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EXPERIMENTAL DETERMINATION OF DIFFUSION COEFFICIENTS IN GAS MIXTURES IN A LABORATORY OF TRANSPORT PHENOMENA

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ABSTRACT

The experimental determination of certain variables such as the diffusivity allows the student of chemical engineering to understand its meaning and significance in the mass transfer operations. This article presents an apparatus with which students determine this important variable.

KEYWORDS: Diffusion, mass transfer, experimentation.

1.- INTRODUCTION

In the laboratory of Chemical engineering of the Faculty of chemistry at the Universidad Nacional Autónoma de México, (UNAM) about one hundred students of Chemical engineering, apply their knowledge in Transport Phenomena. This laboratory has been built deliberately, with appliances and equipment in which experiments are performed to clarify the knowledge presented in the lectures. In that laboratory teachers have implemented a series of experiments since they think it is important that students develop through experimentation, models representing different phenomena. In the experiments students must face up to the problem and develop mathematical models of the phenomenon under study and from them perform experiments that lead to the obtaining of the required data. One of these experiments deals with the diffusion coefficients

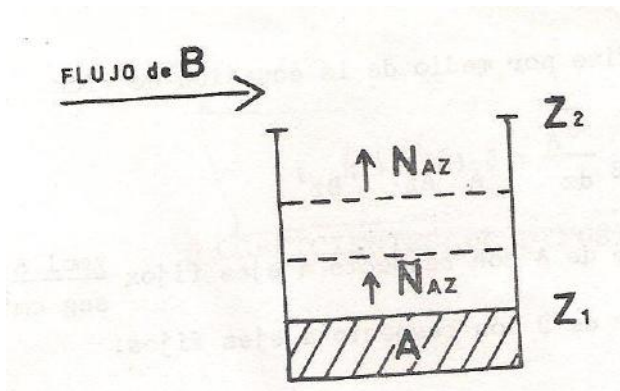
2. DIFFUSIVITY

The motion of molecules regardless of any global movement of the fluid is called molecular diffusion. This movement is inherent to molecules and depends on temperature and pressure. In the broadcast each molecule behaves independently of other molecules, although clearly there are continuous clashes between them and as a result the molecules move through a zigzag movement. To move a molecule carries with it mass, energy and momentum.

The molecular transport of matter can be described using the Fick law. Fick's law indicates that the mass flow of the component A, per unit of cross-sectional to the direction of the flow area and per unit time is proportional to the gradient of concentrations:

$$\tilde{J}_A = -D_{AB} \frac{d\tilde{c}_A}{dz} \quad (1)$$

Where \tilde{J}_A is the flow-molar mass of substance A in the direction is z, only due to molecular motion and D_{AB} is the diffusivity coefficient of mass or diffusion. According to this expression, the mass A. Fig. 1 will move in the direction in which decreases the concentration of the substance .



Fig

$$\tilde{J}_A = \tilde{C}_A(u_A - \tilde{V})(2)$$

$$\therefore \tilde{J}_A = \tilde{C}_A(u_A - \tilde{V}) = -D_{AB} \frac{d\tilde{C}_A}{dz} (3)$$

$$\tilde{J}_A = \tilde{C}_A u_A - \tilde{C}_A \tilde{V} = -D_{AB} \frac{d\tilde{C}_A}{dz} (4)$$

1 pero :

$$\tilde{V} = \frac{\tilde{C}_A u_A + \tilde{C}_B u_B}{\tilde{C}_T} ; \quad \frac{\tilde{C}_A}{\tilde{C}_T} = \tilde{x}_A$$

$$\tilde{C}_A u_A = -D_{AB} \frac{d\tilde{C}_A}{dz} + \tilde{x}_A (\tilde{C}_A u_A + \tilde{C}_B u_B) (5)$$

$$\tilde{N}_A = -D_{AB} \frac{d\tilde{C}_A}{dz} + \tilde{x}_A (\tilde{N}_A + \tilde{N}_B) (6)$$

This is another way of expressing the law of Fick, which says that molecules that pass through a point with fixed coordinates are due to the movement of the molecules and the current drag.

Diffusivity or diffusion coefficient is a measure of the resistance to the diffusion of A through the component B. Knowledge of the diffusion coefficient is very important in mass transfer, since it is used in almost all correlations that have to do with the sizing of the equipment.

