

MAGNETOHYDRODYNAMIC OPTIMIZATION OF THE FLUID FLOW DURING THE SOLIDIFICATION OF BINARY MIXTURES IN ENCLOSURES

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Abstract. *In this paper we propose a multilevel approach based on our previously developed hybrid optimizer to solve a double-diffusive fluid flow, during the phase-change, in the presence of magnetic body forces. The problem consists of a square cavity subjected to a thermosolutal flow where the patterns of the isoconcentration are prescribed. Thus, the optimization problem is formulated in terms of the magnetic boundary conditions that must induce such prescribed concentration profile. The optimizer is based on several deterministic and evolutionary algorithms with automatic switching among them, combining the best features of each one. The code was validated, in some previous work, against transient benchmark results for thermosolutal problems with and without phase change.*

Keywords: *Hybrid Optimization, Phase-Change, Magnetohydrodynamics, Thermo-solutal flow*

1. Introduction

Solid-liquid phase-change (solidification or melting) in multi-component systems plays important roles in engineering and in environmental and material processing, such as metal castings, crystal growth, welding, polymer production, freezing in oceans, and so on.

In liquids containing a solute, natural convection driven by both temperature and solute concentration gradients in the liquid phase has a considerable influence on the solidification process in multi-component systems. Temperature gradients may be externally imposed (i.e. by heating/cooling) and are caused internally by the latent heat release or absorption within the mushy zone. The solubility of a component may be variable in solid and liquid phases for multi-component solutions. Thus, during solidification, a component may be incorporated or rejected, therefore inducing local compositional gradients at the solid-liquid interface. This convective flow, driven by both thermal and solutal buoyancy forces, is commonly recognized as double-diffusive natural convection in solidification. Diverse double-diffusive convection patterns can be generated in the liquid because of different molecular diffusivities of heat and species for most fluids. Variations arise from the boundaries of the moving of the mushy region, the interactions among the heat and mass transfer, fluid flow, and involvement of two distinct phases which have different thermo physical properties.

Many research groups have contributed to this area by studying experimentally (Cao et al., 1990; Chellaiah, 1991; Beckermann and Viskanta, 1989; Wang et al., 1999a, 1999b; Skudarnov et al., 2002; Ghenai et al., 2003; Mergui et al., 2004), analytically (Chakraborty and Dutta, 2002) and numerically (Fleming et al., 1967; Kaviany, 1991; Ni and Beckermann, 1991; Ni and Incropera, 1995a, 1995b; Bennon and Incropera, 1988; Sampath and Zabaras, 2001; Heinrich and Poirier, 2004) the solidification process in rectangular, trapezoidal, and V-shaped enclosures. Experimental methods play important roles in investigating the solidification process. Mathematical numerical modeling has been and continues to be a powerful tool in improving the understanding of the solidification process.

1.1 Objectives

The objective of this work is to explore the feasibility of a concept of specifying a desired pattern of concentration distribution of impurities, dopants or micro-particles in liquids undergoing thermo circulation. For example, when growing single crystals from a melt it is desirable that any impurities that originate from the walls of the crucible do not migrate into the mushy region and consequently deposit in the crystal. On the other hand, it is highly desirable to achieve a distribution of dopants in the crystal that is as uniform as possible (Motakeff, 1990; Hirtz and Ma, 2000). Similarly, microsegregation results in the interdendritic spaces when freezing a solute-enriched liquid. It does not constitute a major quality problem of the cast part, since the effects of microsegregation can be removed during

subsequent soaking and hot working. Macro-segregation, on the other hand, causes non-uniformity of composition in the cast section on a larger scale (Ghosh, 2001). Another example is in the manufacturing of composites and functionally graded materials when it would be highly desirable to have the ability to manufacture composite parts with specified distributions of concentration of micro-fibers or nano-particles.

This control of the distribution of a solute in a thermo-convective flow could be achieved by applying appropriate distributions of magnetic and/or electric fields (Dulikravich et al., 2003) acting on the electrically conducting fluid containing the solute (Colaço and Dulikravich, 2005a).

