GASEOUS DIFFUSION OF A VOLATILE LIQUID IN AIR

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ABSTRACT

This study presents three different methods to determine the diffusion coefficient of a gas by evaporation from a liquid surface.

Acetone is chosen as a volatile liquid, while air is considered as the gas. The methods are compared among each other based on their accuracy and the experimental are considered as a reference for comparison. An experimental apparatus is used to determine the diffusivity of the vapour of acetone in air. The result of testing the chosen methods proved that their accuracies are fair enough with the exception of Hirsch spots method which gave the best result.

Key words: diffusivity , Vapour of volatile liquid in air, concentration at the interface of volatile liquid.

INTRODUCTION

When a concentration gradient exists within a fluid consisting of two or more components, there is a tendency for each constituent to flow in such a direction as to reduce the concentration gradient.

When a liquid evaporates into gas, vapor is transferred from the surface to the bulk of the gas as the result of the concentration gradient, the process continues until the whole liquid is evaporated or until the gas is saturated and the concentrated gradient is reduced to zero.

The importance of diffusion as a controlling factor for chemical mobilization and transformation, the important interaction between the diffusion-controlled and convection - transport domains have been acknowledged, for both liquid and gaseous phase transport (1, 2).

The diffusion coefficient by definition provides basic information about the effective, tortuous pathway of the liquid or gas phase (3, 4). Recently, a number of conceptually based, predictive models for the solute and gas diffusion coefficients in soils have been presented (5, 6, and 7).

Moldrup et al, (8) studied three analysis concerning diffusive and convective transport parameters in the soil liquid and gaseous phases. The analysis based on the classical definition of porous media tortousity (9).

In the first analysis, the predictive solute and gas diffusivity models together with the measured data for different textured soils were used to compare the tortousities in the soil liquid and gaseous phases. In the second analysis, gas diffusivity and air permeability are linked together in a classical transport model (10) to establish a conceptually based model to describe soil structure – forming potential. In the third analysis, the Campbell type constitutive parameter model (11) was applied for gas and soluble diffusivities to illustrate difference between the diffusive and convective transport parameters in the soil gaseous and liquid phases.

THE AIM

The aim of this work is to test three different methods to determine the diffusion coefficent of a gas by evaporation from a liquid surface , where the experimental value is chosen as an exact value for comparison.

Summary of Theory

The diffudsivity of the vapour of a volatile liquid in air can be conveniently determined by Winklemanns method in which liquid is contained in a narrow diameter vertical tube, maintained at a constant temperature. An air stream passed over the top of the tube to ensure that the partial pressure of the vapour is transferred from the surface of the liquid to the air stream by molecular diffusion.

The rate of mass transfer is given by:

$$N_A = D \cdot \left[\frac{C_A}{L}\right] \frac{C_T}{C_{Bm}} \qquad (1)$$

Where

D = Diffusivity (m^2/sec)

C_A= Saturation concentration at interface ($Kmol/m^3$)

L = Effctive distance of mass transfer (mm)

C_{Bm} = Logarithmic mean molecular concentration of vapour ($kmol/m^3$)

C_T = Total molar concenration = C_A+C_{Bm} ($kmol/m^3$)

Considering the evaporation of the liquid :

$$N_A = \frac{P_L}{M}\left[\frac{dl}{dt}\right] \qquad (2)$$

P_L Where is the density of the liquid :

$$\left[\frac{P_L}{M}\right]\frac{dl}{dt} = D \cdot \left[\frac{C_T}{L}\right]\left[\frac{C_T}{C_{BM}}\right] \qquad (3)$$

Inegrating and putting $L = L_0$ at $t = 0$

$$L^2 - (L_0)^2 = \left[\frac{2M.D}{P_L}\right]\left[\frac{C_A.C_T}{C_{BM}}\right] \cdot t \qquad (4)$$

Note : L_0 and L cannot be measured accurately but L - L_0 can be measured accurately using the vernier of the microscope.

$$(L - L_0)\cdot(L - L_0 + 2L_0) = \left[\frac{2M.D}{P_L}\right]\left[\frac{C_A.C_T}{C_{BM}}\right]\cdot t$$

or

$$\frac{t}{(L - L_0)} = \left[\frac{P_L}{2.M.D}\right]\cdot\left[\frac{C_{BM}}{C_A.C_T}\right]\cdot(L - L_0) + \left[\frac{P_L.C_{BM}}{M.D.C_T.C_A}\right]\cdot L_0 \qquad \textbf{(5)}$$

where M = molecular weight (kg/mol)
t = time (sec)

if is the slope of graph of $\frac{t}{(L - L_O)}$ against $(L - L_O)$

$$s = \left[\frac{p_L.C_{BM}}{M.D.C_T.C_A}\right] \textit{or} \quad D = \frac{1}{s}\left[\frac{P_L\cdot C_{BM}}{M\cdot D\cdot C_T\cdot C_A}\right]L_0 \qquad \textbf{(6)}$$

