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NUMERICAL SIMULATION OF CONVECTIVE FLOWS OCCURING DURING *AL-4.1WT%CU* SOLIDIFICATION

Mechighel F.*[1,2], EL Ganaoui M.[2], Pateyron B.[2] and Kadja M.[3]
[1]University of Annaba, Department of Mechanical Engineering,
Annaba, 23000, Algeria,
[2]University of Limoges, SPCTS UMR 6638 CNRS, Faculty of Sciences and Technology,
87060, Limoges, France;
[3]University of Constantine, Department of Mechanical Engineering,
Constantine, 25000, Algeria,
*E-mail: f_mechighel@yahoo.fr

ABSTRACT

This study presents a numerical simulation of the convective laminar flow, driven by combined thermo-solutally buoyancy forces, under a uniform horizontally applied magnetic field, held during the solidification of a molten alloy *Al- 4.1wt%Cu* filled in a rectangular cavity. The continuum model, of Bennon and Incropera [1], was used in the development of the mathematical model, representing the solidification phenomena. Following this model, the alloy solidification process is governed by continuity, Navier-Stokes, energy, species and electrical potential conservation equations. Here solved by using finite volume method. The effect intensity of the magnetic field on convective flow has been investigated. The governing equations are firstly non-dimensionalized and are approximated by using a finite volume method.

INTRODUCTION

Solidification occurs in many metals growth processes, like foundry, welding, ingot casting, crystal growth, laser processing etc. The main feature in the solidification of a metallic alloy is the liquid-solid interface phase change associated with the release of latent heat and the solute redistribution.

In recent years, numerical simulations have shown the ability of macroscopic solidification models to predict the effects of convection in the mushy zone and bulk liquid on the development of an irregular liquidus front, flow channels in the mushy zone, local remelting of solid, and complicated macrosegregation for the solidification of a variety of binary alloys.

The cause of macrosegregation is the long-range advection of alloy species due to the relative movement or flow of segregated liquid and solid during solidification. There are numerous causes of fluid flow and solid movement in casting processes: flow that feeds the solidification shrinkage and the contractions of the liquid and solid during solidification; buoyancy forces induced thermo-solutal (double-diffusive) convection flows due to thermal and solutal gradients in the liquid; these forces can either aid or oppose each other, depending on the direction of the thermal gradient and whether the rejected solutes cause an increase or a decrease in the density of the liquid [2, 3].

NOMENCLATURE

u , v	[m/s]	Velocity vector components
h	[J/K]	Enthalpy
C	[wt%]	Solute concentration
T	[K]	Temperature
p	[N/m^2]	Pressure
x , y	[m]	Cartesian axis directions
t	[s]	Time
ν	[m^2/s]	Kinematical viscosity
ε		Volume faction
f		Mass fraction
U ,V		Dimensionless velocity vector components
H		Dimensionless enthalpy
X		Dimensionless Solute concentration
Φ		Dimensionless electrical potential
Θ		Dimensionless temperature
P		Dimensionless Pressure
X, Y		Dimensionless Cartesian axis directions
τ		Dimensionless time
ρ		Dimensionless density

Subscripts

c	Characteristic scale
ini , f	Initial (reference), fusion
e	Eutectic
*, ad	Dimension, dimensionless
s , l	Solid, liquid phase
c,h	cold, hot boundary
sol , liq	Solidus, Liquidus line in phase diagram

To prevent macrosegregation all efforts are aimed at controlling fluid flow and solid movement for example: include adjustments to the alloy composition or thermal gradients to induce stable density stratification in the liquid; include centrifugal forces, or electromagnetic fields to redistribute the flow, [2].

