Resolution of thermal energy transfer by diffusion and by convection

Resolução da transferência de energia térmica por difusão e por convecção

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Rodrigo Daher
Universidade Federal de Uberlândia, Av. João Naves de Ávila, 2121 - Santa Mônica,
Uberlândia - MG, 38408-100
E-mail: rodrigo.daher@ufu.br

ABSTRACT
Transfer of thermal energy is present all around us, it can be used to analyse systems such as our body, a launching rocket, a heating pan, refrigeration systems, engines and so on. A solid comprehension of how the thermal energy convection works in a simpler body is very important to guarantee a correct understanding and development of more complex real life engineering problems. The main subject of this paper is to study the transfer of thermal energy by diffusion and by convection and create an algorithm that can realize the simulation of this transfer of thermal energy in a bidimensional domain. To reach this goal, firstly was studied the physical model of the transfer of thermal energy. After that, the finite-difference numerical technique to spatial discretization was used to create the mesh of the body and two different methods - explicit and implicit - were used to discretize in time. To accomplish the numerical analysis, a Fortran90 algorithm was developed for each method in order to simulate the thermal energy transfer by diffusion and by convection given the boundaries conditions. Lastly, the results were quantitative validated by the manufactured method solution to ensure the code is functional. As a conclusion, the code showed up to be consistent, returning quantitative and qualitative validated results.

Keywords: thermal energy transfer, diffusion equation, numerical analysis, advection, convection

RESUMO
A transferência de energia térmica está presente à nossa volta, pode ser utilizada para analisar sistemas como o nosso corpo, um foguete de lançamento, uma panela de aquecimento, sistemas de refrigeração, motores e assim por diante. Uma compreensão sólida de como funciona a convecção de energia térmica num corpo mais simples é muito importante para garantir uma correcta compreensão e desenvolvimento de problemas de engenharia mais complexos da vida real. O assunto principal deste trabalho é estudar a transferência de energia térmica por difusão e por convecção e criar um algoritmo que possa realizar a simulação desta transferência de energia térmica num domínio bidimensional. Para atingir este objectivo, estudou-se em primeiro lugar o modelo físico da transferência de energia térmica. Depois disso, foi utilizada a técnica numérica de diferença finita à discretização espacial para criar a malha do corpo e dois métodos diferentes - explícito e implícito - foram utilizados para discretizar no tempo. Para realizar a análise numérica, foi desenvolvido um algoritmo Fortran90 para cada método, a fim de
INTRODUCTION

This paper has the objective to simulate the thermal energy transfer by diffusion and by convection in a bidimensional domain. First of all, usually advection is called wrongly as convection, but convection is comprised of two mechanism. Convection is the joint random molecular motion (diffusion), and bulk motion (advection).

According to Incropera et al. (2007), diffusion is given by the random molecular motion. In thermal energy transfer it happens when exists a difference of temperatures, the higher temperatures are associated with molecules that has higher energy. When the molecules collide, a transfer of energy happens from the more energetic to the less energetic.

Advection, usually wrongly called as convection, is the transfer of energy by bulk motion. In thermal energy transfer, this means a large number of molecules are moving collectively. This motion in the presence of temperature gradient contributes to the thermal energy transfer.

In this paper the problem to be solved is the thermal energy transfer by pure diffusion and by convection in a bidimensional domain. It is very useful to develop canonical problems, such as in this paper, to understand the physical characteristics in the thermal energy transfer behavior when imposed the boundary conditions. To reach this goal, numerical techniques were used.

Sometimes it is not possible to reach an exact answer to a thermal energy transfer problem, so usually it is used numerical methods in order to find a solution. To validate the numerical method, in this paper were used a synthesised solution, which means it is possible to resolve the thermal energy transfer analytically and compare with the numerical results.
2 MATHEMATICAL MODEL

The thermal energy diffusion equation is a partial differential equation. For a temperature function $T(x, y, t)$, it is usually compacted as shown in Equation 1, where $t$ represents time, $2$ is the Laplace operator and $\alpha$ is the thermal diffusivity coefficient.

\[
\frac{\partial T}{\partial t} = \frac{1}{\alpha} \nabla^2 T
\]  

(1)

In this study it is considered a bidimensional domain, so the thermal energy diffusion equation can be written as in Eq. 2

\[
\frac{\partial T}{\partial t} = \frac{1}{\alpha} \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right].
\]  

(2)

