Homework 1

Q1: Determine the real root of $f(x) = 5x^3 - 5x^2 + 6x - 2$:

(a) Graphically.

(b) Using bisection to locate the root in the range 0 < x < 1, iterate until the estimated error ε_a falls below a level of 0.5 % .

Q2: Find the root of $f(x) = x^2 - x - 2 = 0$ in the range 1 < x < 3, using the secant method.

Q3: The heat capacity of carbon dioxide as a function of tempeature is given by:

$$Cp = 1.716 - 4.257 \times 10^{-6} T - \frac{15.04}{\sqrt{T}}$$

Where the units of Cp are (kJ/kg K) and the unit of temperature T is (K). Find the temperature which yields a heat capcity 1 (kJ/kg K).

a-Using secant method with initial quess of 400 K and 600 K.

b-Use Newton-Raphson method with initial quess of 400 K.

Q4: Solve $f(x) = x^3 + 4x^2 - 10$ using the *Newton-Raphson* method for a root in [1, 2].

Q5: Calculate the Bubble point of ternary system (liquid composition: Pentane 9 mol%, Hexane 57 mol% and Heptane 34 mol%). The vapor pressure of these components is calculated by the following Antoine equations:

Pentane P^o_1=exp(13.8183-2477.07/(T+233.21))

Hexane P^o_2=exp(13.8216-2697.55/(T+224.37))

Heptane P^o_3=exp(13.8587-2911.32/(T+216.64))

Where: $K_i = P^o_i/Pt$

Pt=760 mm hg

$y_i = K_i \times x_i$

At bubble point $\sum y_i = \sum K_i \times x_i = 1$

Homework 2

Q1: a-Use a first and second order Lagrange interpolating polynomials to evaluate the density of unused motor oil at T=15 ^{O}C based on the following data:

$T_1 = 0$ $f(T_1) = 950$

$T_2 = 20$ $f(T_2) = 933$

$T_3 = 40$ $f(T_3) = 912$

b-Use Matlab to plot the experimental results vs results predicted from first and second order polynomial (Note: divide the temperature range into 10 points using linspace command)

Q2: The following data are taken from the steam table:

Temp ^{o}C	150	160	170	180
Pressure	4.854	6.502	8.076	10.225

a) Use Lagrange interpolating polynomials to correlate the pressure as a function of temperature.

b) Find the pressure at temperature T = 175 ^{o}C

Q3: Following table gives the chemical dissolved in water.

Temperature °C	15	20	25	30	35
Solubility	21.5	22.4	23.5	24.6	25.8

Find a polynomial of solubility as a function of temperature by Newton's divided difference formula.

Homework 3

Q1: It is required to estimate the relationship between the percentage of ammonia that escapes unabsorbed and the temperature of the cooling water at a plant for making nitric acid by the oxidation of ammonia. Data collected on 10 days of operation are as follows (y = % ammonia, x = temperature in °C):

x	23	24	21	22	20	18	25	26	22	24
y	2.6	2.5	1.0	2.0	1.5	1.1	2.5	3.2	1.4	2.2

a) Fit the results to a first-order polynomial $y = A + Bx$.

b) What do you predict the % unabsorbed ammonia to be when the temperature is 19 °C?

c) Use the ***polyfit*** function to check your results:

Q2: The vapor pressure of n-butane, determined experimentally at various temperatures, is presented in the following table:

T (K)	292.94	302.22	309.83	316.33	322.04	327.22
P_{vap} (atm)	2.0414	2.7218	3.4023	4.0827	4.7632	5.4437

The dependence of the vapor versus temperature can be represented by the Antoine equation:

$$\ln P_{vap} = A - \frac{\Delta H_{vap}}{R \cdot T}$$

where R = 1.98 kcal / kmol / K is the gas constant

Estimate the enthalpy of vaporization, ΔH_{vap} of n-butane

Q3: Fit (a) a quadratic (2^{nd} degree) polynomial and (b) a cubic (3^{rd} degree) polynomial, to the following data

x	3	4	5	7	8	9	11	12
y	1.6	3.6	4.4	3.4	2.2	2.8	3.8	4.6

Use the ***polyfit*** function to check your results:

Homework 4

Q1: Evaluate the following integrals using 6 subintervals Trapezoidal Rule

$$I = \int_3^6 (3x^2 + 5)^3 dx$$

$$I = \int_2^5 \int_3^4 (x^2 + y^2 + 1)^{2.5} dxdy$$

Q2: Evaluate $\int_0^6 \frac{1}{1+x^2} dx$ by using

a) 7 points Trapeziodal rule,

b) 7 points Simpson's 1/3 rule

c) 7 points Simpson's 3/8 rule.

