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NUMERICAL AND THERMAL ANALYSIS OF THE ENTHALPY-POROSITY TECHNIQUE FOR APPLICATION IN METAL WELDING PROCESSES.

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Abstract. *The enthalpy-porosity technique for modeling convection-diffusion phase change with application to melting a pure gallium is presented in this work. To solve this classical thermal problem, it was considered a bidimensional two-phase numerical model for convection-dominated melting and solidification. Based on a fixed grid, a computational algorithm was implemented in C++. In this work the thermal properties of the pure gallium was considered constant. Adopting a fully implicit control volume, the finite volume technique was used to solve the energy, mass conservation and momentum equations. The SIMPLE algorithm is employed to determine the velocity and pressure field. The upwind scheme was introduced for the convection term. The liquid mass fraction is determined iteratively from the solution of the enthalpy equation. Based on the results obtained in this work the thermal model will be improved to simulate a Gas Tungsten Arc Welding process (GTAW). Inverse problems will be applied to estimate the heat flux supply to the workpiece during the welding process, and a tridimensional numerical model, based on the enthalpy-porosity technique, will be used to calculate the width and depth of the weld bead.*

Keywords: *enthalpy-porosity technique, heat transfer, phase change.*

1. INTRODUCTION

The heat transfer problem with phase change attracts a considerable attention of mechanical engineering researchers due to its relevance and application in several industrial processes as casting and welding of metallic materials. One of the most widely used welding processes is the GTAW (Gas Tungsten Arc Welding). This process is used with success for stainless steels and non-ferrous materials welding. The welding of workpieces is obtained through a voltaic arc, which is a very intense heat source. The thermal behavior analysis of the physical problem that occurs during the welding process is crucial to understand, for example, the formation of the width and depth of the weld, microstructure changes and residual tensions. However, the heat flux supplied to the workpiece is unknown and its determination in heat transfer represents an inverse problem.

The difficulty to solve the thermal problem with phase change is related to define a numerical and powerful mathematical methodology to provide with accuracy the solid-liquid phase change according to the model and its physical properties.

The phase change phenomenon involves a system of nonlinear partial differential equations and numerical implementation of moving boundary conditions. Several techniques are available to solve these kinds of problems and a comprehensive review can be found in Crank et al (1984). Basically, the methodologies developed are classified in three groups according to Brent et al. (1988): empirical, classical and enthalpy technique.

Among the available methodologies, the enthalpy technique consists of an alternative approach to classical and empirical method. It allows the use of standard solutions for mass flow and energy with a fixed grid and it does not require mathematical manipulations during the solid-liquid or liquid-solid transition. Basically, the method calculates the latent heat in the energy equation interactively, considering the temperature and the latent nodal heat for each cell of the domain. This technique is quite cited in the literature and it is recognized as satisfactory by several authors, such as: Alexiades and Solomon (1993), Meyer (1978) and Tayler (1975). A problem identified in this kind of technique is to fix the condition of zero velocity when a solid region becomes liquid or vice versa. A suitable approach was presented by Gartling (1980), in which was introduced the concept of mass fraction. In this case, the viscosity of a cell is driven to a very large value when the mass fraction of liquid tends to zero. This increased viscosity provides the necessary coupling between physical state and fluid flow equations, making the velocity in the cells tends to zero.

Voller and Markatos (1985) examined several methods to deal with the condition of zero velocity in fixed grids and proposed an alternative approach quite similar to that one used for Gartling (1980). According to the authors, the computational cells undergoing phase change are modeled as pseudo porous media and the mass fraction varies from 0, (fully solid medium) to 1 (fully liquid medium). From this concept emerged the enthalpy-porosity technique that is the base of the present work.

