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Convection Diffusion Equation in Transient Regime with Physical Properties Variable with Temperature using Least Squares Finite Element Method-LSFEM.

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Abstract. *The objective of this work was to solve the convection diffusion equation in transient regime with physical properties varying with temperature via the Least Squares Finite Element Method. For that, a code in C language was developed, two-dimensional elements with eight nodes were used for spatial discretization, the Cranck-Nicolson method for time discretization, the Gauss-Legendre quadrature method for calculating integrals and the conjugate gradients to solve the linear system due to the positive symmetric matrix being obtained. The results showed that as each time step, the thermal diffusivity, $\alpha(T)$, is a very small constant value, $\alpha(T) << 1$ the dominant phenomenon is convection. The most important contribution of this work was to use the second derivative of diffusion without the artifice of lowering its order and also to use the physical properties that vary with temperature in the diffusion convection equation.*

Keywords: *Convection Diffusion Equation , Transient Regime, Least Squares Finite Element Method, Language C.*

1. INTRODUCTION

According Dag *et al.* (2006) the convection diffusion equation model some of the phenomena such as the heat transfer in a draining film, water transfer in soils, spread of pollutants in rivers and streams, contaminant dispersion in shallow lakes, flow in porous media, dispersion of dissolved salts in groundwater, thermal pollution in river systems, etc. According Ferreira (2015) the analytical solutions of the convection diffusion equation when initial and boundary conditions are complicated, then numerical methods are used to obtain the solution. The least squres finite element method - LSFEM presents a unified formulation for the 3 types of partial differential equations, resulting in positive symmetric and defined matrices, which are efficiently solved using the conjugate gradient method.

Romão *et al.* (2011) presents the numerical solution by the Galerkin and Least Squares Finite Element Methods, of the three-dimensional Poisson and Helmholtz equations. The results showed that LSFEM shows better performance when compared to the Galerkin method, when the objective is to obtain the derivative of T (x, y, z). In the work of Pereira *et al.* (2014) the LSFEM was used to solve the three-dimensional diffusion convection equation with Peclet number ranging from 10, 10^2,..., 10^9. The results showed that for low Peclet values, 10 or 10^2 the solutions did not show oscillations, for high values there are oscillations in the solutions due to the mesh refinement limited by the processing capacity. Putri *et al.* (2018) presented the numerical solution of the two-dimensional diffusion convection equation via LSFEM. The results were compared with the analytical solutions of the equation and presented very close values, so the developed code was validated.

Given this contextualization from the analysis of the works presented, it is possible to perceive the great importance of the diffusion convection equation in several applications, especially in the area of heat transfer, the use of LSFEM to solve these problems will provide results that will enrich the literature.

The objective of this work is to resolve convection diffusion equation in transient regime with physical properties variable with temperature using least squares finite element method-LSFEM.

2. FORMULATION MATHEMATICAL

The objective of this work is to solve the diffusion convection equation in transient regime with physical properties that vary with temperature using the least squares finite element method, in a generic domain $\Omega \in R^2$ it is limited and closed, with Dirichlet boundary conditions and initial condition. The partial differential equation for this problem under study is presented in Eq. (1),

$$\frac{\partial T(x,y,t)}{\partial t} + u\frac{\partial T(x,y,t)}{\partial x} + v\frac{\partial T(x,y,t)}{\partial y} = \alpha(T)\frac{\partial^2 T(x,y,t)}{\partial x^2} + \alpha(T)\frac{\partial^2 T(x,y,t)}{\partial y^2} \tag{1}$$

The thermal diffusivity, $\alpha(T)$, which represents the speed at which heat diffuses through a material medium is defined according to the Eq. (2),

$$\alpha(T) = \frac{k(T)}{\rho(T)c_p(T)} \tag{2}$$

where, $\rho(T)$, is the density, $c_p(T)$, is the specific heat, $k(T)$ the thermal conductivity and $\vec{U} = (u, v)$ is the speed field.

2.1 METHOD LEAST SQUARES

The central idea of the method of least squares is to determine u $\in \Omega^e$ for the minimization of the integral of the residue. Defining the quadratic functional as equation (3).

$$I(u) = |[R(u)]|^2 = \int_\Omega R(u)^2 d\Omega \tag{3}$$

with $u \in \Omega^e$={ $u \in H^2$} at where H^2 is the Hilbert space of order 2. To the solution u be a minimizer of the functional given by equation (3) the first variation δI equation (4) it should be zero.

$$\delta I(u) = 2\int_\Omega (\delta R)R(x)d\Omega = 0 \quad \text{or} \quad \delta I(u) = \int_\Omega (\delta R)R(x)d\Omega = 0 \tag{4}$$

Therefore we conclude that the function w_i will be equal to the first variation of the residue δ being the least squares method.

2.2 FORMULATION MATHEMATICAL USING FINITE ELEMENT METHOD OF LEAST SQUARES - LS-FEM

Isolating the transient term of the equation (41) obtains the equation (5).

$$\frac{\partial T(x,y,t)}{\partial t} = \alpha(T)\frac{\partial^2 T(x,y,t)}{\partial x^2} + \alpha(T)\frac{\partial^2 T(x,y,t)}{\partial y^2} - u\frac{\partial T(x,y,t)}{\partial x} - v\frac{\partial T(x,y,t)}{\partial y} \tag{5}$$

The approximate solution $\widetilde{T}(x,y,t)$ is given by equation (6).

$$\widetilde{T}(x,y,t) = \sum_{i=1}^{Nnos} T_i(t)N_i(x,y) \tag{6}$$

From the approach of family θ can approach the transient term adopting $\theta = 0.5$ called a scheme of Cranck - Nicolson.

