

MATERIALS AND MANUFACTURING PROCESSES

Vol. 19, No. 4, pp. 1-24, 2004

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47

Optimization of Intensities and Orientations of Magnets Controlling Melt Flow During Solidification

George S. Dulikravich,^{1,*} Marcelo J. Colaço,² Brian H. Dennis,³
Thomas Martin,⁴ Igor N. Egorov-Yegorov,⁵ and Seungsoo Lee⁶

¹Florida International University, Mechanical and Materials Eng. Dept.,
MAIDROC Lab., Miami, FL, USA

AQ1

²Military Institute of Engineering (IME), Mechanical and Materials Eng. Dept.,
Rio de Janeiro, Brazil

³University of Texas at Arlington, Mechanical and Aerospace Eng. Dept.,
Arlington, TX, USA

⁴Pratt and Whitney Engine Company, Turbine Discipline Engineering and
Optimization Group, East Hartford, CT, USA

⁵Sigma Technology, Moscow, Russia

⁶Inha University, Aerospace Eng. Dept., Incheon, Korea

ABSTRACT

When growing large single crystals from a melt, it is desirable to minimize thermally induced convection effects so that solidification is achieved predominantly by thermal conduction. It is expected that under such conditions any impurities that originate from the walls of the crucible will be less likely to migrate into the mushy region and consequently deposit in the crystal. It is also desirable to achieve a distribution of the dopant in the crystal that is as uniform as possible. A finite volume method and a least-squares spectral finite element method were used to develop accurate computer codes for prediction of solidification from a melt

*Correspondence: Prof. George S. Dulikravich, Florida International University, Mechanical and Materials Eng. Dept., MAIDROC Lab., EC 3474, Miami, FL 33027, USA; E-mail: dulikrav@fiu.edu.

1

DOI: 10.1081/LMMP-200031887
Copyright © 2004 by Marcel Dekker, Inc.

1042-6914 (Print); 1532-2475 (Online)
www.dekker.com

48 under the influence of externally applied magnetic fields. A hybrid constrained
49 optimization algorithm and a semi-stochastic self-adapting response surface opti-
50 mizer were then used with these solidification analysis codes to determine the
51 distributions of the magnets that will minimize the convective flow throughout
52 the melt or in desired regions of the melt only.

AQ2

56 INTRODUCTION

57
58 The objective of this article is to demonstrate the feasibility of determining
59 unknown boundary values of an applied magnetic field that will create user-specified
60 features of the melt flow-field and the melt/solid interface. This article presents a
61 proof-of-concept effort and it does not present the most advanced MHD analysis
62 involving solidification. In this study, all physical properties (density, heat conduc-
63 tivity, heat capacity, electric conductivity, etc.) were treated as constants instead
64 of as functions of temperature. The effects of magnetization were not included. This
65 study does not involve optimization of thermal boundary conditions in MHD
66 solidification.^[1]

67 The latent heat released in the mushy region of a solidifying melt, where
68 $T_{\text{liquidus}} > T > T_{\text{solidus}}$, is assumed to be proportional to the local volumetric liquid/
69 (liquid + solid) ratio.^[2,3]

$$70 \quad f = \frac{V_\ell}{V_\ell + V_s} = \left(\frac{T - T_{\text{solidus}}}{T_{\text{liquidus}} - T_{\text{solidus}}} \right)^n = \tilde{\theta}^n \quad (1)$$

71
72 Here, the exponent n is typically $0.2 < n < 5$, while $f=1$ for $T \geq T_{\text{liquidus}}$ and $f=0$
73 for $T \leq T_{\text{solidus}}$. In all test cases, the non-dimensional temperature is given as

$$74 \quad \theta = \frac{T - T_{\text{solidus}}}{T_h - T_c} \quad (2)$$

75
76 Thus, $\theta=0.0$ corresponds to interface between the solid phase and the mushy region.
77 For relatively small changes of density with temperature, it is justifiable to assume
78 linear variation of density as a function of the temperature.^[4] In the liquid, the
79 density is

$$80 \quad \rho_\ell = \rho_r \left[1 + \left(\frac{\partial(\rho_\ell/\rho_r)}{\partial\theta} \right)_r (\theta - \theta_r) \right] = \rho_r [1 - \alpha_\ell(\theta - \theta_r)] \quad (3)$$

81
82 with a similar expression for the solid phase. Therefore, the liquid-solid mixture
83 density and modified heat capacity can be defined as

$$84 \quad \rho_{\text{mix}} = f\rho_\ell + (1-f)\rho_s \quad (4)$$

$$85 \quad c_{\text{mix}} = f\rho_\ell \frac{\partial(c_\ell\theta_\ell)}{\partial\theta} + (1-f)\rho_s \frac{\partial(c_s^{eq}\theta_s)}{\partial\theta} \quad (5)$$

Optimization of Intensities and Orientations

95 where an enthalpy method^[3] was used to formulate the equivalent specific heat
96 coefficient in the solid phase.

