

# LOW-COST MASS TRANSFER EXPERIMENTS

## Part 6. Determination of Vapor Diffusion Coefficient

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**M**olecular diffusion determines the rate of most mass-transfer operations. Determination of the diffusion coefficient of the key component is very important for predicting rates of mass transfer, and many correlations are reported in the literature for binary and multicomponent systems.<sup>[1-4]</sup>

This paper describes a simple experimental technique for determining binary diffusion coefficients for vapor (A)-gas (B) systems in which the vapor is generated by the evaporation of a pure volatile liquid and the gas is air. The theory is described in many textbooks on mass transfer and unit operations,<sup>[2-4]</sup> and only a brief treatment is given below for immediate reference.

From Fick's first law of diffusion for the case of stagnant B in a binary system, the flux of A at steady state ( $N_{Az}$ ) is given by<sup>[2]</sup>

$$N_{Az} = \frac{D_{AB} p_t}{RTz p_{BM}} (p_{A1} - p_{A2}) \quad (1)$$

where  $D_{AB}$  is the diffusion coefficient,  $R$  is the ideal gas constant,  $T$  is the absolute temperature,  $z$  is the length of the diffusion path,  $p_t$  is the total pressure,  $p_{A1}$  and  $p_{A2}$  are the partial pressures of component A at the two extremes of the diffusion path, and  $p_{BM}$  is the logarithmic mean of the

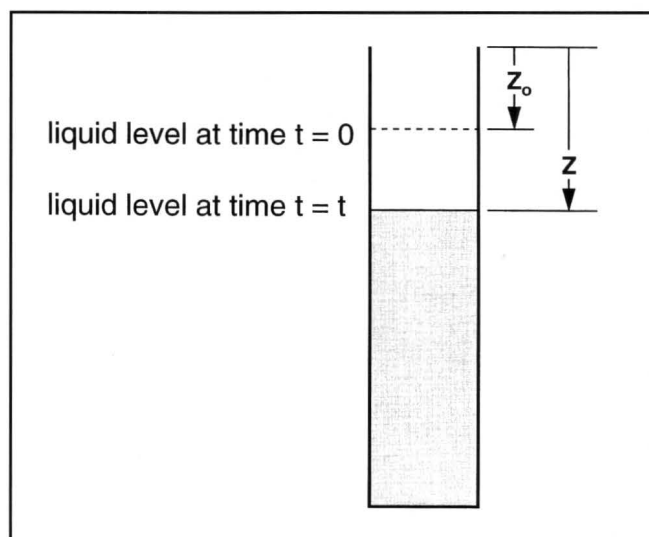
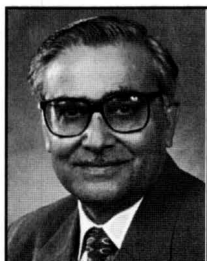


Figure 1. The evaporation tube.

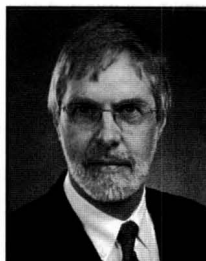
partial pressures of component B at the two ends of the diffusion path.

Let us suppose we have a liquid in a tube (see Figure 1) of cross-section  $a$ , and in time,  $dt$ , the liquid level in the tube

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falls through distance  $dz$ . The volume of liquid evaporated will be given by  $(a \cdot dz)$ . If the density of the liquid is  $\rho_A$  and the molecular weight is  $M_A$ , the molar evaporation of A will be equal to  $\rho_A(a \cdot dz)/M_A$  and the rate of evaporation,  $\rho_A a \cdot dz / M_A dt$ , can be related to the diffusional flux ( $N_{Az} \cdot a$ ) by the following equation:

$$N_{Az} a = \frac{\rho_A a}{M_A} \frac{dz}{dt} \quad (2)$$

Assuming the liquid level drops very slowly and therefore pseudo-steady-state conditions apply,  $N_{Az}$  in Eq. (2) may be substituted for by Eq. (1), giving

$$\frac{\rho_A}{M_A} \frac{dz}{dt} = \frac{D_{AB} p_t}{RT z p_{BM}} (p_{A1} - p_{A2}) \quad (3)$$

which can be rearranged as

$$z \, dz = C \, dt \quad (4)$$

where

$$C = \frac{D_{AB} p_t M_A}{RT p_{BM} \rho_A} (p_{A1} - p_{A2}) \quad (5)$$

Equation (4) can be integrated as

$$\int_{z_0}^z z \, dz = C \int_0^t dt \quad (6)$$

which yields

$$\frac{z^2 - z_0^2}{2} = C t \quad (7)$$

Equation (7) suggests that a plot of  $(z^2 - z_0^2)/2$  vs.  $t$  will be linear, passing through the origin and having a slope  $C$ . The value of  $D_{AB}$  can therefore be calculated from the measured slope  $C$  by rearranging Eq. (5) as

$$D_{AB} = \frac{CRT p_{BM} \rho_A}{p_t M_A (p_{A1} - p_{A2})} \quad (8)$$

It may be noted that  $p_{A1}$  is the vapor pressure of liquid A at  $T$ , and  $p_{A2}$  may be safely assumed to be zero as fresh air flows over the tube.

