the time in hours (correct to 2 decimal places) at which the liquid height z_1 in the cylinder is equal to the liquid height z_2 in the sphere.

56. *Semi-Batch Reactor with a Single 1st-Order Reaction*

Consider the case where a batch reactor is being filled. Assume a single, first-order reaction ($A \rightarrow B$) and a sinusoidal volumetric flowrate into the reactor $F = 4.0 + 2\sin(10t)$ with no flow out of the reactor.



If C_{AF} (feed concentration) = 5 mol/m^3, $k = 1$ hr^{-1}, with $V = 2.0$ m^3 and $C_A = 0$ at $t = 0$, simulate the concentration of A as a function of time using MATLAB. Run the model for 10 hours and plot the concentration profile.

57. *Batch Reactor with a Series Reaction*

Consider the series reaction:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$

(a) Assuming that each of the reactions is first-order and constant volume, write down the modeling equations for C_A, C_B, and C_C, where C_A, C_B, and C_C represent the concentrations (mol/volume) of components A, B, and C, respectively.

(b) Derive a third-order ODE for the concentration of C. That is, your ODE should look like

$$f\left(\frac{d^3C_C}{dt^3}, \frac{d^2C_C}{dt^2}, \frac{dC_C}{dt}, C_C, k_1, k_2, k_3\right) = 0$$

(c) If $k_1 = 1$ hr^{-1}, $k_2 = 2$ hr^{-1}, $k_3 = 3$ hr^{-1}, and $C_{A0} = C_A(t{=}0) = 1$ mol/liter, solve the ODE in Part (b) analytically for the concentration of C at any given time t.

58. *Batch Reactor with a Series Reaction*

Consider a batch reactor with a series reaction where component A reacts to form component B. Component B can also react reversibly to form component C. The reaction scheme can be characterized by:

$$A \xrightarrow{k_1} B \underset{k_{2r}}{\overset{k_{2f}}{\rightleftarrows}} C$$

Here k_{2f} and k_{2r} represent the kinetic rate constants for the forward and reverse reactions for the conversion of B to C, while k_1 represents the rate constant for the conversion of A to B.

(a) Assuming that each of the reactions is first-order and constant volume, write down the 3 modeling equations for C_A, C_B, and C_C, where C_A, C_B, and C_C represent the concentrations (mol/volume) of components A, B, and C, respectively.

(b) Using the following definitions:

Dimensionless time,	$\tau = k_1 t$
Conversion of A,	$x_1 = (C_{A0} - C_A) / C_{A0}$
Dimensionless concentration of B,	$x_2 = C_B / C_{A0}$
Ratio of rate constants,	$\alpha = k_{2f} / k_1$
Ratio of forward and reverse rate constants,	$\beta = k_{2r} / k_1$

Derive a second-order ODE for the dimensionless concentration of B. Your ODE must contain only dimensionless quantities (x_2, τ, α, and β).

(c) Solve the ODE in Part (b) analytically to find x_2 as a function of τ, α, and β.

(d) Using the following data:

$k_1 = 1.0 \ \text{min}^{-1}$ $\quad k_{2f} = 1.5 \ \text{min}^{-1}$ $\quad k_{2r} = 2.0 \ \text{min}^{-1}$

$C_{A0} = C_A (t = 0) = 3.0$ mol/liter

$C_{B0} = C_B (t=0) = 0$ mol/liter

$C_{C0} = C_C (t=0) = 0$ mol/liter

Solve for C_B analytically as a function of time.

(e) Given the data in Part (d), find the maximum concentration of B and the reaction time at this concentration. If no such maximum exists, prove it mathematically. Repeat the above calculations for the case of $k_1 = 3 \ \text{min}^{-1}$, $k_{2f} = 1.5 \ \text{min}^{-1}$, $k_{2r} = 1 \ \text{min}^{-1}$ while the initial conditions remain the same.

