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Computational Solution of One Dimensional Diffusion Equation with Fixed Limits

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Abstract: This paper presents a model for the mathematical description of the diffusion process, as well as an attempt to use Green's function approach to solve the one-dimensional diffusion equation within the necessary bounds. By studying the initial condition for, we will be able to obtain the appropriate solution to this diffusion equation. With a constant diffusion coefficient, this equation represents the rate of change of concentrations of substances in their own lattice or in separate substances. Finally, numerical answers will be obtained via a computational approach. Because we consider t = 0 throughout the equation, the result can also be applied to an isothermal diffusion.

Keywords: Diffusion process, Fick's law, Green's function method, Mathematical modelling of diffusion process, Thermal diffusion.

I. Introduction

In a solute, diffusion refers to the number of atoms that travel across a plane of unit area in a certain amount of time. A flux or current is the name given to the flow of solute atoms. The movement of solute atoms is influenced by a non-uniformity or gradient, which is referred to as a force. In its broadest meaning, it is the movement of foreign or impurity atoms with respect to the atoms of the host crystal, and the force can cause solute atoms to move relative to the host crystals.

Temperature, momentum, and concentration gradients result in related fluxes of thermal energy, momentum, and species quantity. Ordinary diffusion or molecular diffusion is the term used to describe diffusion that is caused by a concentration gradient. These gradients can be used to create a mathematical model. The concentration gradient was also taken into account when creating a model [1]. However, the thermal diffusion is the subject of this study. The transport constitutive equations are the relationships between forces and fluxes: Heat transfer is governed by the Fourier law, fluid mechanics is governed by Newton's (or Stoke's) law, and mass transfer is governed by Fick's law [2]. The goal of this course is to use constitutive equations, as well as specific boundary and beginning conditions, to solve general field balance equations.

Diffusion can occur within gases, liquids, solids, or their interfaces, and it always involves a mixture, which can be any multi-component system including many constituents. It's also possible in two or three dimensions. Grain boundary diffusion is two-dimensional diffusion that occurs on the surface of solids or along interior surfaces that separate grains of polycrystalline solids [3].

The macroscopic, microscopic, and molecular levels are the three levels at which phenomena of transport can be examined [4]. The length scales employed in these three levels of descriptions are obviously different. As a result, a system of differential equations with boundary and contact conditions can be used to explain the problem of mass transfer for diffusion. Several strategies [5] can be used to provide an exact analytical solution to the problem.

Several writers have looked at the mathematical modelling of mass transfer by diffusion in solids as well as the approaches for finding analytical solutions [6]. Simultaneously, a system of n-systems was used to address mathematical modelling of mass transfer in symmetric heterogeneous and non-porous media [7].

II. The Mathematical Model and Formulation

The concentration gradient is used to derive the diffusion equation. Assume that a solute has a concentration of c per unit volume at any moment t. (x,y,z). A flow of solute atoms from higher concentration to lower concentration is caused by the concentration gradient (grad c), which is supplied by the density vector at time j. After that, we have Fick's first law.

$$J = -D\Delta c \tag{1}$$

Negative sign indicates that the flow is in the direction of low concentration.

In the case of a surface S with volume V, the rate of change of the quantity is given by

$$\frac{\partial}{\partial t}\int_V c(x,y,z,t)\,dxdydz \tag{2}$$

S per unit time is the amount of solute that comes out to the surface.

$$\int_S j.\hat{n}dS \quad (3)$$

$\hat{n}$ represents the unit normal vector to the surface.

If there isn't a sink or a source inside the volume, we get equations (2) and (3).

$$\frac{\partial}{\partial t}\int_V c(x,y,z,t)\,dxdydz = -\int_S j.\hat{n}\,dS$$

$$= \int_S (D\,grad\,c).\hat{n}\,dS = \int_V div(D\,grad\,c)\,dxdydz$$

Hence

$$\int_V [\frac{\partial c}{\partial t} - div(D\,grad\,c)]\,dxdydz = 0 \quad (4)$$

The Fick's second law, as equation (4) holds for all volume,

$$\frac{\partial c}{\partial t} = div(D\,grad\,c)$$

Since D is assumed to be a constant and known as diffusion coefficient. We get the diffusion equation

$$\frac{\partial c}{\partial t} = D\Delta^2 c \quad (5)$$

where $\Delta^2 = (\frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} + \frac{\partial}{\partial z^2})$

Hence the equation in one dimensional form becomes,

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial t^2} \quad (6)$$

The equation known as heat conduction equation governing by the temperature gradient, is

$$\frac{\partial T}{\partial t} = \alpha\,\Delta^2 T = \alpha\,\frac{\partial^2 T}{\partial t^2} \quad (7)$$

Here α is represents the *thermal diffusivity* of the substance.