Castings solidification has been reviewed in books dealing with solidification, [4], and the work due to [5]. Likewise, experimental and theoretical studies on solidification of an Aluminum–Copper alloy have been carried out by several researchers [6]. Also, in [7, 8], is modelled horizontal solidification of an Aluminum–Copper alloy under the influence of shrinkage and buoyancy driven convection. Also, in [9], the authors studied the combined effect of thermo-solutal buoyancy and contraction driven flow on macrosegregation during the direct chill casting of a round Al–Cu ingot. In [10, 11], modelling of directional solidification of binary and multi-component alloys is reported in a vertical cavity including effect of gravity and variable cavity on macrosegregation. Motion in liquid phase can be controlled possibly by external forces, such as Lorentz force [2] due to an applied external magnetic field.

This paper focuses on the study of double diffusive convection in the system Al-4.1wt% Cu, induced by thermo-solutal buoyancy forces. Also, the effect of a uniform applied horizontally magnetic field on the flow control is studied.

BASIC CONSIDERATIONS AND GOVERNING EQUATIONS

A square mould, of height and length *L=100 mm*, as shown on Figure 1, is considered filled with a *Al-4.1%wt Cu* alloy liquid system. The thermo-physical properties of the system *Al-4.1%wtCu* [6] are presented in table 1. Initially the molten alloy has the concentration $C_{ini}=4.1\ \%$ and the temperature $T_{ini}=662°C$. The eutectic temperature ($T_e=548°C$). Suddenly, the left wall is cooled to the temperature $T_c=546°C$ and maintained at this temperature. While, the right wall temperature T_h is maintained equal to the initial temperature of the melt. The other top and bottom walls are insulated and adiabatic. Under these conditions the directional solidification commences.

In general, the following assumptions are assumed: the molten *Al-4.1%wtCu* flow is unsteady and laminar, constant viscosity and Newtonian flow in the liquid phase, two-phase flow is described as a mixture of solid and liquid phases, all of the properties of the mixture can be obtained from each phase component properties, equal and constant phase densities except for variations in the buoyancy term (validity of the Boussinesq approximation), stationary solid without deformation and internal stress, isotropic permeability in the mushy zone (using equation of Blake-Kozeny), no Joule heating effects, negligible flow induced by phase transformation shrinkage, local thermal and phase equilibrium in the mushy zone, negligible species diffusion in the solid phase.

In order to control of the melt flow the application of an external uniform magnetic field in order to suppress fluctuations and turbulences. Let assume that the mould is permeated by a uniform horizontally magnetic field $\boldsymbol{B}$ of constant magnitude B_0, Figure 1. Lorentz force $\boldsymbol{F}$ of component ($F_x^* = 0$, F_y^*) drives dynamic convection flow this force is given in [12] with electrically insulated boundaries in the presence of two-dimensional flow the electric potential φ is constant (i.e. $\nabla\varphi = 0$). The dynamical convection is governed by the Hartmann number, $Ha = B_0 L\sqrt{\sigma_e/\mu}$, where σ_e is the electrical conductivity, and μ the dynamic viscosity of the melt.

Using the following dimensionless variables: $X = x/x_c$, $Y = y/x_c$, $U = u/U_c$, $V = v/U_c$, $P = p/P_c$, $\tau = t/t_c$, $\Theta = (T - T_e)/\Delta T$, $H = h/cp_l\Delta T$, $X = C/\Delta C$ and $\Phi = \varphi/\nu B_0$, where $(u,\ v,\ h,\ C, \varphi)$ are the flow dependent variables, p: the pressure, t: time, T: temperature, $(x,\ y)$: Cartesian coordinates. We define characteristic scales for: length, velocity, pressure, time, temperature, enthalpy, species concentration, and electric potential respectively, [13], as following:

$x_c = L$, $U_c = \sqrt{g\beta_T \Delta T\ L}$, $P_c = \rho U_c^2$, $t_c = \sqrt{L/g\beta_T\Delta T}$, $\Delta T = T_h - T_e$, $cp_l\Delta T$, $\Delta C = m^{ad}\Delta T/m$, and νB_0.

