One-dimensional Model of the Diffusion Process Using the Quantum Mechanics Concepts

Raúl C. Pérez, and Robles N.

IEMI, Department of the Basic Subjects, Mendoza Regional Faculty, Technology National University, Argentina

Abstract: The diffusion process are presents in many areas of the sciences and engineering, traversing horizontally the different thematic. It is possible to mention as example, the environmental impacts, and its influence on the chemical, the construction and food industry process, etc. The deep knowledge of the diffusion process, it is possible to make a beneficial use of them in different areas mentioned. So, also using the new knowledge is possible developed a model from the experimental data, that it can simulate all phenomena in which intervene the diffusion process. In order to analytic develop of model, it can use the quantum mechanic formalism to resolve the Fick's equation. With all these acknowledge and de model, it can simulate wished situation of diffusion process to determine parameters and variables necessary in order to make more efficient and beneficial all diffuser process.

Keywords: Model, diffusion process, quantum mechanics concepts

1. Introduction

The diffusion is a physical and chemical process that are present in many areas of the sciences and engineering, traversing horizontally the different thematic.

It is possible to mention as example, the environmental impacts that produce the acid rain, its roll on the cloud drop formation [1]. As well also, the influence on the chemical, the construction and food industry, etc.

With the deep knowledge of the diffusion process, it is possible to make beneficial use of them in different areas of the science, the engineering and the industry.

1.1 Diffusion Theory

It is known as diffusion to the thermal motion of all particles in liquid or gas state, at determinate temperature T, entering another diffuser material. The speed of this movement is function of the temperature, the viscosity and the mass of the particles. The diffusion phenomenon is to describe the net flow of the molecules from a region of higher concentration to a region of lower concentration, due to the pressure difference between them. Of course, if the concentrations are equals, the molecules keep moving, but the pressure gradient is null, then the diffusion process finish. The particles motion is governed to equilibrium process of auto diffusion due at the molecular random motion.

The result of the diffusion process is a gradual mix of matter, in such a way that the distribution of molecules is uniform.

On the equilibrium situation, the molecular motion is called "dynamic equilibrium".

The molecular diffusion is usually formalized mathematically using the Fick's diffusion laws. These laws are the quantitative nature, formally represented to differential equations that describe these phenomena. Adolf Fick (1829-1901).

(1) First Fick's Law

This law established the relation between the perpendicular diffusive flow at the determinate area, and the concentration in stationary state. The particle flux goes from the high concentration region to the

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Corresponding author: Raúl C. Pérez, Dr., Professor, research fields: theoretical physics, noelia robles, chemical engineering.

lower concentration area, with a magnitude that is proportional at the concentration gradient.

In such case, under these concepts, the first Fick's law has the mathematical form:

$$J = -D\nabla C \qquad (1)$$

Where:

D represents the proportionality constant, whose physical means are the properties of the diffuser material, it is known as diffusion coefficient.

J is the particles diffusion flow, perpendicular to a certain area of the interesting study.

∇C is the concentration gradient.

(2) Second Fick's Law

Under the same concepts explained in the first Fick's law, but operating mathematically, under the considerations of the mass conservation in all chemical reactions, it will obtain:

$$\frac{\partial C}{\partial t} = D\nabla^2 C \qquad (2)$$

The last Eq. (2) is very util to get its analytics solutions, conveniently applying the initials and boundary conditions.

It is interesting to see, that the Eq. (2) had a full analogy with the Schrödinger's differential equation of the quantum mechanics, to the free motion of the particles, whose expression is:

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\nabla^2 \Psi \qquad (3)$$

The squared value of the solution function Ψ of the differential Eq. (3) physically represents the most probable value that the particles is in a determinate position at a given time.

This analogy opens an important door to approach the study of the diffusion process using the formalism and concepts of the quantum mechanics. This situation to allow to develop a new way to study the diffusive phenomena.

2. Hypothesis

For the exposed above, it is possible to study the diffusion process using the conceptual formalism of quantum mechanic. Particularly to the one-dimensional simple case of the particles flux when penetrate a diffuser material traversing the potential energy barrier.