III. Analytic Description of Diffusion Process

Consider the atom distribution between substances A and B. The Gaussian function, which specifies the normal distribution probability function as, can be used to calculate diffusion from any point of an individual material,

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\xi)^2}{2\sigma^2}} \quad (8)$$

σ is the standard deviation defined in $\sigma \in [0, +\infty)$.

When $\sigma \to 0$ to $P(x) \to \delta(\xi)$, where δ defines the Dirac delta function. The method of Green's function can be used to evaluate the solution of diffusion equation, which is of the following form

$$T(x,t) = \int_{-\infty}^{+\infty} G(x,\xi,t)\,f(\xi)\,d\xi \quad (9)$$

where $G(x,\xi,t) = \frac{1}{\sigma(t)\sqrt{2\pi}} e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}}$, known as the kernel.

Function $\sigma(t)$ is the or diffusion radius or depth of individual elementary species, for diffusion from one point.

Now from equation (8) and (9)

$$T(x,t) = \int_{-\infty}^{+\infty} \frac{1}{\sigma(t)\sqrt{2\pi}} e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}} f(\xi)\,d\xi \quad (10)$$

Hence, $\frac{\partial^2 T}{\partial x^2} = \frac{1}{\sigma^5(t)\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}} [(x-\xi)^2 - \sigma^2(t)] f(\xi) d\xi$

(11)

$$\frac{\partial T}{\partial t} = \frac{\sigma'(t)}{\sigma^4(t)\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}} [(x-\xi)^2 - \sigma^2(t)] f(\xi) d\xi$$

(12)

Also, from equation (10) we have, by taking t = 0

$$T(x,0) = \int_{-\infty}^{+\infty} \delta(\xi) f(\xi) d\xi = f(\xi) \quad (13)$$

Since $\int_{-\infty}^{+\infty} \delta(\xi) d\xi = 1$

Equation (11) & (12) along with (7), we get

$$\sigma'(t) \int_{-\infty}^{+\infty} e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}} [(x-\xi)^2 - \sigma^2(t)] f(\xi) d\xi$$

$$= \frac{\alpha}{\sigma(t)} \int_{-\infty}^{+\infty} e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}} [(x-\xi)^2 - \sigma^2(t)] f(\xi) d\xi$$

It gives, $\sigma'(t) = \frac{\alpha}{\sigma(t)}$ (14)

& $\sigma(t) = \sqrt{2\alpha t}$, (15)

Hence, $T(x,t) = \frac{1}{\sqrt{4\pi\alpha\,t}} \int_{-\infty}^{+\infty} e^{-\frac{(x-\xi)^2}{4\alpha\,t}} f(\xi) d\xi$ (16)

This is the elementary solution or fundamental solution of diffusion equation for infinite interval. Also c(x, t) is an analytic function of x & t and is positive for every x.

Initial and final conditions for $t = 0$ are defined as-

$T(x, 0) = t_0$ (const.) for $a < x < b$

$= 0$ for outside (17)

By taking equations (13) & (17) together, we have

$$f(\xi) = t_0 \quad \text{for} \quad \xi \le 0$$
$$= 0 \qquad \text{for} \quad \xi > 0 \tag{18}$$

Equation (10) can be rewritten with (15) and (18) as,

$$T(x,t) = \frac{t_0}{\sqrt{4\pi\alpha t}} \int_a^b e^{-\frac{(x-\xi)^2}{4\pi t}} d\xi \tag{19}$$

Introducing the new independent variable η, defined as-

$$\eta = -\frac{(x-\xi)}{\sqrt{4\alpha t}}, \text{ Hence } \quad d\xi = \sqrt{4\alpha t}\, d\eta$$