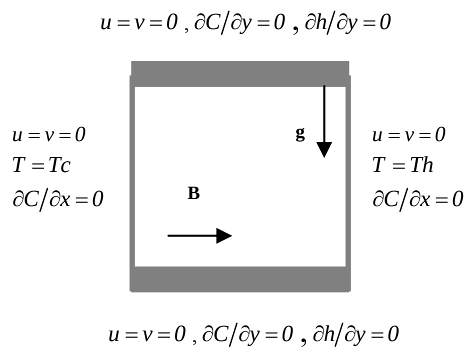

Figure 1 Mould geometry

Governing equations for alloy solidification, based on the continuum model [1], are represented by: the mass, momentum, energy, species and electrical potential conservation equations, written in dimensionless form are given, as following:

$$\frac{\partial\rho}{\partial\tau} + \nabla\cdot\left(\rho\vec{V}\right) = 0 \tag{1}$$

$$\begin{aligned}\frac{\partial(\rho U)}{\partial\tau} + \nabla\bullet\left(\rho\vec{V}U\right) = -\frac{\partial P}{\partial X}\\ + \frac{1}{Gr^{0.5}}\nabla\bullet\left(\rho\nabla U\right) - \frac{1}{Da\ Gr^{0.5}}\frac{\left(1-\varepsilon_l\right)^2}{\varepsilon_l^{\ 3}}\rho U + F_x\end{aligned} \tag{2}$$

$$\frac{\partial(\rho V)}{\partial \tau}+\nabla \bullet\left(\rho \vec{V} V\right)=-\frac{\partial P}{\partial Y}$$
$$+\frac{1}{Gr^{0.5}} \nabla \bullet(\rho \nabla V)-\frac{1}{Da\, Gr^{0.5}} \frac{\left(1-\varepsilon_l\right)^2}{\varepsilon_l{}^3} \rho V$$
$$+\left(\Theta+N X_l\right)+F_y \tag{3}$$

$$\frac{\partial(\rho H)}{\partial \tau}+\nabla \bullet\left(\rho \vec{V} H\right)=\frac{1}{Pr\, Gr^{\frac{1}{2}}} \nabla \bullet\left(\frac{1+\varepsilon_s(Rk-1)}{CP} \nabla H\right)$$
$$+\frac{1}{Pr\, Gr^{\frac{1}{2}}} \nabla \bullet\left(\frac{1+\varepsilon_s(Rk-1)}{CP} \nabla\left(H_l-H\right)\right)$$
$$-\nabla \bullet\left[f_s \rho \vec{V}\left(H_l-H_s\right)\right] \tag{4}$$

$$\frac{\partial(\rho X)}{\partial \tau}+\nabla \bullet\left(\rho \vec{V} X\right)=\frac{1}{Sc\, Gr^{\frac{1}{2}}} \nabla \bullet\left(\left(1-f_s\right) \rho \nabla X\right)$$
$$+\frac{1}{ScGr^{\frac{1}{2}}} \nabla \bullet\left(\left(1-f_s\right) \rho \nabla\left(X_l-X\right)\right)$$
$$-\nabla \bullet\left[f_s \rho \vec{V}\left(X_l-X_s\right)\right] \tag{5}$$

$$\nabla^2 \Phi=0 \tag{6}$$

where: $\vec{V}$ is the dimensionless velocity vector. And the resulting dimensionless quantities: the Grashof number *Gr*, the Prandtl number *Pr*, the Darcy number *Da*, the Schmidt number *Sc*, the Stefan number *Ste* and the Hartmann number *Ha*. Moreover, other dimensionless parameters include: $CP = cp_s/cp_l$, $Rk = k_s/k_l$ and $N = \beta_s \Delta C/\beta_T \Delta T$, respectively, are listed on Table 2.

