Finite difference method applied to heat transfer in polymers

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Abstract. The study of efficient solution methods for mathematical models from physics is important for the purpose of making predictions. In the study of the equations of mathematical physics, the heat equation has an important place. Techniques for studying heat transfer include topics such as Fourier analysis, Bessel functions, Legendre polynomials, etc. Throughout this article we will study the heat equation from the point of view of calculating its solutions. For this reason, the solution of the heat equation is proposed by the Fourier method and the explicit numerical method. In the last part of the article studies the accuracy of the numerical method in relation to heat transfer in a spherical polymer and raises the advantage of working with numerical methods to solve mathematical models derived from conservative laws.

1. Introduction

The discovery of differential calculus allowed new possibilities for the mathematical modeling of physical phenomena. Partial differential equations have their conceptual basis in integration and differentiation. Some extremely important examples in the application of mathematical models that use partial differential equations to encode physical phenomena are electromagnetic theory, the general theory of relativity and the mathematical foundation of quantum mechanics. The development of the theory of partial differential equations has relevance as a line of research oriented to develop diverse methods that allow solving the equations of mathematical physics [1].

In relation to the advances of engineering the use of mathematical models with partial differential equations it is directly related to the study of the mathematical theory of heat conduction [2]. Studying techniques to solve the heat equation has been a relevant chapter in the theory of partial differential equations. The first method to solve the heat equation was proposed by Fourier in 1812 [3] and since then the Fourrier theory has been an area of mathematical physics with a growing interest in researchers.

With the formulation of the first theoretical model of computing by Alan Turing [4] the numerical calculation of the solutions of differential equations is a field of study of great interest [5] due to the speed of calculation of the solutions and the precision of the results in relation to the traditional solution methods. With the previous idea as the main motivation this article investigates the numerical calculation of the solution of the heat equation in the context of heat conduction. The advantage of this approach lies in the simplicity of the method along with the accuracy of the results. To support the numerical approach used to solve the heat equation the research relies on the experimental data of [6] in which the phenomenon of heat transfer in a spherical polymer is modeled by the use of Fourier theory.
This article is organized with a first section where it is proposed to describe the traditional method to solve the mathematical model of heat transfer in a spherical polymer, also describes in detail the numerical method to solve the physical model. The second section compares the fourier method against the numerical method in relation with the data of [6]. In the last section, the mathematical reasons for the accurate of the results, by the numerical method, is analysed.

In addition to the above, this work is the result of the continuity of research [7-9] conducted at the Universidad Francisco de Paula Santander, Seccional Ocaña in the study of thermal processes in brick factories in Norte de Santander, Colombia.

2. Mathematical model of heat transfer

An important set of the partial differential equations of mathematical physics are based on the conservation laws. A conservation law is the mathematical formulation of the physical principle that states that the rate of change of a quantity within a region is equal to the rate of change of the flow of the quantity in the region's boundary. Equation (1) represents the mathematical formulation of the conservation principle [10].

\[
\frac{d}{dt} \int_V T \, dV = - \int_{\partial V} \Phi \, dS + \int_B \Phi \, dV.
\] (1)

By applying Fourier's law and the divergence theorem to Equation (1), the heat transfer model (Equation (2)) is derived [10].

\[
\nabla^2 T = \left( \frac{1}{k} \right) \frac{\partial T}{\partial t},
\] (2)

where \(k\) represents the constant of diffusion. Because of the nature of the heat transfer is in a spherical polymer the appropriate coordinates to represent the heat equation are the spherical coordinates [11]. This fact can be specified in the Equation (3).

\[
\frac{\partial^2 T}{\partial r^2} = \frac{1}{r} \frac{\partial T}{\partial r} \quad (0 \leq r \leq a).
\] (3)

The following subsections aim to calculate the classical and numerical solution of the Equation (3). In the case of the numerical methods, a detailed study of the solution will be carried out.

2.1. Fourier method

The analytical method to solve Equation (3) using the separation method [6], the temperature function is represented by the Equation (4).

\[
T(r, t) = \frac{2aT(0)}{r \pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin \frac{n \pi}{a} \, e^{-\frac{kn^2 \pi^2 t}{a^2}}.
\] (4)

The value \(T\) at the center as \(r \to 0\) is given by the Equation (4).

\[
\frac{T_c - T_s}{T_0 - T_s} = 2 \sum_{n=1}^{\infty} (-1)^{n+1} e^{-\frac{kn^2 \pi^2 t}{a^2}}.
\] (5)

The Equation (5) calculates the temperature of the polymer. The complexity of the expression it allows to think in a different point if view. The next section develops a new perspective to solve the differential Equation (3).
2.2. Numerical solution
The idea of the finite difference method is to substitute a continuous differential equation in a discrete algebraic problem that can be solved in a finite number of steps. The numerical solution only approximates a finite number of points in the region. The Taylor’s theorem of ensures that for values close to \( x \), a function \( f(x) \) can be expanded as indicated by Equation (6).

\[
f(x + h) = f(x) + f'(x)h + \cdots + \frac{1}{n!}f^{(n)}(x)h^n.
\]  