2.1 Objectives

To develop an analytic model of the diffusion process using the quantum mechanics formalism, especially to the study of the behavior of the diffusion coefficient.

To resolve the Fick's equation to the diffusive phenomena, to get a diffusion coefficient behavior and analytic model using the quantum mechanics concepts.

3. Development

It is possible to perform an analogy between the potential barrel model of the quantum mechanics [2] and the diffusion phenomena, to the case when the diffusive particles break through the boundary of diffuser material.

For simplicity, a one-dimensional model will be developed, that which coincides with the average general motion of the particle flow.

3.1 One-Dimensional Model of the Potential Barrier

Each particle of the diffusive substance that penetrate the diffuser material, they move with energy E, to surface that separate the free region 1 (x < 0) of the diffuser material region 2 (x ≥ 0) as show the Fig. 1.

To can penetrate, the particles should break through the barrier of the potential energy V_0 on the position x = 0.

The Schrödinger's Eq. (3) to stationary states of the particles that are moving with energy E into the potential energy field $V(x)$ has a form:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x)\Psi = E\Psi \qquad (3)$$

In this equation, Ψ(x, t) is the wave function, solution of the Schrödinger's differential equation, whole square value has the physical mean of the
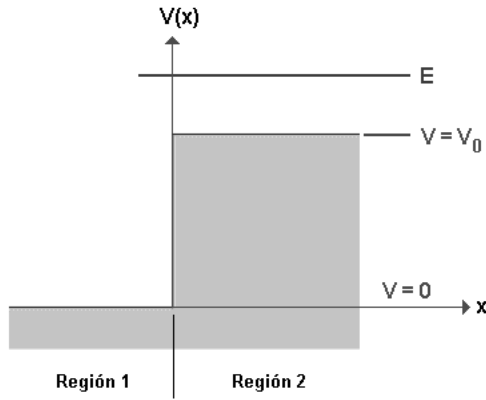
Fig. 1 Graphic of the energy of the particles in position function. In the origin x = 0 exist a potential energy step with height V(x) = V_0.

probability of the particles of being in a position x at the time t determinate, respect a framework determinate.

To the case of study of the diffusion process, into the region 1 (to see Fig. 1), the particles of the flux move freely ($V(x) = 0$) with energy E. So that, the Schrödinger equation take de form:

$$\frac{d^2\Psi_1}{dx^2} + k_1^2\Psi_1 = 0 \quad (x < 0) \tag{4}$$

Its solution is:

$$\Psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$$

With $k_1^2 = \frac{2mE}{\hbar^2}$

In this result $A_1 e^{ik_1 x}$ represent the wave function of the particles moving from the left to the right toward the potential barrier. However, $B_1 e^{-ik_1 x}$ correspond at the wave function of those particles that before whip back, they are moving to left in the region 1.

On the same way, into the region 2, the particles that get through the potential barrier, they diffused to the right moving with energy ($E-V_0$); and its Schrödinger equation will be:

$$\frac{d^2\Psi_2}{dx^2} + k_2^2\Psi_2 = 0 \quad (x > 0) \tag{5}$$

And its solution is:

$$\Psi_2(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x} \tag{6}$$

With $k_2^2 = \frac{2m(E-Vo)}{\hbar^2}$

$A_2 e^{ik_2 x}$ should be understood as the wave function of the particles that are diffused into the region 2; and they are moving to the right of the x axis.

However, $B_2 e^{-ik_2 x}$ correspond at the wave function of the particles that are moving to the left into the same region to different reasons.

3.2 The Diffusion Coefficient D

Of the density of the particles flux J_0 that arrive over the potential barrier from the right, a certain fraction them get to penetrate at the region 2 inside of the diffuser material.

The quantum expression to the density of the particles flux J_0 is [2]:

$$J_0 = \frac{\hbar k}{m}|A_1|^2 \tag{7}$$

In the case that the energy E of the incident particles on the potential barrier is greater than the potential energy of the barrier V_0, then these particles penetrate at the zona 2 of the diffuser material.

