Diffusion Model for Fe-Mg in Planetary Materials: A Mathematical Approach

[1]Mustakahmed Badi, [2]Amit Basu Sarbadhikari, [3]Charmy Patel
[1]M.E. Research Scholar, [2]Scientist, [3]Associate Professor
EC Department, V.V.P. Engineering College, Rajkot, Gujarat, India

ABSTRACT: **A major objective of understanding planetary formation & evolution processes is to determine absolute or relative time scale of respective processes or part of the complex processes. It is shown that the Diffusion Modeling is a powerful tool for this purpose. Understanding that how the processes happen in a Broad range of Spatial and temporal scales is important. Diffusion model will be defined using different types of planetary samples & useful techniques. This work is concentrated on studying diffusion concentration profile, calculating Diffusion time, diffusion distance & the choice of suitable boundary conditions. Diffusion model can be implementing using finite difference methods for 1D and 2D module.**

KEYWORDS: **diffusion, olivine, diffusive coefficient, concentration gradient, diffusion time, 1D diffusion model**

1. INTRODUCTION

Diffusion is a fundamental physical process, in this process atoms migrate from matter based on difference of concentration gradient. This is also referred to as the movement of a substance down a concentration gradient, resulting into the uniform distribution of all substance gradients means the value of change in value of one quantity with respect to another quantity. Diffusion can occur in any materials like gaseous, solid or liquid. The function diffusion model is too used to estimate the relative time for the isotopes to create in mineral. Diffusion is a process of a random movement of substance; hence this is statistical problem of mathematical analysis.

The phase of any matter always depends on the surrounding conditions of the environment, e.g. temperature and pressure. A Good knowledge of the timescales is mostly necessary to understand a broad range of diffusion phenomena, the time of magma transport through the crust, and mixing, to the processes that occur right before an eruption.

2. RELATED WORK

An overview of the basic concepts of diffusion, Mathematics of diffusion, various form of diffusion equation is explained in earlier study [1]. In this research paper also various kinds of diffusion types were described. The description of the dynamic environment, rate of homogenization processes, formation of rock and other things for Diffusion modeling was given in [2]. Like any other kinetics process diffusion also has only one mathematical law which obtained from Fick's law, in which the concentration profile was used to understand the time scale of magmatic process to understand compositional zoning of major and trace element or isotopic composition in igneous mineral, melts and crystals in [3]. The idea for residence time modeling of the compositional zoning of trace element in particular certain thermodynamic and kinetics aspects were provided in [4]. The development and evaluation of compositional profiles within crystal depends on thermodynamic variable. In [5] authors defined the diffusion process in specific natural samples, which can be used to extract time and temperature information for variety of geochemical and geological processes. They also explained diffusion equation for different coordination systems. In further discussion they included different types of diffusion pathways in geological media like volume or lattice, grain-boundary, defect and surface diffusion. In geological systems, the relative important of this classical path depends upon the process of interest. An understanding of how different processes occur in combination on a wide range of spatial and temporal scales to produce a stable dynamic planetary processes were explained [6]. Compositional zoning in minerals or planetary materials is like decoded the tracks with suitable technology for CD.

3. 1-D DIFFUSION MODEL

The mathematical analysis of diffusion process is complex but an excellent theoretical approach was provided by Crank in 1975. The German physiologist A. Fick investigated diffusion law.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \quad (1)$$

Where C = Concentration, t = Time, x = Distance, D = Diffusion Coefficient.

We follow a forward modeling approach to obtain information on time by modeling concentration gradients observed in natural crystals. Petrological constraints and intuition are applied to infer an initial concentration distribution, and the suitable form of the continuity equation.

The 1-D diffusion equation (2) can be implement using the first step is to discretize the space and time coordinates into finite but small increments to make a grid. We have a step size Δx on the space coordinate, and Δt on the time coordinate. In the simplest implementations these square measure taken to be constants, however don't seem to be needed. These define the little variations that will be recognized by the computing algorithms at that specific purpose of time and space.

$$C_{i,j+1} = C_{i,j} + D * \Delta t * \left(\frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{(\Delta x)^2}\right) \quad (2)$$

Equation (2) is an explicit finite difference of the equation (1). The equation (2) can be used as iterative procedure to obtain the concentration profile at different time.