$$\begin{aligned}\frac{\widetilde{T}_n^{s+1} - \widetilde{T}_n^s}{\Delta t} &= \theta\left\{\alpha(T)\frac{\partial^2\widetilde{T}}{\partial x^2} + \alpha(T)\frac{\partial^2\widetilde{T}}{\partial y^2} - u\frac{\partial\widetilde{T}}{\partial x} - v\frac{\partial\widetilde{T}}{\partial y}\right\}^{s+1} + (1-\theta)\left\{\alpha(T)\frac{\partial^2\widetilde{T}}{\partial x^2} + \alpha(T)\frac{\partial^2\widetilde{T}}{\partial y^2} - u\frac{\partial\widetilde{T}}{\partial x}\right. \\ &- \left. v\frac{\partial\widetilde{T}}{\partial y}\right\}^s \\ &= 0.5\left\{\alpha(T)\frac{\partial^2\widetilde{T}}{\partial x^2} + \alpha(T)\frac{\partial^2\widetilde{T}}{\partial y^2} - u\frac{\partial\widetilde{T}}{\partial x} - v\frac{\partial\widetilde{T}}{\partial y}\right\}^{s+1} + 0.5\left\{\alpha(T)\frac{\partial^2\widetilde{T}}{\partial x^2} + \alpha(T)\frac{\partial^2\widetilde{T}}{\partial y^2} - u\frac{\partial\widetilde{T}}{\partial x}\right. \\ &- \left. v\frac{\partial\widetilde{T}}{\partial y}\right\}^s\end{aligned} \tag{7}$$

The residue $R(x,y)$ is given by equation (8).

$$\begin{aligned}R(x,y) &= \frac{\widetilde{T}^{s+1}}{\Delta t} - \frac{\widetilde{T}^s}{\Delta t} - 0.5\left\{\alpha(T)\frac{\partial^2\widetilde{T}}{\partial x^2} + \alpha(T)\frac{\partial^2\widetilde{T}}{\partial y^2} - u\frac{\partial\widetilde{T}}{\partial x} - v\frac{\partial\widetilde{T}}{\partial y}\right\}^{s+1} - 0.5\left\{\alpha(T)\frac{\partial^2\widetilde{T}}{\partial x^2} + \alpha(T)\frac{\partial^2\widetilde{T}}{\partial y^2}\right. \\ &- \left. u\frac{\partial\widetilde{T}}{\partial x} - v\frac{\partial\widetilde{T}}{\partial y}\right\}^s\end{aligned} \tag{8}$$

Grouping the terms in time s and time $s+1$ it has equation (9).

$$\begin{aligned} R(x,y) &= \left\{\frac{\widetilde{T}}{\Delta t} - 0.5\alpha(T^s)\frac{\partial^2\widetilde{T^s}}{\partial x^2} - 0.5\alpha(T^s)\frac{\partial^2\widetilde{T^s}}{\partial y^2} + 0.5u\frac{\partial\widetilde{T}}{\partial x} + 0.5v\frac{\partial\widetilde{T}}{\partial y}\right\}^{s+1} + \left\{-\frac{\widetilde{T}}{\Delta t} - 0.5\alpha(T^{s-1})\frac{\partial^2\widetilde{T}}{\partial x^2}\right. \\ &- \left. 0.5\alpha(T^{s-1})\frac{\partial^2\widetilde{T}}{\partial y^2} + 0.5u\frac{\partial\widetilde{T}}{\partial x} + 0.5v\frac{\partial\widetilde{T}}{\partial y}\right\}^{s} \end{aligned} \tag{9}$$

Therefore:

$$\begin{aligned} R(x,y) &= \left\{\frac{1}{\Delta t}\sum_{i=1}^{Nnos} T_i^{s+1}N_i - 0.5\alpha(T^s)\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial^2 N_i}{\partial x^2} - 0.5\alpha(T^s)\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial^2 N_i}{\partial y^2} + 0.5u\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial N_i}{\partial x}\right. \\ &+ \left. 0.5v\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial N_i}{\partial y}\right\} + \left\{-\frac{1}{\Delta t}\sum_{i=1}^{Nnos} T_i^{s}N_i - 0.5\alpha(T^{s-1})\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial^2 N_i}{\partial x^2} - 0.5\alpha(T^{s-1})\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial^2 N_i}{\partial y^2}\right. \\ &+ \left. 0.5u\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial N_i}{\partial x} + 0.5v\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial N_i}{\partial y}\right\} \end{aligned} \tag{10}$$

The first variation δR the residue equation (10) is given by:

$$\begin{aligned} \delta R &= \frac{\partial R}{\partial T_i}\delta T_i = \left(\frac{1}{\Delta t}\sum_{i=1}^{Nnos} N_i - 0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial x^2} - 0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial y^2} + 0.5u\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial x}\right. \\ &+ \left. 0.5v\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial y}\right)\delta T_i \end{aligned} \tag{11}$$

Applying the method of least squares equation (12).

$$\begin{aligned} \int_\Omega R(x,y)\delta R d\Omega &= \int_\Omega\left\{\left(\frac{1}{\Delta t}\sum_{i=1}^{Nnos} T_i^{s+1}N_i - 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial^2 N_i}{\partial x^2} - 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial^2 N_i}{\partial y^2}\right.\right. \\ &+ \left. 0.5u\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial N_i}{\partial x} + 0.5v\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial N_i}{\partial y}\right) + \left(-\frac{1}{\Delta t}\sum_{i=1}^{Nnos} T_i^{s}N_i - 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial^2 N_i}{\partial x^2}\right. \\ &- \left.\left. 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial^2 N_i}{\partial y^2} + 0.5u\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial N_i}{\partial x} + 0.5v\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial N_i}{\partial y}\right)\right\}\left\{\frac{1}{\Delta t}\sum_{i=1}^{Nnos} N_i\right. \\ &- \left. 0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial x^2} - 0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial y^2} + 0.5u\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial x} + 0.5v\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial y}\right\}\delta T_i d\Omega = 0. \end{aligned} \tag{12}$$

as $\delta T_i \neq 0$.