3. DIFFUSION COEFFICIENT IN GASES

It has been obtained experimentally that the diffusion in gases increases with temperature and decreases with pressure and it is also depending on the size of the molecules, since larger molecules spread at a slower rate. There are numerous data on the diffusion coefficient of a gas into another, but the results are usually presented at given temperature and pressure. The diffusion coefficient is a constant very employed in mass transfer operations, so that when it is not possible to make experiments, there are correlations that give us the approximate values of the diffusion coefficients..

3.1 Obtaining experimental diffusion coefficient:-

The diffusion coefficient can be obtained through a cell of Arnold, Figure 1. The cell consists of a glass tube that is partially filled with liquid that is going to evaporate. By the top of the cell flows a stream of gas that carries the vapour formed in the tube. The gas that passes through the upper part is insoluble in liquid and therefore the flow into the fluid will be null.

Of equation (6)

$$\tilde{N}_A = -D_{AB} \frac{d\tilde{C}_A}{dz} + \tilde{x}_A (\tilde{N}_A + 0) \quad (07)$$

If we make suitable amendments and separate the variables and integrate within limits: z_1, \tilde{y}_{A1} to z_2, \tilde{y}_{A2} It is obtained:

$$\tilde{N}_{Az} = D_{AB} \frac{\tilde{C}}{z_2 - z_1} \frac{\tilde{y}_{A1} - \tilde{y}_{A2}}{\tilde{y}_{B1} \ln} \quad (08)$$

In the cell of Arnold the liquid level does not change, however in the cell used in this practice the level if it varies, Fig 2, so the above equation must be modified.

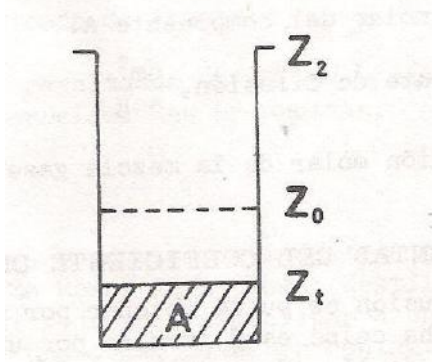


Fig. 2.

The flow in this case is a function of height.

$$\tilde{N}_{Az} = D_{AB} \frac{\tilde{C}}{z} \frac{\tilde{y}_{A1} - \tilde{y}_{A2}}{\tilde{y}_{B1} \ln} \quad (10)$$

And is related to a quantity of substance leaving the liquid phase.

$$\tilde{N}_{Az} = \tilde{C}_{AL} \frac{dz}{d\theta} \quad (11)$$

Equating equations (10) and (11)

$$\tilde{C}_{AL} \frac{dz}{d\theta} = D_{AB} \frac{\tilde{C}}{z} \frac{\tilde{y}_{A1} - \tilde{y}_{A2}}{\tilde{y}_{B1} \ln} \quad (12)$$

Separating variables and integrating between the limits, Z_0, θ_0 to Z_θ, θ .

It is obtained:

$$D_{AB} = \frac{\tilde{C}_{AL}}{\tilde{C}} \frac{\tilde{y}_{B1} \ln}{(\tilde{y}_{A1} - \tilde{y}_{A2})} \frac{Z_\theta^2 - Z_0^2}{2\theta} \quad (13)$$

That is the equation which is applied to the calculation of diffusion coefficients in the cell used in this practice. Where:

\tilde{C}_{AL} = molar concentration of the liquid. mol/cm³

\tilde{C} = Molar concentration of the gas mixture, mol/cm³.

Z_θ = distance from the top of the cell to the level of the liquid at the time θ , cm.

Z_0 = distance from the top of the cell to the level of the liquid at the time 0, cm.

θ = time, sec.

D_{AB} = coefficient of diffusion or difusividad.cm²s.

The diffusion which is carried out in this case, is also called diffusion through a stationary gas stationary, this type of diffusion is present in the unit operations absorption and humidification

In gases:

$$D_{AB} = D_{BA} \quad (14)$$

If you want data to other conditions, it is possible to calculate them using the equation:

$$D_{AB,T_2,P_2} = D_{AB,T_1,P_1} \left(\frac{P_1}{P_2} \right) \left(\frac{T_2}{T_1} \right)^{\frac{3}{2}} \quad (15)$$

In the literature there are several correlations to calculate these coefficients among them are those of Gilliland (2), Slattery, (3) Hirschfelder (4), Fuller (5), etc.