Where :

$$C_T = \left[\frac{1}{Kmol.vol}\right]\times\left[\frac{T_{abs}}{T_a}\right]\ldots\ldots\ldots\ldots\left[K_{mol.vol}\frac{m^3}{K_{mol}}\right]$$

$$C_{B_1} = C_T$$

$$C_{B_2} = \left[\frac{P_A - P_V}{P_a}\right].C_T$$

$$C_{Bm} = \frac{(C_{B1} - C_{B2})}{In\left[\frac{C_{B1}}{C_{B2}}\right]}$$

$$C_A = \left[\frac{p_V}{p_a}\right].C_T$$

then:

THE FIRST METHOD[12]

This method was based on generalized equation to predict the diffusivity's of a gas.

The equation is:

$$D_{AB} = \frac{0.0018158\, T^{3/2}}{P.(\sigma_{AB})^2 \Omega_0}\left[\frac{(M_A + M_B}{M_A.M_B}\right]^{1/2} \qquad (7)$$

Where

D_{AB} = diffusivity, cm²/s

T = Temperature, K

M_A, M_B = Molecular weight of components A and B

P = Pressure, atm

$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2}$ effective collision diameter

Ω_D = Collision integral = f (KT/ε_{AB})

K = Boltzman`s constant

ε = Lennard – Jones force constant for

$$\varepsilon_{AB} = \sqrt{\varepsilon_A \varepsilon_B}$$

THE SECOND METHOD [13]

This method based on consideration of kinetic theory of gases. This method is recommended for mixtures of non polar gases or of a polar with a non polar gas.

$$D_{AB} = \frac{(0.0016 - 0.000246\sqrt{\frac{1}{M_A}+\frac{1}{M_B}})T^{3/2} \cdot \sqrt{\frac{1}{M_A}+\frac{1}{M_B}}}{P_t(\gamma_{AB})^2[F(KT/\varepsilon_{AB})]} \quad \textbf{(8)}$$

T = absolute temperature,K

P_t= absolute pressure, atm

γ_{AB} = molecular separation of collision $= \frac{\gamma_A + \gamma_B}{2}$

$ergs = \sqrt{\varepsilon_A \varepsilon_B}$

ε_{AB} = energy of moleculer separation interaction,

k = boltzmann`s constant

f (kt / ε_{AB}) = collision function.

M_A , M_B = Molecular weight of A and B, respectively.

THE THIRD METHOD (14)

This method considered the following equation:

$$D_{AB} = \frac{0.01498\,T^{1.81}\left[\frac{1}{M_A}+\frac{1}{M_B}\right]^{0.5}}{P(T_{CA}T_{CB})^{0.1405}(V^{0.4}_{CA}+V^{0.4}_{CB})^2} \quad \textbf{(9)}$$

T_{CA}, T_{CB} = critical temperature of material A and B

V_{CA}, V_{CB} = critical molar volumes A and B cm^3/g_{mol}

P = pressure, atm

EQUIPMENT SET-UP:

The apparatus is equipped with the following devices:

Thermometer.-

-Capillary tube.

-Vernier height gauge.

-Microscope

-Temperature controller.
-Heater switch.
-Air pump switch.
-Earth leakage circuit breaker.

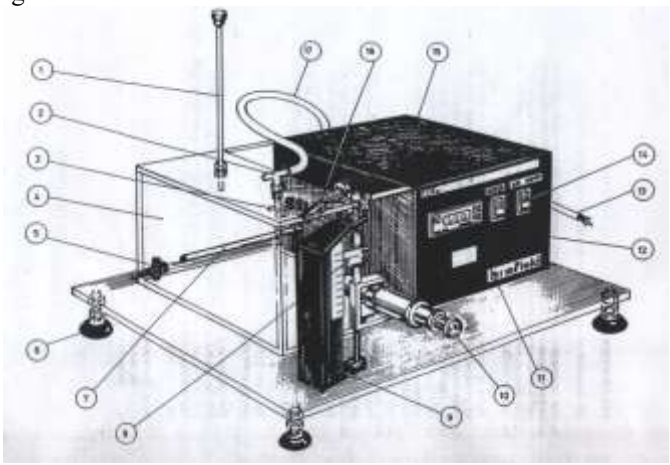

Fig (1) The used apparatus

PROCEDURE

Partially fill the capillary tube with Acetone to a depth of approximately 35 mm. Remove top nut from the metal fitting. Carefully, insert capillary tube through the rubber at the top of the tube rests on the top of the nut. Gently screw this assembly onto the top plate, with the "T" piece normal to the microscope. Connect flexible air tube to one end of the "T" piece. With the microscope set up as shown, adjust the object lens to within 20-30mm from the tank.