Now equation (19) becomes,

$$T(x,t) = \frac{t_0}{\sqrt{\pi}} \int_{(a-x)/\sqrt{4\alpha t}}^{(b-x)/\sqrt{4\alpha t}} e^{-\eta^2} d\eta =$$

$$\frac{t_0}{2}\left[\frac{2}{\sqrt{\pi}} \int_0^{(b-x)/\sqrt{4\alpha t}} e^{-\eta^2} d\eta - \frac{2}{\sqrt{\pi}} \int_0^{(a-x)/\sqrt{4\alpha t}} e^{-\eta^2} d\eta\right] \tag{20}$$

Now define the error function as,

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\eta^2} d\eta$$

So, the equation in (20) becomes,

$$T(x,t) = \frac{t_0}{2}\left[erf\left(\frac{b-x}{\sqrt{4\alpha t}}\right) - erf\left(\frac{a-x}{\sqrt{4\alpha t}}\right)\right]$$
$$where\, \alpha = Thermal\ diffusivity \tag{21}$$

If we replace heat by concentration, the result can be restated as,

$$C(x,t) = \frac{c_0}{2}\left[erf\left(\frac{b-x}{\sqrt{4Dt}}\right) - erf\left(\frac{a-x}{\sqrt{4Dt}}\right)\right]$$
$$where\, D = Diffusion\ coefficient \tag{22}$$

IV. Numerical Results

Because the related fluxes in amount of species and thermal energy are defined by the gradient of concentration and temperature, they are referred to as ordinary diffusion and thermal diffusion, respectively. The graphs below show a correlation between the two outcomes in equations (21) and (22) that produce the temperature and concentration values, respectively. Heat conduction in fluids can be thought of as molecular energy transmission insofar as the underlying process is the mobility of the constituent molecules. Some materials, such as metals, transfer heat quickly, while others, like wood, operate as thermal insulators. The physical property that describes the rate at which heat is conducted is thermal conductivity (κ) and in addition the thermal diffusivity α is defined in terms of thermal conductivity (κ) as where is the heat capacity at constant pressure per unit mass. Also, when constant physical parameters are assumed, the quantity i.e. thermal diffusivity exists in the equation of change for momentum and energy transfer in the same way as kinematics viscosity with the same dimensions (length^2/time). It may also be observed that the thermal conductivity of low-density gases increases with increasing temperature, but the graphs in this work are created by assuming density as a constant parameter, whereas the thermal conductivity of most liquids decreases with increasing temperature. If thermal conductivities in solids are to be considered, they must be tested experimentally. They are difficult to forecast or measure because they are dependent on several elements that are difficult to predict or measure. In crystalline materials, the phase and crystalline size are important; nevertheless, in amorphous solids, the degree of molecular orientation is important. The pore size vacancy fraction and the fluid within the pores have a significant impact on porous materials' thermal conductivity. The graphs clearly show that as the value of spatial coordinate(x) increases, the concentration and temperature increase continuously, and that both concentration (C) and temperature (T) are highly dependent on initial concentration and initial temperature, respectively, and that both quantities increase in a constant manner as the initial values increase, resulting in the same shapes of variations for different parameters appearing in the solutions. Fig(s). 1, 2, 3, and 4 indicate that as the diffusion coefficient and the initial concentration are increased, the concentration increases. With increasing initial temperature, the same findings are obtained for the varied thermal diffusivities in Fig(s). 4, 5, 6, 7, and 8.