ISSN 2176-5480

In this sense, the objective of this work is to develop a technique to obtain the location of melting front, velocity fields and temperature of a metal during phase change. Based on a fixed grid, the enthalpy-porosity technique treats as a porous media the whole field of cells which are located in the solid-liquid interface. In relation to the cells that are fully located in solid regions, the mass fraction suppresses velocity vectors in momentum equations. The benefit of this methodology is to simulate simultaneously solid and liquid regions considering energy, mass and momentum equations.

2. THERMAL PROBLEM

The objective of this work is initially to understand the difficulties related to the algorithm development and simulation of this kind of problem to further apply the knowledge in the study of three-dimensional problems of engineering, such as those related to welding processes. In this sense, a classical thermal problem involving melting of pure gallium in a rectangular cavity was studied in this work. This problem was chosen because the material thermo-physical properties are well known and in literature there are several scientific information to help in the solution of the thermal problem, such as: Voller and Markatos (1985), Voller and Prakash (1987), Kim et al. (2001), among others.

Gallium has a melting point close to the room temperature in tropical regions (29,78°C) and comprehensive and accurate experimental results about its melting or freezing front can be found in scientific literature. Such information are going to be used to validate de thermal model presented in this work.

Figure 1. Melting of pure gallium at room temperature (infoescola, 2012).

Figure 2 shows the physical model and boundary conditions.

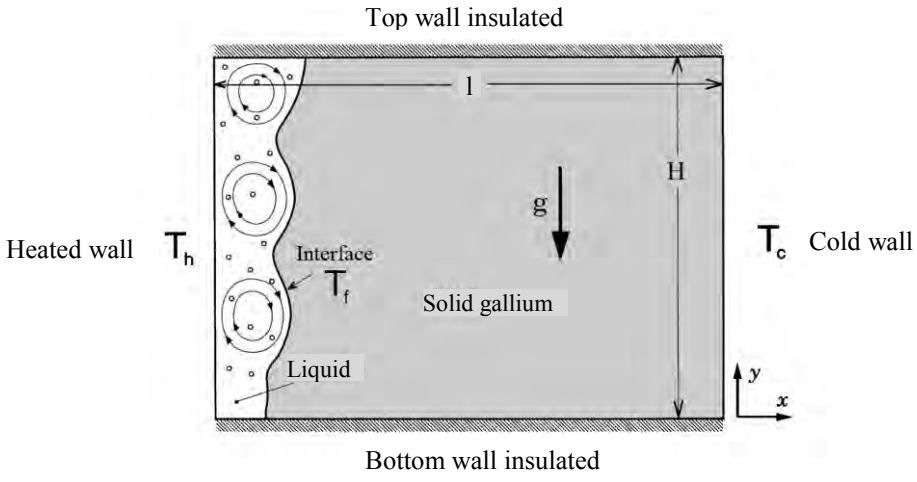


Figure 2. Physical model and boundary conditions.

The model represents basically a two-dimensional thermal problem in which is prescribed temperature in the left and right walls, and thermal insulation in the top and bottom walls.

The dimensions of the thermal problem and gallium thermal properties are presented in Tab. 1.

ISSN 2176-5480

Table 1. Properties of pure Gallium and input data of the simulation.

Parameters	Symbol	Value	Unit
Density (Liquid)	ρ	6093	$\mathrm{kg}\,m^{-3}$
Reference density	ρ_{ref}	6095	$\mathrm{kg}\,m^{-3}$
Specific heat	c	381,5	$\mathrm{J}\,kg^{-1}K^{-1}$
Thermal conductivity	k	32	$\mathrm{W}\,m^{-1}K^{-1}$
Volumetric thermal expansion coefficient of liquid	β	$1{,}2\cdot10^{-4}$	
Latent heat of fusion	L	80160	$\mathrm{J}\,kg^{-1}$
Melting point	T_m	29,78	ºC
Reference temperature	T_{ref}	29,78	ºC
Temperature of the right side	T_h	38	ºC
Temperature of the left face	T_c	28,3	ºC
Cavity length	l	0,0889	m
Cavity Height	H	0,0635	m
Acceleration due to gravity	g	9,8	$\mathrm{m}\,s^{-2}$
Rayleigh number	Ra	$7\cdot10^{5}$	
Stefan number	St	0,046	
Prandtl number	Pr	0,0216	
Mass fraction	f	0 to 1	

