Research Assistants

Elvan Konuk Tokak
Neslişah Ulus

DETERMINATION OF DIFFUSION COEFFICIENT FOR LIQUIDS AND GASES

1. INTRODUCTION

Molecular diffusion, often called simply diffusion, is the thermal motion of all (liquid or gas) particles at temperatures above absolute zero. The rate of this movement is a function of temperature, viscosity of the fluid and the size (mass) of the particles, but is not a function of concentration[1]. Diffusion explains the net flux of molecules from a region of higher concentration to one of lower concentration, but it is important to note that diffusion also occurs when there is no concentration gradient. The result of diffusion is a gradual mixing of material. In a phase with uniform temperature, absent external net forces acting on the particles, the diffusion process will eventually result in complete mixing[2].

The kinetic theory of the gases provides a means of visualizing what occurs, and indeed it was the success of this theory in quantitatively describing the diffusion phenomena which led to its rapid acceptance. In the case of a simplified kinetic theory, a molecule is imagined to travel in a straight line at a uniform velocity until it collides with another molecule, whereupon its velocity changes both in magnitude and direction. The average distance the molecule travels between collisions is its mean free path, and the average velocity is dependent upon the temperature. The molecule thus travels a highly zigzag path, the net distance in one direction which it moves in a given time, the rate of diffusion, being only a small fraction of the length of its actual path. For this reason the diffusion rate is very slow, although we can expect it to increase with decreasing pressure, which reduces the number collisions and with increased temperature, which increases the molecular velocity[4].

Diffusion is quite different from the movement of molecules when a fluid is flowing. In this case movement is not random; all molecules are moving together and in the same direction[3].

In biological systems, diffusion plays an essential role in the transport, over short distances (for example across cell membranes), of molecules such as nutrients, respiratory gases (carbon dioxide and oxygen)[3].

One application of diffusion is the separation of isotopes, particularly those of uranium. When uranium hexafluoride diffuses through a porous plate, the ratio of the 235 and 238 isotopes is changed slightly. With sufficient number of passes, the separation is nearly complete. There are large plants in the USA and UK for obtaining enriched fuel for fast nuclear reactors and the fissile uranium-235, originally required for the first atom bombs. Another application is the diffusion pump, used extensively in vacuum work, in which the gas to be evacuated diffuses into a chamber from which it is carried away by the vapour of a suitable medium, usually oil or mercury[3].

2. THEORY

When there is a concentration gradient in a multicompartment thermodynamic system, a matter irreversible flux starts from the high concentrations to the low ones. This flux is called **"diffusion".** The diffusion tends to give back the system to its balance state, of constant concentrations. Fick's Law describes the diffusion. For the statement of such law, binary mixes will be only considered, although possible similar developments are possible for multicomponent mixes[5].

2.1 Fick's Law of binary mixes

Let's consider the system represented on Figure 2.1. In such system, a liquid A evaporates in an insoluble pure gas B.

At the same time, the liquid A comes out very slowly by the bottom of the system, as it is shown on the Figure 2.1. The vapors do the same when they are removed by a draft of gas B that flows by the top of the system.

In view of the circumstances regarding the concentration differences of A between the gas in contact with liquid and the gas in the top, there will be constantly a movement of the vapors through the narrow tube to the top. On the other hand, the gas mix will move globally to downward, because of the liquid emptiness. If this emptiness is slow enough, the net movement of A will be upward.

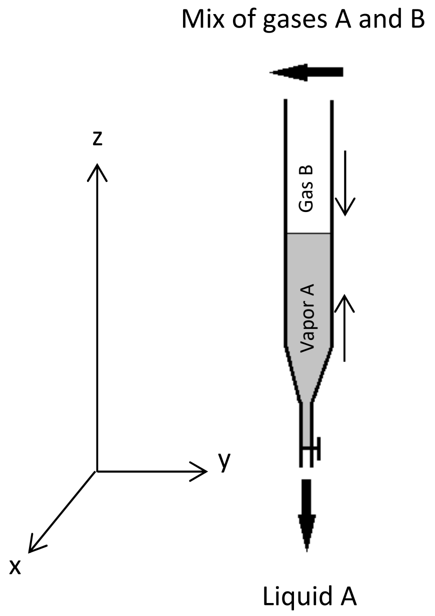

Figure 2.1. Diffusion of a vapor A in a gas B, which is insoluble in the liquid phase A

The experimental Fick's Law of the diffusion establishes that in a system in which there is concentration gradient, the component A moves, regarding the mixing global movement, taking the direction of the concentration negative gradient C_A, according the following equation.

$$J_A = -D_{AB}.\nabla C_A \tag{1}$$

where;

J_A = Molar flux of A (kgmol A/s.m^2)

D_{AB} = Diffusion coefficient, molecular diffusivity of the molecule A in B (m^2/s)

C_A = Concentration of A (kg/m^3)

∇C_A = gradient operator applied to concentration of A (kg/m^3)

The equation (1) is not the usual form of Fick's Law, since the coefficient D_{AB} depends on the system concentration. That is why the next expression is preferred:

$$J_A = -C.D_{AB}.\nabla x_A \tag{2}$$

where;

x_A = Mole fraction of A

This equation represents the so-called **Fick's Law** of the diffusion. In this case, the diffusivity D_{AB} is almost independent of the system concentration.

