The diffusion problem

E V Volodina¹ and E A Mikishanina²

¹ Department of Higher Mathematics and Theoretical Mechanics, Chuvash State University, Moscow avenue, 15, Cheboksary, 428015, Russia
² Department of Actuarial and Financial Mathematics, Chuvash State University, Moscow avenue, 15, Cheboksary, 428015, Russia

E-mail: evg_volodina@mail.ru, evaeva_84@mail.ru

Abstract. The study of diffusion processes is relevant in various fields: chemistry, physics, metallurgy, medicine, and others. The paper considers and solves the problem of diffusion of charged particles under the action of an electromagnetic field in a semi-infinite thin tube. The mathematical formulation is a boundary value problem for an inhomogeneous partial differential equation of the parabolic type. To obtain an accurate analytical solution, the operator method is used. The solution is initially obtained in the form of an image, and then the solution of the original problem is obtained using the inverse Laplace transform. The solution of the test example is obtained, a graphical image of the desired function is constructed in the MatLab software package.

1. Introduction

Diffusion is the transfer of matter caused by the disordered thermal motion of diffusing particles and the ordered motion of charged particles under the action of an electromagnetic field.

The development of the diffusion process leads to the formation of a diffusion layer, which is understood as a layer of the material of the part (or base) at the saturation surface, which differs from the original one in chemical composition, structure and properties. This so-called near-surface layer can provide the necessary technological properties for the cutting tool. In the case of saturation of the surface layer of the product with metals, the process is often called diffusion metallization. The phenomenon of diffusion is especially relevant when it is necessary to obtain materials with improved properties (increased strength, resistance to oxidation, thermal stability) in mechanical engineering, medicine (traumatology, surgery, orthopedics). It is also noted that as a result of diffusion, water is able to penetrate under high pressure into such high-strength materials as glass. This is evidenced by the study of Bridgman [1], which he described in his work "The latest research in the field of high pressures".

The simplest mathematical formulation of the diffusion problem leads to the solution of the boundary value problem for a partial differential equation of the parabolic type:

\[
\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2}.
\]

The boundary conditions will be determined by the features of the simulated scenario. Here the function \(T(x,t)\) is an unknown function of the coordinates \(t, x\), where the coordinate \(t\) in particular can refer to time, the coordinate \(x\) can refer to the direction in space. The constant \(D\) is called the diffusion coefficient.
and is determined by the physical properties of the material in which the diffusion occurs. Parabolic partial differential equations are found in problems where some dissipative mechanisms are involved, such as viscous stress, or thermal conductivity. A differential equation that defines a solution in more than one spatial direction and is parabolic with respect to time (or to a coordinate of the time type) becomes elliptical in a stationary state (if a stationary solution exists).

There are a sufficient number of methods for solving this equation. One of the most common methods of analytical solution of the diffusion equation is the method of separation of variables - the Fourier method [2]. The equation of nonstationary diffusion in a flat unbounded plate has the form (1), its solution is sought as the sum of an infinite series of terms of the form

$$c_m = \alpha_m f_n(x) g_m(t).$$

The specified method for the case of an unbounded plate ($x \in (-\infty, +\infty)$) can be generalized by presenting the solution as a Bohr-Fourier series:

$$T(x,t) = \sum_{n=1}^{\infty} a(\lambda_n, t) e^{i\lambda_n x},$$

where a set of numbers $\{\lambda_n\}_{n=1}^{\infty}$ is a countable set of real numbers that have no limit at point 0, $|a(\lambda_n, t)| < \alpha_n$, $\sum_{n=1}^{\infty} |\alpha_n| < \infty$, for any $t$ from a certain interval $t \in [0, t_0]$. The boundary conditions must also be almost periodic. The desired function (2) will be called almost-periodic [3].

The apparatus of almost-periodic functions (periodic functions) together with the generalized discrete Fourier transform [4] was used in solving a large number of physical problems [5-8]. The use of almost-periodic functions in this problem may be due to the unevenness of the diffusion process itself, the disparity of physical properties at different points of the plate.