2.1 Governing Equations

The mathematical formulation was presented by Brent et al. (1988) and it is based on the enthalpy-porosity technique. The model is bidimensional, incompressible, laminar and the thermo-physical properties are considered constant. Eq. (1) to (4) presents the mass conservations, momentum and energy equations:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \tag{1}$$

$$\frac{\partial u}{\partial t}=-\frac{1}{\rho}\frac{\partial P}{\partial x}-\left(u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right)+\upsilon\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)+S_u \tag{2}$$

$$\frac{\partial v}{\partial t}=-\frac{1}{\rho}\frac{\partial P}{\partial y}-\left(u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right)+\upsilon\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)+\rho_{ref}g\beta(T-T_{ref})+S_v \tag{3}$$

$$\rho c\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}\right)=k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)-\rho L\left(\frac{\partial f}{\partial t}\right) \tag{4}$$

where u and v are the velocity vectors, T is the temperature, P pressure vector, x and y are the coordinate axis and t is the time.

It is proposed in this work to treat each finite volume as a porous element, with porosity represented trough the mass fraction. Thus, when a finite volume changes from solid to liquid the mass fraction gradually changes from zero to one. The source terms in momentum equations (S_u and S_v) suppress the velocity vector when a finite volume is solid

ISSN 2176-5480

and gradually, when mass fraction varies from 0 to 1, velocity field arises in liquid region. The source term S takes the appropriate form of Carman-Kozeny (Eq. 5) as presented by Voller and Prakash (1987).

$$\vec{S} = -C\left(\frac{(1-f)^2}{f^3+b}\right)\vec{V} \tag{5}$$

where C is a constant large enough to dissipate cell velocity but not so large to cause numerical instability, V is the velocity vector and b is merely a computational constant introduced to avoid division by zero.

2.2 Numerical Model

Based on fully implicit scheme, finite volume technique was used to solve mass conservation, momentum and energy equations. The SIMPLE algorithm is employed to determine the velocity and pressure field. The upwind scheme was introduced to solve the convection terms. The liquid mass fraction is determined iteratively from the solution of the energy equation. It is based on the numerical discretization of energy equation as presented in Eq. (6) to (15).

$$a_p T_p^{t+\Delta t} + a_e T_e^{t+\Delta t} + a_w T_w^{t+\Delta t} + a_s T_s^{t+\Delta t} + a_n T_n^{t+\Delta t} = a_{po} T_p^t + b_p - a_{po}\frac{L}{c} f_p^{n+1} \tag{6}$$

Table 2 shows the coefficients of Eq. (6) after discretization.

Table 2. Coefficient values in Eq 6.

$a_p = \frac{pc}{\Delta t} + \frac{2\beta\rho cu}{\Delta x} + \frac{2\beta\rho cv}{\Delta x} + \frac{2k}{(\Delta x)^2} + \frac{2k}{(\Delta y)^2}$	
$a_{po} = \frac{pc}{\Delta t}$	$b_p = a_{po}\frac{L}{c} f_p^t$
$a_e = \left(\frac{1}{2} - \Phi_x\right)\frac{pcu}{\Delta x} - \frac{k}{(\Delta x)^2}$	$a_w = -\left(\frac{1}{2} + \Phi_x\right)\frac{pcu}{\Delta x} - \frac{k}{(\Delta x)^2}$
$a_n = \left(\frac{1}{2} - \Phi_y\right)\frac{pcv}{\Delta y} - \frac{k}{(\Delta y)^2}$	$a_s = -\left(\frac{1}{2} + \Phi_y\right)\frac{pcv}{\Delta y} - \frac{k}{(\Delta y)^2}$

where Φ is a constant useful in upwind scheme, according to the value the finite volume it values ½ or - ½.