$$\begin{aligned} \int_\Omega R(x,y)\delta R d\Omega &= \int_\Omega\left\{\left(\frac{1}{\Delta t}\sum_{i=1}^{Nnos} T_i^{s+1}N_i - 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial^2 N_i}{\partial x^2} - 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial^2 N_i}{\partial y^2}\right.\right. \\ &+ \left. 0.5u\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial N_i}{\partial x} + 0.5v\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial N_i}{\partial y}\right) + \left(-\frac{1}{\Delta t}\sum_{i=1}^{Nnos} T_i^{s}N_i - 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial^2 N_i}{\partial x^2}\right. \\ &- \left.\left. 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial^2 N_i}{\partial y^2} + 0.5u\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial N_i}{\partial x} + 0.5v\sum_{i=1}^{Nnos} T_i^{s}\frac{\partial N_i}{\partial y}\right)\right\}\left\{\frac{1}{\Delta t}\sum_{i=1}^{Nnos} N_i\right. \\ &- \left. 0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial x^2} - 0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial y^2} + 0.5u\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial x} + 0.5v\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial y}\right\}d\Omega = 0. \\ &= \int_\Omega\left(\frac{1}{\Delta t}\sum_{i=1}^{Nnos} T_i^{s+1}N_i - 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial^2 N_i}{\partial x^2} - 0.5\alpha(T)\sum_{i=1}^{Nnos} T_i^{s+1}\frac{\partial^2 N_i}{\partial y^2}\right. \end{aligned}$$

$$
\begin{aligned}
&+ \quad 0.5u\sum_{i=1}^{Nnos}T_i^{s+1}\frac{\partial N_i}{\partial x}+0.5v\sum_{i=1}^{Nnos}T_i^{s+1}\frac{\partial N_i}{\partial y}\Bigg)\Bigg(\frac{1}{\Delta t}\sum_{i=1}^{Nnos}N_i-0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial x^2}\\
&- \quad 0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial y^2}+0.5u\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial x}+0.5v\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial y}\Bigg)d\Omega+\int_\Omega\Bigg(-\frac{1}{\Delta t}\sum_{i=1}^{Nnos}T_i^sN_i\\
&- \quad 0.5\alpha(T)\sum_{i=1}^{Nnos}T_i^s\frac{\partial^2 N_i}{\partial x^2}+0.5\alpha(T)\sum_{i=1}^{Nnos}T_i^s\frac{\partial^2 N_i}{\partial y^2}+0.5u\sum_{i=1}^{Nnos}T_i^s\frac{\partial N_i}{\partial x}\\
&+ \quad 0.5v\sum_{i=1}^{Nnos}T_i^s\frac{\partial N_i}{\partial y}\Bigg)\Bigg(\frac{1}{\Delta t}\sum_{i=1}^{Nnos}N_i-0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial x^2}-0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial y^2}\\
&+ \quad 0.5u\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial x}+0.5v\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial y}\Bigg)d\Omega=0.
\end{aligned}
\tag{13}
$$

Because the values of T_i^s are known:

$$
\begin{aligned}
&\int_\Omega\Bigg(\frac{1}{\Delta t}\sum_{i=1}^{Nnos}T_i^{s+1}N_i \quad - \quad 0.5\alpha(T)\sum_{i=1}^{Nnos}T_i^{s+1}\frac{\partial^2 N_i}{\partial x^2}-0.5\alpha(T)\sum_{i=1}^{Nnos}T_i^{s+1}\frac{\partial^2 N_i}{\partial y^2}+0.5u\sum_{i=1}^{Nnos}T_i^{s+1}\frac{\partial N_i}{\partial x}\\
&\qquad + \quad 0.5v\sum_{i=1}^{Nnos}T_i^{s+1}\frac{\partial N_i}{\partial y}\Bigg)\Bigg(\frac{1}{\Delta t}\sum_{i=1}^{Nnos}N_i-0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial x^2}-0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial y^2}\\
&\qquad + \quad 0.5u\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial x}+0.5v\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial y}\Bigg)d\Omega\\
&= - \quad \int_\Omega\Bigg(-\frac{1}{\Delta t}\sum_{i=1}^{Nnos}T_i^sN_i-0.5\alpha(T)\sum_{i=1}^{Nnos}T_i^s\frac{\partial^2 N_i}{\partial x^2}+0.5\alpha(T)\sum_{i=1}^{Nnos}T_i^s\frac{\partial^2 N_i}{\partial y^2}+0.5u\sum_{i=1}^{Nnos}T_i^s\frac{\partial N_i}{\partial x}\\
&+ \quad 0.5v\sum_{i=1}^{Nnos}T_i^s\frac{\partial N_i}{\partial y}\Bigg)\Bigg(\frac{1}{\Delta t}\sum_{i=1}^{Nnos}N_i-0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial x^2}-0.5\alpha(T)\sum_{i=1}^{Nnos}\frac{\partial^2 N_i}{\partial y^2}+0.5u\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial x}\\
&+ \quad 0.5v\sum_{i=1}^{Nnos}\frac{\partial N_i}{\partial y}\Bigg)d\Omega
\end{aligned}
\tag{14}
$$

Rearranging the equation (14) get the linear system equation (15).