The units in the international system for the diffusion coefficient (D_{AB}) are [m^2/s], although, frequently, they are expressed in [cm^2/s]. The diffusivity numerical values change a lot depending on the system that is considered. This variation is especially important when the different states of matter aggregation are considered thus, the gases diffusivities change usually at the interval from 10^{-5} to 10^{-4} [m^2/s], whereas for the liquids the variation is found at the interval from 10^{-10} to 10^{-9} [m^2/s]. The diffusivity in the solids varies a lot from a system to another one, and their values are much smaller, approximately from 10^{-34} to 10^{-14} [m^2/s].

Although the gases kinetic theory is very simple, it is interesting to watch a gas diffusivity dependence with the pressure and the temperature. The diffusion coefficient increases with the temperature and decreases with the pressure[5].

Another very useful form to express the first Fick's Law is:

$$N_A = x_A(N_A + N_B) - C.D_{AB}\nabla x_A \qquad (3)$$

where;

N_A, N_B = Rate of convective mass transfer (kgmol/m^2.s)

x_A = Mole fraction of A

D_{AB} = Molecular diffusivity of the molecule A in B (m^2/s)

C = Concentration (kg/m^3)

Equation (3) is the final general equation for diffusion plus convection which can be said as the "combined flux". "$x_A(N_A + N_B)$" term indicates the "convective flux" and "$C.D_{AB}\nabla x_A$" indicates the "molecular flux"[5].

2.2 Applicaton of Fick's Law for the Diffusivity Determination.

The experimental determination of the diffusion coefficient, D_{AB}, for a binary mixing can be made through a device similar to the one shown on Figure 2.2. Let's consider indeed a test tube with dimensions such that the effects in the system limits can be disregarded. Let's suppose likewise that inside a pure liquid A evaporates slowly and continuously; and that its vapors are spreaded over B, an inert gas in rest. During the experiment, the temperature and the pressure are kept constant. On the other hand, the diffusion will be only considered in the direction of the axis "z". If the evaporation is slow enough, the surface level will remain almost constant, and as a result, there will be no flow of B in the test tube inside. That is to say, $N_B=0$ (the gas is insoluble in the liquid)[4].

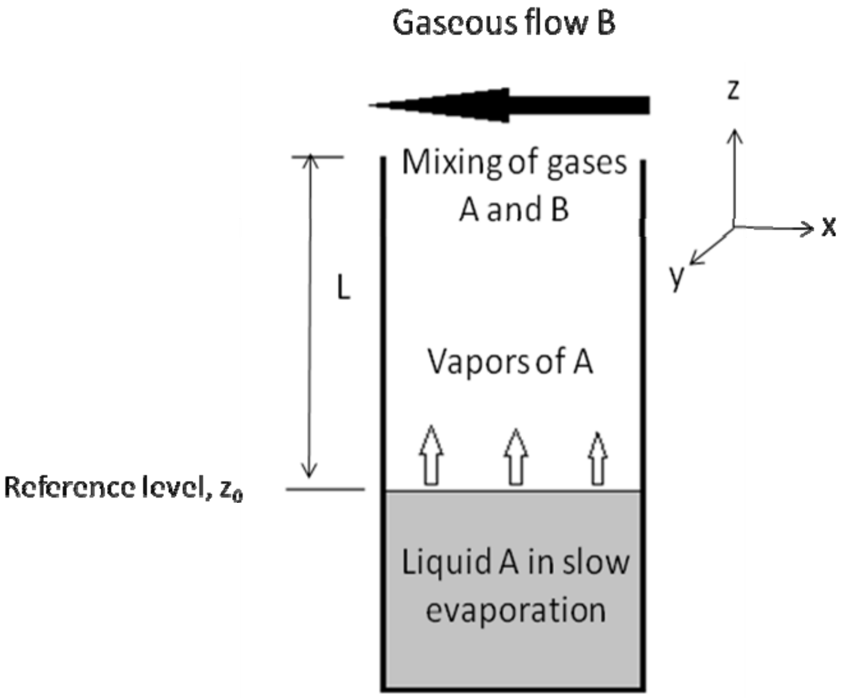

Figure 2.2 Device to measure the diffusivity for a gaseous environment

Regarding this hypothesis goodness, it is useful to remind that, in normal conditions, the volume of an evaporated gaseous mass is hundreds of times above the volume occupied in the liquid phase.