Adjust the vertical height of the microscope until the capillary tube is visible, if the capillary tube is not visible, adjust the distance from the object lens to the tank until it is visible. For a clearer and well defined view of the meniscus inside the capillary tube, adjust the position of the viewing lens in or out of the microscope body as necessary. Note that when viewing the capillary tube the image will be upside down, so that the bottom of the tube is at the top of the image. When the meniscus has been determined, the sliding vernier scale should be aligned with the suitable graduation on the fixed scale. Switch on air pump and then record the level inside the capillary tube. Switch on the temperature controller water bath (adjust the set point on the controller to 40 centigrade) and obtain a steady temperature. After approximately 60 minutes switch off the water bath (to prevent air bubbles from obscuring the reading) and record the change in level inside the capillary tube. Switch on bath and repeat the procedure approximately every 60 minutes.

RESULT AND DISCUSSION

The table shows the experimental results were ($t/L - L_0$) is drawn against ($L - L_0$) and determines the gradient s from the graph, then these results used to determine the diffusivity.

Time from commencement of experiment	**Liquid level $L - L_0$**	**$t / L - L_0$**
ks	**mm**	**ks/mm**
0	0	0
3.6	2.2	1.636
7.2	4.2	1.714
11.16	6.3	1.771
15.9	8.8	1.807
19.98	10.8	1.85
23.4	12.4	1.887
78.78	34.5	2.233
83.52	36.1	2.313
87.24	37.3	2.339
91.8	38.9	2.36
97.32	40.8	2.385
101.0	42.0	2.407

Table [1]: Experimental results showing the liquid level for different time.

This data is typical result for this experiment at steady state taken in the following conditions:
Temperature 313K.-
-Pressure is atmospheric.

Now the computer program of math cad is used to obtain the slope for the given data to determine the best fit line for the data.

Graphical Calculation

The data in Table (1) are used to determine the gradient using the fig (2) and then there results were used to determine the diffusivity. Fig (2) represents the data and from the by it can be fond that:

Slope (x,y) = 0.018 intercept (x,y) = 1.638

$$\text{Line}(x,y) = \begin{pmatrix} 1.638 \\ 0.018 \end{pmatrix}$$

So, the slope is 0.018 and the intercept is 1.638; therefore, the values give the factors for the best-fit line for the data, and is given by the equation for the straight line :

$$Y = 0.018x + 1.638$$

The line is shown in fig. (2) in a solid line associated with the line for the given data and is represented by (f(s),s) in the graph.

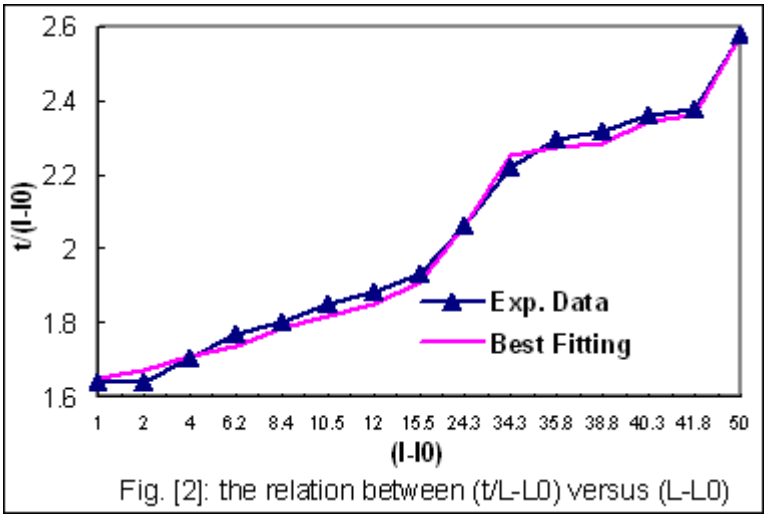

Fig. [2]: the relation between (t/L-L0) versus (L-L0)