The use of the Fourier and Bohr-Fourier methods in solving the diffusion problem has one significant drawback. The solution is an infinite sum of the series. The question arises about the convergence of the resulting series and about the sufficient number of terms that must be taken to obtain an answer with the specified accuracy. Therefore, the question arises of using an alternative analytical method or alternative numerical methods.

To obtain an approximate numerical solution, the finite difference method is used, which includes the construction of an algorithm for the numerical solution of the diffusion equation. The diffusion equation contains the same dissipative mechanism that is found in the study of problems of thermal conductivity or fluid mechanics with a significant influence of viscosity. When using numerical methods, first of all, accuracy suffers, since there is an increase in the error in the numerical calculation of derivatives.

The solution of the diffusion problem by the operator method allows us to obtain an exact solution in the form of an image, then return to the original solution by the inverse Laplace transform. This method will be discussed in the next section. The great advantage of this method is that it is an accurate analytical method. Namely, analytical methods are the first methods of choice.

2. Setting and solving the problem
Consider the problem for a thin semi-infinite tube $x \in [0, +\infty)$ isolated from the sides and the left end. In it, under the influence of an electromagnetic field, charged particles move, for example $N^+$, which reach the base and penetrate inside, that is, diffusion occurs according to the type of implantation.

The Fokker-Planck and Fick laws lead to a mathematical model of the following form:
This is an inhomogeneous nonstationary problem under zero boundary conditions. To solve this problem, we will replace the variables in order to obtain a homogeneous equation under inhomogeneous conditions:

\[
\begin{align*}
\frac{\partial c}{\partial t} &= D \frac{\partial^2 c}{\partial x^2} + f(t), 0 < x, t < +\infty, \\
c(0, t) &= 0, 0 \leq t < +\infty, \\
c(x, 0) &= 0, 0 \leq x < +\infty. 
\end{align*}
\]

(3)

Note that the function \( \mu(t) \), based on the physical meaning, satisfies the conditions \( \mu(0) = 0 \) and \( \mu(t) \to \text{const} \) for \( t \to \infty \), that is, there is saturation.

To solve this problem, we use the Laplace transform with respect to the variable \( t \). Given the properties of this transformation, we will have:

\[
\begin{align*}
c_i(x, t) &= C(x, p), \\
c_i(x, t) &= pC(x, p), \\
c_{xx}(x, t) &= C_{xx}(x, p).
\end{align*}
\]

Then equation (6) is transformed to the form

\[
pC(x, p) = DC_{xx}(x, p)
\]

or

\[
C_{xx}(x, p) - \frac{p}{D} C(x, p) = 0.
\]

This is an ordinary second-order differential equation for the variable \( x \) (\( p \) plays the role of a parameter). There are two additional conditions, namely: the value of the function \( C(x, p) \) for \( x = 0 \) is known, which follows from the boundary condition of problem (6).

Denote by \( M(p) \) the image of the function \( \mu(t) \), that is \( \mu(t) = M(p) \). Further, from the physical meaning of the problem, it is obviously necessary to assume that \( C(\infty, p) = 0 \). Then we come to the next problem:

\[
\begin{align*}
C_{xx}(x, p) - \frac{p}{D} C(x, p) &= 0, 0 \leq x < +\infty, \\
C(0, p) &= M(p), \\
C(\infty, p) &= 0.
\end{align*}
\]

Let's make a characteristic equation
\[ k^2 - \frac{p}{D} = 0, \]

from which

\[ k = \pm \frac{\sqrt{p}}{\sqrt{D}}. \]

Then

\[ C(x, p) = B_1 e^{\frac{p}{\sqrt{D}} x} + B_2 e^{-\frac{p}{\sqrt{D}} x}, \]

where \( B_1(p) \) and \( B_2(p) \) are arbitrary functions. It is clear that \( B_1 = 0 \), since \( C(x, p) \to \infty \) for \( x \to \infty \) and \( B_2 \neq 0 \).