In this work, we will demonstrate the use of magnetic fields only. Then, the task is to determine the proper strengths, locations, and orientations of magnets that will have to be placed along the boundaries of the container so that the resulting magnetic forces will interact with thermal buoyancy and concentration buoyancy forces to cause such a thermo-convective motion of the fluid that will create the solute concentration pattern that coincides with the specified (desired) pattern of the solute distribution.

Mathematical models for the combined electro-magneto-hydro-dynamics (EMHD) became available only recently (Dulikravich, 1999; Ko and Dulikravich, 2000). Numerical simulation using these advanced models is still impossible because of the unavailability of the large number of physical properties that still need to be evaluated experimentally. Consequently, the complete EMHD model has traditionally been divided into two sub-models (Dulikravich and Lynn, 1997a; 1997b): a) magnetohydrodynamics (MHD) that models incompressible fluid flows under the influence of an externally imposed magnetic field, while neglecting any electric fields and electrically charged particles, and b) electro-hydro-dynamics (EHD) that models the incompressible fluid flows under the influence of an externally imposed electric field, while neglecting any magnetic fields. These simplified analytical sub-models have recently been used to numerically demonstrate feasibility of solving inverse problems in thermo-convection involving optimized magnetic and electric fields. That is, this novel manufacturing concept involves the numerical solution of MHD model and application of a constrained optimization algorithm that is capable of automatically determining the correct strengths, locations, and orientations of a finite number of magnets that will produce the magnetic field force pattern that will create the specified concentration pattern in the fluid.

2. General Model

The physical problem considered here involves the laminar magnetohydrodynamic (MHD) natural convection of an incompressible Newtonian binary mixture. The fluid physical properties are assumed constant. The energy source term resulting from viscous dissipation is neglected and buoyancy effects are approximated by the Oberbeck-Boussinesq hypothesis. Radiative heat transfer, Soret and Dufour effects are neglected.

For the columnar dendritic zone, a porous media model (Voller et al., 1989; Swaminathan and Voller, 1997; Zabarar and Samanta, 2004; Voller et al., 2004) must be employed such that the velocity of the solid phase is imposed as zero. Also, the dissipative interfacial stress is usually modeled in an analogy with Darcy law, where the permeability is commonly approximated using the Kozeny-Carman equation (Voller et al., 1989; Zabarar and Samanta, 2004). This porous media model will not be utilized in this work. In this work, we will use the so-called mushy zone model (Ghosh, 2001; Voller et al., 1989), which is applicable to amorphous materials (waxes and glasses), and the equiaxed zone of metal casting. In this model, the solid is assumed to be fully dispersed within the liquid and the velocity within the solid phase is reduced by imposing a large difference of viscosity between the solid and liquid phases.

The modifications to the Navier-Stokes equations for the MHD fluid flow with heat transfer come from the electromagnetic force on the fluid where all induced electric field terms have been neglected (Dulikravich, 1999; Ko and Dulikravich, 2000; Dulikravich and Lynn, 1997a; 1997b). Then, the Navier-Stokes and the Maxwell equations for the MHD model can be written, for the Cartesian coordinate system as

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = S \quad (1)$$

$$Q = \lambda \phi \quad E = \lambda u \phi^* - \Gamma \frac{\partial \phi^{***}}{\partial x} \quad F = \lambda v \phi^{**} - \Gamma \frac{\partial \phi^{****}}{\partial y} \quad (2.a-c)$$

where t is the physical time, x and y are the Cartesian coordinates, u and v are the components of the velocity field in the x and y directions and the other quantities, S , λ , ϕ , ϕ^* , ϕ^{**} , ϕ^{***} and Γ , are given in Tab. 1 for the equations of conservation of mass, species, x -momentum, y -momentum, energy, magnetic flux in the x -direction and magnetic flux in the y -direction.