4. DESCRIPTION OF THE CELL USED

The device used to determine the coefficients of diffusion was proposed by Tapia, (1975) and consists of the following parts:

- (a) An U-shaped glass cell which has a graduated capillary tube in one of the branches. At the bottom of the cell is a valve that facilitates the circulation of fluid or prevents it. The cell is surrounded by an jacket of glass through which passes a liquid that keeps the cell at a constant temperature. Fig. 3.
- (b) A thermal bath that maintains the selected temperature in the water that circulates through the cell. Fig.4
- (c) A compressor that makes the air to pass through the top of the cell.
- (d) A cathetometer which is used to measure the height of the liquid in the cell.

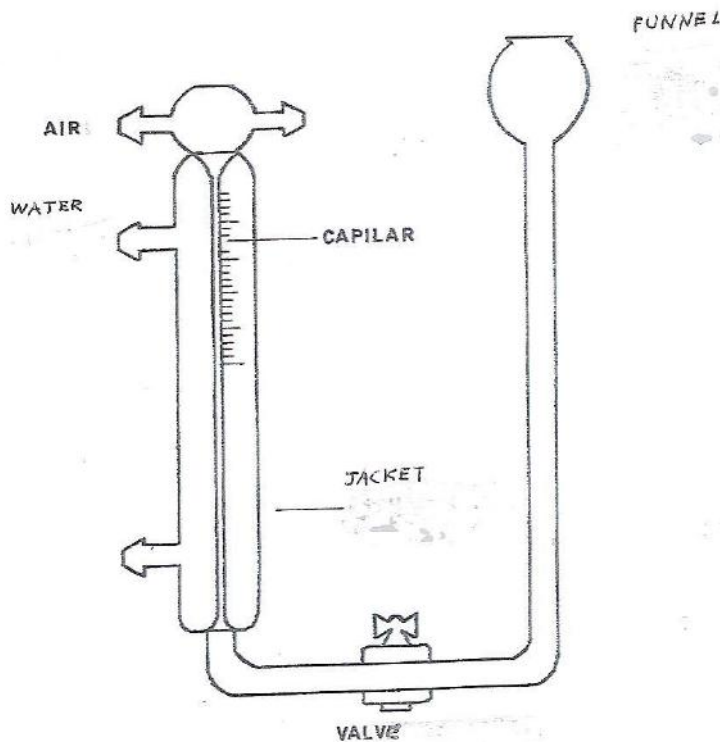


Fig. 3.

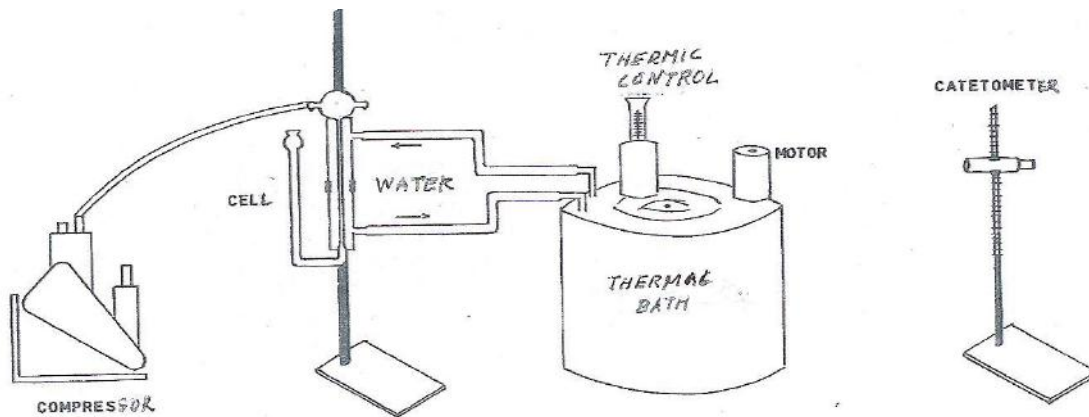


Fig.4

5. EXPERIMENTAL DEVELOPMENT

So that students can make the required experiments they should follow the following steps:

- 1.- Wash the cell perfectly and filled it with the fluid that is going to evaporate.
- 2.- Close the valve that connects two branches of the cell and place the cell with a pin in a support.
- 3.-Connect the upper part of the cell to a compressor and the jacket to the thermal bath.
- 4.-Select the working temperature.
- 5 -Startup the thermal bath and the compressor.
- 6.-Measure the initial height of the liquid in the cell with the cathetometer, generally the level must be 1.5 or 2 cm from the top of the cell.