Applying the continuity boundary conditions on the frontier between region 1 and region 2 ($x = 0$) to the quantum mechanics:

$$\Psi_1(0) = \Psi_2(0) \text{ and } \frac{d\Psi_1(0)}{dx} = \frac{d\Psi_2(0)}{dx}$$

Then in these cases it had obtainedthat[2]:

$$A_2 = A_1 + B_1 \text{ and } k_1(A_1 - B_1) = k_2 A_2$$

Solving and rearranging the before expression, it gives:

$$B_1 = \frac{k_1-k_2}{k_1+k_2} \quad \text{y} \quad A_2 = \frac{2.k_1}{k_1+k_2} \tag{8}$$

The reason of the particles density flux that get to enter J_D at the region 2 over the density of the incident particles flux J_0 is known as *transmission coefficient D*, or *diffusion coefficient*.

If is taken in account the Eq. (8), the expression to D is[2]:

$$D = \frac{J_D}{J_0} = \frac{4k_1.k_2}{(k_1+k_2)^2} \tag{9}$$

Replacing the expression of the k_1 and k_2 (4) and (6) into the Eq. (9), is obtained that:

$$D = 4.\frac{\sqrt{E.(E-V_0)}}{2E-V_0+2.\sqrt{E.(E-V_0)}} \qquad (10)$$

The expression of the Eq. (10) shown that only those particles with energy E greater than the potential energy V_0 of the barrier, it can be penetrated at region 2; in other case, the value of the square root will be imaginary, and the diffusion coefficient has not a real value.

If it is considered that the energy of the movement of the particles with one free degree can be expressed as $E = \frac{1}{2}.K.T$, (K is the Boltzmann's constant, with a value equal at $1,830649.10^{-23}$ J/K).

T is the temperature in Kelvin degree. Replacing this equality into the Eq. (10) and operating, it found that:

$$D = 4.\frac{\sqrt{\frac{1}{2}.k.T\left(\frac{1}{2}.k.T-V_0\right)}}{k.T-V_0+2.\sqrt{\frac{1}{2}.k.T.\left(\frac{1}{2}.k.T-V_0\right)}} \qquad (11)$$

In accord with the obtained Eq. (11), the diffusion coefficient value depends on the two parameters: the temperature T of the diffusion process and the potential energy V_0 of the barrier.

3.3 Calculation of the potential Energy of the Barrier V_0

To can use the Eq. (11) in order to calculate de diffusion coefficient D, it is necessary to determinate the energy value V_0 of the potential barrier. So, combining the relations (8) and operating them, it is possible find:

$$A_2 k_2 = 2.k_1 - A_2 k_1 \qquad (12)$$

Replacing the expression of k_1 y k_2 respectively and combining them, it is possible to obtain:

$$A_2.\sqrt{(E-V_0)} = \sqrt{E}.(2-A_2) \qquad (13)$$

Replacing E for $\frac{1}{2}.k.T$ into the Eq. (13) and clearing the potential energy of the barrier V_0:

$$V_0 = E - E\left(1-\frac{2}{A_2}\right)^2 = E.\frac{4}{A_2}\left(1-\frac{1}{A_2}\right) = \frac{2kT}{A_2}\left(1-\frac{1}{A_2}\right) \quad (14)$$

It is possible to get a A_2 value through of the experimental measurement. In the case of diffusion process, it can have the value of the diffusive substance concentration into the inner of the diffuser material (region 2), at any distance $x > 0$.

With de measured data, and the temperature value of diffusion process; it is possible to use the Eq. (14) to calculate the potential energy of the barrier.

Once the V_0 of the potential barrier value is calculated, it can used to calculate the diffusion coefficient through of the Eq. (11).