The thermal energy convective equation is similar to the Eq. 2. The difference is that the convective equation has the advective terms. The thermal energy convective equation is shown in Eq. 3:

\[
\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{1}{\alpha} \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right].
\]  

(3)

The boundaries conditions set were: the left side of the square has temperature $T_1$, the right side has temperature $T_2$ and both up and down sides have a linear behavior from $T_1$ to $T_2$, as shown in Eq. 4. Also, in the center of the geometry there is an area with more energy than the rest of the domain, with $T_1$ of temperature. In this case, $T_1$ is 200 oC and $T_2$ is 0 oC. The energy dissipation was disconsidered.

\[
\begin{align*}
T(x, y, 0) &= 0 \\
T(0, y, t) &= T_1 \\
T(L, y, t) &= T_2 \\
T(L, y, t) &= T_2
\end{align*}
\]  

(4)

Figure 1 shows the scheme of the boundary condition.
3 NUMERICAL ANALYSIS

Usually it is not possible to solve the thermal energy transfer analytically, so it is necessary to study numerical methods to reach this goal.

In this paper the numerical analysis is separated in 3 subsections. First will be discussed the finite-difference technique, for the spatial discretization and the creation of the mesh. For the time discretization was used two different methods, the first is the explicit method and the last the implicit method.

A Fortran90 algorithm was developed to compute the numerical calculus for each method. This programming language is used due to its ability of working with arrays - extremely important in the implicit method- and fast processing time, unlike high-level programming languages, that are easier to write but takes more computational process.

TecPlot360®c is used for the graphic interface to visualize the obtained transient data and analyse it qualitative.

3.1 FINITE-DIFFERENCE TECHNIQUE

Unlike the analytical solution, the numerical solution only enables the determination of the temperature in discrete points. As proposed by Ferziger et al. (2019) to select these points, it is necessary to divide the medium of the body in small regions and refer them with the point in the center. This reference point is usually called node and the group of all points is named as mesh, or even nodal network. The x and y coordinates are designated by i and j indices.

Doing so, the computer is capable to calculate the temperature of each cell at each instant. The more fine the mesh is, more accuracy the results have. However, the computational cost is huge depending on how small the regions are, which imply more time running the code and more data to deal with.
Equations 5 and 6 show the finite-difference approximation.

\[
\frac{\partial T}{\partial x}
\bigg|_{i-1/2,j} = \frac{T_{i,j} - T_{i-1,j}}{\Delta x}
\]  \hspace{1cm} (5)

\[
\frac{\partial T}{\partial x}
\bigg|_{i+1/2,j} = \frac{T_{i+1,j} - T_{i,j}}{\Delta x}
\]  \hspace{1cm} (6)

Equation 7 presents the approximation with finite-difference for the second derivative \( \frac{\partial^2 T}{\partial t^2} \).

\[
\frac{\partial^2 T}{\partial x^2}
\bigg|_{i,j} \approx \frac{\partial T/\partial x|_{i+1/2,j} - \partial T/\partial x|_{i-1/2,j}}{\Delta x}
\]  \hspace{1cm} (7)

Equation 8 is obtained substituting the Eq. 5 and Eq. 6 into Eq. 7. It demonstrates the second derivative approximation used in the code.

\[
\frac{\partial^2 T}{\partial y^2}
\bigg|_{i,j} \approx \frac{T_{i+1,j} + T_{i-1,j} - 2T_{i,j}}{(\Delta y)^2}
\]  \hspace{1cm} (8)

The process is analogous for the y direction, as showed in the Eq. 9.

\[
\frac{\partial^2 T}{\partial y^2}
\bigg|_{i,j} \approx \frac{T_{i+1,j} + T_{i-1,j} - 2T_{i,j}}{(\Delta y)^2}
\]  \hspace{1cm} (9)

This numerical technique is used to discretize the mathematical model in space. Now it is possible to write the mathematical model in a numerical way. To conclude the numerical analysis, it is required to discretize in time. For this, it is used two different methods.