7.-After a certain time, usually an hour, measure the level of the liquid in the cell.

5.1 Experimental data:-

In an particular experiment the students obtained the following data: (Table 1)

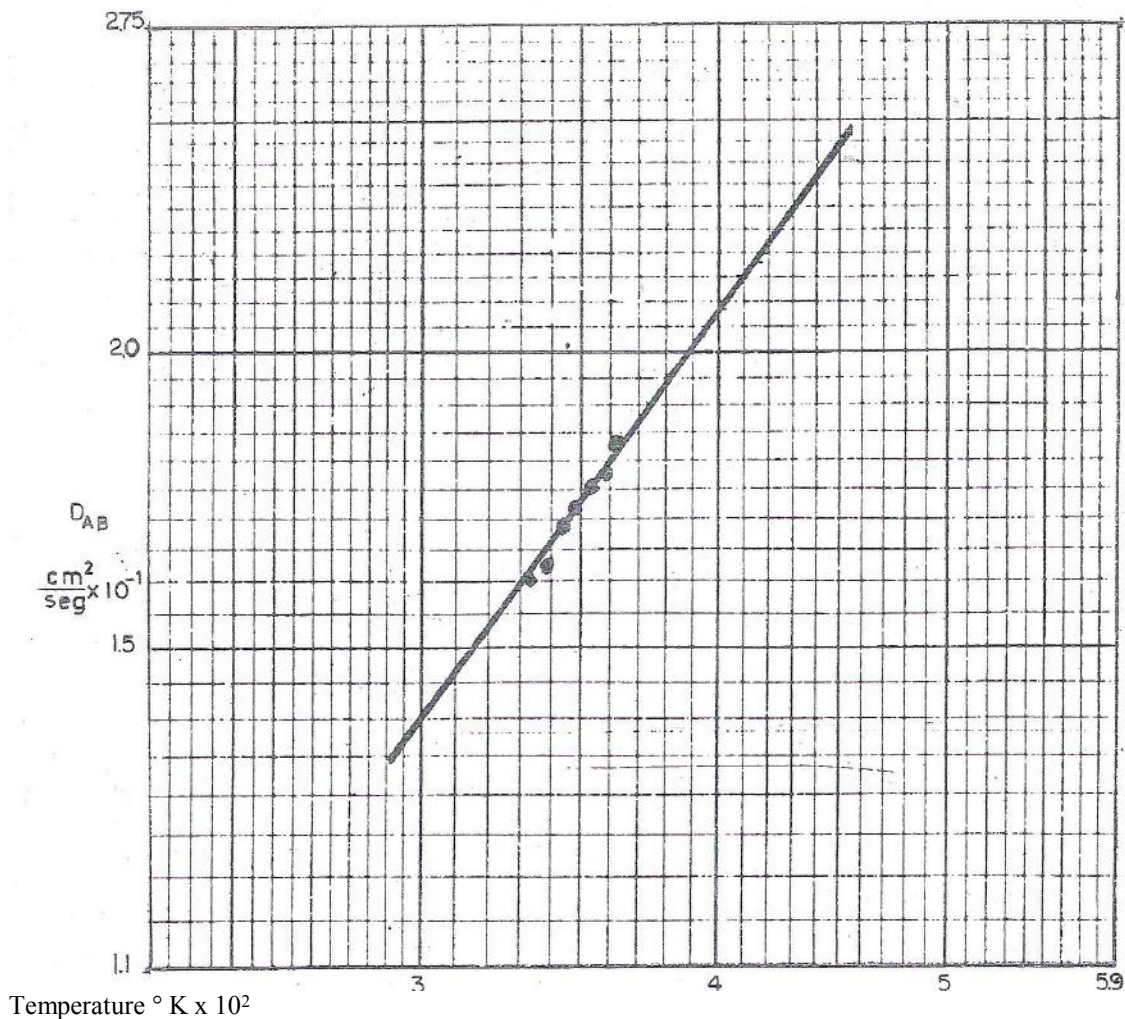
Table 1.-Air-acetic acid system.

D_{AB} cm^2/s	0.16	0.162	0.169	0.172	0.175	0.176	0.184		
$T^\circ \text{K}$	333	338	343	348	353	358	363		

The above data are presented in graph 1.

Graph 1

Variation of the diffusion coefficient with temperature for acetic acid system - air at the pressure of 586 mm of Hg (pressure in the city of Mexico).