(f) Validate your analytical solutions by solving the differential equations in Part (a) with MATLAB and plot the time profiles of components A, B, and C. Use both sets of rate constants (i.e. $k_1 = 1.0 \ \text{min}^{-1}$, $k_{2f} = 1.5 \ \text{min}^{-1}$, $k_{2r} = 2.0 \ \text{min}^{-1}$ and $k_1 = 3.0 \ \text{min}^{-1}$, $k_{2f} = 1.5 \ \text{min}^{-1}$, $k_{2r} = 1.0 \ \text{min}^{-1}$).

59. *Modeling Two Reactions in Series in a Batch Reactor*

Consider the following two reactions in series:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

The orders of the two reactions do not follow the stoichiometry but instead can be described by the following modeling equations. i.e. the first reaction is 3rd-order while the second reaction is 0th-order:

$$\frac{dC_A}{dt} = -k_1 C_A^3 \qquad \frac{dC_B}{dt} = k_1 C_A^3 - k_2 \qquad \frac{dC_C}{dt} = k_2$$

(a) Derive an exact (analytical) expression of C_A as a function of time in terms of k_1, given that at t = 0, $C_A = C_{A0}$, and C_B = 0. Then use the analytical solution to determine C_A at t = 1.0 hour if k_1 = 2.0 (gmol/liter)$^{-2}$-hour^{-1} and C_{A0} = 2.0 gmol/liter and C_{B0} = 0.

C_A (t = 1.0 hour) = _______________ gmol/liter

(b) Derive an exact (analytical) expression of C_B as a function of time in terms of k_1 and k_2, given that at t = 0, $C_A = C_{A0}$, and C_B = 0. Simplify your final expression as much as possible. Then use the analytical solution to determine C_B at t = 1 hour, given that k_1 = 2.0 (gmol/liter)$^{-2}$-hour^{-1}, k_2 = 0.5 gmol/liter-hour, C_{A0} = 2.0 gmol/liter, and C_{B0} = 0.

C_B (t = 1.0 hour) = _______________ gmol/liter

(c) Calculate $C_{B,max}$ and the time at which C_B is at maximum based on the exact solution in Part (b).

$C_{B,max}$ (t = __________ hour) = _______________ gmol/liter

(d) Suppose the two reactions in series now follow the following modeling equations. Repeat Part (a).

$$\frac{dC_A}{dt} = -k_1 \sqrt{C_A} \qquad \frac{dC_B}{dt} = k_1 \sqrt{C_A} - k_2 C_B \qquad \frac{dC_C}{dt} = k_2 C_B$$

C_A (t = 1.0 hour) = _______________ gmol/liter

(e) Repeat Part (b) with the new modeling equations.

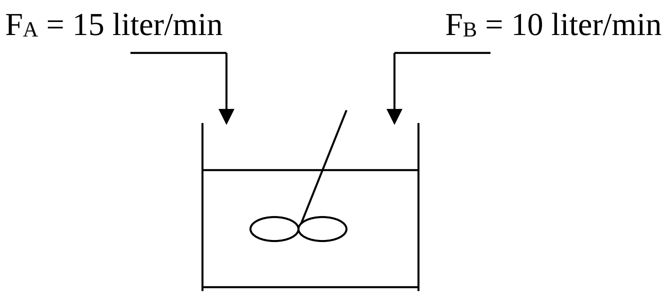
C_B (t = 1.0 hour) = _______________ gmol/liter

(f) Repeat Part (c) with the new modeling equations.

$C_{B,max}$ (t = __________ hour) = _______________ gmol/liter

60. *Isothermal Semi-Batch Reactor*

(a) Consider an isothermal semi-batch reactor where a single reaction takes place in a solvent S, which is inert. In this reaction, 2 moles of component A react with one mole of component B to form one mole of component C: $2A + B \xrightarrow{k_1} C$. The reaction rate does not conform to the stoichiometry but is 1st-order with respect to each reactant as follows: $r_A = -k_1 C_A C_B$



Initially (t = 0 min), the reactor contains 100 liters of solution and 300 moles of A. Assuming that all components have the same density of 60 mol/liter, derive 3 ODE equations needed to compute C_A, C_B, and C_C, the concentrations (moles/liter) of A, B, and C, respectively. Use *ode45* in MATLAB to solve for and plot (in a single graph) the concentrations of the 3 components. Run the model for 20 minutes with an increment of 0.5 minute.

