Lab Report 3

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Problem Statement 1:

Methanol (A) is evaporated into a stream of dry air (B) in a cylindrical tube at 328.5 K. The distance from the tube inlet to the liquid surface is z_2-z_1 = 0.238 m. At 7=328.5 K, the vapor pressure of methanol is P_{A0} = 68.4 kPa and the total pressure is P = 99.4 kPa. The binary molecular diffusion coefficient of methanol in air under these conditions is DAB = 1.991 x 10-5 m/sec. The temperature profile in the tube exhibits a linear characteristic from the liquid surface (T= 328.5 K) to the tube inlet (T= 295 K). Calculate the molar flux of methanol within the tube and plot the mole fraction profile of methanol from the liquid surface to the flowing air stream.

Multicomponent Diffusion

• For multicomponent diffusion in gases at low density to the positive z direction, the Maxwell–Stefan equation can be expressed as

$$\frac{dC_i}{dz} = \sum_{i=1}^{n} \frac{x_i N_i - x_j N_j}{D_{ij}}$$

where

C_i, (kg mol/m*) is the concentration of species i

x_i is the mole fraction of species i

N_i, (kg mol/(m2 sec)) is the mole flux of species i

D_{ij} (m/sec) is the molecular diffusivity of i in j

n is the number of components

For gas mixture of three components (A, B, C) the Maxwell-Stefan equation yields

$$\frac{dC_A}{dz} = \sum_{i=1}^{n} \frac{x_A N_B - x_B N_A}{D_{AB}} + \frac{x_A N_C - x_C N_A}{D_{AC}}$$

$$\frac{dC_B}{dz} = \sum_{i=1}^{n} \frac{x_B N_A - x_A N_B}{D_{AB}} + \frac{x_B N_C - x_C N_B}{D_{BC}}$$

$$\frac{dC_C}{dz} = \sum_{i=1}^{n} \frac{x_C N_A - x_A N_C}{D_{AC}} + \frac{x_C N_B - x_B N_C}{D_{BC}}$$

where $D_{ij} = D_{ji}$ (i,j=A,B,C)

Solution:

Algorithm/strategy-

At $z = z_1$, $x = P/P_{A0}$. We guess N_A, solve the differential equation $dx_A/dz = -(1-x_A)N_A/_{DAB}C$, and check whether the condition $x_{A2} = 0$ is satisfied. If $x_{A2} \neq 0$, the calculation procedure is repeated by using another initial guess of N_A. The bisection method can be effectively used in the iterative calculation procedure.

The built-in function ode45 is used to solve the ode and the obtained value is compared wrt the convergence criteria which is set to 1e-11, if the solution hasn't converged yet a new guess value is obtained by the bisection method which divides the range of solution by half at every iteration.

Code-

```
Dab = 1.991e-5; T = 328.5; R = 8.314; P = 99.4; Pa0 = 68.4; Tf = 295;
z2 = 0.238; z1 = 0; zv = [z1 z2];
C = P/(R*T); x0 = Pa0/P; critN = 1e-11; errN = 1;
Na1 = 3.5e-6; Na2 = 3.6e-6;
while errN > critN
 Nam = (Na1+Na2)/2;
 [z x1] = ode45(@xaz,zv,x0,[],Na1,Dab,C);
 [z x2] = ode45(@xaz,zv,x0,[],Na2,Dab,C);
 [z xm] = ode45(@xaz,zv,x0,[],Nam,Dab,C);
  if x1(end)*xm(end) < 0
  Na2 = Nam;
  else
  Na1 = Nam;
  end
  errN = abs(Na1 - Na2);
end
xblm = x0/(log(1/(1-x0)));
Nanal = Dab*C*x0/((z2-z1)*xblm);
fprintf('Estimated Nab = %e, xA = %8.6f\n',Nam, xm(end));
```

```
fprintf('Analytic Nab = %e\n',Nanal);
figure(1)
plot(z,xm), xlabel('z(m)'), ylabel('x_A'), axis tight
function dxdz = xaz(z,x,Na,Dab,C)
dxdz = -(1-x)*Na/Dab/C;
end
```

Problem Statement 2:

Gases A and B are diffusing through stagnant gas C at a temperature of 55°C and a pressure of 0.2 atmospheres from point 1 (z1) to point 2 (z2). The distance between these two points is 0.001 m. The molar flux of B was measured to be NB = − 4.143 x 10−4 kg mol/(m2 .sec) (i.e., gas B diffuses from z2 to z1). The gas mixture is assumed to be ideal gas. Estimate the molar flux of A (NA).Data: CA1 = 2.229 x 10^{-4} , CA2 = 0, CB0 = 0, CB2 = 2.701 x 10^{-3} , CC1 = 7.208 x 10^{-3} , CC2 = 4.730 x 10^{-3} , DAB = 1.47 x 10^{-4} , DAC = 1.075 x 10^{-4} , DBC = 1.245 x 10^{-4}

Solution:

Algorithm/strategy-

Since component C is stagnant, N_C= 0. A simple way to solve this problem is first to assume the value of N_A, solve the differential equations, and check whether the concentration conditions at z_2 are satisfied. The initial guess for N_A can be determined by $N_A = -D_{AC}(C_{A2}-C_{A1})/L$ assuming the gas is a binary mixture of A and C. This procedure is repeated using updated N_A until the concentration conditions at z_2 are satisfied. The bisection method can be used to update N_A. The total concentration is given by C_t = n/V = P/RT from ideal gas law.