Table 1 - Parameters for the Navier-Stokes and Maxwell equations

Conservation of	λ	ϕ	ϕ^*	ϕ^{**}	ϕ^{***}	Γ	S
Mass	ρ	1	1	1	1	0	0
Species	ρ	C	C	C	C	D	$\nabla \cdot [f_s \rho_s D_s \nabla (C_s - C)] + \nabla \cdot [f_l \rho_l D_l \nabla (C_l - C)]$
x-momentum	ρ	u	u	u	u	μ	$-\frac{\partial P}{\partial x} - \frac{B_y}{\mu_m} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]$
y-momentum	ρ	v	v	v	v	μ	$-\frac{\partial p}{\partial y} - \rho g [1 - \beta(T - T_0) - \beta_s(C - C_0)] + \frac{B_y}{\mu_m} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]$
Energy	ρ	h	h	h	T	k	$\frac{C_p}{\sigma \mu_m^2} \left[\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y} \right]^2$
Magnetic x-flux	1	B_x	0	B_x	B_x	$\frac{1}{\mu_m \sigma}$	$\frac{\partial (u B_y)}{\partial y}$
Magnetic y-flux	1	B_y	B_y	0	B_y	$\frac{1}{\mu_m \sigma}$	$\frac{\partial (v B_x)}{\partial x}$

In Tab. 1, B_x and B_y are the magnetic flux components in the x and y -direction, respectively. C is the concentration of the solute, C_p is the specific heat at constant pressure, D is the mass diffusion coefficient of the solute, g is the acceleration of gravity, h is the enthalpy per unit mass, k is the thermal conductivity, p is the pressure, t is the time, T is the temperature, u and v are the velocity components in the x and y -direction, respectively. x and y are the Cartesian coordinates, β is the thermal expansion coefficient, β_s is the solute expansion coefficient, μ is the fluid viscosity, μ_m is the magnetic permeability, σ is the electric conductivity, ρ is the fluid density, f is the mass fraction. The subscripts 0, l, s, e, m are related to reference value, liquid phase, solid phase, eutectic point and melting point, respectively. The concentration of the solid phase is related to the concentration of the liquid phase, within the mushy region, through the partition coefficient K as $C_s = K C_l$.

Note that we used the Oberbeck-Boussinesq approximation for the variation of the density with temperature and concentration in the y -momentum conservation equation. Also note that in the energy conservation equation, the term $C_p T$ was replaced by the enthalpy, h , per unit mass. This is useful for problems dealing with phase change where we could use the enthalpy method (Voller et al., 1989). The above equations were transformed from the physical Cartesian (x, y) coordinates to the computational coordinate system (ξ, η) and solved by the finite volume method. The SIMPLER method (Van Doormal and Raithby, 1984) was used to solve the velocity-pressure coupling problem. The WUDS interpolation scheme (Raithby and Torrance, 1974) was used to obtain the values of u , v , h , B_x and B_y as well as their derivatives at the interfaces of each control volume. The resulting linear system was solved by the GMRES method (Saad and Schultz, 1985).

Details on the derivation of the general model, as well as the concentration and energy equations can be found in (Dulikravich et al., 2003; Dulikravich et al., 2004; Colaço and Dulikravich, 2005b).

The MHD analysis code was validated against available analytical and experimental benchmark test cases (Colaço and Dulikravich, 2005a, 2005b; Dulikravich et al., 2004). They involved forced convection in regular and irregular channels, natural convection in regular and irregular cavities, forced convection in the presence of magnetic fields (Pouiseuille-Hartmann Flow), phase change in heat conduction and heat convection problems, natural convection in the presence of magnetic fields, steady-state cooperating thermosolutal convection in enclosures, transient cooperating thermosolutal convection in enclosures and transient phase change of the binary mixture in enclosures.

3. Multilevel Hybrid Optimizer

A hybrid optimization is a combination of the deterministic and the evolutionary/stochastic methods, in the sense that it utilizes the advantages of each of these methods (Dulikravich et al., 1999). The hybrid optimization method usually employs an evolutionary/stochastic method to locate a region where the global extreme point is located and then automatically switches to a deterministic method to get to the exact point faster. The hybrid optimization method used here is quite simple conceptually, although its computational implementation is more involved. The global procedure is illustrated in Fig. 1. It uses the concepts of four different methods of optimization, namely: the Broyden-Fletcher-Goldfarb-Shanno (BFGS) quasi-Newton method (Broyden, 1987), the particle swarm method (Kennedy and Eberhart, 1995), the differential evolution method (Storn and Price, 1996) and the simulated annealing method (Corana et al., 1987).