97
98
$$c_s^{eq} = c_s - \frac{1}{S_{TE}} \frac{\partial L}{\partial \theta}$$
 99 (6)

100 Here, the specific heat coefficient accounts for the latent heat release in the mushy
101 region. The non-dimensional numbers used in magneto-hydrodynamics (MHD)
102 modeling are as follows:

103 Reynolds hydrodynamic Prandtl hydrodynamic Eckert number

104
105
$$R_e = \frac{\rho_r v_r \ell_r}{\mu_{vr}} \quad P_R = \frac{\mu_{vr} c_r}{\kappa_r} \quad E_c = \frac{v_r^2}{c_r \Delta T_r}$$
 106 (7a-c)

107
108 Grash of number Prandtl magnetic Hartmann number

109
110
$$G_R = \frac{\rho_r^2 \alpha_r g_r \Delta T_r \ell_r^3}{\mu_{vr}^2} \quad P_m = \frac{\mu_{vr} \sigma_r \mu_r}{\rho_r} \quad H_T = \ell_r \mu_r H_r \left(\frac{\sigma_r}{\mu_{vr}} \right)^{1/2}$$
 111 (7d-f)

112
113 Stefan number Froude number Rayleigh number

114
115
$$S_{TE} = \frac{c_r \Delta T_r}{L_r} \quad F_R = \frac{v_r^2}{g_r \ell_r} \quad R_a = \frac{\rho_r^2 \alpha_r c_r g_r \Delta T_r \ell_r^3}{\kappa_r \mu_{vr}}$$
 116 (7g-i)

117 Using these parameters, the non-dimensional formulation of the Navier-Stokes
118 subsystem of the MHD equations for phase-changing mixtures of two liquids has
119 been formulated.^[5-7] In this formulation, the solid phase is treated as the second
120 liquid with extremely high viscosity. Assuming that both phases have the same local
121 velocity, the non-dimensional form of mass conservation is obvious.

122
123
$$\nabla \cdot \underline{v} = 0$$
 124 (8)

125 Each phase could have been modeled with its own velocity, which would yield a
126 more complicated expression for multi-component mass conservation.^[8] The non-
127 dimensional version of linear momentum conservation for two-phase MHD flows
128 with thermal buoyancy, and magnetic force is

129
130
$$\rho_{mix} \frac{\partial \underline{v}}{\partial t} + f \rho_\ell \nabla \cdot (\underline{v} \underline{v} + \hat{p}_\ell \underline{I}) + (1-f) \rho_s \nabla \cdot (\underline{v} \underline{v} + \hat{p}_s \underline{I})$$

131
132
$$= f \left\{ \nabla \cdot \left[\frac{\mu_{v\ell}}{R_e} (\nabla \underline{v} + (\nabla \underline{v})^*) \right] + \frac{G_R}{R_e^2} \rho_\ell \alpha_\ell \theta \underline{g} + \frac{H_T^2}{P_m R_e^2} \mu_\ell (\nabla \times \underline{H}) \times \underline{H} \right\}$$

133
134
$$+ (1-f) \left\{ \nabla \cdot \left[\frac{\mu_{vs}}{R_e} (\nabla \underline{v} + (\nabla \underline{v})^*) \right] + \frac{G_R}{R_e^2} \rho_s \alpha_s \theta \underline{g} + \frac{H_T^2}{P_m R_e^2} \mu_s (\nabla \times \underline{H}) \times \underline{H} \right\}$$
 135 (9)
136

137 where the non-dimensional hydrodynamic, hydrostatic, and magnetic pressures were
138 combined to give

139
140
$$\hat{p}_\ell = \frac{p}{\rho_\ell} + \frac{\varphi}{F_R^2} + \frac{H_T^2}{P_m R_e^2} \mu_\ell \underline{H} \cdot \underline{H} \quad \text{and} \quad \hat{p}_s = \frac{p}{\rho_s} + \frac{\varphi}{F_R^2} + \frac{H_T^2}{P_m R_e^2} \mu_s \underline{H} \cdot \underline{H}$$
 141 (10)

142 Here, φ is the non-dimensional gravity potential defined as $\underline{g} = -\nabla\varphi$. Then, the
143 non-dimensional form of energy conservation for incompressible phase-changing
144 MHD flows including Joule heating can be written as^[6]

$$\begin{aligned}
 & c_{\text{mix}} \frac{\partial \theta}{\partial t} + f \rho_\ell \nabla \cdot (c_\ell \theta \underline{v}) + (1-f) \rho_s \nabla \cdot (c_s^{eq} \theta \underline{v}) \\
 & = f \left[\frac{1}{R_e P_R} \nabla \cdot (\kappa_\ell \nabla \theta) + \frac{1}{\sigma_\ell P_m^2 R_e^3} H_7^2 E_c (\nabla \times \underline{H}) \cdot (\nabla \times \underline{H}) \right] \\
 & + (1-f) \left[\frac{1}{R_e P_R} \nabla \cdot (\kappa_s \nabla \theta) + \frac{1}{\sigma_s P_m^2 R_e^3} H_7^2 E_c (\nabla \times \underline{H}) \cdot (\nabla \times \underline{H}) \right] \quad (11)
 \end{aligned}$$