Since there is only flow in the direction of the axis “z”, the matter microscopic balance for the component A in a stable state and in absence of chemical reaction will be:

$$\frac{d(N_A)z}{dz} = 0 \qquad (4)$$

where;

N_A = Rate of convective mass transfer (kgmol/m^2.s)

z = Distance from reference level z_0 (m)

Therefore, integrating;

$$N_{Az} = C_1 \qquad (5)$$

And C_1 is an integration constant. This last equation shows that the molar flow density of A in the direction of the axis “z” is constant, that is to say, the molar flow that goes through any section is the same one.

Applying Fick’s Law in its form expressed by the equation (3) and formulating properly the component “z” of the gradient operator in cylindrical coordinates, the result will be:

$$N_{Az} = x_A\,(N_{Az} + N_{Bz}) - C.\,D_{AB}\,\frac{dx_A}{dz} \qquad (6)$$

And, since there is no flow of component B, it will be possible to write:

$$N_{Az}.\,dz = -C.\,D_{AB}.\frac{dx_A}{1-x_A} \qquad (7)$$

Differential equation which integral is obtained directly, being constants N_{Az} and c are ideal when the pressure and the temperature are constant. Likewise, D_{AB} is considered invariable. Thus:

$$N_{Az}.\,z = C.\,D_{AB}.\ln(1 - x_A) + C_2 \qquad (8)$$

where C_2 is a new integration constant. On the other hand, there are two boundary conditions, which the composition of the gas must comply with; on the first place, if in the interface gas-liquid it is admitted that the partial pressure of A, p_A, the vapor pressure for the pure component to the temperature of the experiment, and Dalton's Law is fulfilled, the result will be:

For z= 0 $$x_A = \frac{p_A}{P} = x_{A,0} \qquad (9)$$

Being p the total pressure of the system, and

For z= L $$x_A = x_{A,L} \qquad (10)$$

Where L (m) is the length of the test tube (Figure 2.2) that contains the gaseous mixing and $x_{A,L}$ is the molar fraction of A in the gaseous flow A-B that circulates on the upper part of the test tube.

Applying both boundary conditions to the integrated equation, the result, easily obtained, will be an expression for the diffusivity calculation:

$$D_{AB} = \frac{N_{Az}.L}{C} \cdot \frac{1}{ln\frac{1-x_{A,L}}{1-x_{A,0}}} \qquad (11)$$

If it is preferred, this last equation can be written according to the partial pressures of the gases A and B. Thus, if it is indicated by p_{BL} to the partial pressure of the gas B on the upper part of the test tube, and through p_{B0} to the partial pressure of this gas in the interface, having in mind that for an ideal gas, C= P/RT, it is obtained:

$$D_{AB} = \frac{N_{Az}.L.R.T}{P.\ln\left(\frac{p_{BL}}{p_{B0}}\right)} \qquad (12)$$

This equation allows the estimation of diffusivities if the user knows the total pressure P, the temperature T and the values for the partial pressures of B in the interface and on the upper part of the test tube. N_{Az} is calculated by a weighing or by lectures of level from the evaporated moles of A (m_{ev}) (kg) in a certain period of time (t_k) (s), knowing, of course, the cross sectional area of the test tube, A^*:

$$N_{Az} = \frac{n_{ev}}{t_k A^*} \qquad (13)$$

From the developed equations, it is possible to estimate a concentration profile for A or for B.

Applying the first condition limit to the equation (8), it is obtained:

$$N_{Az}.z - C.D_{AB}.ln\frac{1-x_A}{1-x_{A,0}} \qquad (14)$$

As a result, it is obtained:

$$x_A = 1 - (1 - x_{A,0}).e^{N_{Az}.z/C.D_{AB}} \qquad (15)$$

It is an equation that relates the concentration variation (x_A) with the position z. That is to say, it is the expression of the concentration profile. On the other hand, from the equation (11) and (14), another alternative expression obtained for such profile:

$$\frac{z}{L} = \frac{\ln[\frac{1-x_A}{1-x_{A,0}}]}{\ln[\frac{1-x_{A,L}}{1-x_{A,0}}]} \qquad (16)$$

As a result, it is deduced that:

$$x_A = 1 - (1 - x_{A,0}).(\frac{1-x_{A,L}}{1-x_{A,0}})^{z/L} \qquad (17)$$

It is a similar equation to the (15) one, but according to both boundary conditions.