3.2 EXPLICIT METHOD

The explicit method consists in calculate all the temperatures based on the previous temperatures. Equation 10 shows the finite-difference approximation to the time derivative.

\[
\frac{\partial T}{\partial t}
\bigg|_{i,j} \approx \frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t}
\]  \hspace{1cm} (10)
Where \( n+1 \) is the actual time and \( n \) is the previous time. This problem is a transient problem, so it calculates the temperature successively separated by the interval \( \Delta t \). So the total amount of time the code runs is the product between

\[
\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} = \frac{1}{\alpha} \left[ \frac{T_{i+1,j}^n + T_{i-1,j}^n - 2T_{i,j}^n}{\Delta x^2} + \frac{T_{i,j+1}^n + T_{i,j-1}^n - 2T_{i,j}^n}{\Delta y^2} \right]
\]  

(11)

Equation 12 represents the thermal energy transfer convective equation with the finite-difference technique for spatial discretization and the explicit method for the time.

\[
\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} + u \frac{T_{i+1,j}^n - T_{i-1,j}^n}{\Delta x} + v \frac{T_{i,j+1}^n - T_{i,j-1}^n}{\Delta y} = \frac{1}{\alpha} \left[ \frac{T_{i+1,j}^n + T_{i-1,j}^n - 2T_{i,j}^n}{\Delta x^2} + \frac{T_{i,j+1}^n + T_{i,j-1}^n - 2T_{i,j}^n}{\Delta y^2} \right]
\]  

(12)

Equation 13 shows the Eq. 11, isolating the \( n + 1 \) term and considering \( \Delta x = \Delta y \).

\[
T_{i,j}^{n+1} = F_o(T_{i+1,j}^n + T_{i-1,j}^n + T_{i,j+1}^n + T_{i,j-1}^n) + (1 - 4F_o)T_{i,j}^n
\]  

(13)

Equation 14 shows the Eq. 12, isolating the \( n + 1 \) term and considering \( \Delta x = \Delta y \).

\[
T_{i,j}^{n+1} = F_o(1 - u)T_{i+1,j}^n + (1 - v)T_{i,j+1}^n + (1 + u)T_{i-1,j}^n + (1 + v)T_{i,j-1}^n) + (1 - 4F_o)T_{i,j}^n
\]  

(14)

The Fourier number, the \( F_o \) term showed in Eq. 13 and 14 is represented in Eq. 15.

\[
F_o = \frac{\alpha \Delta t}{(\Delta x)^2}
\]  

(15)

The Fourier number, the \( F_o \) term showed in Eq. 13 and 14 is represented in Eq. 15.

\[
F_o = \frac{\alpha \Delta t}{(\Delta x)^2}
\]  

(15)

With the boundaries conditions given, the temperature of all nodes are available in the initial time, \( t = 0 \). These temperatures are used to calculate the nodal temperature in the new time \( t = \Delta t \). Now that the temperature of all nodes in the time \( t = \Delta t \) are available, these new temperatures are used to calculate the nodal temperatures in \( t = 2\Delta t \). This process goes on until it reaches the convergence.

The accuracy of the finite-difference increases as the value of \( \Delta t \) and \( \Delta x \) decreases. The values for those parameters have to be chosen wisely to be accurate enough for reach the convergence but not to small, so it is possible to run in domestic computers.

Unlike the next numerical method, the explicit method can show some oscillations that are not befitting with the physical reality, and those oscillations can make the method become unstable according to time, making the result diverges. So the explicit method has a stable criteria which consists in maintaining the Fourier number greater than or equal to zero. It has to adapt as \( (1 - 4F_o) \geq 0 \). The Inequality 16 represents the stable criteria that the explicit method must follow.
The implicit method, differently than the explicit method, calculate all the temperatures simultaneously. So it has a linear equations system to be solved at the same time to estimate all the temperatures.

The finite-difference equation for the implicit method, discretize the Eq. 2 and Eq. 3 at the actual time, n + 1 insted of the previous time, n.

Equation 17 shows the implicit thermal energy transfer diffusion equation.

\[
\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} = \frac{1}{\alpha} \left[ \frac{T_{i+1,j}^{n+1} + T_{i-1,j}^{n+1} - 2T_{i,j}^{n+1}}{\Delta x^2} + \frac{T_{i,j+1}^{n+1} + T_{i,j-1}^{n+1} - 2T_{i,j}^{n+1}}{\Delta y^2} \right]
\] (17)

Equation 18 shows the implicit thermal energy transfer convective equation.

\[
\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} + u \frac{T_{i+1,j}^{n+1} - T_{i-1,j}^{n+1}}{\Delta x} + v \frac{T_{i,j+1}^{n+1} - T_{i,j-1}^{n+1}}{\Delta y} = \frac{1}{\alpha} \left[ \frac{T_{i+1,j}^{n+1} + T_{i-1,j}^{n+1} - 2T_{i,j}^{n+1}}{\Delta x^2} + \frac{T_{i,j+1}^{n+1} + T_{i,j-1}^{n+1} - 2T_{i,j}^{n+1}}{\Delta y^2} \right]
\] (18)