According to Voller and Brent (1989) the mass fraction "*f*" is iteratively determined from the solution of energy equation. The author presents three approaches to iteratively estimate the mass fraction. This study applies one of the techniques proposed by the author, in which the mass fraction vector is estimated at each instant of time. In this case, the mass fraction is calculated using Eq. (7).

$$f_p^{n+1} = f_p^n + \lambda.cor \tag{7}$$

where "λ" is a sub-relaxation coefficient to be adjusted (0 < λ <1), "*n*" is the iteration and "*cor*" is the correction for f_p^{n+1}. Furthermore, the following relations are valid:

$$f_p^{n+1} < 0 \Rightarrow f_p^{n+1} = 0 \tag{8}$$

$$f_p^{n+1} > 1 \Rightarrow f_p^{n+1} = 1 \tag{9}$$

To obtain the correction value "*cor*" in the Eq. (7) Voller and Brent (1989) propose that:

$$a_p T_p^{t+\Delta t} + \text{Terms} = a_{po} T_p^t + b_p - a_{po}\frac{L}{c} f_p^{n+1} \tag{10}$$

ISSN 2176-5480

where

$$\text{Terms} = a_e T_e^{t+\Delta t} + a_w T_w^{t+\Delta t} + a_s T_s^{t+\Delta t} + a_N T_N^{t+\Delta t} \tag{11}$$

When occurs phase change in a given cell the term $T_p^{t+\Delta t}$ in Eq.(10) assumes the value T_m, namely melting temperature. Then:

$$a_p T_m + \text{Terms} = a_{po} T_p^t + b_p - a_{po} \frac{L}{c} f_p^{n+1} - a_{po} \frac{L}{c} cor \tag{12}$$

Subtracting Eq. (12) of Eq. (10) follows that

$$-a_p (T_p^{t+\Delta t} - T_m) = -a_{po} \frac{L}{c} cor \tag{13}$$

Then,

$$cor = \frac{ca_p}{La_{po}} (T_p^{t+\Delta t} - T_m) \tag{14}$$

Finally, substituting Eq. (14) in Eq. (7), the mass fraction can be interactively estimated according to the following equation

$$f_p^{n+1} = f_p^n + \lambda \frac{ca_p}{La_{po}} (T_p^{t+\Delta t} - T_m) \tag{15}$$

Figure 3 shows the computational algorithm to solve partial differential equations presented in this work.