(6)

The approximation error of Equation (6) is of the order \( O(h^{n+1}) \). Approximations of the derivatives can be generated by Taylor's theorem. Solving Equation (3) numerically is equivalent to calculating finite-difference approximations for the function \( T \). Taylor's theorem for multivariate functions has the form of the Equation (7).

\[
T(x + h, t) = T(x, t) + T_x(x, t)h + \frac{1}{2}T_{xx}(x, t)h^2 + \frac{1}{3!}T_{xxx}(x, t)h^3 + O(h^4).
\]  

(7)

By using Equation (7) the explicit approximations of Equations (8) and Equation (9) are generated.

\[
T_t(r_j, t_{n+1}) = \frac{T(r_{j, t_{n+1}}) - T(r_{j, t_{n}})}{\Delta t},
\]  

(8)

\[
T_{xx}(x_j, t_{n}) = \frac{T(x_{j-1, t_{n}}) - 2T(x_{j, t_{n}}) + T(x_{j+1, t_{n}})}{(\Delta x)^2}.
\]  

(9)

By substituting Equation (8) and Equation (9) in Equation (3) we get Equation (10) which represents the finite model of heat transfer in the spherical polymer.

\[
\frac{T(r_{j, t_{n+1}}) - T(r_{j, t_{n}})}{\Delta t} = \frac{T(x_{j-1, t_{n}}) - 2T(x_{j, t_{n}}) + T(x_{j+1, t_{n}})}{(\Delta x)^2}.
\]  

(10)

From Equation (10) the recurrent formulas: Equation (11), Equation (12) and Equation (13) are deduced.

\[
T_t^{k+1} = s(T_x^k + T_0^k) + (1 - s)T_t^k,
\]  

(11)

\[
T_j^{k+1} = s(T_{j+1}^k + T_{j-1}^k) + (1 - s)T_j^k,
\]  

(12)

\[
T_n^{k+1} = s(T_{n+1}^k + T_{n-1}^k) + (1 - s)T_n^k.
\]  

(13)

It is important to note that the Equations (11), Equation (12) and Equation (13) represents the temperature in different nodes and they represent a system of equation. Look at the Equation (14) by the case \( n = 3 \).

The Equation (14) is the key for the numerical solution of Equation (3) by the use of computer simulation.

\[
\begin{pmatrix}
1 - 2s & s & 0 \\
s & 1 - 2s & s \\
0 & s & 1 - 2s
\end{pmatrix}
\begin{pmatrix}
T_t^k \\
T_2^k \\
T_3^k
\end{pmatrix}
= \begin{pmatrix}
(1 - s)f(t_0) \\
0 \\
sg(t_0)
\end{pmatrix},
\]

(14)
3. Results and discussion

To validate the numerical solution the research proposes to check the numerical model, Equation (10), with the experimental data of [6], where an experiment is performed to measure the temperature of a spherical polymer designed in the laboratory. The design of the polymer [6] allowed uniform use of the diffusion constant throughout the cooling process. This fact is reflected in the smoothness of the solution.

The Figure 1 and Figure 2 show the temperature profile generated by applying the numerical scheme of the Equation (11), Equation (12) and Equation (13) to the Equation (3).

Figure 1 and Figure 2 show a decrease in temperature from 150° to 30°, which is consistent with the experimental data from [6] and the physical theory of the heat transfer phenomenon [12]. The behavior of the curve in Figure 1 as a decreasing function that has a behavior that tends to an asymptote in 30°, shows that the explicit numerical method for calculating the temperature of the spherical polymer is relevant. The mathematical reasons for the good fit of Figures 1 and 2 to the physical phenomenon of heat transfer are as follows. The code designed to solve the system of equations 10 and therefore calculate the temperature verifies the stability condition \( k \leq \frac{1}{2} \). The previous condition of stability is a necessary and sufficient condition to guarantee the convergence of the numerical solutions generated by the explicit method, Equation (10) to Equation (14), in addition to guaranteeing the adjustment of the numerical solution and the analytical solution, Equation (5). A detailed mathematical development of the stability conditions of the explicit numerical method can be found in [13]. The solution by numerical methods has the advantage of reducing a calculation problem in partial derivatives to a calculation problem of solutions of a system of linear equations. The study of linear equation systems by computational methods is the subject of a large group of research work [14]. The importance for mathematical physics of numerical methods is to transfer a problem from the physics of the continuous medium to a simple mathematical problem.

4. Conclusion

The explicit numerical method proposed from Equation (10) to Equation (14) to solve the differential Equation (3) of mathematical physics that models the physical phenomenon of heat transfer proved to be efficient from different points of view. First, the curve generated by the solution of the linear system of the Equation (14) fits the physical phenomenon of the experiment of Unsworth J and Duarte F 1979. Secondly, the development of the numerical scheme is conceptually simple and reduces the problem of continuous analysis to the study of solving a system of linear equations. Finally, this article raises the study of differential equations from the numerical point of view and how this perspective can be relevant when studying mathematical models of physics through the use of computational methods.
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