The following experimental data have been obtained for this reaction when carried out in a batch reactor:

Time(minute)	0	5.0	7.5	12.0	15.5	25.0	32.0	40.0
C_A(mol/liter)	2.0	1.65	1.52	1.40	1.28	1.17	1.10	1.06
C_B(mol/liter)	0.5							

(b) At the end of 20 minutes, the 2 feeds to the reactor are suddenly shut off, and 4,500 moles of a new component called D (same density as components A, B, and C) are charged to the reactor. That is, the reactor now operates in a batch mode. Component D reacts with component C to form A and B, and the reaction now looks as follows:

$$2A + B \overset{k_1}{\rightleftarrows} C + D$$

k_2

with a reaction rate of $r_A = -k_1C_AC_B + k_2C_D$ (2nd -order forward and 1st-order reverse). The value of k_2 has been measured to be 1.0 min^{-1}. Derive analytically the concentration of A as a function of time, and compute C_A at steady state based on your derived equation. Your final expression should be simplified as much as possible and should not contain any parameters except *t* (time) and C_A.

Useful Integrals: $$\int \frac{dx}{x(a+bx)} = -\left(\frac{1}{a}\right)\ln\left(\frac{a+bx}{x}\right)$$

$$\int \frac{dx}{B} = \begin{cases} +\dfrac{2}{\sqrt{\gamma}}\tan^{-1}\left(\dfrac{\omega}{\sqrt{\gamma}}\right) & if \quad \gamma > 0 \\ -\dfrac{2}{\omega} & if \quad \gamma = 0 \\ -\dfrac{2}{\sqrt{-\gamma}}\tanh^{-1}\left(\dfrac{\omega}{\sqrt{-\gamma}}\right) & if \quad \gamma < 0 \end{cases}$$

where $B = a + bx + cx^2$
$\gamma = 4ac - b^2$
$\omega = b + 2cx$

61. *Determination of Reaction Kinetics*

(a) The following laboratory data were obtained for the irreversible reaction under isothermal constant-volume conditions:

$$2A \rightarrow B + C$$

Time (min)	0	3.2	5.0	9.6	12.5	18.4	25.0
[A] (mol/liter)	0.1345	0.0772	0.0602	0.0352	0.0261	0.0168	0.0110

Determine the kinetics to explain these data (i.e. find the order of the reaction and its rate constant).

(b) The following laboratory data were obtained for the irreversible reaction under isothermal constant-volume conditions:

$$A + B \rightarrow C + D$$

Time (sec)	0	2790	7690	9690	14000	19100
[A] (mol/liter)	0.1908	0.1833	0.1745	0.1719	0.1682	0.1650
[B] (mol/liter)	0.0313	0.0238	0.0150	0.0123	0.0086	0.0055

Determine the kinetics to explain these data.

62. *Isothermal Batch Reactor with a Series Reaction*

Consider an isothermal batch reactor with a series reaction where 2 moles of component A react to form one mole of component B. Component B also reacts to form component C. The reaction scheme can be characterized as follows:

$$2A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

Initially (t = 0 hr), $C_A = C_{A0}$, $C_B = 0$, and $C_C = 0$, where C_A, C_B, and C_C represent the concentrations (mol/liter) of components A, B, and C, respectively.

(a) Assume constant volume and that the first reaction $2A \rightarrow B$ is one-half order and the second reaction $B \rightarrow C$ is first-order, i.e.

$$dC_A/dt = -k_1 C_A^{1/2}$$

$$dC_B/dt = \frac{k_1}{2} C_A^{1/2} - k_2 C_B$$

Derive an analytical expression for C_B as a function of time.

(b) The following experimental data were obtained for component C_A:

Time(hr)	0	0.05	0.15	0.35	0.60	0.85	1.0
C_A(mol/liter)	1.0	0.93	0.79	0.54	0.30	0.13	0.06

C_B was also measured to be 0.11 mol/liter at t = 1 hr. Determine the values of k_1 and k_2 and the time t_{max} at which C_B is at its maximum. **Hint**: Use *Polyfit* function in MATLAB to help determine k_1 and k_2.