The mushy zone is modeled by means of an isotropic model. We have used the Blake–Kozeny equation for calculating the permeability in the mushy zone which is given as: $K = K_0\, \varepsilon_l{}^3/(1-\varepsilon_l)^2$, where K_0 is given, in [3], such as: $K_0 = \lambda_2^2/180$. And for the components of the Lorentz force, in dimensionless form: where the Lorentz force $\boldsymbol{F}$ is applied horizontally: $F_x = 0$ and $F_y = -Ha^2/Gr^{0.5}\left[(\sigma_e V)\right]$

All boundaries, except the upper, are assumed to be rigid, no-slip conditions being imposed for velocities: $U = V = 0$ on X=0, 1 and $U = V = 0$ on $Y=0, 1$.

The following boundary conditions are used for the energy equation: $\Theta = 0$ on $X = 0$; $\Theta = 1$ on $X = 1$ and $\partial\Theta/\partial Y = 0$ on $Y = 0,1$.

Thermodynamic equilibrium

Since it is assumed that the local thermodynamic equilibrium exists between the solid and liquid phases, thermo-physical properties of each phase are constant (but different from each other), and the liquidus and solidus lines on the equilibrium phase diagram are linear.

With the full coupling, in the mushy zone, of the temperature field and species concentration through thermodynamic equilibrium requirements temperature and concentration is represented through the following equation: $T = T_f + mC$. Therefore, the dimensionless form Θ_f of the melting point of the pure material T_f is defined as: $\Theta_f = \left(T_f - T_e + mC\right)/\Delta T$.

Therefore, on the dimensionless diagram, the liquidus and solidus lines are given as following: $\Theta_{liq} = \Theta_f + m^{ad} X$, $\Theta_{sol} = \Theta_f + m^{ad}\, X/kp$, respectively. While, dimensionless enthalpies associated with solidus and liquidus temperatures are, respectively, $H_s = CP\,\Theta_{sol}$, $H_l = \Theta_{liq} + Ste$.

Table 1: Thermo-physical Properties for Al-4.1% Cu From [6]

Symbol	Quantity	Value
ks	thermal conductivity of solid	0.19249 kW/m °C
kl	Thermal conductivity of liquid	0.08261 kW /m °C
cps	specific heat of solid	1.0928 kJ/kg °C
cpl	specific heat liquid	1.0588 kJ/kg °C
L_H	Latent heat	397.5 kJ/kg
kp	partition coefficient	0.17
β_T	thermal expansion coefficient	4..95 × 10^{-5} °C^{-1}
β_S	Solutal expansion coefficient	-2.0 wt $\%^{-1}$
$\rho*$	density, assumed here to be constant	2400 kg/ m^3
μ	Dynamical viscosity	0.003 kg/m s
T_{ini}	Initial melt temperature	662 °C
T_c	cold wall temperature	546 °C
T_h	hot wall temperature	662 °C
T_e	eutectic temperature	548 °C
T_f	Pure Al fusion temperature	660 °C
C_{ini}	initial concentration	4.1wt%
C_e	Eutectic concentration	33wt%
D_l	Melt diffusivity	3.0 × 10^{-9} m^2/s
m	liquidus slope assumed from binary diagram	-353 K/ wt%
λ_2	Secondary dendrite spacing assumed, [14]	161 × 10^{-6} m

Table 2: Dimensionless quantities for *Al-4.1% Cu*

Symbol	Quantity	Value
Gr	Grashof number	3.16996416 10^7
Pr	Prandtl number	0.03845
Da	Darcy number [14]	1.55 10^{-9}
Sc	Schmidt number	416.67
Ste	Stefan number	0.2717
Ha	Hartman number (imposed)	0.0 or 300
CP	Specific heat ratio	1.032
Rk	Thermal conductivity ratio	2.33
N	buoyancy ratio	-114.47