Equation 19 shows the Eq. 17, isolating the known temperatures and considering \(\Delta x = \Delta y\).

\[
(1 + 4Fo)T_{i,j}^{n+1} - Fo(T_{i+1,j}^{n+1} + T_{i-1,j}^{n+1} + T_{i,j+1}^{n+1} + T_{i,j-1}^{n+1}) = T_{i,j}^n
\] (19)

Equation 20 shows the Eq. 18, isolating the known temperatures and considering \(\Delta x = \Delta y\).

\[
Fo[1 - u]T_{i+1,j}^{n+1} + (1 - v)T_{i,j+1}^{n+1} + (1 + u)T_{i-1,j}^{n+1} + (1 + v)T_{i,j-1}^{n+1}] + (1 - 4Fo)T_{i,j}^{n+1} = T_{i,j}^n
\] (20)

The actual temperature for i, j node depends on the actual temperatures of the side nodes, but all those temperatures are unknown. So all of them has to be solved simultaneously. In this paper, the method to solve this linear equations system is Gauss-Seidel method.

3.4 GAUSS-SEIDEL METHOD

The numerical method to solve the linear equation systems is the Guass-Seidel method. The convergence condition is that the coefficient matrix is strictly diagonal dominant. A linear equation system can be written in the matrix mode as represented in Eq. 21.

\[
A \cdot T = B
\] (21)
Where A represents the coefficient matrix, T represents the temperature vector and B represents the result vector. The coefficient matrix is a pentagonal matrix, which consists in the coefficients that follow the temperatures terms, represented in the temperatures vector. Lastly, the results vector is the temperatures that the values are already known.

Equation 22 represents the method to solve the linear equation system in an iterative way, where k is the number of the iteration.

\[ T_i^{(k+1)} = \frac{1}{Aii} \left( B_i - \sum_{j<i} A_{ij} T_j^{(k+1)} - \sum_{j=i} A_{ij} T_j^{(k)} \right), \quad i = 1, 2, ..., n \]  

(22)

The Gauss-Seidel method runs into a loop in the algorithm until the difference between the previous iteration temperature from the actual iteration tends to zero. This means the solution of the linear equations system converges and it is possible to continue the simulation.

The implicit method consumes a lot of computational process, once it is a loop running into another loop. Even if the implicit model is more accurate and stable, it consumes more computational process and the programmer has to be careful creating the algorithm. Otherwise the code takes too much time to achieve the convergence.

4 RESULTS

There are two different results obtained. Firstly is presented the pure diffusion simulations results. Lastly is presented the convective simulation results. In both cases were used the explicit and the implicit method.

The software used to plot the results was TecPlot360 due to its simplicity and good graphic results.
4.1 THERMAL ENERGY TRANSFER BY PURE DIFFUSION

To simulate the thermal energy transfer with only diffusion, it is used both Eq. 11 and Eq. 17 in the Fortran90 algorithm. They are the same equations then the convective equations, but without the presence of advection so velocities $u$ and $v$ are equal to zero. There are no advection velocity once it is being considerate only diffusion.

All the figures are from the explicit method.

In both methods, explicit and implicit, the intermediate conditions are possible to see the transfer of thermal energy from the most energetic molecules to the less energetic. When it reaches the convergence state, it is remarkable the linear behavior. That is expected, once the up and down boundary conditions are a linear behavior from $T_1$ to $T_2$.

Both methods show consistent behavior qualitative, transferring thermal energy from the most energetic to the less, it also represent the linear behavior all over the domain.

4.2 THERMAL ENERGY TRANSFER BY CONVECTION

To simulate the thermal energy transfer with the presence of diffusion and advection, it was used the both Eq. 12 and Eq. 18 in the algorithm. Unlike the last section,
the u and v velocities have both value of 5 m/s. Now with the presence of advection, there is a bulk motion to the up-right direction.

Figure 8 shows the initial condition of the problem. Figures 9 and 10 represent the intermediate conditions. Figure 11 demonstrates when the problem achieves the convergence state. All the figures are from the explicit method.

![Figure 8. Initial Condition.](image1)

![Figure 9. Intermediate Condition 1.](image2)

![Figure 10. Intermediate Condition 2.](image3)

![Figure 11. Final Condition.](image4)

Figures 6 and 7 represent an intermediate and the final condition, respectively. Both figures are from the implicit method.

