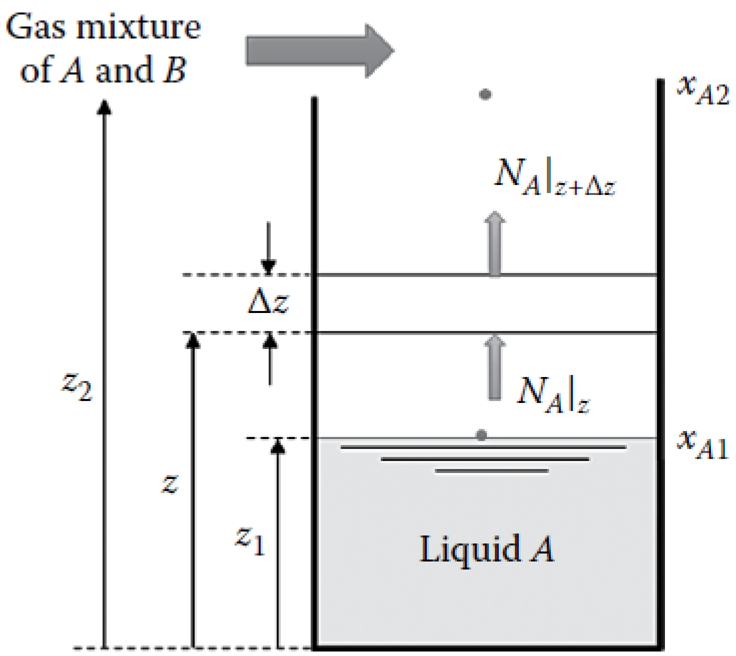
DIFFUSION

ONE DIMENSIONAL DIFFUSION



Gas phase diffusion of A through gas mixture of A and B

$$\frac{dN_a}{dz} = 0 \qquad \frac{dx_A}{dz} = -\frac{(1-x_A)N_a}{D_{AB}C}$$

C *is the total concentration* $(kg\ mol / m^3)$

D_{AB} *is the molecular diffusivity of A in B* $(m^2 / \sec)$

N_a *is the mole flux of A* $(kg\ mol / (m^2 / \sec)$

$x_A = C_A / C$ *is the mole fraction of A*

At $z = z_1, x_A = x_{A1} = P_{A0} / P$. *The gas mixture is assumed to be ideal gas*

Total concentration $C = P / RT$

$$\frac{1-x_A}{1-x_{A1}} = \left(\frac{1-x_{A2}}{1-x_{A1}}\right)^{\frac{(z-z_1)}{(z_2-z_1)}}, N_{AZ}\Big|_{z=z_1} = D_{AB}C\frac{(x_{A1}-x_{A2})}{(z_2-z_1)(x_B)_{lm}}$$

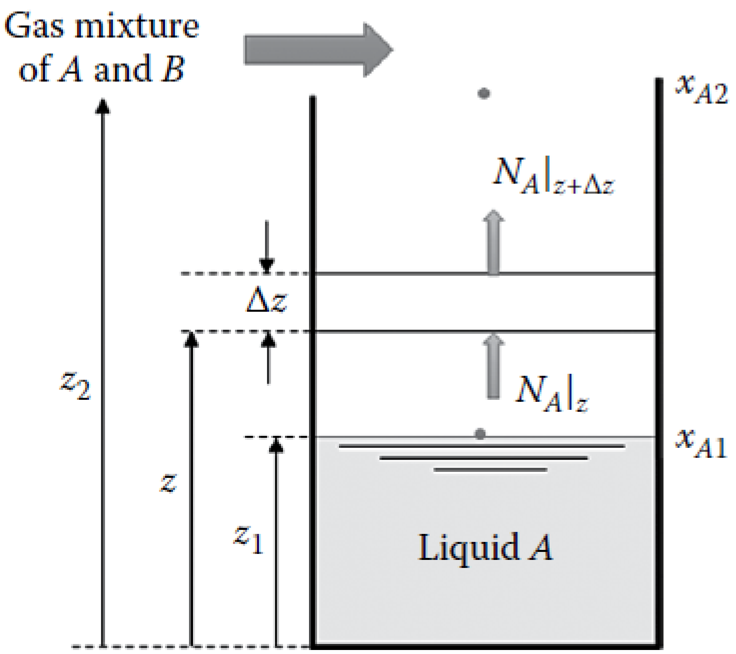
$$where \quad (x_B)_{lm} = \frac{(x_{B2}-x_{B1})}{\ln(x_{B2}/x_{B1})} = \frac{(x_{A1}-x_{A2})}{\ln\left(\dfrac{1-x_{A2}}{1-x_{A1}}\right)}$$

If the diffusivity at T_1 *is known, the diffusivity at* T *may be approximated by*

$$D_{AB} = D_{AB}\Big|_{T1}\left(\frac{T}{T_1}\right)^{1.75}$$

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 T=328.5 K, the vapor pressure of methanol in 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 D_{AB}=1.991x10^{-5} m^2/sec. Calculate the constant molar flux of methanol within the tube at steady state and plot the mole fraction profile of methanol from the liquid surface to the flowing air stream. Compare the calculated molar flux with that obtained from the equation

$$N_{AZ}\Big|_{z=z_1} = D_{AB}C\frac{(x_0)}{(z_2-z_1)(x_B)_{lm}}, (x_B)_{lm} = \frac{x_0}{\ln(1/(1-x_0))}$$