NUMERICAL METHOD

The governing equations in the continuum model were posed into a general advection-diffusion form in order to utilize the control-volume based, finite difference SIMPLER algorithm due to Patankar [15]. The general form is

$$\frac{\partial(\rho\phi)}{\partial t}+\nabla\cdot\left(\rho\vec{V}\phi\right)=\nabla\cdot(\Gamma\nabla\phi)+\left(S_c+S_P\,\phi\right)$$

where ϕ is a general scalar quantity which represents dependent variables (U, V, H, X, and Φ) for the problem, Γ is the diffusion coefficient, and $\left(S_c+S_p\,\phi\right)$ is a source term linearized. For the discretization of the advection term, since it has been known that the numerical instabilities of the Central Difference Scheme (CDS) are great for the solidification problem, which has large source-driven liquid concentration gradients, Prescott and Incropera, [16], rather than CDS, an alternative high order scheme, called QUICK [17], was implemented for the energy and species equations. However, since the momentum equation requires special, treatment in the SIMPLER algorithm, it was discretized, using the CDS.

For the resolution of the algebraically system equations obtained the Thomas Algorithm (TDMA) is used.

For solving the problem of unsteady coupled Thermo-solutal convection, the selected mesh size should only be viewed as a compromise between accuracy and computational cost associated with such simulations. Therefore, all calculations carried out in this work are based on 100×100 nodes. A constant dimensionless time step of $\Delta\tau$ =0.005 is used.

RESULTS AND DISCUSSION

The laminar convective flow of *Al-4.1wt% Cu* in two-dimensional square mould was numerically simulated.

Case where no magnetic field is applied

Convective fluid flow field

As we know a horizontal temperature gradient always causes thermal convection [14, 18]. The intensity and mode (steady, periodic, quasi-periodic or chaotic) of convection depends on the degree of horizontal temperature gradient imposed. Also, compositional gradient in the liquid can lead to a segregation of solute across the interface, which leads to solutal convection. Horizontal temperature gradient causes a counterclockwise fluid flow in liquid phase, and cause a downward motion in the interdendritic liquid, in the mushy zone. Also, the advancing solid-liquid interface is rejecting solute i.e. causes concentration gradient, which decreases with increasing distance from the interface.

Figure 2.a illustrates fluid flow at the time of 15. As the solidification process has proceeded for this time, the temperature gradient has been established and the solidification occurs. At the beginning the fluid is superheated and the fluid flow is affected almost only by temperature gradient because the permeability keeps maximum everywhere in the casting. The downward flow, provoked by thermal gradient, occurs along the side wall of the casting formed, i.e. in the mushy zone, where the horizontal temperature gradients exist (see streamlines).

With the solidification proceeding, the fluid flow is affected by not only the temperature but also the solid fraction and the solute concentration. The solid fraction affects the fluid flow by changing the permeability in the mushy zone.

For *Al-4.1 wt% Cu* alloy, the primary solid phase is Aluminum-rich, whereas the interdendritic liquid becomes enriched in Copper, the heaver of the two constituents and hence the buoyancy force due to the segregation (rejection) of solute acts in the direction to the thermal buoyancy [2]. So the flow is weak in the depth of the mushy zone though in which the gradient of temperature is very high. The effect of the solute concentration is strong in the mushy zone because (buoyancy ratio is *N=-114*). In the mushy zone the gradient of solute concentration is very large, for such system. So the fluid is mainly driven by the temperature and concentration fields and affected by solid fraction changes.

Temperature distribution

Figure 2.b illustrates the isotherms at the previous time of solidification, in the casting (solid formed) the isotherms is regular and along of the profile of casting. The temperature gradients centralize along the sides of the casting and the temperature in the interior of casting is planar, which signified that only conduction is presented in casting.

In the melt, the isotherms are not planar, which signified the presence of the convection. The temperature decreases since the solidification front advances.

Solute distribution field

In solute concentration, on Figure 2.c, we can see levels where the solute is rejected in the mushy zone. The rejected solutes are due to irregularities in liquid concentrations, which caused a decrease in the density of the liquid and provoked solutal buoyancy forces acting on fluid convective flow. Also, these rejected solutes lead to a shaped interface form see figure 2.d (liquid isocompositions). This is due essentially to the system chosen in this study. For this system the Lewis number is extremely high (*Le=10837*), where the solutal mushy boundary layer (solid/liquid interface) is extremely thin and concentration gradients are very high close to the interface, which lead to an increase of the rejected solute in the mushy. The interfacial fluid having an increasing composition varies from the initial value (0.14), towards to the eutectic value (1.14), (see figure 2.d). However, the bulk mass fraction of the solid formed; need not be eutectic because of the presence of the thin thickness mushy layer and is instead controlled by mass transfer within the fluid.