Actually, n_{ev} is the number of evaporated moles; remaining that the number of moles is the mass, n_{ev}, divided by the molecular weight, M_A, and the result is:

$$N_{Az} = \frac{n_{ev}}{t_k.A^*} = \frac{m_{ev}}{M_A.t_k.A^*} \qquad (18)$$

where;

m_{ev} = Evaporated mass of A (kg)

M_A= Molecular weight of A (kg/kgmol)

And to find the value of the mass:

$$m_{ev} = N_{Az}.M_A.t_k.A^* \qquad (19)$$

Finding the value of the unknown quantity and taking the derivative of the mass regarding the time:

$$\frac{\partial m_{ev}}{\partial t} = N_{AZ}\,.M_A\,.A^* \tag{20}$$

On the other hand, the mass flow equals:

$$\dot{m} = \rho.v.A^* \tag{21}$$

where;

$\dot{m}$= Mass flow rate (kg/s)

ρ = Density (kg/m^3)

v = Linear velocity (m/s)

As the mass flow is the change of the mass regarding the time, and the velocity is the change of the space regarding the time, the result will be:

$$\frac{\partial m_{ev}}{\partial t} = \rho.A^*.\frac{\partial z}{\partial t} \tag{22}$$

If the equations (20) and (22) are made equal, the result will be :

$$N_{AZ}\,.M_A\,.A^* = \rho.A^*.\frac{\partial z}{\partial t} \tag{23}$$

Deleting the common elements:

$$N_{AZ}\,.M_A = \rho.\frac{\partial z}{\partial t} \tag{24}$$

Substituting N_{AZ} by its value obtained from the equation (14), $N_{AZ}.z = C\,D_{AB}\ln\frac{(1-x_A)}{(1-x_{A,0})}$,

the result will be:

$$\frac{C\,D_{AB}\ln\frac{(1-x_A)}{(1-x_{A,0})}}{z}.M_A = \rho.\frac{\partial z}{\partial t} \tag{25}$$

Tidying up some terms:

$$\frac{C\, D_{AB} \ln\frac{(1-x_A)}{(1-x_{A,0})}}{\rho} . M_A\, \partial t = z . \partial z \tag{26}$$

By grouping the constant terms in only one term which will be called α, and having in mind that for an ideal gas, C= P/RT, it is obtained :

$$\alpha = \frac{C \ln\frac{(1-x_A)}{(1-x_{A,0})}}{\rho} . M_A = \frac{P.M_A}{R.T.\rho} . \ln\frac{(1-x_A)}{(1-x_{A,0})} \tag{27}$$

Substituting:

$$\alpha . D_{AB} . \partial t = z . \partial z \tag{28}$$

Taking the integral:

$$\alpha . D_{AB} . \int_0^t \partial t = \int_{z_0}^{z} \partial z \tag{29}$$

where; z_0 is the reference level to compare with the point z.

The result is:

$$\alpha . D_{AB} . t\Big]_0^t = \frac{z^2}{2}\Big]_{z0}^{z} . \partial z \tag{30}$$

Operating :

$$\alpha . D_{AB} . (t-0) = \frac{(z^2 - z_0^2)}{2} = \frac{(z-z_0)(z+z_0)}{2} \tag{31}$$

Developing the differences of squares:

$$\alpha.D_{AB}.t = \frac{(z-z_0)(z+z_0)}{2} \tag{32}$$

Tidying up:

$$2\alpha.D_{AB}.t = (z-z_0)(z+z_0) \tag{33}$$

Operating

$$\frac{t}{(z-z_0)} - \frac{1}{2\alpha.D_{AB}}(z+z_0) - \frac{1}{2\alpha.D_{AB}}(z-z_0+z_0-z_0) \tag{34}$$

Grouping again:

$$\frac{t}{(z-z_0)} = \frac{1}{2\alpha.D_{AB}}(z-z_0+2z_0) \tag{35}$$

Finally, the final expression is:

$$\frac{t}{(z-z_0)} = \frac{1}{2\alpha.D_{AB}}.(z-z_0) + \frac{(z_0)}{\alpha.D_{AB}} \tag{36}$$

to which corresponds an equation of a straight line with the form:

$$y = a.x + b \tag{37}$$

Thus, representing $\frac{t}{(z-z_0)}$ regarding (z-z$_o$) the diffusivity D_{AB} can be obtained from the slope of straight line[1].

2.3 Prediction of diffusivities for binary solutions

Since the theory for diffusion in liquids is not very well established as yet, the equations for predicting diffusivities in liquids are by neccessity semiemprical.

However, we shall review briefly the basic theoretical equations from which the final semi empirical equations are derived[6].

Basic theoretical equations for dilute solutions

The Stokes-Einstein equation, one of the first theories, was derived for a very large spherical solute particle(A) diffusing through a liquid solvent (B) of small particles. The Stokes law was used to describe the drag on solute particle as it moved. The equation is:

$$D_{AB} = \frac{9.96x10^{-16}T}{\mu_B V_A{}^{1/3}} \qquad (38)$$

where D_{AB} is diffusion coefficient (m^2/s) μ_B is the viscosity and V_A is the molar volume of solute.This equation applies very well to very large unhydrated molecules of about 1000 molecular weight and greater in low-molecular-weight solvents or where the molar volume V_A of the solute is above about 500 cm^3/g mole[7].