In order to speed-up the optimization task, a multilevel approach is utilized, where the procedure illustrated on the left side of Fig. 1 is repeated over several levels of grid refinement (showed on the right side of Fig. 1). Thus, the optimization procedure starts with a very coarse grid and it goes to a finer grid as the iteration continues. In this paper

we used a four-level optimization approach. Thus, Fig. 1 shows a different grid size used in each of the optimization levels.

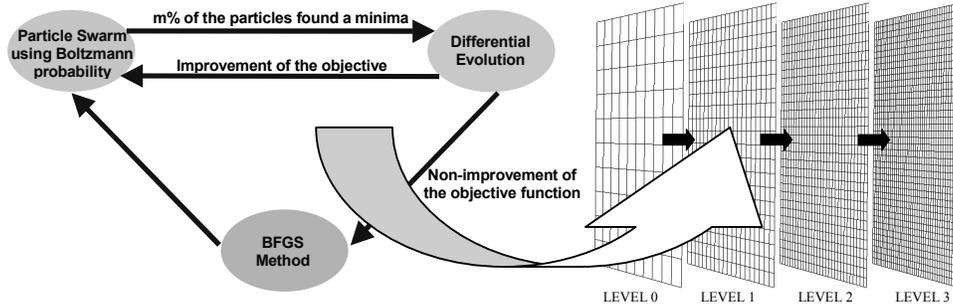


Figure 1. Global Procedure for the Multilevel Hybrid Optimization Method.

The driven module is the particle swarm method, which performs most of the optimization task. The particle swarm method is a non-gradient based optimization method created in 1995 by an electrical engineer (Russel Eberhart) and a social psychologist (James Kennedy) (Kennedy and Eberhart, 1995) as an alternative to the genetic algorithm methods. This method is based on the social behavior of various species and tries to equilibrate the individuality and sociability of the individuals in order to locate the optimum of interest. The original idea of Kennedy and Eberhart came from the observation of birds looking for a nesting place. When the individuality is increased the search for alternative places for nesting is also increased. However, if the individuality becomes too high the individual might never find the best place. In other words, when the sociability is increased, the individual learns more from their neighbor's experience. However, if the sociability becomes too high, all the individuals might converge to the first place found (possibly a local minimum).

In the hybrid optimizer, when a certain percentage of the particles find a minimum, the algorithm switches automatically to the differential evolution method and the particles are forced to breed. If there is an improvement in the objective function, the algorithm returns to the particle swarm method, meaning that some other region is more prone to having a global minimum. If there is no improvement on the objective function, this can indicate that this region already contains the global value expected and the algorithm automatically switches to the BFGS method in order to find its location more precisely. In Fig. 1, the algorithm returns to the particle swarm method in order to check if there are no changes in this location and the entire procedure repeats itself. After some maximum number of iterations is performed (e.g., five) the process stops. Details of this hybrid optimizer as well of other optimizers can be found in two recent tutorials (Colaço et al., 2004; Colaço et al., 2005c).

4. Results

In this paper we deal with the inverse determination of the magnetic boundary conditions that interact with thermal and concentration buoyancies and create such a fluid flow that gives some pre-specified concentration distribution of the solute within some region. The geometry considered is a square cavity, whose height and length are equal to 150 mm. The top, bottom and right walls were kept thermally insulated. The left wall was kept at a "cold" temperature, lower than the eutectic temperature. All boundaries are impermeable both to the velocities and to the concentration. The initial conditions were taken as above the melting point for the temperature and below the eutectic point for the concentration. Thus, a solidification front starts from the left wall and a combined buoyancy force due to the thermal and solutal gradients cause the fluid flow.