The thermal convection cell; confining the Al-rich fluid at the top, see figure 2.c. While the Cu-rich fluid, is confined, at the bottom. An accumulation of Al-rich fluid at the top causes a decrease in the liquidus temperature (see isotherms figure 2.b), which retards the growth of liquidus front at the mould top. Thus, the solid and mushy zone thickness becomes non-uniform.

Case where a horizontally magnetic field is applied

For the second case, the solidification system is subjected to a strong horizontally external magnetic field characterized by *Ha=300*. Streamlines for the convective flow field, isotherms, solute concentration liquid, and liquid isocompositions corresponding to the stage of the solidification process, at time τ =15, are presented in figure 3.

We remark that the flow intensities become lower that the previous case. The application of the externally magnetic field reduces the velocity vector magnitudes and leads to damping out instable flows, thereby improving the homogeneity of the solid formed.

CONCLUSION

In the present paper, a problem on coupled effects of electromagnetic and buoyancy forces driven convection, in the molten *Al-4.1wt%Cu* alloy filled in a rectangular mould has been investigated numerically by employing a finite volume method. Obtained results, have been shown the benefit effect of the external magnetic field. This field has been instabilities thresholds reducing.

Magnetic field enhances micro-structural properties through melt flow control, thereby improving the homogeneity of the solid formed.

Finally, it requires to be mentioned that solutions of the present problem could be investigated other binary systems, for the case where the mould has a top free surface. Also, for cases where the magnetic field; is applied, in other directions.

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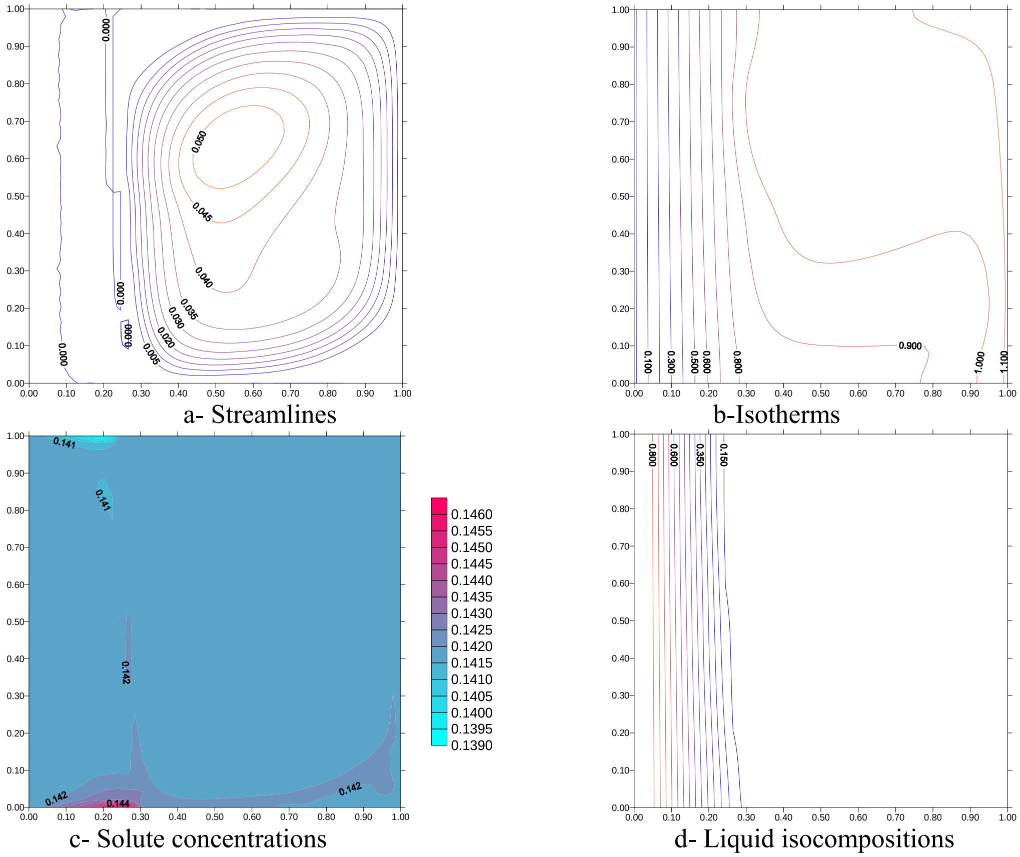