Compare the results with its actual value.

Q3: The volume of reactor is given by following expression: $V = \frac{F_{A0}}{CA_o} \int_0^{0.9} \frac{d\,x_A}{k(1 - x_A)}$

With $k = 2.7 \times 10^7 \exp(-6500/T) \min^{-1}$ and $T = 325 + \frac{19000\,x_A}{120.35x_A + 143.75}$ using

F_{A0} = 1500 mol/min, CA_0 =2.5 mol.L^{-1}, ε = -0.2

Calculate the volume of the reactor using Simpsons rule with five points (4 steps).

Q4: The flow rate of an incompressible fluid in a pipe of radius 1m is given by:

$$Q = \int_0^r 2\pi r U.dr$$

Where *r* is the distance from the centre of the pipe and U is the velocity of the fluid. Use the trapezoidal rule to estimate the value of Q for the following tabulated velocity measured at different radius r :

U (m/s)	1.0	0.99	0.96	0.91	0.84	0.75	0.64	0.51	0.36	0.19	0.0
r (m)	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0

Homework 5

Q1: Use central difference approximation to find dy/dx and d^2x/dx^2 at x = 52 from the following data.

x	50	51	52	53	54	55	56
y	3.684	3.7084	3.7325	3.7563	3.7798	3.8030	3.8259

Compare the results with the exact values of derivatives for the function $y = x^{1/3}$.

Q2: Given the following pairs of values of x and y.

x	0.7	0.8	0.9	1.0	1.1	1.2	1.3
y	0.644218	0.717356	0.783327	0.841471	0.891207	0.932039	0.963558

Use Forward difference approximation to numerically determine the first, second and third derivatives at x = 1.

Q3: Use forward, backward and central difference approximations to estimate the first derivative of $f(x)=e^{2x}+1$ at x=2 using a step size h=0.2. Compare the results with the exact.

Q4: Derive the expressions for $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ up to the fourth order derivatives at $x = x_n$ using backward difference approximation.

Homework 6

Q1: Solve the system of equations by Gaussian Elimination.

a)
$$x + 3y + 3z = 4$$
$$2x - 3y - 2z = 2$$
$$3x + y + 2z = 5$$

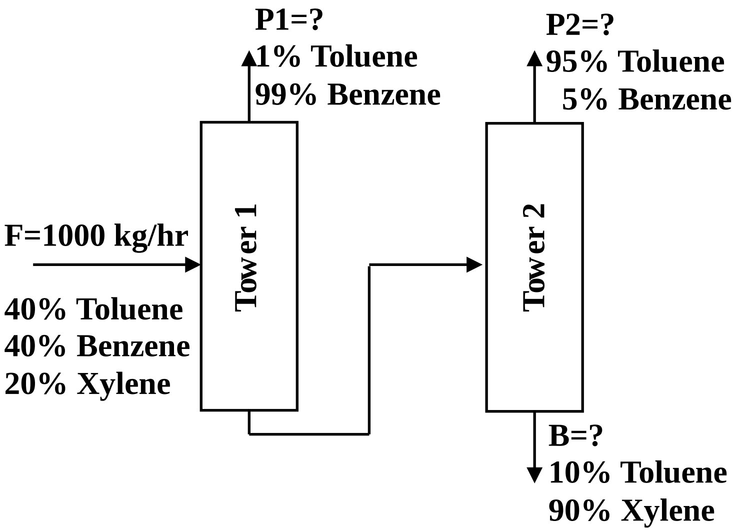
b)
$$8x_1 + 4x_2 + 2x_3 = 24$$
$$4x_1 + 10x_2 + 5x_3 + 4x_4 = 32$$
$$2x1 + 5x2 + 6.5x3 + 4x_4 = 26$$
$$4x_2 + 4x_3 + 9x_4 = 21$$

Q2: Solve the system of linear equations, using Gauss-Jordan elimination:

a)
$$4x + 8y - 4z = 4$$
$$3x + 8y + 5z = -11$$
$$-2x + y + 12z = -17$$

b)
$$a + b + c + d = 5$$
$$4a + 3b - c + 5d = 2$$
$$2a + 5b - 7c - 9d = 0$$
$$a + 2b + 3c + 4d = 10$$

Q3: Write a program to calculate the values of the unknown flow rates P1, P2, P3 by Gauss-Jordan method.