The theory of absolute reaction rates by Eyring [Geancoplis, Perkins]. Has also been used to predict viscosity, thermal diffusivity, and molecular diffusion coefficients. The liquid is treated as a lattice like array of molecules, which is imperfect because of holes or vacancies. The solute molecules carrying momentum, heat or mass migrate or jump from one hole or equilibrium position to another. As the molecules migrates, it actually carries momentum, heat or thermal energy, and mass-a different species of meterial. However, heat and momentum can also be transported by an additional mechanism by actual collision with adjacent molecules without migrating to a "hole". Hence, the mass diffusivity will be the smallest of the three. For example, in water at ºC the self-diffusivity of water , D_{AA}, is $1.35x10^{-5}$ cm^2/s, thermal diffusivity α ($k\rho/C_p$) is $142x10^{-5}$ cm^2/s, and momentum diffusivity μ/ρ is $1790x10^{-5}$ cm^2/s. Hence, actual migration mechanism is small compared to the collision mechanism in liquids. The final equations of the absolute reaction rate theory paralel those by the Stokes-Einstein method and do not predict the diffusivities for liquids well. Arnold [Thakar] applied the kinetic theory of gases to the liquid state and predicted the diffusivity to be proportional to $1/\mu^{0.5}$ [7]

Estimation of diffusion coefficients in dilute solutions

The Wilke-Chang correlation can be used for most general purposes where the solute (A) is dilute in the solvent (B):

$$D_{AB} = 1.173x10^{-16}(\varphi M_B)^{\frac{1}{2}}(T/\mu_B V_A{}^{0.6}) \qquad (39)$$

where M_B is the molecular weight of B, μ_B is the viscosity of B in Eq.(39),V_A is the solute molar volume at the boiling point, and φ is an “association parameter” of the solvent, where φ is 2.6 for water, 1.9 for methanol,1.5 for ethanol and for benzene, ether, heptane or other unassociated solvents. When molar volumes are above about 400 cm^3/g mole in low-molecular-weight solvent, the Stokes-Einstein equation should be used. When water is the solute, the values predicted from Eq. (39) should be multiplied by a factor of 1/2.3. Eq. (39) predicts the diffusivities with a mean deviation of about 10-15 percent for aqueous solutions but only to about 25 percent in nonaqueous solvents. Data indicate that the temperature correction of D_{AB} proportional to T/μ_B may over correct. The equation should be used with caution outside the temperature range of 5 to 40 °C. Perkins and Geancoplis state that for highly viscous liquids of hydrocarbons and glycerol the viscosity exponent should be less than 1.0 and between 0.5 and 1.0 [6].

Othmar and Thakar give a simple equation for solutes (A) in water (B), which is as accurate as Eq. (39)

$$D_{AB} = \frac{14x10^{-5}}{\mu_B^{1.1} V_A^{0.6}} \tag{40}$$

where μ_B is again cp. This equation is often preferred for water as the solvent.

2.4 Prediction of diffusivity for gases

The diffusivity of a binary gas mixture in the dilute gas region, that is low pressures near atmosheric, can be predicted using the kinetic theory of gases. The gas is assumed to consist of rigid spherical particles that are completely elastic on collision with another molecule, which imlies that momentum is conserved[8].

In a simplified treatment it is assumed that there are no attractive or repulsive forces between the molecules. The derivation uses the mean free path λ, which is the average distance that a molecule has traveled between collisions.

The final equation is:

$$D_{AB} = \frac{1}{3} v\lambda \tag{41}$$

where D_{AB} is the diffusivity in m^2/s, v is the average velocity of the molecules[8].

Semi emprical method of Fuller, which is more convenient to use is often preferred. The equation was obtained by correlating many recent data and uses atomic volumes.

The equation is:

$$D_{AB} = \frac{1.00x10^{-7} T^{1.75} (1/MA + 1/MB)^{1/2}}{P[(\sum VA)^{1/3} + (\sum VB)^{1/3}]^2} \quad (42)$$

where D_{AB} is the diffusivity in m^2/s, T temperature in K, M_A is the molecular weight of A in kg/kg mol M_B is the molecular weight of B, P absolute pressure in atm, $\sum VA$ sum of structural volume increments for A, $\sum VB$ sum of structural volume increments for[8].

The equation shows that D_{AB} is proportional to 1/P and $T^{1.75}$. If an experimental value of D_{AB} is available at a given T and P and it is desired to have a value of D_{AB} at another T and P, one should correct the experimental value to the new T and P by means of relationship $D_{AB} \alpha T^{1.75}/P$ [8].

3. EXPERIMENTAL PROCEDURE

3.1 SAFETY

People who work in laboratories are exposed to many kinds of hazards. However, many accidents in the laboratory can be prevented if each person in the laboratory observes a set of common precautions and uses proper experimental techniques and procedures at all times.

Please follow these instructions when you came across an accidental situation.