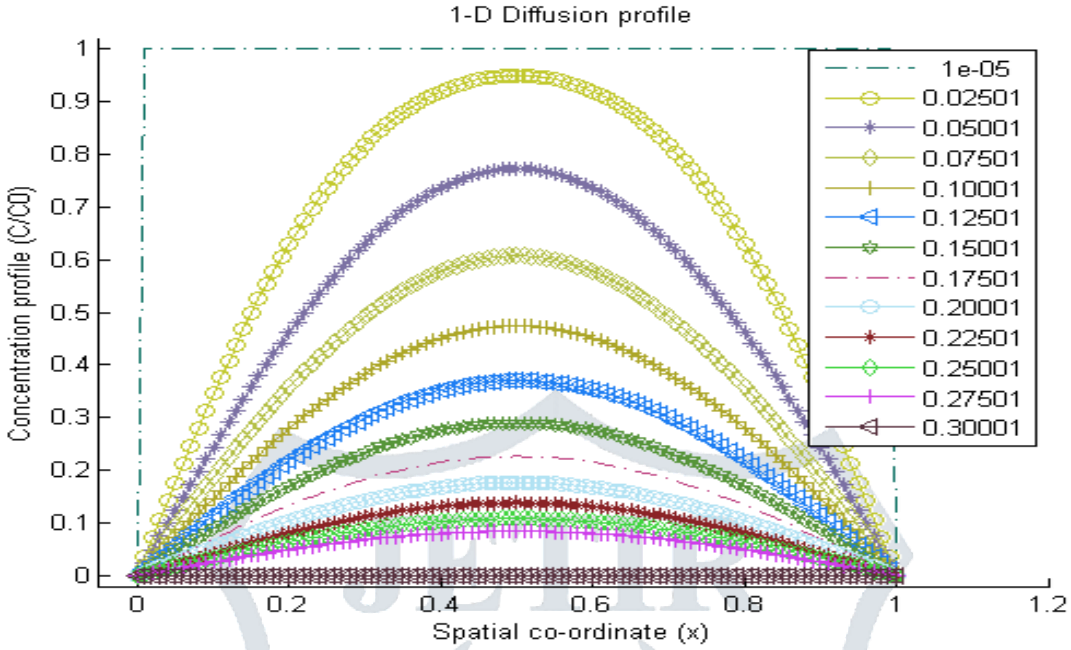

Figure 1:-Diffusion Profile for 1-D

Figure 1 is representing the 1-D diffusion profile for the Fe-Mg. It represents how the concentration will be change with time and space. Hear initial concentration is homogeneous and diffusion is driven by the change in composition at the boundary.

This is the common distance a carrier will move from purpose of generation till it diffused. Diffusion length is that the average length a carrier moves between generations and diffused [9]. Semiconductor materials that area unit heavily doped have larger recombination rates and consequently, have shorter diffusion lengths. A higher diffusion length is indicative of materials with longer lifetimes, and is thus a very important quality to contemplate with semiconductor materials [9].

A minority carrier with a specific life time (t) will be found at an average distance (L) from the point where it was generated given as (3), Where L is the diffusion length in meters, D is the diffusivity in m²/s and t is the lifetime in seconds.

$$L = \sqrt{D * t} \quad (3)$$

4. 2-D DIFFUSION MODEL

As explained above for the 1-D diffusion model similarly we explain the 2-D model for diffusion concentration. The two dimensional diffusion equation can be written as

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} \quad (4)$$

Now consider the discretized domain as the *i* is the column number which represents the spatial discreitization of the domain in *x* direction. Similarly, *j* is the row number which represents the spatial discretization in *y* direction and *n* is the temporal discretization. Now, we can discretize the diffusion equation as follows.

$$C_i^{n+1} = \left\{C_{i,j}^n + \frac{\Delta t}{(\Delta x)^2} * \left(C_{i+1,j}^n + C_{i-1,j}^n + C_{i,j+1}^n + C_{i,j-1}^n - 4C_{i,j}^n\right)\right\} \quad (5)$$

This is an explicit finite difference form of the equation (4). The equation (5) can be used to obtain the concentration at different time steps using iterative procedure as shown in fig. 2.

