Applications of the Poisson and diffusion equations to materials science

C Nolasco\textsuperscript{1}, N J Jácome\textsuperscript{2}, and N A Hurtado-Lugo\textsuperscript{3}

\textsuperscript{1} Grupo de Investigación de la Facultad de Educación, Artes y Humanidades, Universidad Francisco de Paula Santander, Seccional Ocaña, Colombia
\textsuperscript{2} Grupo de Investigación de la Facultad de Ciencias Administrativas, Universidad Francisco de Paula Santander, Seccional Ocaña, Colombia
\textsuperscript{3} Grupo de Investigación de la Facultad de Ciencias Agrarias, Universidad Francisco de Paula Santander, Seccional Ocaña, Colombia

E-mail: cnolascos@ufpso.edu.co

\textbf{Abstract.} The scope of a variety of experiments involving the transfer of heat in engineering applications is evident in research on thermal studies throughout the department of Norte de Santander, Colombia. From the energy optimization processes in the brickworks of the province of Ocaña to the didactic use in the Universidad Francisco Santander, Ocaña, Colombia. In this sense, mathematical models will be a fundamental tool in the understanding of thermal transfer processes. The aim of this work is to establish a mathematical model by numerical methods to determine the physical process of heat transfer in liquid crystal. For the data acquisition, an experiment that measures thermal properties on an aluminum plate was designed. We proceed to propose a mathematical model that uses the Poisson equation. Also, we proceed to calculate the solution of the equation by the finite difference method and then make a comparison with the analytical solution and the experimental data.

1. Introduction

In Universidad Francisco de Paula Santander, Ocaña, Colombia, research is understood as a transversal tool that defines work inside and outside the classroom, seen in a methodological, applied and critical way that points to the problems that arise within the academy and the outside world, under the premise of being the transforming bridge where the new knowledge points to the intellectual, scientific and technological development of the student, teachers and the institution to achieve their mission and vision, seen from the continuous improvement of the communities [1]. To this end, research is defined in innovative concepts, in new techniques, in freedom of thought, respect for values and principles, as well as the ability to develop alternative solutions to the multiple problems that society demands.

In this broad sense, in the Universidad Francisco de Paula Santander, Ocaña, Colombia, research activities have been developed that point to the aforementioned. A sample of this work is exemplified by the contributions of a variety of researchers [2-4] of the university in the understanding of the processes of energy optimization in the brickworks of the province of Ocaña, Colombia.

Recently [5] he has described experimental designs that investigate thermal conduction by applying the Laplace equation. Experiments study heat conduction using a sensitive liquid crystal film. This article describes a heat transfer experiment that extends the use of liquid crystal films as a temperature sensor. The experiment describes the thermal transfer in a stable state and makes use of the Poisson
equation for its theoretical description [6]. The research interest is practical and pedagogical and makes use of mathematical tools that describe a variety of physical phenomena.

The study of mathematical models with numerical methods to explain heat transfer in the context of liquid crystals is little known. The main contribution of this work is to show the simplicity of the numerical method used to model the transference phenomenon in contrast to the analytical method that usually appears in the specialized works [7]. The proposed numerical method will allow the understanding of heat conduction with the help of a computer program. In section 2 of the work a description of the experiment [7] that models the thermal transfer is made. Section 3 presents a general description of the heat equation; with some additional hypotheses the Poisson equation is derived [6]. In section 4, the Poisson equation is solved by analytical and numerical methods. Finally, the solutions are compared and the next phase in the investigation is proposed.

2. Methodology
The experimental design [7] consists of attached metal support with two arms. The first arm has an opening diameter of 0.7 cm at the top a plate with a liquid crystal film is placed at a temperature 29 °C - 35 °C. The second arm is placed in the lower part of the support in which it places a heat lamp connected to a Variac. Heat radiates evenly over the opening area. The plate temperature is measured by the color change observed on the liquid crystal film. The temperature distribution is radial. The position of the four temperatures characteristic of particular film are measuring using the color transitions and a traveling microscope positioned above the film.