$$[A]\{T^{s+1}\}=[b]\{T^s\} \tag{15}$$

where

$$
\begin{aligned}
A_{i,j} \quad &= \quad \int_\Omega\left(\frac{1}{\Delta t}N_i-0.5\alpha(T)\frac{\partial^2 N_i}{\partial x^2}-0.5\alpha(T)\frac{\partial^2 N_i}{\partial y^2}+0.5u\frac{\partial N_i}{\partial x}+0.5v\frac{\partial N_i}{\partial y}\right)\left(\frac{1}{\Delta t}N_j-0.5\alpha(T)\frac{\partial^2 N_j}{\partial x^2}\right.\\
&- \quad \left.0.5\alpha(T)\frac{\partial^2 N_j}{\partial y^2}+0.5u\frac{\partial N_j}{\partial x}+0.5v\frac{\partial N_j}{\partial y}\right)d\Omega
\end{aligned}
\tag{16}
$$

$$
\begin{aligned}
b_i \quad &= \quad -\int_\Omega\left(-\frac{1}{\Delta t}N_i-0.5\alpha(T)\frac{\partial^2 N_i}{\partial x^2}+0.5\alpha(T)\frac{\partial^2 N_i}{\partial y^2}+0.5u\frac{\partial N_i}{\partial x}+0.5v\frac{\partial N_i}{\partial y}\right)\left(\frac{1}{\Delta t}N_j-0.5\alpha(T)\frac{\partial^2 N_j}{\partial x^2}\right.\\
&- \quad \left.0.5\alpha(T)\frac{\partial^2 N_j}{\partial y^2}+0.5u\frac{\partial N_j}{\partial x}+0.5v\frac{\partial N_j}{\partial y}\right)d\Omega
\end{aligned}
\tag{17}
$$

3. METHODOLOGY

For resolve the equation of convection - diffusion two dimensional using least squares finite element method - LSFEM a code in C language was implemented quadratic two - dimensional elements with 8 nodes were used for spatial discretization. The Cranck-Nicolson method was used to discretize the time, the method of Gaussian Quadrature - Legendre are used for the calculation of the integrals, the solving the linear system obtained will be used the method of conjugate gradients why the global matrix is symmetric and positive definite sparse result of using LSFEM.

3.1 Discretização Espacial

In the context of the finite element method, there are two basic types of coordinate systems, the local coordinate system where coordinates are expressed in terms of (ξ, η) this being the domain of the reference element Ω^r and the global coordinate system where the coordinates are expressed in terms of the Cartesian coordinates (x, y) this being the domain of the global element Ω^e. The transformation from the global coordinates (x, y) to the local coordinates (ξ, η) is done through the change presented below according to Reddy (1993, p. 421).

$$x = \sum_{i=1}^{Nnos} x_i N_i(\xi, \eta) \qquad y = \sum_{i=1}^{Nnos} y_i N_i(\xi, \eta) \tag{18}$$

where $(x_i,\, y_i)$ are the global coordinates of the i -th node of the global element Ω^e and $N_i(xi, \eta)$ are the interpolation functions of the Ω^r reference element. The $N_i(x, y)$ interpolation functions can be expressed as a function of the local coordinates (ξ, η),

$$N_i(x, y) = N_i(x(\xi, \eta), y(\xi, \eta)) \tag{19}$$

Usando a regra da cadeia para a função $N_i(x, y)$, obtem- se $\partial N_i/\partial \xi$ and $\partial N_i/\partial \eta$, Eq. (20),

$$\frac{\partial N_i}{\partial \xi} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \xi} \qquad \frac{\partial N_i}{\partial \eta} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \eta} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \eta} \tag{20}$$

in matrix notation, Eq.(21)

$$\left\{ \begin{array}{c} \partial N_i/\partial \xi \\ \\ \partial N_i/\partial \eta \end{array} \right\} = \underbrace{\left[\begin{array}{cc} \partial x/\partial \xi & \partial y/\partial \xi \\ \\ \partial x/\partial \eta & \partial y/\partial \eta \end{array} \right]}_{J} \left\{ \begin{array}{c} \partial N_i/\partial x \\ \\ \partial N_i/\partial y \end{array} \right\} \tag{21}$$

From Eq. (21) we obtain the relationship between the global coordinates (x, y) and the local coordinates (ξ, η) of the first order partial derivatives of the interpolation functions $N_i(x, y)$. Matrix J is the Jacobian matrix of the transformation. Showing the first order partial derivatives of $N_i(x, y)$ as a function of the global coordinates (x, y), Eq.(22),

$$\left\{ \begin{array}{c} \partial N_i/\partial x \\ \\ \partial N_i/\partial y \end{array} \right\} = J^{-1} \left\{ \begin{array}{c} \partial N_i/\partial \xi \\ \\ \partial N_i/\partial \eta \end{array} \right\} = \frac{1}{|det(J)|} \left[\begin{array}{cc} \partial y/\partial \eta & -\partial y/\partial \xi \\ \\ \partial x/\partial \eta & \partial x/\partial \eta \end{array} \right] \left\{ \begin{array}{c} \partial N_i/\partial \xi \\ \\ \partial N_i/\partial \eta \end{array} \right\} \tag{22}$$

For the first order partial derivatives to exist in relation to the global coordinates (x, y) of the interpolation functions $N_i(x, y)$ it is necessary and sufficient that there is the inverse of the Jacobian matrix J, for that this occurs the determinant $det(J)$ must be non-null for all points (ξ, η) in Ω^e, that is,

$$det(J) = \frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial x}{\partial \eta} \neq 0. \tag{23}$$

Then the first order partial derivatives in relation to the global coordinates (x, y) of the $N_i(x, y)$ interpolation functions will be, Eq.(24),

$$\frac{\partial N_i}{\partial x} = \frac{1}{|J|}\left[\frac{\partial y}{\partial \eta}\frac{\partial N_i}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial N_i}{\partial \eta}\right] \qquad \frac{\partial N_i}{\partial y} = \frac{1}{|J|}\left[-\frac{\partial x}{\partial \eta}\frac{\partial N_i}{\partial \xi} + \frac{\partial x}{\partial \xi}\frac{\partial N_i}{\partial \eta}\right] \tag{24}$$