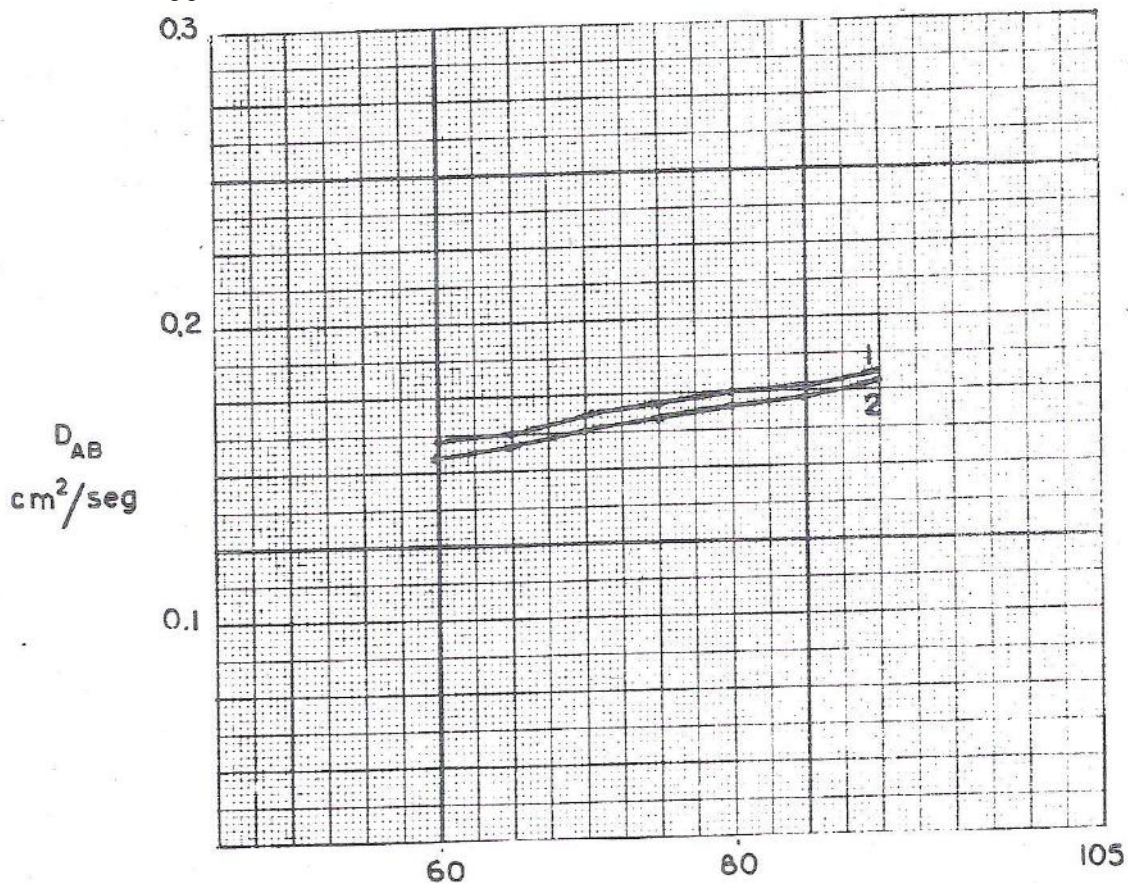
The slope obtained was 1.4 compared to the theoretical of 1.5.

The students also compared their results with those that can be obtained through theoretical equations such as the Gilliland [2], and obtained the following graph:

$$D_{AB} = \frac{0.0043 T^{\frac{3}{2}} \left(\frac{PM_A + PM_B}{PM_A \times PM_B} \right)^{\frac{1}{2}}}{P \left(V_{bA}^{\frac{1}{3}} + V_{bB}^{\frac{1}{3}} \right)^2} \quad (16)$$

Graph 2

Comparison of the experimental results with those obtained from the equation of Gilliland. Air-acetic acid system 586 mm Hg pressure



Temperature in °C

D_{AB} experimental curve 1

D_{AB} Gilliland curve 2

6. CONCLUSIONS

Through the experimental determination of the diffusion coefficients the students can understand what this means and how it behaves with the temperature. The experiments carried out by the students shows coefficients similar to which can be predicted by means of certain correlations. The apparatus proposed for the determination of these coefficients is reliable, cheap, and simple to operate.

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