The four walls were subjected to unknown magnetic field distributions whose directions were made orthogonal to each wall. In order to satisfy the magnetic flux conservation equation

$$\nabla \cdot \mathbf{B} = 0 \quad (3)$$

the following periodic conditions were imposed

$$B_1(y = 0 \text{ mm}) = B_2(y = 150 \text{ mm}) \quad \text{and} \quad B_3(x = 0 \text{ mm}) = B_4(x = 150 \text{ mm}) \quad (4.a,b)$$

The objective was to minimize the natural convection effects by reducing the gradient of concentration along the y direction, thus attempting to obtain a concentration profile similar to those obtained for pure conduction over the entire time of simulation. The objective function to be minimized is then formulated as

$$F = \int_{t=0}^{t_f} \sqrt{\frac{1}{\#cells} \sum_{i=1}^{\#cells} \left(\frac{\partial C_i}{\partial y_i} \right)^2} dt \quad (5)$$

The magnetic field boundary conditions were discretized at six points equally spaced along the $x = 0.0$ and along $y = 0.0$ boundaries and interpolated using B-splines for the other points at those boundaries. The magnetic boundary conditions at $x = 150$ mm and $y = 150$ mm were then obtained using periodic conditions from Eqs. (4.a) and (4.b).

The initial thermal condition was set equal to 1685.04 K throughout the container. At time zero, left wall temperature was set equal to 1624.96 K. The initial condition for the concentration was set equal to 0.1 kg m⁻³. The eutectic temperature and concentration were set to 1681 K and 0.8 kg m⁻³, respectively, while the melting temperature was set to 1685 K. The equilibrium partition coefficient K was set to 0.3 and the final time of the simulation was 1 hour.

The physical properties were taken for molten silicon (Colaço et al., 2003) as

$\rho_l = 2550 \text{ kg m}^{-3}$	$\rho_s = 2550 \text{ kg m}^{-3}$	$k_l = 64 \text{ W m}^{-1} \text{ K}^{-1}$	$k_s = 64 \text{ W m}^{-1} \text{ K}^{-1}$
$C_{pl} = 1059 \text{ J kg}^{-1} \text{ K}^{-1}$	$C_{ps} = 1059 \text{ J kg}^{-1} \text{ K}^{-1}$	$\mu_l = 0.0032634 \text{ kg m}^{-1} \text{ s}^{-1}$	$\mu_s = 326.34 \text{ kg m}^{-1} \text{ s}^{-1}$
$\sigma_l = 12.3 \times 10^5 \text{ 1/m } \Omega$	$\sigma_s = 4.3 \times 10^4 \text{ 1/m } \Omega$	$\beta = 1.4 \times 10^{-4} \text{ K}^{-1}$	$\beta_s = 0.0875$
$D_l = 6.043 \times 10^{-9} \text{ kg m}^{-1} \text{ s}^{-1}$	$D_s = 0 \text{ kg m}^{-1} \text{ s}^{-1}$	$g = 9.81 \text{ m s}^{-2}$	$\mu_m = 1.2566 \times 10^{-5} \text{ T m A}^{-1}$
$L = 1.8 \times 10^6 \text{ J/kg}$			

Figure 2 shows the calculated iso-void and the iso-concentration profiles predicted for this test case without any magnetic field applied for four different times: $t = 15$ min., 30min., 45min., and 60min. One can see the large curvature profile for both the void fraction and the concentration lines. A void fraction equals to one represents a pure solid, while a void fraction equals to zero represents a pure liquid. It is worth to note that the solid phase rejects solute to the liquid phase, as the solidification front propagates upwards, as one can see on the bottom of Fig. 2.