(c) Now, suppose the order of the above series reaction conforms to the stoichiometry, derive analytically a 1^{st}-order ODE for C_B, i.e.

$$dC_B/dt + p(t)C_B = q(t)$$

but do not solve this ODE.

(d) When the reaction order conforms to the stoichiometry, the following experimental data were obtained for C_A:

Time(hr)	0	0.03	0.06	0.10	0.15	0.20	0.30
C_A(mol/liter)	1.0	0.76	0.63	0.51	0.39	0.33	0.25

It was also observed that C_B reached a maximum of 0.14 mol/liter at t = 0.1 hr. Determine the values of k_1 and k_2.

63. *Maximizing Product Yield in an Isothermal Batch Reactor*

Consider an isothermal batch reactor with the following series of two reactions:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

Chemical *B* is the desirable product. The two reactions do not follow the stoichiometry. Instead, the first reaction is one-halfth-order while the second reaction is first-order with respect to the reactant, i.e.

$$\frac{dC_A}{dt} = -k_1 C_A^{1/2}$$

$$\frac{dC_B}{dt} = k_1 C_A^{1/2} - k_2 C_B$$

(a) Given that at $t = 0$, $C_A = C_{A0}$ and $C_B = 0$, derive analytically an expression of C_B as a function of time. Note that your final equation for C_B must be expressed in terms of C_{A0}, k_1, and k_2.

(b) It is obvious that the concentration of product *B* will go through a maximum. Determine the time at which the concentration of *B* is at the maximum if $C_{A0} = 1.0$

kmol/liter, k_1 = 1.5 kmol$^{1/2}$/liter$^{1/2}$-hour, and k_2 = 2.0 hour^{-1}. Also, calculate this maximum concentration.

<u>Answer the following questions</u>:

t_{max} = ____________________ hour $C_{B,max}$ = __________________ kmol/liter

64. ***Modeling an Isothermal Reversible Reaction and Determining Rate Constants***

Consider an isothermal batch reactor with the following reversible reaction:

$$A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$$

The reversible reaction does not follow the stoichiometry. Instead, the forward reaction is zeroth-order while the backward reaction is second-order with respect to the reactant, i.e.

$$\frac{dC_A}{dt} = -k_1 + k_2 C_B^2$$

$$\frac{dC_B}{dt} = k_1 - k_2 C_B^2$$

(a) Given that at t = 0, $C_A = C_{A0}$ and $C_B = C_{B0}$, derive analytically an expression of C_B as a function of time. Note that your final equation for C_B must be expressed in terms of C_{B0}, k_1, and k_2.

(b) Based on the result in Part (a), derive now an analytical expression of C_A as a function of time. Again, your final equation for C_A must be expressed in terms of C_{A0}, C_{B0}, k_1, and k_2.

(c) The following data are available from experiments:

t (hour)	0	0.05	0.15	0.30	0.40	0.55	0.70
C_B (mol/liter)	6.0	4.40	3.10	2.36	2.20	2.08	2.03
C_A (mol/liter)	6.0						

Also, it was observed that at steady-state, C_B = 2.0 mol/lier. Determine the values of the two rate constants k_1 and k_2.

Answer the following questions:

k_1 = _______________ mol/hr k_2 = ______________ liter^2/mol-hr

65. *Modeling Three Reactions in Series*

Consider the following three reactions in series:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$

The orders of the three reactions do not follow the stoichiometry but instead can be described by the following modeling equations:

$$\frac{dC_A}{dt} = -k_1 C_A^{3/2} \qquad \frac{dC_B}{dt} = k_1 C_A^{3/2} - k_2$$

$$\frac{dC_C}{dt} = k_2 - k_3 C_C \qquad \frac{dC_D}{dt} = k_3 C_C$$

(a) Derive an exact (analytical) expression of C_B as a function of time. Note that your final equation for C_B must be expressed in terms of k_1, k_2, C_{A0}, and C_{B0}, and that C_{B0} is not necessarily equal to zero.

(b) Also derive an exact (analytical) expression of C_D as a function of time in terms of k_2, k_3, C_{C0}, and C_{D0}. Note that C_{C0} and C_{D0} are not necessarily equal to zero.