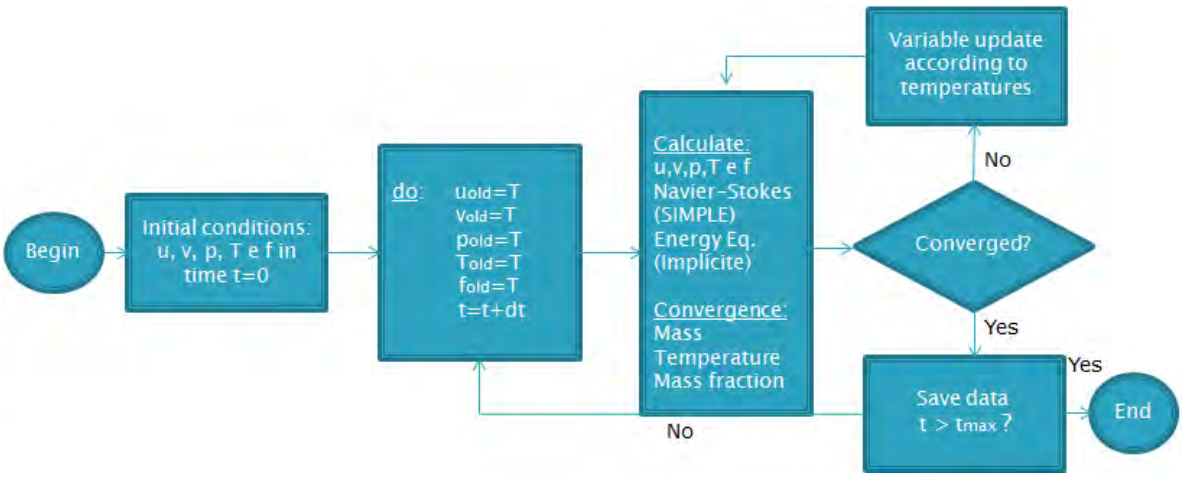


Figure 3. Computational algorithm

The convergence criteria of the numerical solution were based on both mass and energy conservation, reflecting the convergence of the flow and temperature field, respectively.

ISSN 2176-5480

3. RESULTS

Figure 4 shows the convergence of the thermal model according to the refinement of the numerical mesh. In this case it was analyzed the temperature and mass fraction along the cavity length "l" at the coordinate y = 0.03 m at the time of 3 min.

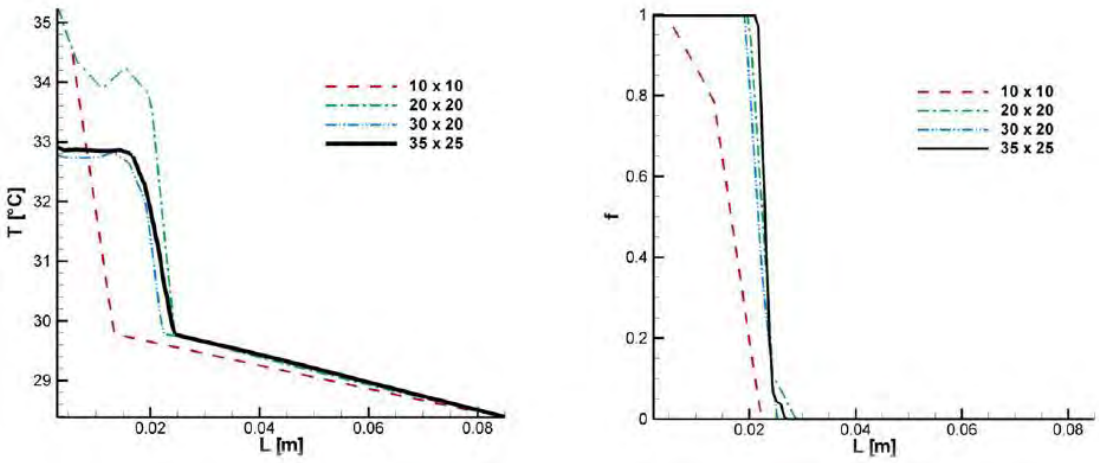


Figure 4. Convergence analysis of the thermal problem: a) Temperature and b) mass fraction along the cavity length "l" at the coordinate y = 0.03 m at the time of 3 min

Analyzing Figure 4 it is noted that from meshes with 30 x 20 and 35 x 25 nodes the results are quite similar. Therefore, in this work it was adopted the mesh with 35 x 25 nodes in the solution of the thermal problem.

The position of the melt front, temperature fields, mass fraction distribution and streamlines at 3 minutes are show in Fig. 5. As noted by Brent et al. (1988) and Voller and Brent (1989) the melt front is virtually planar after 3 minutes as the natural convection field has just begun to develop.