- If you receive a chemical splash (NaCl solution) to your eyes, immediately flush eyes with plenty of water at least 15 minutes, lifting upper and lower eyelids occasionally[9].
- Inhalation of asetone vapors irritates the respiratory tract. It may cause coughing, dizziness, dullness, and headache. If you come across high concentration of acetone vapor, come out to take fresh air [9].
- Spills shall be cleaned immediately. Small spills of liquids on bench tops shall be cleaned immediately with personal protective equipment (gloves) to prevent contact with skin or clothing.
- Your hands and the buttons of the device have to be dry when you working with an electrical device.
- It is the responsibility of everyone working in the laboratory to make certain that the laboratory is left clean after work is performed.

3.2 PART I Diffusion in Liquids

The unit which is used during the experiment (Figure 3.1) consists of :

- A liquid tank
- A magnetic stirrer and magnet
- A conductimeter
- A conductivity sensor
- A diffusion cell (capillaries number (N)= 317 capillary length (x)= 5 mm)
- Thermostatic bath (water bath, resistance, level switch, temperature sensor)
- A console that includes:

- ✓ Temperature digital indicator
- ✓ Digital controller of the water temperature
- ✓ Heating resistor switch
- ✓ Level switch
- ✓ Water temperature sensor
- ✓ General switch

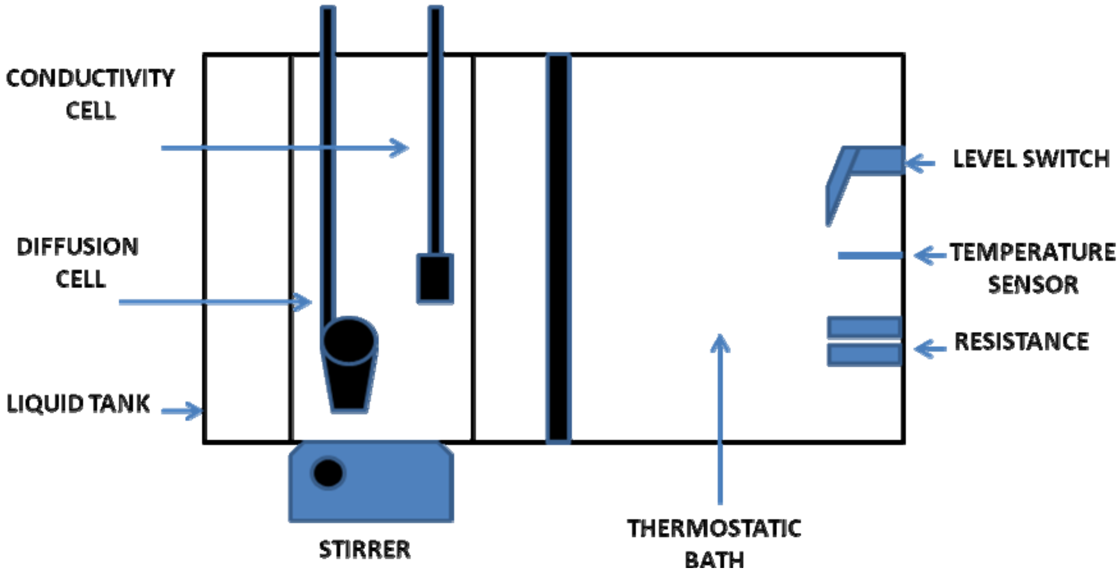

Figure 3.1. “Liquid diffusion” experiment system

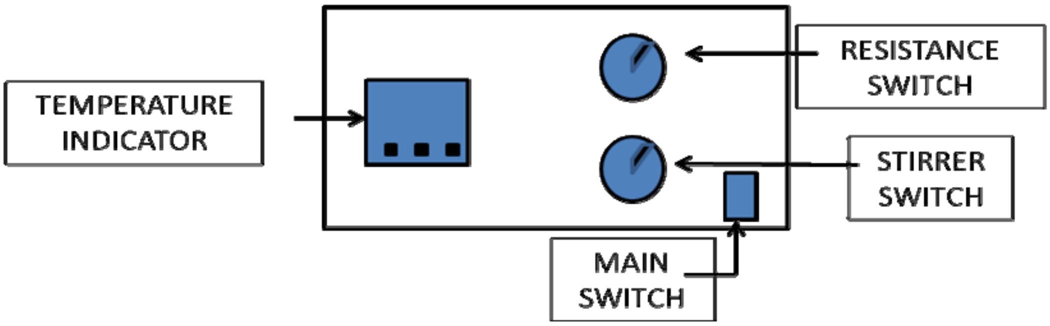

Figure 3.2. Control console of “liquid diffusion” experiment system

The electrical conductivity of aqueous solutions is governed by the presence and concentration of ions in solution. Therefore, pure water does not conduct an electrical current well since the concentrations of hydrogen and hydroxide ions are very small. Solutes whose solutions are conductive are called electrolytes and a solute is considered a strong electrolyte if it dissociates completely into its constituent ions e.g. NaCl and KI aqueous solutions. Thus, if concentration is higher, that means more ions are present per volume of water and the conductivity of the solution will be higher. Conductivity has the SI units of siemens per metre ($S \cdot m^{-1}$) and cgs units of inverse second (s^{-1}).