The data acquisition system for the aluminum plate was designed, following the technique of recollecting data in [7] to record the temperatures monitored by thermometers. The method to establish the mathematical model consisted in modeling the temperature through the use of the Poisson equation.

3. Mathematical model
The foundation of the Poisson equation is the Fourier law and the law of conservation of energy as evidenced in [8]. Let \( \Omega \) be a region in space where a heat flux is located and \( T(x,y,z,t) \) represents the temperature over time at the point \( (x,y,z) \) en \( \Omega \). it is assumed that the region is homogeneous and is characterized by specific heat \( c \) and the density constant \( \rho \). Let \( B \) be an arbitrary sphere contained in \( \Omega \).

When applying the principle of energy balance to \( B \), it is necessary that the rate of change of the total amount of caloric energy contained in \( B \) must be equal to the rate of change of heat flux that crosses the border of \( B \) plus the rate of change of the heat energy produced by any source in \( B \). The amount of heat in a small volume \( dV = dx dy dz \) is \( cpT dV \), thus the amount of caloric energy in \( B \) is given by the integral in three dimensions \( \int_B cpT dV \).

We assume that the heat produced by the sources is given by the function \( f = f(x,y,z,t) \), where \( dV \) the reason that heat is generated in \( dV \). Therefore, the reason at which heat is generated in all of \( B \) is \( \int_B dV \).

Note that \( f \) has energy dimensions per unit volume per unit time. Next, the heat flux vector function is introduced \( \phi(x,y,z,t) \). The reason at which the flow crosses an oblique surface element \( dA \) oriented by a unit vector \( n \) is \( \phi \cdot ndA \). Consequently, the rate of change in the flow of energy that crosses the border of \( B \), denoted by \( \partial B \), is the surface integral \( \int_{\partial B} \phi \cdot ndA \). In this context the conservation law translates into the Equation (1).

\[
\frac{d}{dt} \int_B c \rho T dV = -\int_{\partial B} \phi n dA + \int_B f dV.
\] (1)

The negative sign of equality indicates that the energy network on the left side of the equation decreases, which is correct. Using the divergence theorem in Equation (1) allows us to rewrite the flow integral as a volume integral, in Equation (2).

\[
\int_B \nabla \phi dV = \int_{\partial B} \phi \cdot ndA.
\] (2)
Remember that if \( \phi = (\phi_1, \phi_2, \phi_3) \), so its divergence is the scalar function defined in the Equation (3).

\[
\text{div}\phi = \frac{\partial \phi_1}{\partial x} + \frac{\partial \phi_2}{\partial y} + \frac{\partial \phi_3}{\partial z}
\]  

(3)

By applying Equation (2) and Equation (3), Equation (1) can be written as Equation (4).

\[
\frac{d}{dt} \int_B \rho T dV = -\int_B \text{div}\phi dV + \int_B f dV
\]  

(4)

Due to the homogeneity conditions applied to Equation (4), it is possible to introduce the derivative under the sign of the integral on the left side and reorganize the terms under the volume integral as Equation (5).

\[
\int_B (\rho c_T + \text{div}\phi - f) dV = 0
\]  

(5)

This balance law must be taken for every sphere \( B \) contained in \( \Omega \), therefore the integral can be neglected, giving the differential Equation (6).

\[
\rho c_T \frac{dT}{dt} + \text{div}\phi = f
\]  

(6)

For everything \( t \) and everything \( (x, y, z) \in \Omega \). The differential Equation (6) contains two unknown functions, the scalar temperature \( T \) and the vector heat flux \( \phi \). Fourier's law of heat conduction establishes a relationship between \( T \) and \( \phi \), namely Equation (7).

\[
\phi = -K \text{grad}T = -K(T_x, T_y, T_z)
\]  

(7)

Where \( K \) is the thermal conductivity constant. By replacing Equation (7) in Equation (6) and using the identity \( \text{div}\text{grad}T = T_{xx} + T_{yy} + T_{zz} \), the heat equation for temperature \( T(x, y, z, t) \) in three dimensions is obtained Equation (8).

\[
\rho c_T \frac{dT}{dt} - K(T_{xx} + T_{yy} + T_{zz}) = f
\]  