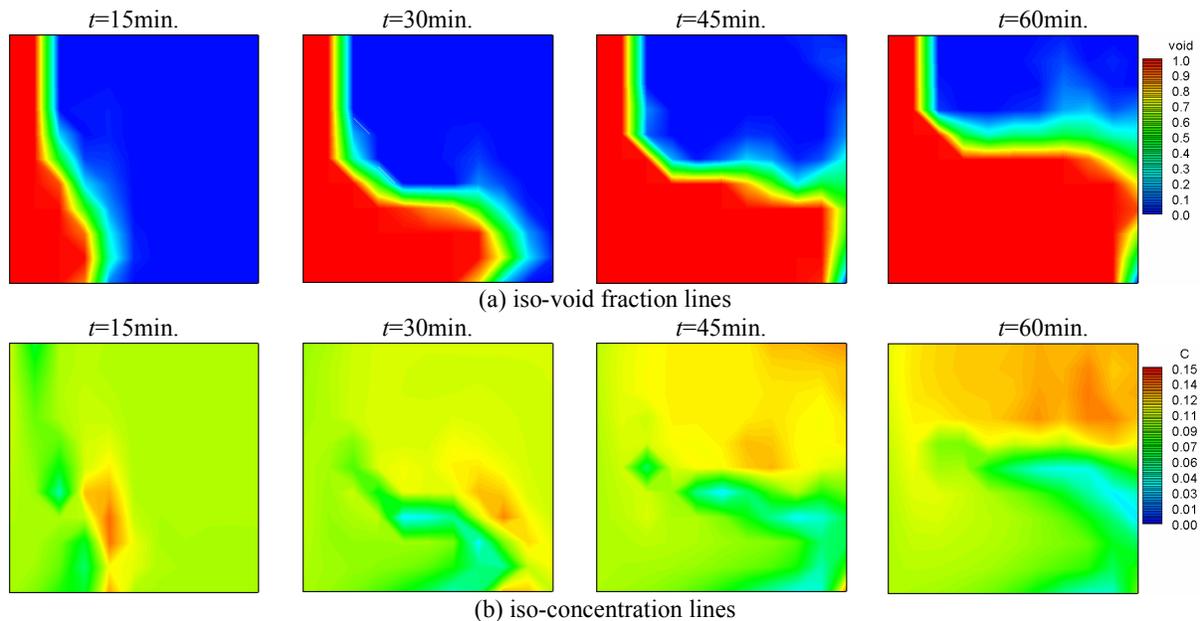


Figure 2. Iso-void fraction patterns (a), and iso-concentration patterns (b) with no applied magnetic field ($B = 0$).

Figure 3 shows iso-void and the iso-concentration profiles resulting from six optimized terms in the B-spline on each boundary for the estimation of the magnetic boundary conditions for four different times. Under the influence of the magnetic field, both the iso-concentration and iso-void fraction profiles are more flat. In fact, the magnetic field “freezes” the solidification process, so that the void fraction profile practically does not change after $t = 15$ min. One can see that the gradients of concentration in the y direction are reduced significantly. Using more design variables (B-spline control points) in the optimization could create even better results where the gradients of concentration in the y direction would be further reduced. The optimization task was performed on a 96 CPU parallel computer located in the MAIDROC Lab at the Florida International University.