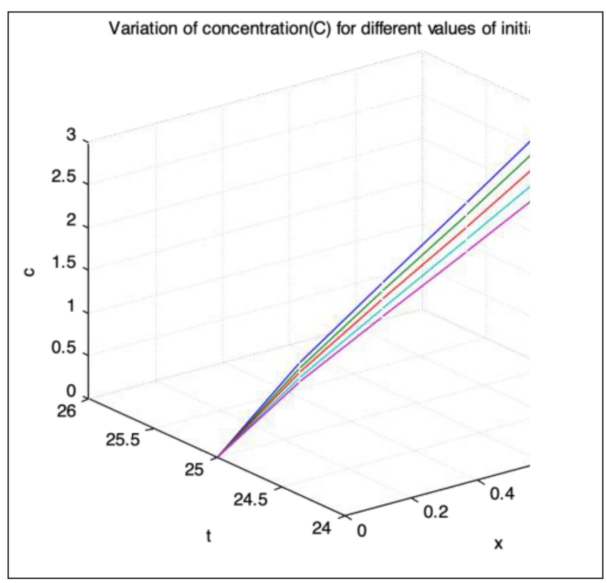

Fig. 1

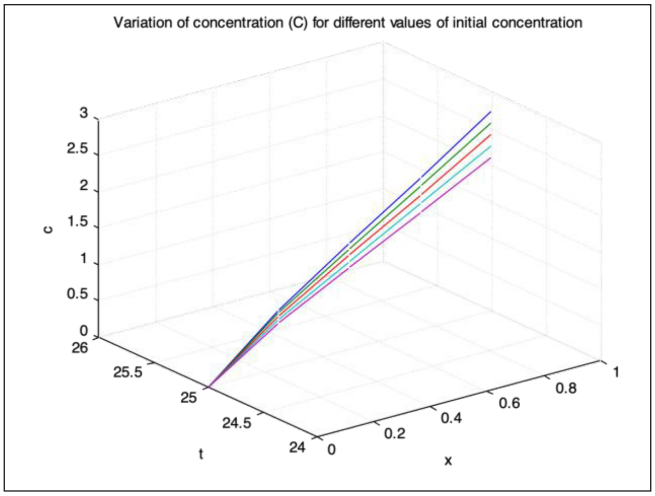

Fig. 2

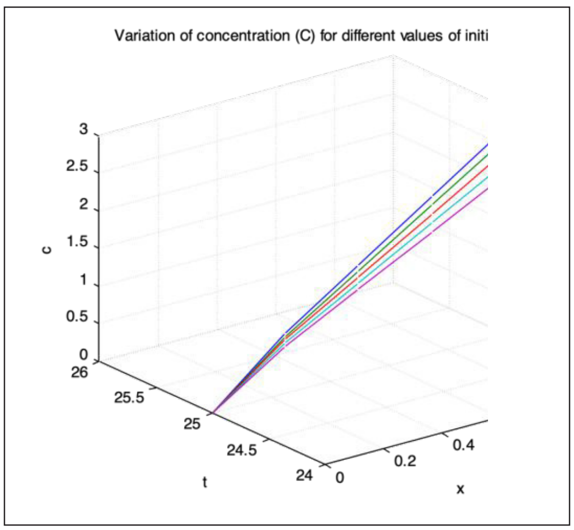

Fig. 3

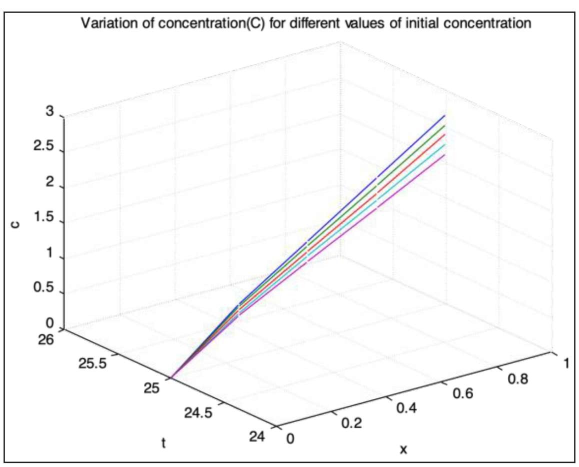

Fig. 4

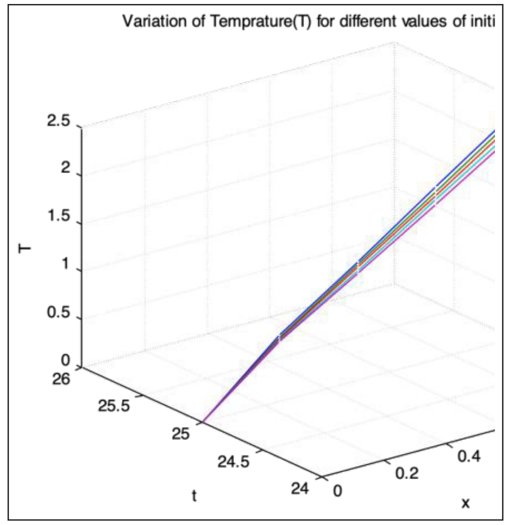

Fig. 5

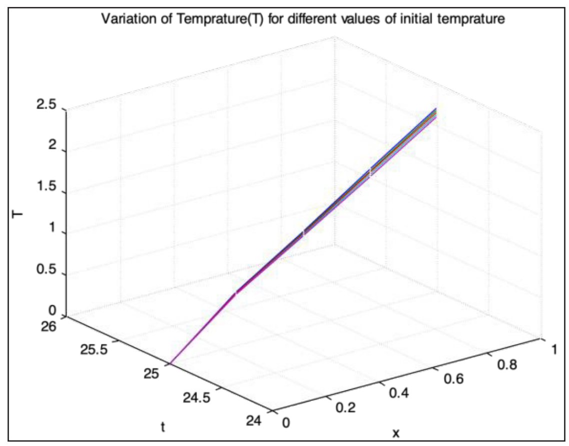

Fig. 6

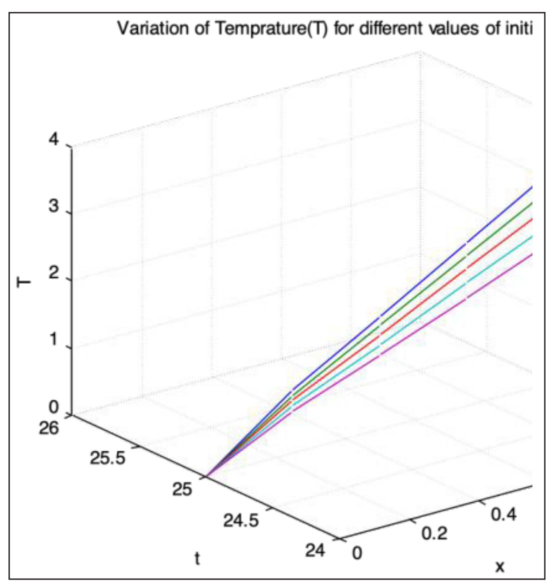

Fig. 7

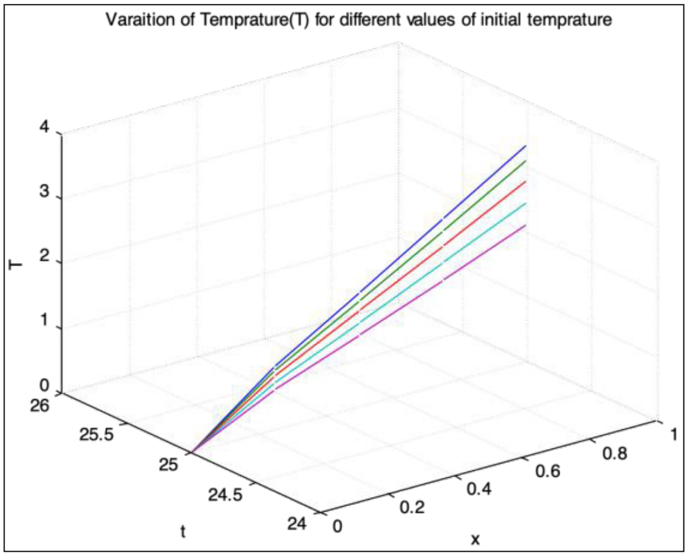

Fig. 8

V. Conclusion

The Fick's second law, which was solved by the applicability of the Green's function, can be used to mathematically model the diffusion process in substances. Equation (21), solved with t = 0 as the initial condition, is the final result of equation (6), and equation (6) was restated in a parallel form in terms of temperature (21). The complementary error function utilised in the final result [equation (20)] has the property of efficiently limiting solute penetration to depths less than or equal to twice the diffusion depths. When the thickness of the blocks of the solid is some necessary finite value of solid thickness, this condition serves to limit the anneal time in diffusion studies. We use t = 0 as a constant throughout the process so that we may use the end result in isothermal diffusion, which is a physical process in which the temperature remains constant throughout.

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