(8)

The expression \( T_{xx} + T_{yy} + T_{zz} \) is called the Laplacian of \( T \) and is denoted by \( \Delta T \). Therefore, \( \Delta T = T_{xx} + T_{yy} + T_{zz} \). Finally, Equation (8) can be written as the Equation (9):

\[
T_t - k \Delta T = \frac{1}{c_p} f
\]  

(9)

Where \( k = \frac{K}{c_p} \) is called the diffusion constant. As a particular case of study, the Poisson equation represented in Equation (10).

\[
-(T_{xx} + T_{yy}) = f
\]  

(10)

By experimental design, Equation (10) is reduced to Equation (11) with a change in polar coordinates.
− \left( \frac{1}{r} \right) \left[ \frac{d}{dr} \left( \frac{d}{dr} \right) \right] \frac{T(r)}{dr} = \frac{-Q_0}{\kappa} \tag{11}

Equation (11) is transformed into Equation (12).

\left( \frac{d^2 T}{dr^2} \right) + \left( \frac{1}{r} \right) \left( \frac{dT}{dr} \right) = \frac{-Q_0}{\kappa} \tag{12}

Subject to the initial conditions reflected in the Equation (13).

\begin{align*}
T(0) &= 31.0, \quad T'(0) = 0
\end{align*} \tag{13}

4. Solution of the Poisson equation

In this section, the solution of the differential Equation (12) is calculated, subject to boundary conditions of the Equation (13) by numerical methods using the techniques of [9] and the analytical solution is calculated.

4.1. Solution by numerical methods

In order to solve the differential Equation (12), subject to the boundary conditions (13) the equality is written by the Equation (14).

\left( \frac{d^2 T}{dr^2} \right) = \frac{-Q_0}{\kappa} - \left( \frac{1}{r} \right) \left( \frac{dT}{dr} \right) \tag{14}

The numerical method for solving Equation (14) subject to boundary conditions Equation (13) is the Runge-Kutta method. For this reason, the functions are introduced \( u_1(r) \) and \( u_2(r) \) in Equation (15).

\begin{align*}
\frac{d}{dr} u_1(r) &= T(r) \quad \text{and} \quad \frac{d}{dr} u_2(r) = u_1'(r) \tag{15}
\end{align*}

Therefore, Equation (14) when applying Equation (15) is transformed into Equation (16).

\begin{align*}
u_1'(r) &= u_2(r) \quad \text{and} \quad u_1'(r) = \frac{-Q_0}{\kappa} - \left( \frac{1}{r} \right) u_2(r)
\end{align*} \tag{16}

The system of Equations (16) is solved by the Runge-Kutta method where \( f_1(r, T, T') = u_2(r) \) and \( f_2(r, T, T') = \frac{-Q_0}{\kappa} - \left( \frac{1}{r} \right) u_2(r) \).

4.2. Analytical solution of the Poisson equation

For the experimental design, the situation is analogous to the electrical potential inside a uniformly charged cylinder, for a detailed study of the calculation see reference [10]. The analytical solution is given by Equation (17).

\begin{align*}
T(r) &= -\left( \frac{Q_0}{4\kappa} \right) r^2 + T(0)
\end{align*} \tag{17}

By replacing the initial conditions of Equation (13) in Equation (17) the analytical solution is generated Equation (18).

\begin{align*}
T(r) &= -40.1r^2 + 31.0
\end{align*} \tag{18}
5. Results
The mathematical model to validate the results of the experiment presented in section 2 in this paper has its basis in the mathematical model of the Equation (17). In order to validate the numerical model of Equation (16), for the process of heat transfer for the aluminum plate, we proceed to build a mesh on the aluminum plate and calculate the temperature on each of the nodes. The previous validation is developed through the implementation of a program [11]. Table 1 contains the data used in the program that implements the Runge-Kutta method to solve system of Equations (16).

| Parameters                      | Data   |
|---------------------------------|--------|
| $Q_0$ (initial / constant transfer volume) | 160    |
| $T_0$ initial temperature       | 31 ºC  |
| $T_i$                           | 0 ºC   |

The program designed with the data from Table 1 simulates the experiment effect of heat transfer for the aluminum plate. Figures 1 shows the results of applying the Runge-Kutta method to the Equation (16) to calculate the temperature function. Figure 1 prove that the temperature decreases. Figure 2 shows the temperature function of Equation (18), that is constructed from the analytical methods, is a decrease function.