(c) Component *B* is the desired product whose concentration should be maximized. Given that k_1 = 0.5 liter$^{1/2}$/gmol$^{1/2}$-hr, k_2 = 2.0 gmol/liter-hr, and C_{A0} = 10 gmol/liter, and C_{B0} = 3.0 gmol/liter, determine the maximum C_B and the time at which this maximum occurs.

(d) Given that C_{C0} = 1.0 gmol/liter, C_{D0} = 0, and k_3 = 1.0 hr^{-1}, compute the concentration of *A*, *B*, *C*, and *D* after 1 hour. What is the domain of this modeling problem, i.e. how long should the reactions be simulated? Why?

Answer the following questions:

$C_A(t = 1\text{ hr})$ = _______________ gmol/liter $C_B(t = 1\text{ hr})$ = _______________ gmol/liter

$C_C(t = 1\text{ hr})$ = _______________ gmol/liter $C_D(t = 1\text{ hr})$ = _______________ gmol/liter

$C_{B,\,max}$ = ______________ gmol/liter t_{max} = _______________ hours

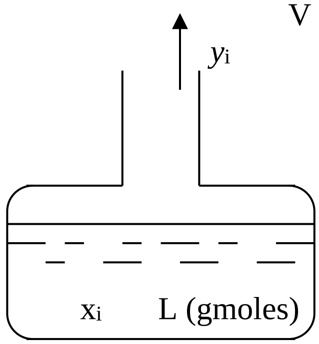
Domain of this modeling = ____________ hours

Reason: ____

____

66. *Batch Distillation, I*

A liquid mixture containing 70.0 mole% n-pentane and 30.0 mole% n-hexane is distilled in a batch still, and is initially charged with 100 gmoles of the mixture.



(a) The equilibrium relationship between the mole fraction *x* of n-pentane in the liquid and that in the vapor *y* is of the form

$$y_{C5} = x_{C5}\left(a + \frac{b}{1 + x_{C5}^2}\right)$$

Note that this equation is only valid for n-pentane, and not necessarily for n-hexane. Assuming ideal gas and ideal liquid and given

For n-pentane, $\log_{10} P^{VAP} = 6.85221 - \dfrac{1064.630}{T + 232.00}$

For n-hexane, $\log_{10} P^{VAP} = 6.87776 - \dfrac{1171.53}{T + 224.366}$

P^{VAP} in mmHG
T in °C

Calculate the mole fraction of pentane in the vapor phase in equilibrium with the 70 mole% pentane-30 mole% hexane mixture at the initial system temperature of 46 °C. Also, calculate the coefficients *a* and *b* in the n-pentane *x*-*y* relationship.

(b) At any given instant, the vapor leaving the still may be considered to be in equilibrium with the remaining liquid. Assuming that the values of *a* and *b* do not change with time and that vapor and liquid phases are constantly in equilibrium with each other, derive an analytical equation relating L, the amount of liquid left in the still, to x, the mole fraction of n-pentane in this liquid, i.e.

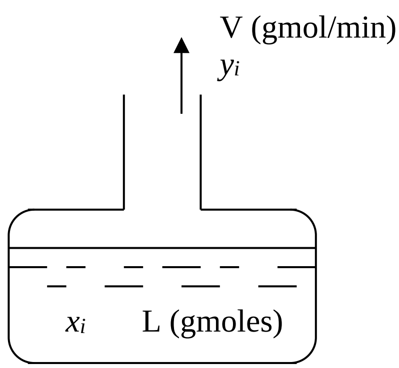
$$L = \text{function}(x_{C5})$$

67. *Batch Distillation, II*

A liquid mixture containing 60.0 mole% n-pentane and 40.0 mole% n-hexane is to be distilled in a batch still, and is initially charged with 100 gmoles of the mixture. The equilibrium relationship between the mole fraction *x* of n-pentane in the liquid and that in the vapor *y* has been correlated to the following equation:

$$y = 1.8804\,x - 0.8804\,x^2$$

Note that this equation is only valid for n-pentane, and not necessarily for n-hexane.