Diffusion in Liquids

- Prepare NaCl solutions at different concentrations (2 M, 1.5 M, 1M).
- Fill up completely the cell with NaCl solutions (1M, 1.5 M, and 2 M, respevtively) and clean up any excess from the solution of the cell outside and from the capillary ends using filter paper.
- Put the cell in its position within the receptacle.
- Fill the receptacle of the measurement unit with distilled water.
- Turn on the magnetic stirrer at a not very quick speed.
- Turn on the conductimeter and measure the conductivity every 30 seconds.
- Turn on the resistance when the cell was filled up with 2M NaCl solutions and repeat the same measurements at 50°C.

3.3 PART II Diffusion in Gases

The unit which is used during the experiment (Figure 3.3) consists of :

- A narrow vertical tube with a known inside diameter
- An air pump
- An air optical system, with a precision focusing adjustment, assembled on an element of vertical movement with a capiler and a vernier
- A water bath to regulate the volatile liquid temperature
- A console that includes:
    - ✓ Temperature digital indicator
    - ✓ Digital controller of the water temperature
    - ✓ Heating resistor switch
    - ✓ Air pump switch
    - ✓ Level switch
    - ✓ Water temperature sensor
    - ✓ General switch

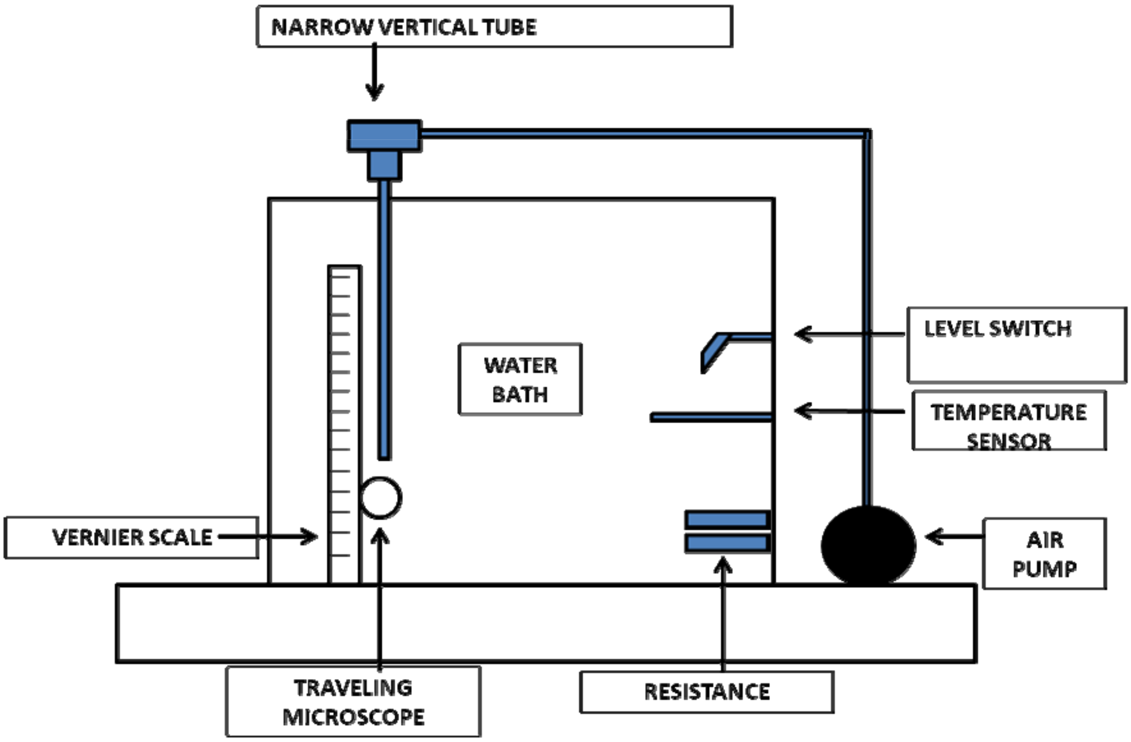

Figure 3.3. “Gas diffusion” experiment system

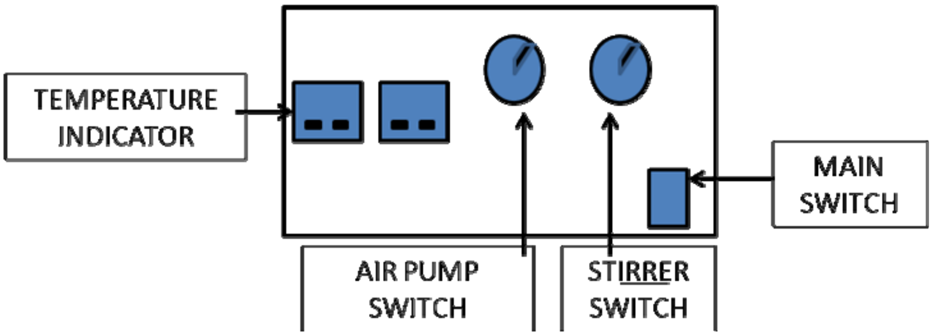

Figure 3.2. Control console of “gas diffusion” experiment system

Diffusion in Gases

- Fill up the capillary tube with acetone and note of acetone highness.
- Take note of acetone highness every 60 minutes.
- Turn on the resistance and perform the same experiment at 45°C.