The system of 3 odes are solved using the built in ode45 function with initial guesses, the solution has at each iteration is compared for convergence wrt convergence criteria, i.e, concentration at z_2, here critN = 1e-10, ensures that. If the solutions have converged we stop else we take new initial guesses by bisection method which reduces the range of solutions at each iteration by half.

Code-

```
Ca1=2.229e-4; Cb1=0; Cc1=7.208e-3; Ca2=0; Cb2=2.701e-3; Cc2=4.73e-3;
D1=1.075e-4; D2=1.245e-4; D3=1.47e-4;
P=0.2;T=328; R=82.057e-3; Ct = P/(R*T);
L=0.001; Nb=-4.143e-4; Nc=0; Na=-D3*(Ca2-Ca1)/L;
zspan = [0 L]; c0 = [Ca1 Cb1 Cc1]; critN = 1e-10; errA = 1;
Na1 = Na/2; Na2 = 2*Na; iter = 1;
while errA > critN
 Nam = (Na1+Na2)/2;
 [z c1] = ode45(@mdif,zspan,[Ca1,Cb1,Cc1],[],D1,D2,D3,Na1,Nb,Nc,Ct);
  [z c2] =
ode45(@mdif,zspan,[Ca1,Cb1,Cc1],[],D1,D2,D3,Na2,Nb,Nc,Ct);
```

```
  [z cm] = ode45(@mdif,zspan,[Ca1,Cb1,Cc1],[],D1,D2,D3,Nam,Nb,Nc,Ct);
  if c1(end,1)*cm(end,1) < 0 % check whether Ca(z2)=0 is satisfied
  Na2 = Nam;
  else
  Na1 = Nam;
  end
  errA = abs(Na1 - Na2); iter = iter+1;
end
c = cm; xa = c(:,1)/Ct; xb = c(:,2)/Ct; xc = c(:,3)/Ct;
figure(2)
plot(z,xa,z,xb,':',z,xc,'.-'), legend('x_A','x_B','x_C')
xlabel('Distance z(m)'), ylabel('Mole fraction')
iter, Na = Nam
function dcdz = mdif(z,c,D1,D2,D3,Na,Nb,Nc,Ct)
% c1=Ca, c2=Cb, c3=Cc, D1=Dab, D2=Dbc, D3=Dac
xa = c(1)/Ct; xb = c(2)/Ct; xc = c(3)/Ct;
dcdz = [(xa*Nb-xb*Na)/D1 + (xa*Nc-xc*Na)/D3;
(xb*Na-xa*Nb)/D1 + (xb*Nc-xc*Nb)/D2;
(xc*Na-xa*Nc)/D3 + (xc*Nb-xb*Nc)/D2];
end
```

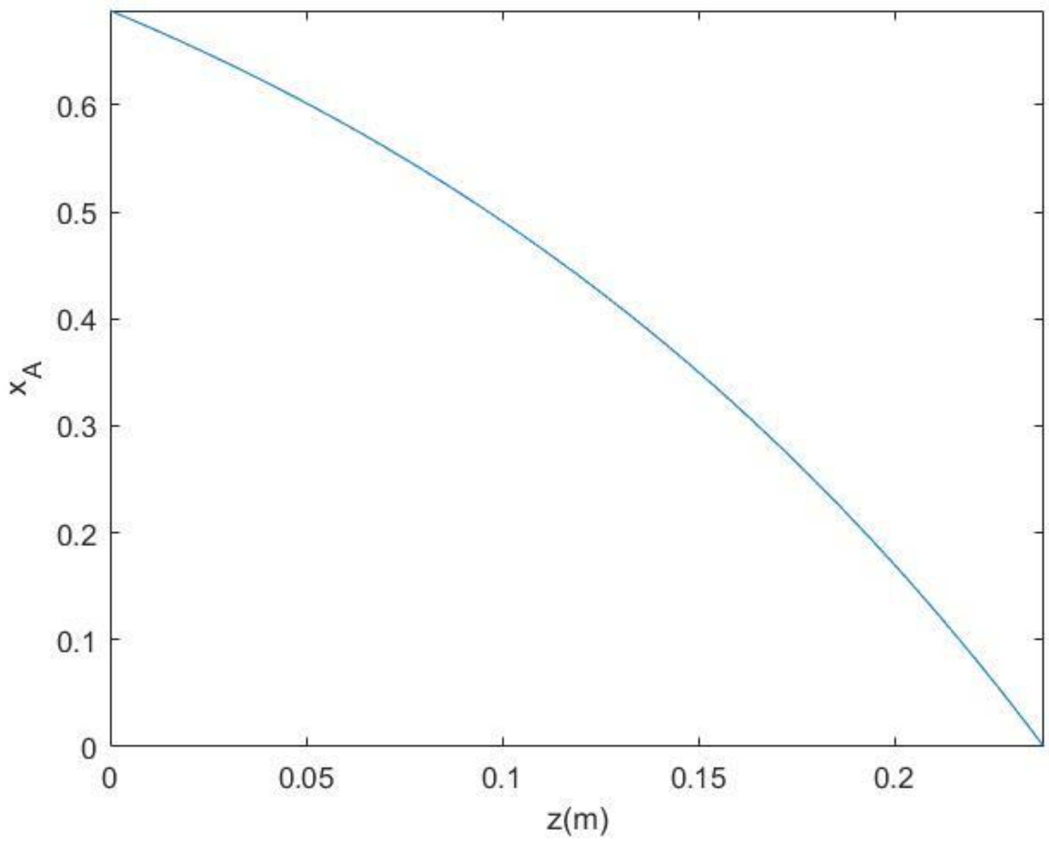
Results:

For problem 1:-

Estimated Nab = 3.547504e-06 m^2/s, x_A = -0.000000

Analytic Nab = 3.547502e-06 m^2/s.

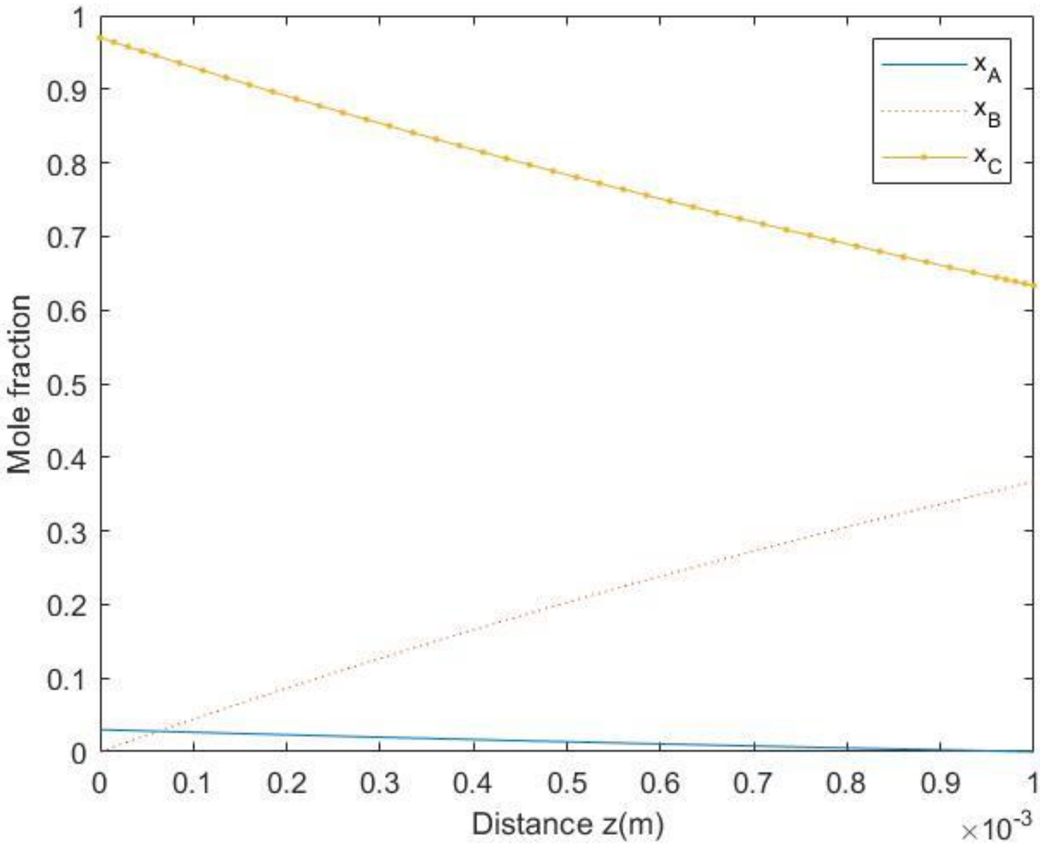
Plot of mole fraction profile of methanol from the liquid surface to the flowing air stream:



For problem 2:-

Estimated Molar flux of A (NA)= 2.3471e-05 m^2/s. after n=20 iterations of computation.

Plot of mole fractions of the components A, B and C v/s z:



Mole fraction
Distance z(m)
×10^-3
x_A
x_B
x_C
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1