(a) Calculate the system temperature at which the above equilibrium relationship was established for the given liquid mixture (i.e. determine T in °C at which the above equation is valid). Also, compute the total system pressure P at the system temperature.

Assume ideal gas and ideal liquid, and the vapor pressures of the two components are:

For n-pentane, $$\log_{10} P^{VAP} = 6.85221 - \frac{1064.630}{T + 232.00}$$

For n-hexane, $$\log_{10} P^{VAP} = 6.87776 - \frac{1171.53}{T + 224.366}$$

P^{VAP} in mmHG
T in °C

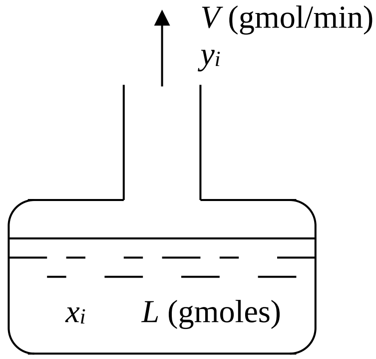
(b) Derive an analytical expression relating the amount of liquid left in the batch still L as a function of *x* (mole fraction of n-pentane in the still) and compute the value of *x* after 90% of liquid has been vaporized.

68. *Batch Distillation, III*

An equimolar liquid mixture of ethanol and water is to be distilled in a batch still at 1 atm and is initially charged with 100 gmoles of the mixture. Because water and ethanol forms a rather nonideal solution, Raoult's Law which fails to predict the azeotrope of the mixture cannot be used for vapor-liquid equilibrium calculations. Instead, the equilibrium relationship between the mole fraction x of ethanol in the liquid and that in the vapor y is correlated to the following empirical equation:

$$y = ax^3 + bx^2 + cx$$

where a, b, and c are constants, which can be determined from experimental data. Note that the empirical equilibrium equation must and does satisfy the two end-points of the x-y curve at $x = 0$ and $x = 1$. The following two pairs of data are known about the mixture: the azeotrope occurs at 89.43 mol% ethanol and when $x = 0.1661$, $y = 0.5089$.



Derive an analytical expression relating the amount of liquid left in the batch still L as a function of x (mole fraction of ethanol in the still).

<u>Answer the following questions</u>:

(i) Compute the value of x after 75% of liquid has been vaporized: x = ____________

(ii) How much liquid is left when $y = 0.70$? L = ____________ gmol

Carry four decimal places in your hand calculations. You may use MATLAB to solve any linear or nonlinear equations you encounter during your derivation of the analytical solution.

69. *Batch Distillation of a Water/Acetic-Acid System*

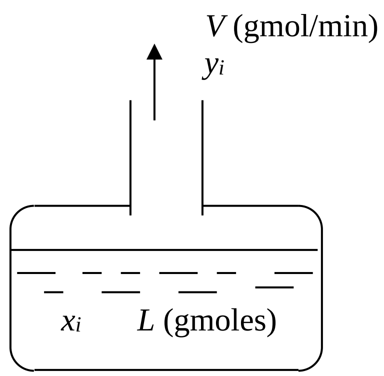
The following vapor-liquid equilibrium data (mole fractions) are available for the water/acetic-acid binary system at 25 °C.

x_{water}	y_{water}	x_{water}	y_{water}
0	0	0.6	0.6993
0.1	0.2329	0.7	0.7770
0.2	0.3558	0.8	0.8530
0.3	0.4517	0.9	0.9274
0.4	0.5379	1.0	1.0
0.5	0.6198		

First, we will use the *Polyfit* function in MATLAB to fit the above data to a quadratic polynomial in the form of

$$y = ax^2 + bx + c$$

The water-acid system is distilled in a batch still as shown, which is initially charged with 100 gmoles of the mixture. The heating of the batch still is controlled such that it vaporizes 5 gmoles of the liquid every minute.



It has also been observed that it takes exactly 10 minutes to distill the mixture to reach 50 mole% water in the liquid. Without using the *ode* solver in MATLAB (although you may use it to verify your answer), compute analytically the initial composition of the liquid mixture.

<u>Answer the following question</u>:

Initial mole fraction of water in the liquid mixture = ________________