Second order partial derivatives in relation to the global coordinates (x, y) of the $N_i(x, y)$ interpolation functions are presented in Eq. (25) e Eq. (26),

$$\begin{aligned} \frac{\partial^2 N_i}{\partial x^2} &= \frac{1}{|J|^2}\left[\left(\frac{\partial y}{\partial \eta}\right)^2 \frac{\partial^2 N_i}{\partial \xi^2} - 2\left(\frac{\partial y}{\partial \eta}\frac{\partial y}{\partial \xi}\frac{\partial^2 N_i}{\partial \xi \partial \eta}\right) + \left(\frac{\partial y}{\partial \xi}\right)^2 \frac{\partial^2 N_i}{\partial \eta^2}\right. \\ &+ \left.\left(\frac{\partial y}{\partial \eta}\frac{\partial^2 y}{\partial \xi \partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial^2 y}{\partial \eta^2}\right)\frac{\partial N_i}{\partial \xi} + \left(\frac{\partial y}{\partial \xi}\frac{\partial^2 y}{\partial \xi \partial \eta} - \frac{\partial y}{\partial \eta}\frac{\partial^2 y}{\partial \xi^2}\right)\frac{\partial N_i}{\partial \eta}\right] \\ &- \frac{1}{|J|^3}\left[\left(\frac{\partial y}{\partial \eta}\right)^2 \frac{\partial |J|}{\partial \xi}\frac{\partial N_i}{\partial \xi} - \frac{\partial y}{\partial \eta}\frac{\partial y}{\partial \xi}\frac{\partial |J|}{\partial \eta}\frac{\partial N_i}{\partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial y}{\partial \eta}\frac{\partial |J|}{\partial \xi}\frac{\partial N_i}{\partial \xi}\right. \\ &+ \left.\left(\frac{\partial y}{\partial \eta}^2\right)\frac{\partial |J|}{\partial \eta}\frac{\partial N_i}{\partial \eta}\right] \end{aligned} \tag{25}$$

$$\begin{aligned}
\frac{\partial^2 N_i}{\partial y^2} &= \frac{1}{|J|^2}\Bigg[\left(\frac{\partial x}{\partial \eta}\right)^2\frac{\partial^2 N_i}{\partial \xi^2} - 2\left(\frac{\partial x}{\partial \eta}\frac{\partial x}{\partial \xi}\frac{\partial^2 N_i}{\partial \xi \partial \eta}\right) + \left(\frac{\partial x}{\partial \xi}\right)^2\frac{\partial^2 N_i}{\partial \eta^2} \\
&+ \left(\frac{\partial x}{\partial \eta}\frac{\partial^2 x}{\partial \xi \partial \eta} - \frac{\partial x}{\partial \xi}\frac{\partial^2 x}{\partial \eta^2}\right)\frac{\partial N_i}{\partial \xi} + \left(\frac{\partial x}{\partial \xi}\frac{\partial^2 x}{\partial \xi \partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial^2 x}{\partial \xi^2}\right)\frac{\partial N_i}{\partial \eta}\Bigg] \\
&- \frac{1}{|J|^3}\Bigg[\left(\frac{\partial x}{\partial \eta}\right)^2\frac{\partial |J|}{\partial \xi}\frac{\partial N_i}{\partial \xi} - \frac{\partial x}{\partial \eta}\frac{\partial x}{\partial \xi}\frac{\partial |J|}{\partial \eta}\frac{\partial N_i}{\partial \eta} - \frac{\partial x}{\partial \xi}\frac{\partial x}{\partial \eta}\frac{\partial |J|}{\partial \xi}\frac{\partial N_i}{\partial \xi} \\
&+ \left(\frac{\partial x}{\partial \eta}^2\right)\frac{\partial |J|}{\partial \eta}\frac{\partial N_i}{\partial \eta}\Bigg] \qquad (26)
\end{aligned}$$

where

$$\begin{aligned}
\frac{\partial |J|}{\partial \xi} &= \frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial x}{\partial \eta}\right) \\
&= \frac{\partial^2 x}{\partial \xi^2}\frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \xi}\frac{\partial^2 y}{\partial \xi \partial \eta} - \frac{\partial^2 y}{\partial \xi^2}\frac{\partial x}{\partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial^2 x}{\partial \xi \partial \eta} \\
\frac{\partial |J|}{\partial \eta} &= \frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial x}{\partial \eta}\right) \\
&= \frac{\partial^2 x}{\partial \xi \partial \eta}\frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta}\frac{\partial^2 y}{\partial \eta^2} - \frac{\partial^2 y}{\partial \eta \partial \xi}\frac{\partial x}{\partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial^2 x}{\partial \eta^2} \qquad (27)
\end{aligned}$$