Figure 2: Case where no magnetic field, Ha=0.0

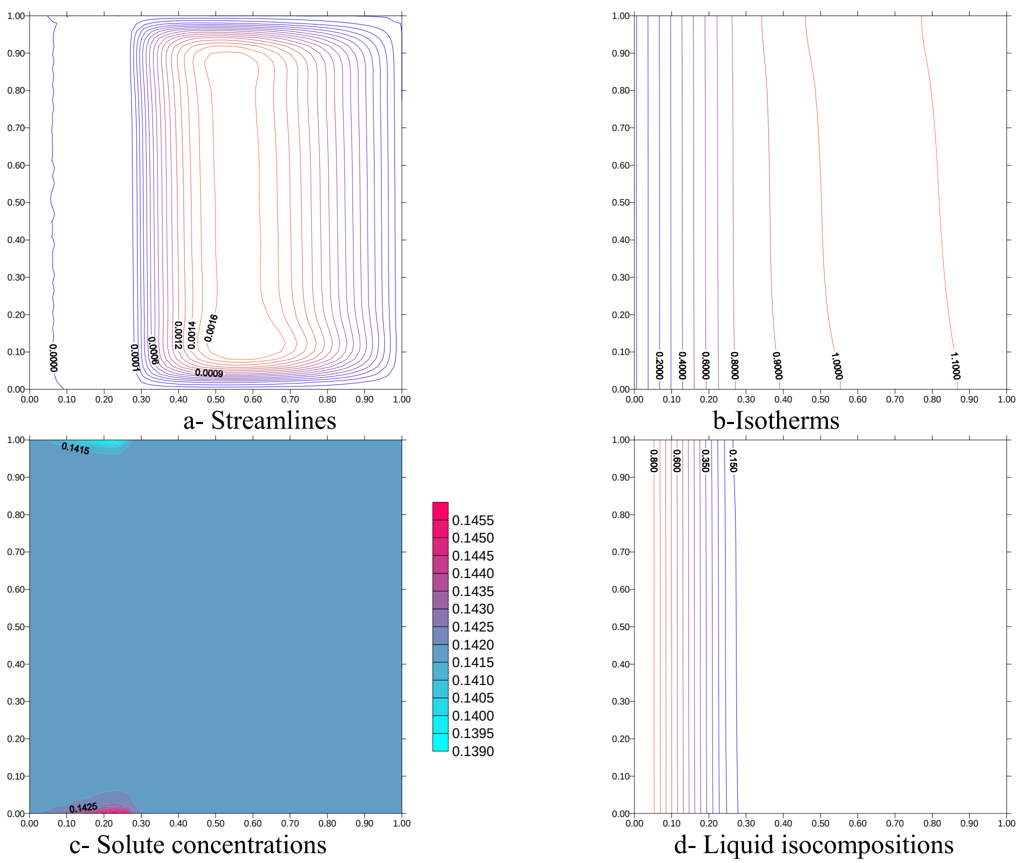

Figure 3: Case where a horizontally magnetic field is applied, Ha=300