![Figure 1. Temperature with the Rungen-Kutta method.](image1)

![Figure 2. Temperature with the explicit solution.](image2)

The results of the figures show an apparent similarity in the results. The numerical method has the advantage of the simplicity of development as well as the method developed in [12]. Analytical techniques show a high level of complexity in their development. For the specific case of Equation (12) and Equation (13) the reference [12] shows the extent of the development of the solutions. From the pedagogical point of view, the numerical method may be more relevant when addressing the solution of differential equations with a relative degree of simplicity.

6. Conclusion
The experiment of heat conduction on the surface of the aluminum plate with the use of crystal liquid film as described in section 2, is modeled by the analytical Equation (18) of the Poisson Equation (12). This research finds another mathematical model based on Runge-Kutta method to describe the experiment in section 2, which has a clear advantage on the mathematical model of Equation (18). First of all, the numerical model is easy to get from the Poisson’s Equation (12) and Equation (13) as verified in sub-section 4.1 and the temperature function can be generated by computational simulation.
The next step in the investigation is to include the effect of transient heat transfer. For this purpose, it is proposed to develop an experimental setup that fits a small modification of the model of this article. The following diffusion Equation (19) is postulated.

$$\left( \frac{d^2 T}{dr^2} \right) + \left( \frac{1}{r} \right) \left( \frac{dT}{dr} \right) - \left( \frac{1}{\rho c} \right) \frac{dT}{dt} = \frac{-Q_s}{K}. \quad (19)$$

To solve Equation (19) it is expected to find a suitable numerical technique that fits this situation.

References
[1] Sánchez Ortiz E A 2013 Proyecto Educativo Institucional (Ocaña: Universidad Francisco de Paula Santander Ocaña)
[2] Guerrero Gómez G, Espinel Blanco H 2013 Comparación del consumo energética y propiedades finales de los productos cocidos entre hornos artesanales a cielo abierto y un horno Hoffman en las Ladrilleras del Municipio de Ocaña en Norte de Santander XX Congreso Peruano de Ingeniería Mecánica, Eléctrica y Ramas Afines (CONIMERA) (Peru: INICTEL)
[3] Guerrero Gómez G, Marrugo Carrazo D E, Gómez Camperos J A 2015 Desarrollo de instrumento virtual enfocado en la adquisición de datos para generar perfiles de temperatura en hornos Revista Ingenio UFPSO 8 47
[4] Guerrero Gómez G, Espinel Blanco E, Sánchez Acevedo H G 2017 Análisis de temperaturas durante la cocción de ladrillos macizos y sus propiedades finales Revista Tecnura 21(51) 118
[5] Canova B P 1990 Laplace’s equation in freshman physics American Journal of Physics 60 135
[6] Feynman R P, Leighton R B, Sands M 1964 The Feynman Lectures in Physics (New York: Addison Wesley)
[7] Bacon M E 1994 Heat, light, and videotapes: Experiments in heat conduction using liquid crystal film American Journal of Physics 63 359
[8] Bulut I 2014 Analytical Solutions of the Steady or Unsteady Heat Conduction Equation in Industrial Devices: A Comparison with FEM Results (Cagliari: Universita degli Studi di Cagliari)
[9] Evans D J, Abdullah A R 1985 A new explicit method for the diffusion-convection equation Computers and Mathematics with Applications 11 145
[10] Logan J D 2004 Applied Partial Differential Equations (USA: Springer Verlag)
[11] Stanoyevitch A 2005 Introduction to Numerical Ordinary and Partial Using Matlab (Hoboken: John Wiley & Sons)
[12] Dehghan M 1999 Fully implicit finite differences methods for two-dimensional diffusion with a non-local boundary condition Journal of Computational and Applied Mathematics 106 25