## EXPERIMENTAL PROCEDURE

The apparatus is quite simple. It consists of a small glass tube of 1- to 2-cm diameter (see Figure 1), a traveling microscope, a source of light to illuminate the liquid meniscus, a thermometer, and a barometer. All these components can be easily found in any chemical engineering laboratory.

The volatile liquids selected should have high vapor pressures to get meaningful results in a reasonable time period—acetone, pentane, and hexane were tested in this study. Tests performed in duplicate indicated that the results were reproducible within the experimental accuracy.

The following procedure is recommended:

1. Fill the tube with the volatile liquid to about 0.5 to 1.0 cm from the top. Care should be taken to pipet the liquid in the tube to avoid wetting the top empty section of the tube with the liquid.
2. Place the tube in a stand and place the stand in an illuminated fume-hood.
3. Note the atmospheric pressure and the temperature in the fume hood.
4. Keep the fume hood fan off and the door fully open (the front glass panel fully raised) to minimize any air turbulence due to suction in the fume hood.
5. Focus the traveling microscope first at the very top of the tube ( $z=0$ ) and then at the liquid meniscus level ( $z=z_0$ ), and immediately start the stopwatch.
6. Record the liquid level ( $z$ ) in the tube with time to obtain a noticeable drop in the liquid depth. This gives the  $z$ -versus- $t$  data.
7. Note the atmospheric pressure and the temperature in the fume hood again.
8. Measure the liquid density at the experimental temperature by weighing a known volume of the liquid.
9. Plot  $(z^2 - z_0^2)/2$  versus  $t$  and obtain the experimental diffusion coefficient from the slope of the plot as per Eq. (8).
10. Predict the diffusion coefficient from the Hirschfelder-Bird-Spotz correlation<sup>[2]</sup> given below and compare with the experimental value obtained in Step 9 above.

$$D_{AB} = \frac{10^{-4} \left( 1.084 - 0.249 \sqrt{\frac{1}{M_A} + \frac{1}{M_B}} \right) T^{3/2} \sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{p_t (r_{AB})^2 f(kt / \epsilon_{AB})} \quad (9)$$

11. Repeat the experiment with a pedestal fan and/or fume hood fan on, and compare the experimental diffusivity values with those with no air circulation in the fume hood.

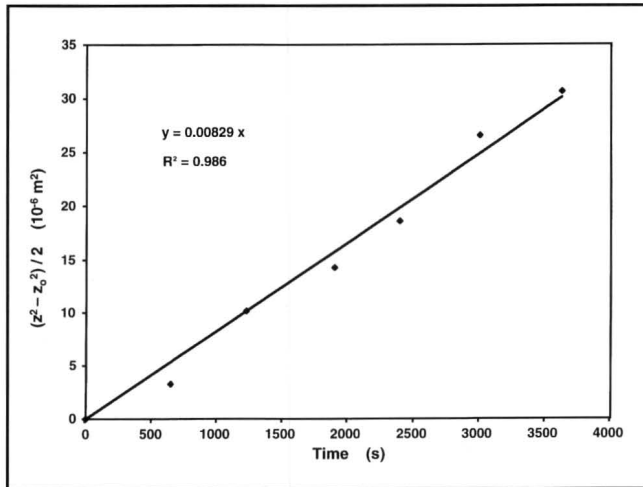


Figure 2. Plot of  $(z^2 - z_0^2)/2$  versus time for acetone vapor diffusing through stationary air.

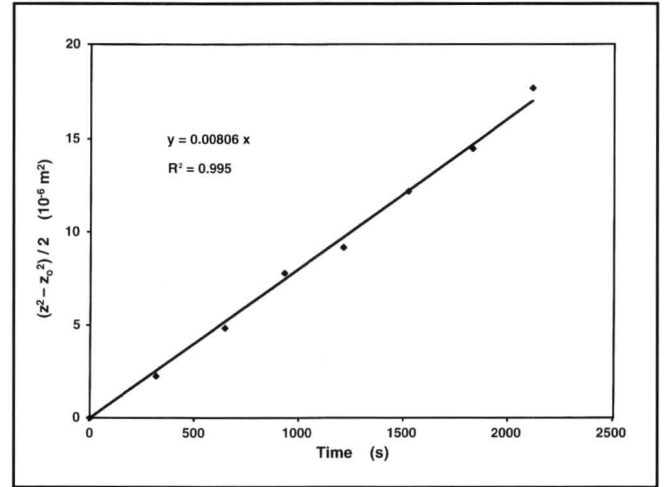


Figure 3. Plot of  $(z^2 - z_0^2)/2$  versus time for hexane vapor diffusing through stationary air.