Solution

Editor - F:\CL 312 Lab\diffusion1.m

diffusion1.m

```matlab
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);
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
```

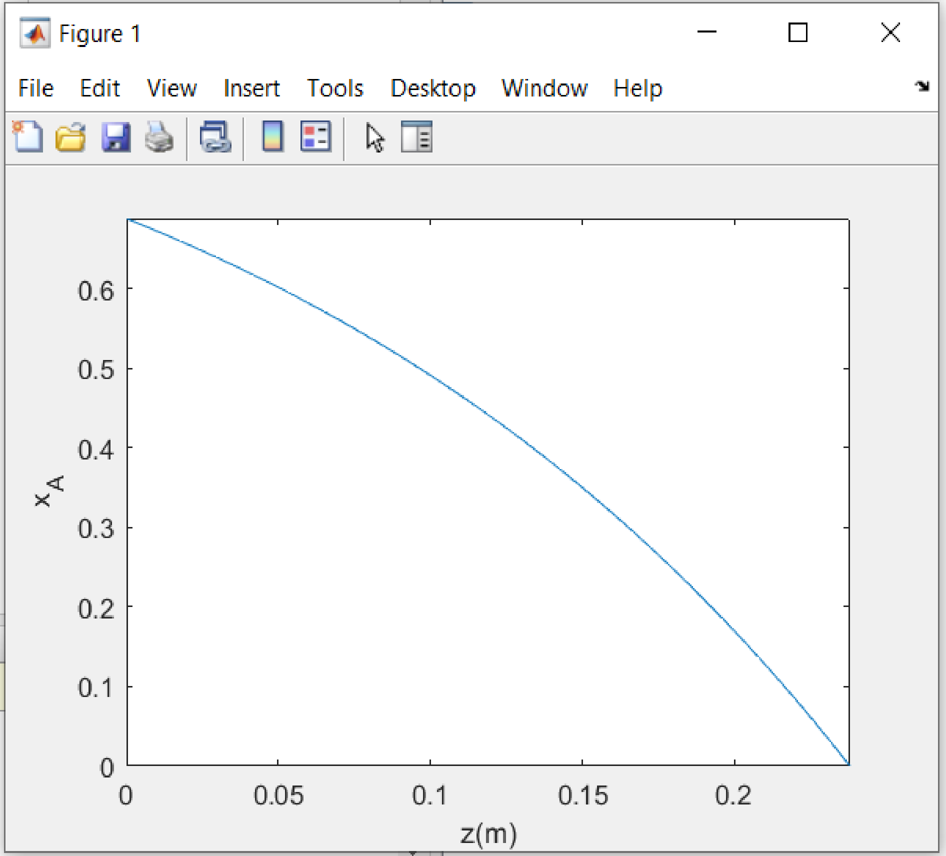
Workspace

Name	Value
C	0.0364
critN	1.0000e-11
Dab	1.9910e-05
errN	6.1035e-12
Na1	3.5475e-06
Na2	3.5475e-06
Nam	3.5475e-06
Nanal	3.5475e-06

Command Window

New to MATLAB? See resources for Getting Started.

```
>> diffusion1
Estimated Nab = 3.547504e-06, xA = -0.000000
Analytic Nab = 3.547502e-06
>>
```



Problem 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 $T = 328.5$ 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 $D_{AB} = 1.991 \times 10^{-5}$ m^2/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^3) is the concentration of species i
x_i is the mole fraction of species i
N_i (kg mol/(m$^2 \cdot$ sec)) is the mole flux of species i
D_{ij} (m^2/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

$$\frac{dC_A}{dz} = \frac{(x_A N_B - x_B N_A)}{D_{AB}} + \frac{(x_A N_C - x_C N_A)}{D_{AC}}$$

$$\frac{dC_B}{dz} = \frac{(x_B N_A - x_A N_B)}{D_{AB}} + \frac{(x_B N_C - x_C N_B)}{D_{BC}}$$

$$\frac{dC_C}{dz} = \frac{(x_C N_A - x_A N_C)}{D_{AC}} + \frac{(x_C N_B - x_B N_C)}{D_{BC}}$$

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

Problem 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 (z_1) to point 2 (z_2). The distance between these two points is 0.001 m.The molar flux of B was measured to be $N_B = -\,4.143 \times 10^{-4}$ kg mol/(m^2.sec) (i.e., gas B diffuses from z_2 to z_1). The gas mixture is assumed to be ideal gas. Estimate the molar flux of A (N_A).*Data*: $C_{A1} = 2.229 \times 10^{-4}$, $C_{A2} = 0$, $C_{B0} = 0$, $C_{B2} = 2.701 \times 10^{-3}$, $C_{C1} = 7.208 \times 10^{-3}$, $C_{C2} = 4.730 \times 10^{-3}$, $D_{AB} = 1.47 \times 10^{-4}$, $D_{AC} = 1.075 \times 10^{-4}$, $D_{BC} = 1.245 \times 10^{-4}$.

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Algorithm/steps for multicomponent diffusion

1. Component C is stagnant, $N_C = 0$
2. The initial guess for $N_A = -D_{AC}(C_{A2} - C_{A1})/L$ assuming the gas is a binary mixture of A and C. The bisection method can be used to update N_A.
3. $N_{A1} = \dfrac{N_{A0} + NC_0}{2} = \dfrac{N_A + 0}{2} = \dfrac{N_A}{2}$
4. Now, consider $N_{A2} = 2 * N_A$
5. The total concentration is given by $C_t = n/V = P/RT$ from ideal gas law.