Therefore

\[ C(x, p) = B_2 e^{-\frac{\sqrt{p}}{\sqrt{D}} x}. \]

Assuming here \( x = 0 \), we get \( C(0, p) = B_2 \). But on the condition \( C(0, p) = M(p) \). This means that \( B_2 = M(p) \). Thus,

\[ c(x, p) = M(p) e^{-\frac{\sqrt{p}}{\sqrt{D}} x}. \]

It remains to return to the original \( c(x, t) \). Let's use the formula

\[ f(t) = 1 - 2 \int_0^a e^{-\frac{x^2}{2\sqrt{\pi}}} \cdot \frac{1}{p} e^{-a\sqrt{p}} = F(p) \quad (D = a^2, \ a > 0). \]

Let's make a replacement \( \frac{\sqrt{D}}{\sqrt{D}} = y \) and get it \( e^{-\frac{\sqrt{D}}{\sqrt{D}} y} = e^{-y\sqrt{p}} \). Find the original for this function using the property:

\[ f(t) = F(p) \int_0^t f(z) dz = \frac{F(p)}{p}. \]

Then we get

\[ e^{-y\sqrt{p}} = \left(1 - 2 \int_0^{\frac{y}{\sqrt{\pi}}} e^{-x^2} dx \right) = \frac{y}{2\sqrt{\pi}} e^{-\frac{x^2}{4t}}, \]

\[ e^{-y\sqrt{p}} = \left( \frac{x}{\sqrt{D}} \right) = \frac{x}{2\sqrt{\pi}\sqrt{D}t} e^{-\frac{x}{4Dt}}, \]

\[ e^{-\frac{\sqrt{p}}{\sqrt{D} t}} = \frac{x}{2\sqrt{\pi}\sqrt{D}t^2} e^{-\frac{x}{4Dt}}. \]
For functions $f_1 = \mu(t)$, $f_2 = \frac{x}{2\sqrt{\pi D t^2}} e^{-\frac{x^2}{4Dt}}$ we apply the convolution theorem:

$$f_1 \cdot f_2 = \int_0^t f_1(\tau) f_2(t-\tau) d\tau = \int_0^t f_1(t-\tau) f_2(\tau) d\tau.$$ 

We get the desired function in the form

$$c(x,t) = \frac{x}{2\sqrt{D \pi}} \int_0^t \frac{\mu(\tau)}{(t-\tau)^2} e^{-\frac{x^2}{4D(t-\tau)}} d\tau.$$ 

So, we have obtained an image of the solution of the diffusion equation taking into account the given initial conditions.

Let's perform a computer simulation to visualize the solution: $D = 1$, $\mu(t) = 1 - e^{-t}$, $0 < x < 10$, $0 < t < 10$. Let's build a graph of the function (figure 1) in the MatLab environment $c(x,t)[9]$.

Figure 1. Graph of the desired function.

3. Conclusion
The problem of diffusion is relevant in many fields of physics, engineering, mechanical engineering, metallurgy, medicine, and chemistry. Both analytical and numerical methods are used to solve the boundary value problem for the diffusion equation. In this paper, the solution of the diffusion equation by the operator method is proposed. The mathematical algorithm of the solution is described. The solutions for the test example are shown. The graph of the desired function is constructed.
References

[1] Bridgmen P 1947 The latest work in the field of high pressures *UFN* 31 pp 210-63

[2] Pikulin V P, Pokhodaev S I 2004 *Practical course on equations of mathematical physics* (Moscow: ICNMO) p 208

[3] Kulagina M F 1995 Construction of almost-periodic solutions of some boundary value problems of mathematical physics *Proceedings of the Russian Association "Women-Mathematicians*" (Voronezh) 3 pp 68-73

[4] Kulagina M F, Mikishanina E A 2015 *Mathematical notes NEFU* 22 11-9

[5] Mikishanina E A 2016 Construction of almost-periodic solutions of some systems of differential equations in the problems of filtration theory *Information Technologies for Intelligent Decision Making Support* 2 (Ufa: Ufa State Aviation Technical University Press) pp 138-41

[6] Mikishanina E A 2020 *Earth and Environmental Science: Conf. series* 421 072003

[7] Kulagina M F, Ivanova V I 2003 *Bulletin of Samara State Technical University. Series: physical and mathematical sciences* 19 pp 89-96

[8] Mikishanina E A 2019 *Earth and Environmental Science: Conf. series* 315 062002

[9] Ketkov Yu L, Ketkov A Yu, Shultz M M 2005 *MATLAB 7: programming, numerical methods* (St. Petersburg: BHV-Petersburg) p 752