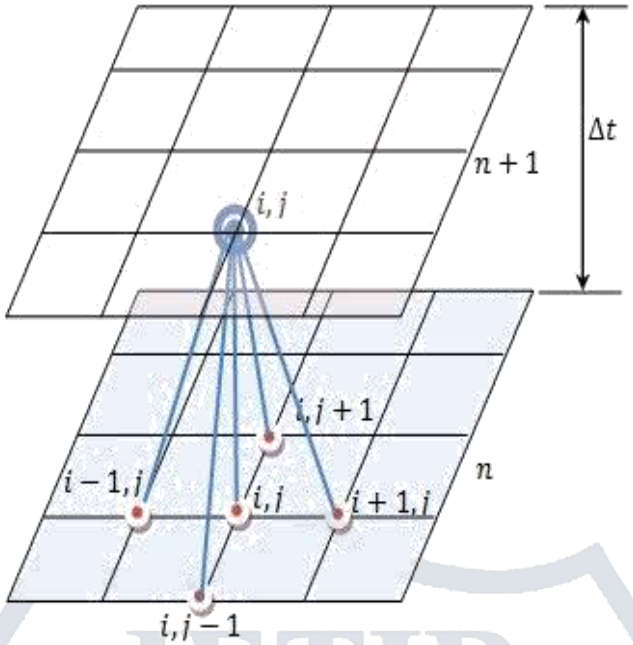

Figure 2: Iterative Procedure for 2-D.

The solution of two dimensional diffusion equation will be shown in fig. 3.

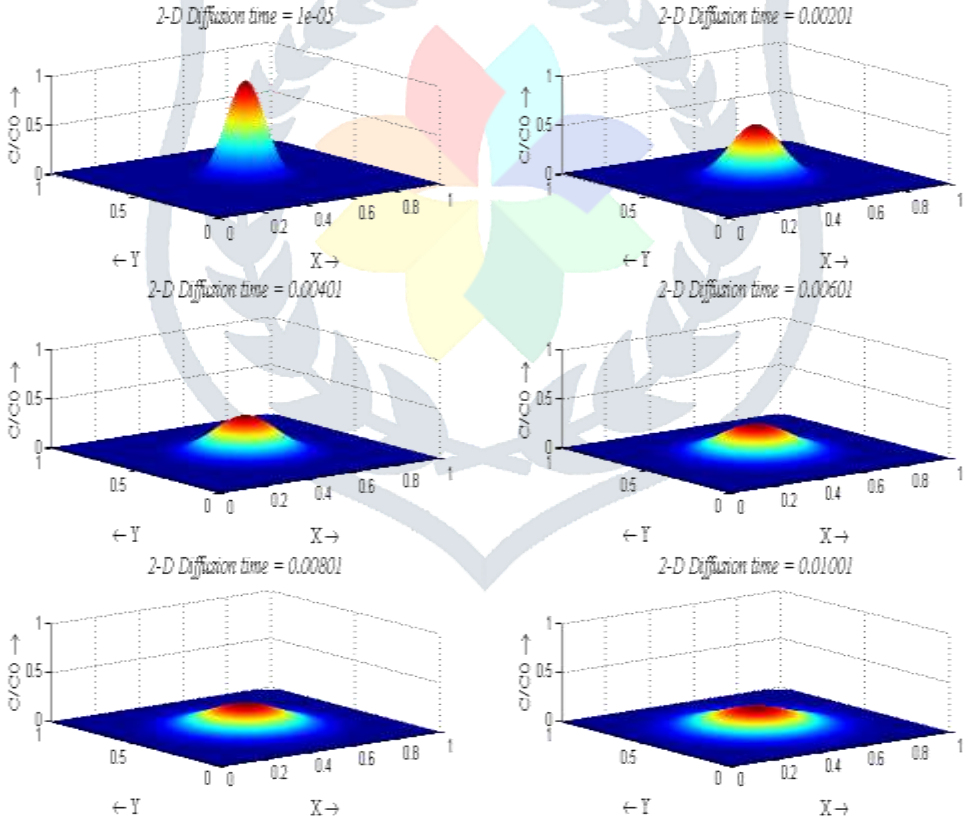

Figure 3 2-D diffusion Profile

From fig. 3, I can analyze that the concentration will remain same in the overall substance and the concentration is maximum at stating of the process and decrease as times goes and concentration profiles will be function of both time and distance from origin. There will be also some time uncertainty in the diffusion times. Therefore, there will be some difficulty to assign best fit to the natural data, so some error analysis of the best time fit will includes those concentration and temperature.

5. CONCLUSION

This conventional method introduced by us with the diffusion model is easy to operate, economical and less time consuming. This conventional method can be applied for calculating relative time for the diffusion of isotopes in mineral too. Diffusion model will help to find out the relative time for planetary processes.

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