with

$$\begin{aligned}
\frac{\partial x}{\partial \xi} &= \sum_{i=1}^{Nnos} x_i \frac{\partial N_i(\xi,\eta)}{\partial \xi} \qquad \frac{\partial x}{\partial \eta} = \sum_{i=1}^{Nnos} x_i \frac{\partial N_i(\xi,\eta)}{\partial \eta} \qquad \frac{\partial^2 x}{\partial \xi^2} = \sum_{i=1}^{Nnos} x_i \frac{\partial^2 N_i(\xi,\eta)}{\partial \xi^2} \\
\frac{\partial^2 x}{\partial \eta^2} &= \sum_{i=1}^{Nnos} x_i \frac{\partial^2 N_i(\xi,\eta)}{\partial \eta^2} \qquad \frac{\partial^2 x}{\partial \xi \partial \eta} = \sum_{i=1}^{Nnos} x_i \frac{\partial^2 N_i(\xi,\eta)}{\partial \xi \partial \eta} \qquad (28)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial y}{\partial \xi} &= \sum_{i=1}^{Nnos} y_i \frac{\partial N_i(\xi,\eta)}{\partial \xi} \qquad \frac{\partial y}{\partial \eta} = \sum_{i=1}^{Nnos} y_i \frac{\partial N_i(\xi,\eta)}{\partial \eta} \qquad \frac{\partial^2 y}{\partial \xi^2} = \sum_{i=1}^{Nnos} y_i \frac{\partial^2 N_i(\xi,\eta)}{\partial \xi^2} \\
\frac{\partial^2 y}{\partial \eta^2} &= \sum_{i=1}^{Nnos} y_i \frac{\partial^2 N_i(\xi,\eta)}{\partial \eta^2} \qquad \frac{\partial^2 y}{\partial \xi \partial \eta} = \sum_{i=1}^{Nnos} y_i \frac{\partial^2 N_i(\xi,\eta)}{\partial \xi \partial \eta} \qquad (29)
\end{aligned}$$

3.2 Method of Gaussian Quadrature - Legendre

The Gaussian Quadrature chooses the points for the calculation in an optimal way instead of being equally spaced as occurs in Newton Cotes' formulas . The points $x_1, x_2, \ldots, x_n$ in the range $[a, b]$ and the weights $w_1, w_2, \ldots, w_n$ are chosen so that the error made in the approximation is minimized, Eq.(30),

$$\int_a^b f(x)dx \simeq \sum_{i=0}^{n} W(x)f(x)dx \simeq \sum_{i=0}^{n} w_i f(x_i). \qquad (30)$$

In the case of the Gauss-Legendre Quadrature the $p_n(x)$ interpolator polynomial is the Legendre polynomial with weight function $W(x) = 1$. Legendre's polynomials are defined by the recurrence formula, Eq. (31),

$$P_n(x) = \frac{(2n-1)xP_{n-1}(x) - (n-1)P_{n-2}(x)}{n} \qquad (31)$$

with $P_0(x) = 1$ e $P_1(x) = x$. The weight functions w_i and the points x_i that are roots of Legrendre's polynomials are tabulated for polynomials of different degrees. The quadrature formula for a quadrilateral element is given by, Eq.(32),

$$\int F(\xi,\eta)d\xi d\eta = \int_{-1}^{1}\left[\int_{-1}^{1} F(\xi,\eta)d\xi\right]d\eta = \int_{-1}^{1}\left[\sum_{j=1}^{N} F(\xi,\eta_j)w_j\right]d\eta$$

$$= \sum_{i=1}^{M}\sum_{j=1}^{N} F(\xi_i,\eta_j)w_i w_j \quad (32)$$

where M and N are called square points in the (ξ,η) directions, with (ξ_i,η_j) gauss points and (w_i,w_j) Gaussian pesos.

3.3 The Cranck-Nicolson method

For the temporal discretization, the θ family method is widely used for the integration of first order differential equations. It is a single step method where the value of T^{n+1} is unknown at time $n+1$, but can be calculated from the value of T^n at time n . In this case, a weighted average is made between T^{n+1} and T^n at the end points of the integration interval.

$$\frac{\partial T}{\partial t} \approx \frac{T^{n+1}-T^n}{\Delta t} = (1-\theta)\frac{\partial T^n}{\partial t} + \theta\frac{\partial T^{n+1}}{\partial t} \quad (33)$$

The time step Δt is kept constant and the parameter θ assumes values within the range $[0.1]$. By varying the values of the parameter θ, different numerical integration schemes are obtained according to Reddy (1993) we have:

$$\theta = \begin{cases} 0, & \text{Differences scheme forward, conditionally stable with precision } O(\Delta t) \\ \frac{1}{2}, & \text{Crank Nicolson scheme, precisely stable } O(\Delta t)^2 \\ \frac{2}{3}, & \text{Galerkin method, stable with precision } O(\Delta t)^2 \\ 1, & \text{Differences scheme backwards, stable with precision } O(\Delta t) \end{cases}$$

3.4 Method of conjugate gradients

The method of conjugate gradients proposed is the most popular iterative method for solving large linear systems where the coefficient matrix is symmetric, sparse and positive, this method proposes a function to be optimized so that the minimum of this function is the solution of the. linear system in question. Given a linear system of the for, Eq. (34).

$$Ax = b \quad (34)$$

with A $\in R^{nxn}$, x $\in R^n$ and b $\in R^n$ The basic idea of an optimization method is to create the optimization function. $F(x): R^n \to R$, because minimizing this function is equivalent to solving the linear system Eq. (34).

4. RESULTS

The results obtained were compared with the analytical solutions via the method of separating the variables to validate the proposed C language code.

4.1 Transient diffusion with constant physical properties

The differential equation for the diffusion problem in transient regime with constant physical properties is presented in Eq. (35),

$$\frac{\partial T(x,y,t)}{\partial t} + k\frac{\partial^2 T(x,y,t)}{\partial x^2} + k\frac{\partial^2 T(x,y,t)}{\partial y^2} = 0. \quad (35)$$

The boundary conditions of the Dirichlet type and the initial conditions are shown in the Eq. (36),

$$\begin{aligned} T(0,y,t) &= 0°\text{C} \quad T(x,0,t) = 0°\text{C} \quad T(1,y,t) = 0°\text{C} \quad T(x,1,t) = 0°\text{C} \quad T(x,y,0) = 100°\text{C} \\ &\text{with} \quad 0 \le (x,y) \le 1 \quad . \end{aligned} \quad (36)$$