Replacing the Eq. (14) in the Eq. (11), another equation is obtained to diffusion coefficient:

$$D = 2.\frac{KT(2-A_2)}{KT(3-A_2)+\frac{4}{A_2}\left(1-\frac{1}{A_2}\right)} \qquad (15)$$

4. Resolution of the Ficks's Equation to the Diffusive Phenomena

The second Fick's law can write to one-dimensional case as:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \qquad (16)$$

To resolve the Eq. (16) using the separable variable method, it is proposed as a solution a function of the type:

$$C(x,t) = X(x).T(t)$$

Where $X(x)$ is a function that depend only on the variable x; and $T(t)$ is a function that depend only on the time. Replacing the $C(x,t)$ expression on the equation (16) and dividing both members for $C(x,t)$, it is obtained de expression:

$$\frac{1}{T}\frac{dT}{dt} = \frac{D}{X}\frac{d^2X}{dx^2} = m^2 \qquad (17)$$

The left member of the Eq. (17) corresponds at the function that depend only on the time, while of the right member is a function that depend only on the spatial variable x, then, only they be equal if both are equal at a constant value, denominated m^2.

So, it has a differential equation system to resolve:

$$\frac{1}{T}\frac{dT}{dt} = m^2 \qquad (17a)$$

$$\frac{D}{X}\frac{d^2X}{dx^2} = m^2 \qquad (17b)$$

To resolve de differential Eq. (17a), it can be

written as:

$\frac{dT}{T} = m^2 dt$; whose solution is:

$$ln\left(T/T_0\right) = m^2 t \text{ or } T(t) = T_0 e^{m^2 t} \qquad (18)$$

Where $T(t)$ is the value of the temporal function at the time t, and T_0 is the initial value of this function ($t = 0$).

Proceeding in the same way to resolve the differential Eq. (17b):

$\frac{d^2 X(x)}{dx^2} = \frac{m^2}{D} \cdot X(x)$. It is proposed as a solution the function:

$$X(x) = A.\cos(k_2 x) \qquad (19)$$

Replacing the Eq. (19) into the differential equation and operating, it is obtained:

$$k_2^2 = \frac{m^2}{D} \text{ or } m^2 = Dk_2^2 \text{ or } m = \mp k_2\sqrt{D}$$

The value of D it is possible to calculated from the Eq. (15); and k_2 value into the region 2 is given to Eq. (6). Then it can be calculated the value of constant m.

With this result obtained, the solution function of the Fick's differential equation is:

$$C(x,t) = e^{k_2^2 Dt}[A_0 \cos(k_2.x) + B_0 \cos(-k_2.x)] \qquad (20)$$

The function solution shows that behavior of the flux the particles is the superposition between stationary plane waves. This behavior is modulated por the temporal factor $e^{k_2^2 Dt}$.

In order to find the value of A_0 and B_0 constant, it is necessary to use the initial and boundary conditions:

Initially, the concentration value of the diffusive substance in the inner of the region 2 is null; it is to say that:

$C(0,0) = 0$, then $A_0 = - B_0$; and so, the Eq. (20) take the form:

$$C(x,t) = A_0 e^{k_2^2 Dt}[\cos(k_2.x) - \cos(-k_2.x)] \qquad (21)$$

If it is possible to measure the value of concentration C_I into the region 2 at the distance $x_I > 0$ at the time t_I, then it can be calculated de value of the coefficient A_0, replacing the x_I and t_I on the Eq. (21) and operating the next expression is obtained:

$$A_0 = \frac{C_1.e^{-k_2^2 Dt_1}}{[\cos(k_2.x_1) - \cos(-k_2.x_1)]} \qquad (22)$$

Now it is possible to model all the one-dimensional diffusion process from a few experimental measurements: The concentration C_I, on the point x_I into the region 2; at the time t_I of the measurement.

5. Results and Conclusions

Given the similarity and analogy between the Schrödinger's equation to the stationary states and the second Fick's law to the diffusion process, it is able use the concepts and results of the quantum mechanics to study the diffusion phenomena, as well also its mathematical formalism.

In fact, it was possible to formalized mathematically the diffusion coefficient D and the potential energy of the barrier V_0.

The results obtained show that it is sufficient to measure the concentration of diffusive substance into a point x_I in the inner the diffuser element, and the time that the measurement was performed, to model all one-dimensional process. Of course, it is necessary also to know the temperature T in Kelvin degree in which take place the diffusion process, to calculate the diffusion coefficient D and the potential energy of barrier V_0.

References

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