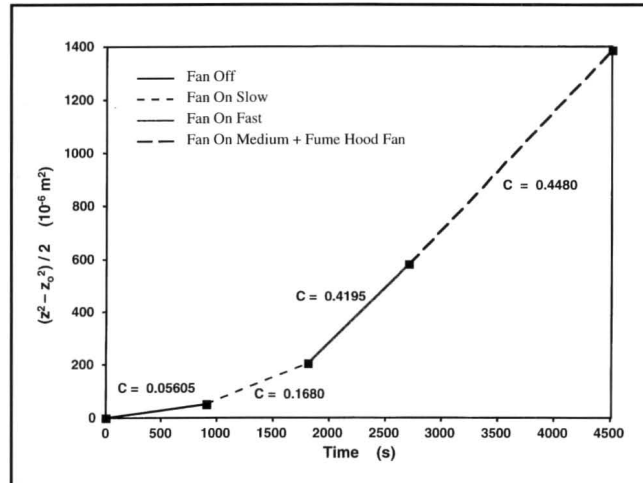


Figure 4. Plot of  $(z^2 - z_0^2)/2$  versus time for pentane-air system with varying levels of air circulation

Vapor	$p_1$ (N/m <sup>2</sup> )	$p_{A1}^5$ (N/m <sup>2</sup> )	Temp. (°C)	Air Flow		Diffusion Coefficient (10 <sup>-6</sup> m <sup>2</sup> /s)		% Deviation
				Fume Hood Fan	Pedestal Fan	Experimental	Predicted	
Acetone	98960	23905	20	Off	Off	10.1	10.8	-6.5
Hexane	99155	16029	19	Off	Off	8.6	8.1	+6.2
Pentane	100616	76500	27	Off	Off	8.5	9.2	-7.6
Pentane	100616	76500	27	Off	Slow	25.5	-	-
Pentane	100616	76500	27	Off	Fast	63.6	-	-
Pentane	100616	76500	27	On	Medium	67.9	-	-

## RESULTS AND DISCUSSION

The results for acetone and hexane at atmospheric pressure, room temperature, and *with no* forced air circulation through the fume hood are plotted in Figures 2 and 3, respectively, and for pentane *without* and *with* forced air flow through the fume hood in Figure 4. As can be noted, the plots of  $(z^2 - z_0^2)/2$  versus  $t$  for acetone and hexane (see Figures 2 and 3, respectively) yield linear lines passing through the origin with a good fit of data points ( $R^2 > 0.986$ ). The experimental and the predicted values of diffusion coefficients, calculated from the slopes of these plots and the first line on Figure 4 for pentane (with no forced circulation in the fume hood), and from the Hirschfelder-Bird-Spotz correlation<sup>[2]</sup> (Eq. 9), respectively, are given in Table 1.

The results suggest that the experimental technique is simple and gives reasonable agreement between experimental and predicted values.

The last three experiments performed with forced air flow in the fume hood (see Table 1 and Figure 4) indicate an increase in the apparent value of  $D_{AB}$ , as expected. These results reflect a very important limitation of this procedure, *i.e.*, for ensuring "stagnant B" conditions (to obtain a good agreement between the experimental and the predicted values of  $D_{AB}$ ) on which the development of Eq. (7) is dependent, undue air turbulence in the fume hood must be absent. Any external turbulence can affect the behavior of the gas mixture in the tube and lead to an increase in the mass-transfer rate.

It may be noted that for this method to work, the density of the vapor (A) should be greater than that of air (B) so that there are no natural convection effects in the tube. This is the case with all common organic liquids.

## CONCLUSIONS

1. Rate of fall in liquid level can be used to determine the diffusion coefficient fairly accurately for vapor-gas systems where the vapor is generated by the evaporation of a pure volatile liquid and the gas is stagnant.
2. Experimental diffusion coefficients are within  $\pm 10\%$  of the predicted values.
3. Turbulence in the experimental area affects the precision of the results.

## GENERAL REMARKS

This laboratory provides students with the opportunity of experiencing how elementary experimental methods can be used to confirm what they read in the classroom. The experiment is extremely simple and can be completed well within the usual three-hour laboratory period. Since linear plots passing through the origin are obtained, only two level readings, about 20 minutes apart, are required for a direct calculation of  $D_{AB}$  through Eqs. (7) and (8).

We recommend that the class be divided into groups and that different groups study the effects of 1) nature of component A, *i.e.*, study different volatile liquids; 2) degree of turbulence in the work station (some effort can be made to quantify the results by measuring air velocity in the fume hood with an anemometer); 3) temperature; and 4) natural convection effects in the evaporation tube (this can be studied with any liquid with a molecular weight lower than that for air—water being the safest). The students should also be asked to review the analysis of sources of error in such a procedure provided by various workers.<sup>[6-8]</sup>

## NOMENCLATURE

a	cross-sectional area of evaporation tube
C	slope of $(z^2 - z_0^2)/2$ vs. $t$ plot
D	diffusion coefficient
f	function
k	Boltzmann's constant
M	molecular weight
$N_{Az}$	steady-state molar flux of A in the z-direction
p	pressure
R	ideal gas constant
r	molecular separation at collision
T	absolute temperature
t	time
z	vertical distance
$\epsilon$	energy of molecular attraction
$\rho$	liquid density

### Subscripts

A	component A
B	component B
AB	components A and B
BM	log-mean average for component B across the diffusion path
0	initial value
t	total
z	in the z-direction
1	beginning of diffusion path
2	end of diffusion path

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