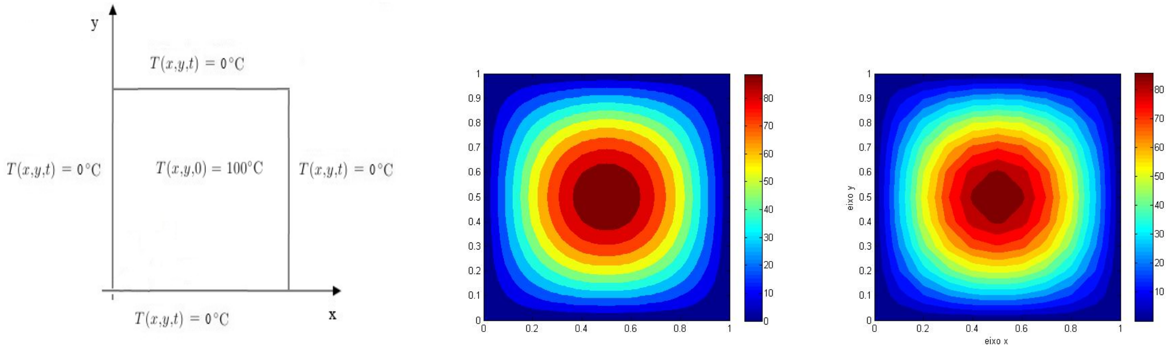
A solução analitica da Eq. (36) é apresentada na Eq.(37),

$$\begin{aligned} T(x,y,t) &= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \frac{400(1-\cos(m\pi)-\cos(n\pi)}{mn\pi^2}\sin(m)\sin(n\pi y)e^{-k\gamma_{mn}^2 t} \\ &+ \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \frac{400(cos(n\pi)\cos(m\pi))}{mn\pi^2}\sin(m)\sin(n\pi y)e^{-k\gamma_{mn}^2 t} \end{aligned} \quad (37)$$

with

$$\gamma_{mn}^2 = \pi^2(m^2+n^2). \quad (38)$$

To obtain the numerical solution, the domain was discretized using 1600 quadrilateral elements with 8 nodes, in temporal discretization a time step $\Delta t = 0.02$ s was used, the value of the thermal conductivity used will be equal to $k =$ 10 W/m.K. The solution analytical, numerical and domain of the problem presented in Eq. (35) presented in the Fig. 1.



(a) Domain. (b) Analytical solution with LSFEM. (c) Numerical solution.

Figure 1. Domain and results for transient diffusion.

For the validation of the numerical solution, a comparison was made between a line of the numerical solution and the analytical solution, shown in Fig. 2, where the biggest difference is equal to approximately 1 %, then it can be concluded that the numerical solution presents a good approximation.

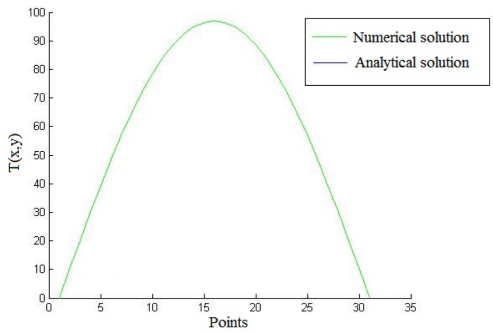


Figure 2. Comparison between numerical and analytical solutions.

4.2 Transient convection with constant physical properties

The differential equation for the transient convection problem is presented in Eq.(39).

$$\frac{\partial T(x,y,t)}{\partial t} + u\frac{\partial T(x,y,t)}{\partial x} + v\frac{\partial T(x,y,t)}{\partial y} = 0. \tag{39}$$

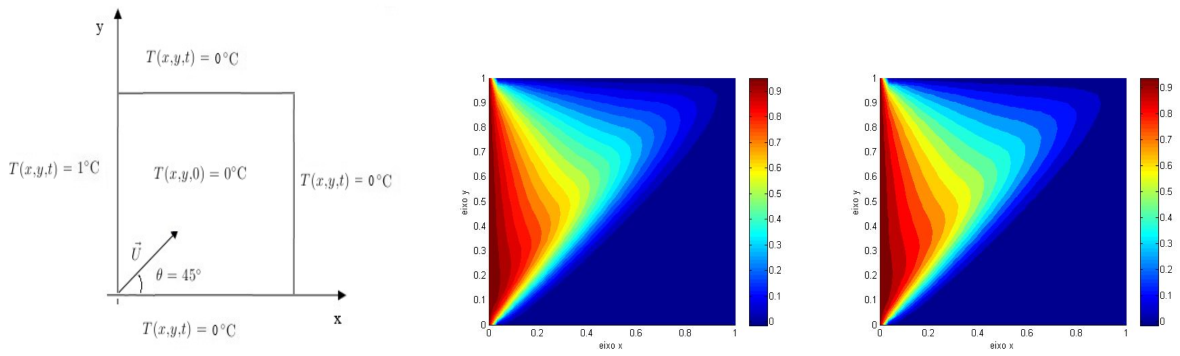
The velocity field $\vec{U} = (u, v)$ is uniform and makes an angle of 45° with Cartesian directions, adopting $u = v = 2$ m/s. The boundary conditions of the Dirichlet type are shown in the Eq. (4.2).

$$\begin{aligned} T(0,y) &= 1^\circ\text{C} \\ T(x,0) &= 0^\circ\text{C} \\ T(1,y) &= 0^\circ\text{C} \\ T(x,1) &= 0^\circ\text{C} \qquad \text{with} \qquad 0 \le (x,y) \le 1. \end{aligned} \tag{40}$$

To obtain the numerical solution, the domain was discretized using 1600 quadrilateral elements with 8 nodes, in temporal discretization a time step $\Delta t = 0.02$ s was used, the value of the thermal conductivity used will be equal to $k =$ 10 W/m.K. The solution analytical, numerical and domain of the problem presented in Eq. (39) presented in the Fig. 3.