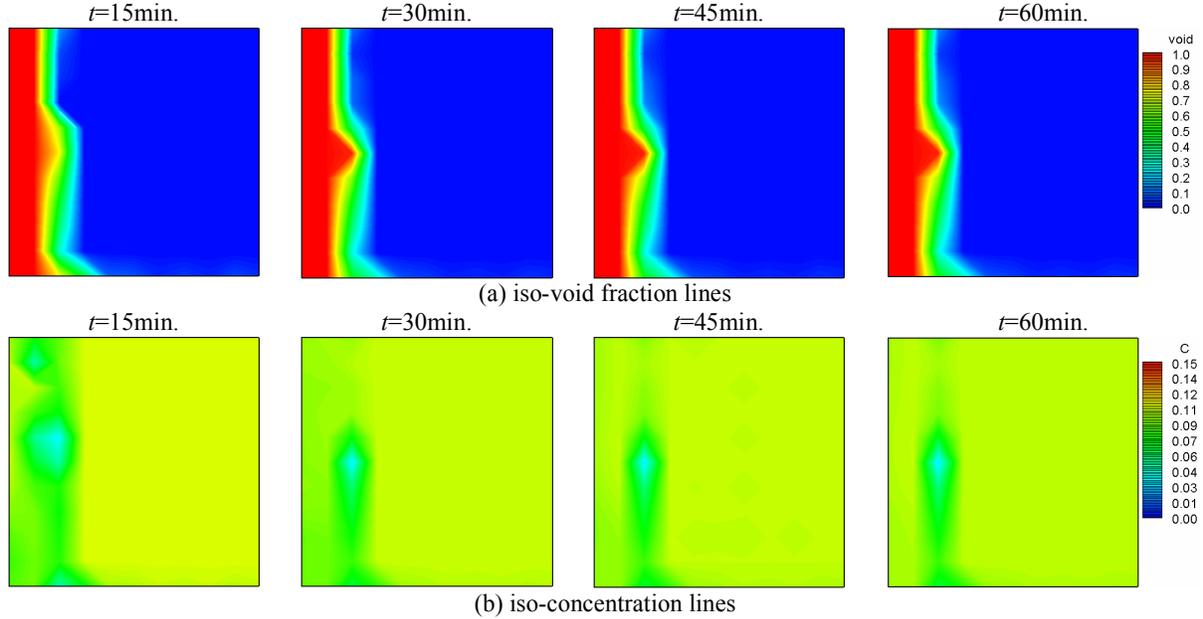


Figure 3. Iso-void fraction patterns (a), and iso-concentration patterns (b) resulting from externally applied magnetic flux B optimized at six points per boundary.

Figure 4 shows the optimized magnetic field boundary conditions for $x = 0$ and $y = 0$. Notice that the strengths of the required magnetic field are very small and could be easily achieved with small permanent magnets. Figure 4 also shows the convergence history of the process of minimizing the objective function (Eq. 5) using the hybrid optimizer with automatic switching among the optimization modules for multi level optimization. Due to the extremely high computational cost, only three levels (levels 0, 1 and 2 in the Fig. 1) were used. These levels represent grid sizes with 10×10 , 20×20 and 30×30 grid cells. The two peaks in the convergence history graphic represent the points where the optimizer changed from one level to another. Since the grid size is different, there is a discontinuity in the objective function calculation and the optimizer uses the last “known to work” parameters as the new estimate.

Although a 30×30 grid size is not fully converged, the results qualitatively show the feasibility of reducing the thermosolutal effects using small optimized magnetic fields.

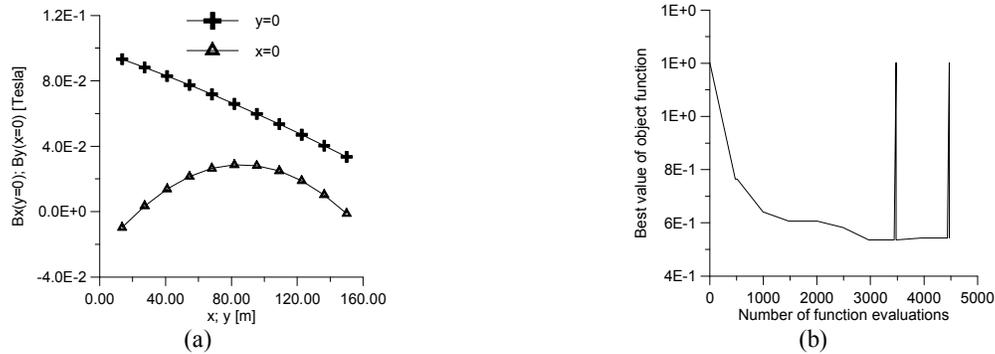


Figure 4. (a) Optimized magnetic boundary conditions at $x = 0$ and $y = 0$ with the estimation of magnetic flux B at six points per boundary. (b) Optimization convergence history for the estimation of magnetic flux B at six points per boundary.

5. Conclusions

In this paper we presented the results of a transient MHD analysis code that is capable of dealing with thermosolutal problems with and without phase change in enclosures. The ability to minimize the natural convection effects in problems dealing with fluid flow of mixtures during phase change was demonstrated by utilizing an optimized distribution of magnetic field along the boundaries of a container. A multilevel hybrid constrained optimization algorithm was used for reducing the concentration gradients to those similar to pure conduction problems. Due to the

extremely high computational cost involved, only qualitative results were shown for a not fully converged calculation. A further investigation is necessary using a finer grid. Also, only a stationary magnetic field was used to minimize a transient shape of the concentration profile. Thus, a transient boundary condition for the magnetic field should be investigated for a more significant reduction of the thermosolutal effects during unsteady solidification of a binary mixture. The three-dimensional cases, involving both MHD and EHD effects should be investigated as well as the study of fluid flows at high Rayleigh numbers involving turbulence.

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