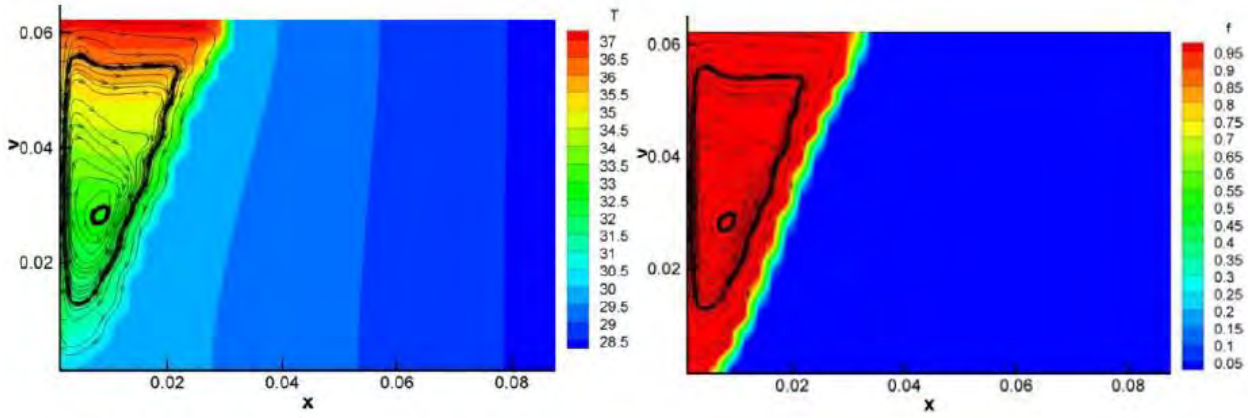
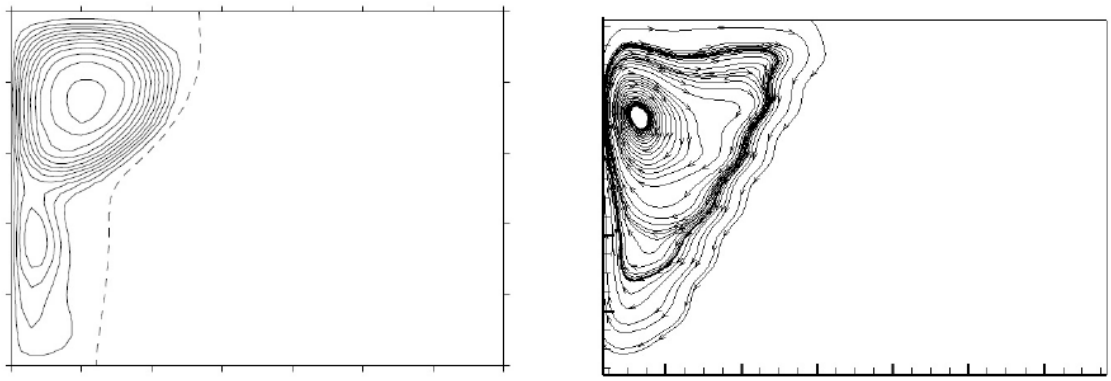


Figure 5. Melt front, temperature field, mass fraction distribution and streamlines after 3 minutes

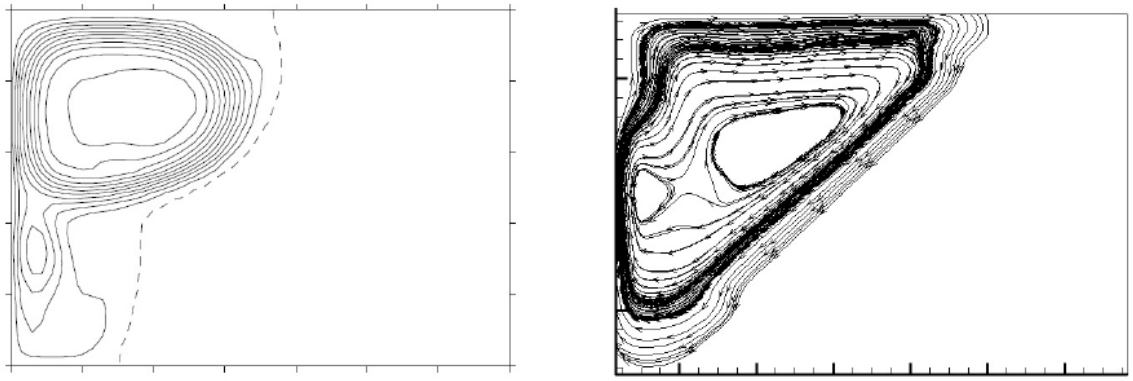
Figures 6 to 8 show a comparison between streamlines at 6, 10, 19 minutes. The results obtained in this work were compared to that one presented by Kim et al. (2001). It was observed that the melt front calculated in this work remains virtually planar during the simulation time and it tends to move more quickly when compared to literature.