As we can see in the Fig. 3 you can see the direction of the fluid flow at 45° and verify that the heat transport occurs correctly from the boundary condition $T(0, y)$ with the highest temperature for the boundary condition $T(x, 1)$ with the lowest temperature occurring a heating of the surface.

Figure 3. Domain and results for transient convection with constant physical properties.



(a) Domain. (b) Numerical. (c) Numerical.

Solving a transient problem tends to solve a permanent problem when $t \to \infty$. The solution is obtained by marching in time from the data at the initial time t_0 until the final time t_f is reached. In practice, when the variation of $T(x, y, t)$ in successive instants of time becomes negligible, it is concluded that the permanent regime has been reached. For the validation of the transient solution, a comparison will be made between a line of the solution in steady state and a line of the solution in a transient regime.

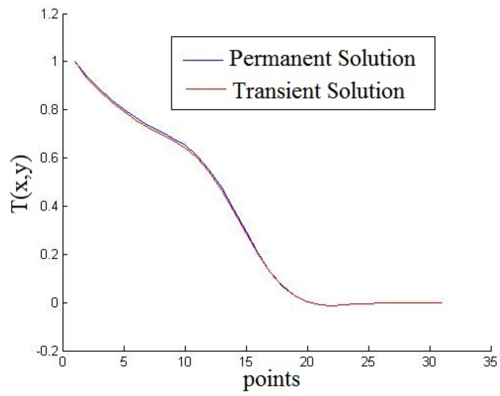


Figure 4. Comparison between Numerical Solutions in Permanent and Transient Regime.

Shown in Fig. 4, where the biggest difference is equal to approximately 1 %, then it can be concluded that the numerical solution presents a good approximation.

4.3 Convection Diffusion Equation in Transient Regime with Physical Properties Variable with Temperature.

The differential equation for the problem of the convection diffusion equation in transient regime with physical properties variable with temperature is presented in Eq. (41),

$$\frac{\partial T(x,y,t)}{\partial t} + u\frac{\partial T(x,y,t)}{\partial x} + v\frac{\partial T(x,y,t)}{\partial y} = \alpha(T)\frac{\partial^2 T(x,y,t)}{\partial x^2} + \alpha(T)\frac{\partial^2 T(x,y,t)}{\partial y^2} \tag{41}$$

The boundary conditions of the Dirichlet type and the initial conditions are shown in the Eq.(42),

$$\begin{aligned} T(0,y,t) &= 1^\circ\text{C} \\ T(x,0,t) &= 0^\circ\text{C} \\ T(1,y,t) &= 0^\circ\text{C} \\ T(x,1,t) &= 0^\circ\text{C} \\ T(x,y,0) &= 0^\circ\text{C} \qquad \text{with} \qquad 0 \le (x,y) \le 1. \end{aligned} \tag{42}$$

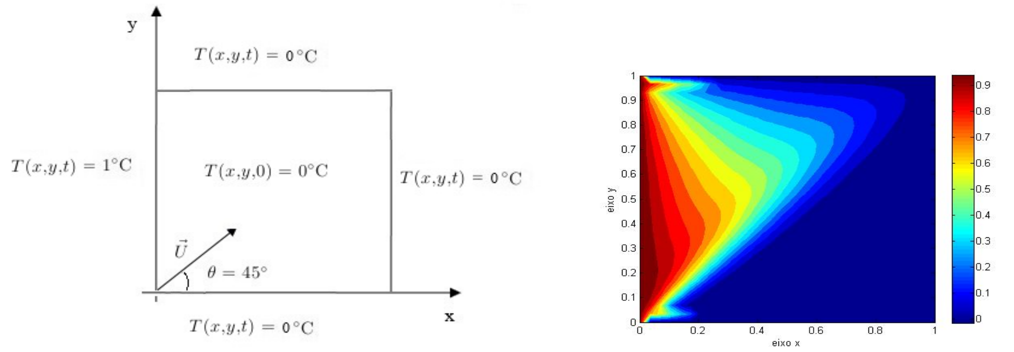
The thermal diffusivity $\alpha(T)$ is a function of the temperature T, being defined according to Eq. (2). The thermal conductivity $k(T)$, the density $\rho(T)$, and the specific heat, c_p, are shown in Eq. (43), Eq. (44) and Eq. (45).

$$k(T) = -9 \times 10^{-6} \cdot T^2 + 0.0021 \cdot T + 0.56. \tag{43}$$

$$\rho(T) = -3.5 \times 10^{-3} \cdot T^2 - 7.3 \times 10^{-2} \cdot T + 1000. \quad (44)$$

$$c_p(T) = -7.5 \times 10^{-10} \cdot T^6 + 1.9 \times 10^{-7} \cdot T^5 - 1.5 \times 10^{-5} \cdot T^4 - 5.3 \times 10^{-5} \cdot T^3 + 0.06 \cdot T^2 - 2.9 \cdot T + 4217. \quad (45)$$

For the calculation of the numerical solution the values of the thermal diffusivity $\alpha(T)$ in the time step t, the value in the time step $t-1$ is used. To obtain the numerical solution, the domain was discretized using 1600 quadrilateral elements with 8 knots. For time discretization, a time step $\Delta t = 0.004$ s was used and $u = v = 20m/s$ and the thermal diffusivity will be a function of the temperature $\alpha(T)$. The solution numerical and domain of the problem presented in Fig. 5.



(a) Domain. (b) Numerical.

Figure 5. Domain and results for convection diffusion equation in transient regime with physical properties variable with temperature.

It can be seen in Fig. 5 that the convection phenomenon was the dominant phenomenon, because the thermal diffusivity $\alpha(T) << 1$.

5. CONCLUSIONS

The most important contribution of this work was the use of the second derivative of diffusion without the artifice to lower its order and also to use the physical properties that vary with temperature in the diffusion convection equation.

6. ACKNOWLEDGEMENTS

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