Homework 7

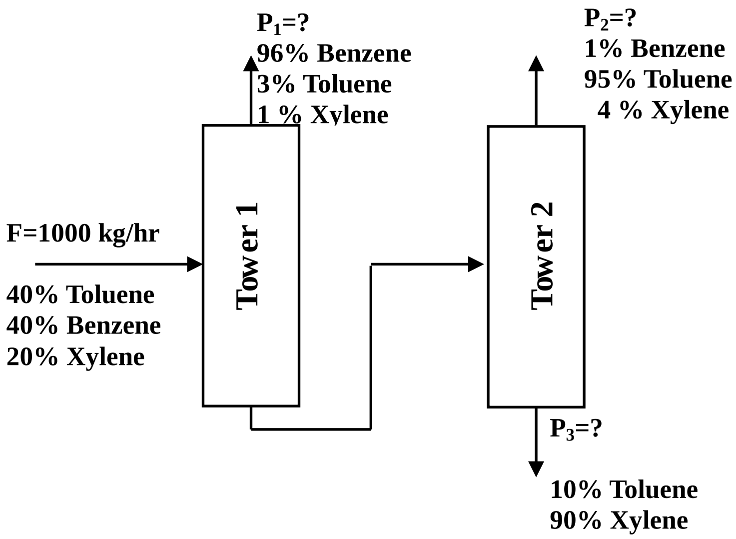
Q1: Solve the system of equations:

$$3a - 0.1b - 0.2c = 7.85$$
$$0.1a + 7b - 0.3c = -19.3\,.$$
$$0.3a - 0.2b + 10c = 71.4$$

a) Using 4 iteration of Jacobi method with the initial values a=0, b=0 and c=0, find the relative error at each iteration.
b) Using 4 iteration of Gauss – Seidel method with the initial values a=0, b=0 and c=0, find the relative error at each iteration.

Q2: For distillation towers shown in figure, use Gauss – Seidel method of 5 iterations to calculate the values of the unknown flow rates P_1, P_2, and P_3.

Note: use initial values $P_1 = P_2 = P_3 = 333.3$



Homework 8

Q1: Solve the system of equations by the substitution method:

$xy = 4$

$x^2 + y^2 = 8$

Q2: Solve the system of equations by the Elimination method

$x^2 - 2y = 8$

$x^2 + y^2 = 16$

Q3: Use 2 iterations of the Newton-Raphson method to approximate the solution to

$x^2 + y^2 = 5$

$y - x^2 = -1$

Use x = y = 1.5 as an initial guess.

Homework 9

Q1: Use the Taylor method to solve the equation $y' = x^2 + y^2$ for $x = 0.2$ given $y(0) = 1$ and $\Delta x=0.05$

Q2: Use Euler's method to solve $y' = 3x^2 + 1$, $y(0) = 2$. Take step size = 0.5 to estimate $y(2)$.

Q3: Find $y(0.1)$ using fourth order Runge-Kutta method when $dy/dx = x^2 + y^2$, $y(0) = 1$ and $h=0.05$.

Q4: For a chemical reaction, the rate of change of the concentration of component A is described by the differential equation:

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

Where

C_A concentration of A (moles/liter)

k_1 rate constant = 2.7 hr^{-1}

k_2 rate constant = 0.8 hr^{-1} $(moles/liter)^{-1}$

The initial concentration of A is: $C_A(0) = 3.0$ mole/liter

Determine the concentration of A at t = 1/4 hr, 1/2 hr, using the forth order Runge-Kutta method, with h = 1/4 hr.

Homework 10

Q1: Using fourth order Runge-Kutta integration method, find y(0.5),z(0.5) from the system of equations

$$\frac{dy}{dx} = x + z$$

$$\frac{dz}{dx} = x - y^2$$

Given y(0)=2 , z(0)=1 , h=0.25.

Q2: Given $y'' + x\,y' + y = 0$, $y(0) = 1$, $y'(0) = 0$, taking h=0.1 find the value of y(0.2) by using fourth order Runge-Kutta method.

Q3: Given the third-order ordinary differential equation and associated initial conditions

$$\frac{d^3y}{dx^3} + 3\frac{d^2y}{dx^2} + 5\frac{dy}{dx} + y = \sin x \quad , \quad y(0) = 4,\ \left.\frac{dy}{dx}\right|_{x=0} = -1,\ \left.\frac{d^2y}{dx^2}\right|_{x=0} = 12$$

a. Write this differential equation as a system of first-order ordinary differential equations

b. Write a required code using ode45 command and plot the values of y for x in the range $0 \le x \le 10$.