ISSN 2176-5480



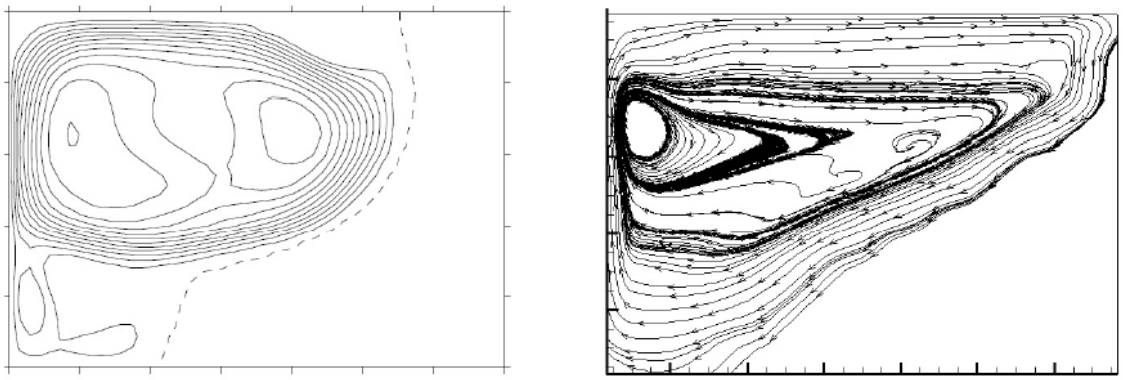
a) b)

Figure 6. Comparison between streamlines at 6 minutes: a) Kin et al. (2001) and b) Present work



a) b)

Figure 7. Comparison between streamlines at 10 minutes: a) Kin et al. (2001) and b) Present work



a) b)

Figure 8. Comparison between streamlines at 19 minutes: a) Kin et al. (2001) and b) Present work

Although the results calculated in this work are not in agreement with literature, the morphology of the melt front is as expected: fluid rising at the heated wall travels across the cavity an impinges on the upper section of the solid front, thereby resulting in a melting area back beyond the mean position of the front.

4. CONCLUSION

The aim of this work was to develop a numerical model to be applied in the study of thermal and fluid-dynamic fields developed during metal heating with phase change. A studied based on the thermal problem with phase-change of gallium in a bidimensional cavity was presented to evaluate the algorithm and the numerical methodology implemented

ISSN 2176-5480

in this work. The future goal is to apply the numerical model and the experience gained in the study of thermal fields developed during a GTAW process.

According to a Cartesian coordinate system a mathematical model was developed. It was based on energy, mass fraction and Navier-Stokes equations. The direct problem was solved with an irregular fixed grid by Finite Volume Method. It was used the enthalpy-porosity technique for simulate the phase change problem. In the numerical solution it was used the upwind scheme for the convective terms and the SIMPLE method was applied to solve Navier-Stokes equations. Simulations were performed to analyze stability, convergence and results provided from the numerical model.

The results calculated in this work are not in agreement with literature. Therefore the next step is to correct the numerical model. As suggested by Brent et al. (1988) and Voller and Brent (1989) the upwind scheme will be removed and Patankar's Power Low Scheme for the convective terms will be implemented. After validating the computational algorithm it is proposed to expand the thermal model to a 3D code and then apply it to the thermal analysis of welding processes.

5. ACKNOWLEDGEMENTS

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