![Figure 12. Intermediate Condition.](image5)

![Figure 13. Final Condition.](image6)
With more iterations is more possible to notice the influence of the bulk motion in the simulation. The first intermediate figure, Fig. 9, is extremely similar to the Fig. 3. But in Fig. 10 shows the influence of the bulk motion very clearly. Figure 12 demonstrates even more clearly the influence of the advection.

In both numerical methods is possible to see the transferring of energy from the higher temperature to the lower. The final condition, differently than the transfer by pure diffusion, is the try of a linear behavior but with the influence of the bulk motion.

5 VERIFICATION

The present section aims at a purely analytical approach of the thermal energy transfer equation with source term

\[
\frac{\partial T}{\partial t} = \frac{1}{\alpha} \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] + f(x, y, t) 
\]
(23)

\[
\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{1}{\alpha} \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] + f(x, y, t) 
\]
(24)

In this case, the source term of the equation is used as a verification technique named Method of Manufactured Solutions (Salari, 2000). The proposed method consists on manufacture an solution, find the source term for the proposed solution and then compare the analytical results with the numerical results.

Equation 25 proposes the \( T_s(x, y, t) \) solution where \( T_0 \) represents the amplitude of \( T_s(x, y, t) \). This choice was made since it is easy to find the source term, once it is trivial to derivate an exponential function.

\[
T_s = T_0 e^{-(x^2 + y^2) + t} 
\]  
(25)

To obtain the source term, it is necessary to change \( T \) for \( T_s \) and isolate \( f(x, y, t) \). As shown in Eq. 26 and Eq. 27.

\[
f(x, y, t) = \frac{\partial T_s}{\partial t} - \frac{1}{\alpha} \left[ \frac{\partial^2 T_s}{\partial x^2} + \frac{\partial^2 T_s}{\partial y^2} \right] 
\]  
(26)

\[
f(x, y, t) = \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} - \frac{1}{\alpha} \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] 
\]  
(27)

After calculating the first and second derivative of \( T_s \) and considering \( T_0 = 1 \) m/s, it is possible to rewrite the final form of the source term as in Eq. 28 and Eq. 29.
This step is important to the computational verification because it allows to indicate if there is any numerical mistake in the algorithm, or some error being propagated (Magalhães et al., 2019). The error was calculated using the L2 norm which is given by Eq. 30. Where \( n \) is the number of cells in the domain, \( x_{\text{numerical}} \) is the numerical value and \( x_{\text{analytical}} \) is the value obtained by both Eq. 24 and Eq. 23.

\[
L_2 = \sqrt{\frac{\sum_{i=1}^{n} (x_{\text{numerical}} - x_{\text{analytical}})^2}{n}}
\]  

Figure 14 shows the logarithm relation between the norm L2 and \( \Delta x \) for the thermal energy transfer by convection. Figure 15 shows the logarithm relation between the norm L2 and \( \Delta x \) for the thermal energy transfer by pure diffusion.

The slope of the adjustment line (m) gives the order of precision of the method. In Figure 14 presents \( m = 1.99999 \) and in Fig. 15 shows \( m = 2.00012 \).

6 CONCLUSION

The main objective of this paper is to simulate the thermal energy transfer by diffusion and by convection. To reach this goal was developed a Fortran90 algorithm to perform the numerical method. After this, using TecPlot360 the
results were plotted, being possible to analyse it qualitative. Lastly, with the MMS was possible to validate quantitative the simulation and analyse the errors.

Two different numerical methods were used in this paper for each simulation. The explicit method, which is faster but less robust and the implicit method, that is much slower but more stable. In both cases, the results are consistent, once it shows the expected behavior, being qualitative validated. It is possible to visualize the qualitative validation in Fig. 5, Fig. 7, Fig. 11 and Fig. 13.

The last step is to quantitative validate the results. To reach this goal, it was used the MMS to calculate the difference between the analytical results and the numerical results from the algorithm used in the simulations. The error was analysed using the norm L2. Figure 14 and Fig. 15 show the slope of the adjustment line close to 2. Since the method is second order, these results supports the consistent of the algorithm used in the simulations.

Regardless, the results were consistent and accurate, the simulations were qualitative and quantitative validated. This paper have achieved its objective, study the thermal energy transfer by diffusion and by convection and successfully simulate those situations in a robust algorithm.

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