From the resulting graph

$$\boldsymbol{s} = 0.018 \cdot 10^{3} \frac{\sec}{\boldsymbol{mm}^{2}}; \qquad \boldsymbol{s} = 18 \cdot 10^{7} \frac{\boldsymbol{s}}{\boldsymbol{m}^{2}}$$

$$\boldsymbol{C_T} = \frac{1}{22.4 \dfrac{\boldsymbol{m}^{3}}{\boldsymbol{Kmol}}} \cdot \frac{273}{313}; \qquad \boldsymbol{C_T} = 0.0389 \frac{\boldsymbol{Kmol}}{\boldsymbol{m}^{3}}$$

$$\boldsymbol{P_L} = 790 \frac{\boldsymbol{Kg}}{\boldsymbol{m}^{3}}; \qquad \boldsymbol{M} = 58.08 \frac{\boldsymbol{Kg}}{\boldsymbol{mol}}$$

$$\boldsymbol{C_{B1}} = 0.389$$

$$\boldsymbol{C_{B2}} = \left[\left(\frac{101.3 - 56}{101.3} \right) \cdot 0.0389 \right] \qquad \boldsymbol{C_{B2}} = 0.0174 \frac{\boldsymbol{Kmol}}{\boldsymbol{m}^{3}}$$

$$\boldsymbol{C_{Bm}} = \frac{(0.0389 - 0.0174}{\boldsymbol{Ln}\left[\dfrac{0.0389}{0.0174} \right]} \qquad \boldsymbol{C_{Bm}} = 0.0267 \frac{\boldsymbol{Kmol}}{\boldsymbol{m}^{3}}$$

From the Equation

$$\boldsymbol{D} = \frac{(\boldsymbol{PL} \cdot \boldsymbol{C_{Bm}})}{\boldsymbol{s} \cdot (2\boldsymbol{M} \cdot \boldsymbol{C_N} \cdot \boldsymbol{C_T})}$$

Then

$$\boldsymbol{D} = \frac{790 \cdot 0.0267}{1.8 \cdot 10^{7} \cdot (2 \cdot 58.08 \cdot 0.0215 \cdot 0.0389)}$$

Hence $$\boldsymbol{D} = 1.206 \cdot 10^{-5} \frac{\boldsymbol{m}^{2}}{\boldsymbol{s}}$$

Analytical results

First method-

On applying the first method which based on an analytical equation (7) , the result showed that the value of the diffusivity is

$D_{AB} = 1.128 \cdot 10^{-5}$ m^2/s

With the accuracy of 93.53 %

- Second method

The second method based on Hirsch felder-Brid- spots method is recommended for mixtures of nonpola gases. On applying equation (8), the result showed the value of the diffusivity is :

$D_{AB} = 1.222 \cdot 10^{-5}$ m^2/s

With the accuracy of 98.67 %

- Third method

Applying equation (9), to determine the diffusivity, the result showed that the value of the diffusivity is :

$DAB = 1.1033 \cdot 10^{-5}$ m^2/s

With the accuracy of 91.48 %

Conclusions

From this study, the following conclusions can be drawn:

* the three methods used in this work to determine the diffusion coefficient of a gas by evaporation from a liquid surface were compared with the experimental results, and their occuracies are almost not far from each other, but as a numerical results the method of hirsch spots gave the best result.
* the microscope was used to adjust the vertical hieght of the liquid and it was adjusted automatically until the cappillary tube is visible.
* the rate of transfer of a smponent in a mixture of two components can be determine not only by the rate of diffusion of the first component but also on the behaviour of the second component.

Nomenclature

C concentration (mol/m^3)
D diffusivity (m^3/sec)
L effective distance of transfer (mm)
M molecular weight (g/g_{mol})
N number of moles (moles)
P pressure (atm)
S slope of straight line in fig (2)
t time (sec)
v critical molar volume (cm^3/g_{mol})

Greek letters

ρ_L density of liquid (gm/cm^3)
б effective collision diameter
ε lennard –johnes force constant of gasses
Ω collision integral
γ molecular separation of collision

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انتشـــار بخـار السوائل المتطايرة في الهـــواء

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الخلاصـــة

في هذه الدراسة تم تطبيق ثلاث طرق نظرية لإيجاد قيمة معامل انتشار الغازات نتيجة التبخر لسوائل متطايرة وتم استخدام مادة الأسيتون كسائل متطاير في الهواء. أيضا تم مقارنة النتائج النظرية المتحصلة من هذه الطرق أعلاه ومقارنتها مع النتائج العملية باستخدام منظومة تطبيقية لقياس معامل الانتشار .

أظهرت النتائج النظرية أن الطرق الثلاثة قد أعطت دقة جيدة وقد تميزت طريقة هيرز سبوتز حيث أعطت دقة أعلى مقارنة بالطرق الأخرى .

الكلمات المفتاحية : الانتشارية. بخار السوائل المتطايرة في الهواء. تركيز الأسطح للسوائل المتطايرة .