4. CALCULATIONS AND DISCUSSION

4.1 Diffusion in Liquids

- Find the ratio between the concentration of a saline solution and the conductivity
- Calculate the diffusion coefficient of 2M saline solution from the conductivity data.
- Calculate the diffusivity of 1.5 M and 1 M NaCl solutions from the conductivity data. Compare the diffusion coefficients of saline solutions at different concentrations. Discuss the effect of concentration in the diffusivity and the reasons of the differences between them.
- Calculate the diffusion coefficient of 2M NaCl solution at 25ºC and 50ºC. Discuss the effect of temperature in the diffusivity and the reasons of the differences between them.

4.2 Diffusion in Gases

- Calculate the diffusivity of acetone and discuss the vapor diffusion of acetone in the air.
- Determine the molar flux density of the volatile liquid.
- Calculate the diffusion coefficient of acetone at 25ºC, 35ºC, 45ºC. Discuss the effect of temperature in the diffusivity and the reasons of the differences between them.
- Represent graphically the concentration profiles of acetone and air.

5. NOMENCLATURE

A^* : Cross sectional area of the tube (m^2)

C : Concentration (kg/m^3)

C_0 : Initial concentration (kg/m^3)

C_A : Concentration of A (kg/m^3)

C_1, C_2 : Integration constant

D : Diameter of a capillary (m)

D_{AB} : Molecular diffusivity of the molecule A in B (m^2/s)

J_A : Molar flux of A (kgmol $A/s.m^2$)

L : Length of test tube (m)

m_{ev} : Evaporated mass of A (kg)

M_A : Molecular weight of A (kg/kgmol)

M_B : Molecular weight of B (kg/kgmol)

n_{ev} : Evaporated mole of A (mol)

N_A : Rate of convective mass transfer (kgmol $A/s.m^2$)

P : Total pressure (N/m^2)

p_A : Partial pressure of A (N/m^2)

p_{B0} : Partial pressure of gas in the interface (N/m^2)

T : Temperature (K)

t_k : Passed time (s)

v : Lineer velocity (m/s)

V_A : Molar volume of the solute (m^3/mol)

VA : Atomic diffusion volumes for gas A to use with Eq. 42

VB : Atomic diffusion volumes for gas B to use with Eq. 42

x_A : Mole fraction of A

z_0 : Reference level of the liquid (m) (Figure 2.2.)

z : Distance from the reference level (m)

ρ_A : Volatile liquid density (kg/m^3)

μ : Viscosity of the solution (kg/m.s)

φ : Association parameter of the solvent

λ : Mean free path

6. REFERENCES

[1] Maton, Anthea; Jean Hopkins, Susan Johnson, David LaHart, Maryanna Quon Warner, Jill D. Wright. Cells Building Blocks of Life. Upper Saddle River, New Jersey: Prentice Hall. pp. 66–67 (1997).

[2] D. Brogioli and A. Vailati, Diffusive mass transfer by nonequilibrium fluctuations: Fick's law revisited, Phys. Rev. E 63, 012105/1-4 (2001).

[3] http://encyclopedia.farlex.com/Fick%27s+first+law+of+diffusion

[4] "Determination of Diffusion Coefficient for Liquids and Gases" Practices Manual, EDIBON, S.A.

[5] Geankoplis, C. J., "Transport Processes and Unit Operations", 3rd Edition, p. 388 (2003).

[6] Wilke, C. R., and Chang, Pin. A.I.Ch.E.J., 1, 264 (1995).

[7] Reid, R. C., Prausnitz, J. M., and Sherwood, T.K. The properties of gases and liquids, 3rd ed. Newyork: McGraw-Hill Book Company, (1977).

[8] Fuller, E.N., Schettler, P.D., and Giddings, J. C. Ind. Eng. Chem., 58, 19 (1996).

[9] http://www.jtbaker.com/msds/englishhtml/a0446.htm

Name Surmane: **Date:**

Asistant:

Group number:

DATA SHEET

1. *Determination of Diffusion Coefficients of Gases*

T (°C) = T (°C) =

Time (min)	Height (mm)

Time (min)	Height (mm)

2. *Determination of Diffusion Coefficients of Liquids*

C = 1 M

Time (min)	Conductivity (S/m)

C = 1,5 M

Time (min)	Conductivity (S/m)

C= 2 M

Time (min)	Conductivity (S/m)