154 The classical modeling of MHD assumes that there are no free electric charges in
155 the fluid.^[5,7] With these assumptions Maxwell's system for steady electro-magnetics
156 of a moving media becomes

$$157 \quad \nabla \cdot \underline{B} = 0 \quad (12)$$

$$159 \quad \nabla \times \underline{H} = \underline{J} \quad (13)$$

$$161 \quad \nabla \cdot \underline{J} = 0 \quad (14)$$

163 Ohm's law relates the induced electric current to the magnetic intensity vector in a
164 moving media.

$$165 \quad \underline{J} = \sigma \underline{v} \times \underline{B} \quad (15)$$

167 If electric conductivity and magnetic permeability are assumed to be constant within
168 each phase, then the following non-dimensionalized magnetic field transport equation
169 for the phase-changing MHD flow can be obtained from Eqs. (12) to (15).
170 It needs to be solved intermittently^[6] with Eqs. (8) through (11).

$$171 \quad \frac{\partial \underline{H}}{\partial t} - \nabla \times (\underline{v} \times \underline{H}) = \frac{f/(\sigma_\ell \mu_\ell) + (1-f)/(\sigma_s \mu_s)}{P_m R_e} \nabla^2 \underline{H} \quad (16)$$

174 The modified magnetic transport equations (16), the continuity equation (8), the
175 modified linear momentum balance equations (9), and the modified energy balance
176 equation (11) were integrated numerically using a finite volume method for
177 structured clustered grids written in terms of non-orthogonal boundary-conforming
178 coordinates.^[9] Artificial density formulation was used to remove the singularity from
179 the Navier-Stokes system, and the artificial time integration was performed using a
180 four-stage Runge-Kutta algorithm.

181
182
183
184 **EXAMPLES OF COMPUTED MHD FLOWS**
185 **WITH SOLIDIFICATION**
186

187 First, let us consider the problem of steady state solidification in two square-
188 shaped containers without any magnetic field. Each container had the following

Optimization of Intensities and Orientations

189
190
191
192
193
194
195
196
197
198
199
200
201
202
203
204
205
206
207
208
209
210
211
212
213
214
215
216
217
218
219
220
221
222
223
224
225
226
227
228
229
230
231
232
233
234
235

Table 1. Physical properties of molten and solid silicon.^[9]

$\rho_\ell = 2550 \text{ kg/m}^3$	$\rho_s = 2330 \text{ kg/m}^3$
$c_{p\ell} = 1059 \text{ J/kg K}$	$c_{ps} = 1038 \text{ J/kg K}$
$\kappa_\ell = 64 \text{ W/m K}$	$\kappa_s = 22 \text{ W/m K}$
$T_\ell = 1685 \text{ K}$	$T_s = 1681 \text{ K}$
$\sigma_\ell = 12.3 \times 10^5 \text{ 1/}\Omega \text{ m}$	$\sigma_s = 4.3 \times 10^4 \text{ 1/}\Omega \text{ m}$
$\mu_{v\ell} = 7.018 \times 10^{-4} \text{ kg/m s}$	$\mu = 7.022 \times 10^{-4} \text{ kg m/A}^2 \text{ s}^2$
$L = 1.803 \times 10^6 \text{ J/kg}$	$\alpha = 1.4 \times 10^{-4} \text{ 1/K}$

Table 2. Parameters for two test cases.

Case 1 (small container)	Case 2 (large container)
$l_r = 0.01 \text{ m}$	$l_r = 0.02 \text{ m}$
$Re = 1000$	$Re = 1000$
$B_r = 0.1 \text{ T}$	$B_r = 0.1 \text{ T}$
$v_r = 2.7522 \times 10^{-2} \text{ m/s}$	$v_r = 1.3761 \times 10^{-2} \text{ m/s}$
$Pr = 1.1613 \times 10^{-2}$	$Pr = 1.1613 \times 10^{-2}$
$Gr = 1.8132 \times 10^5$	$Gr = 1.4506 \times 10^6$
$Ra = 2.1056 \times 10^3$	$Ra = 1.6845 \times 10^4$
$Fr = 8.7870 \times 10^{-2}$	$Fr = 3.1067 \times 10^{-2}$
$Ec = 7.1524 \times 10^{-8}$	$Ec = 1.7881 \times 10^{-8}$
$Ht = 4.1864 \times 10^1$	$Ht = 8.3729 \times 10^1$

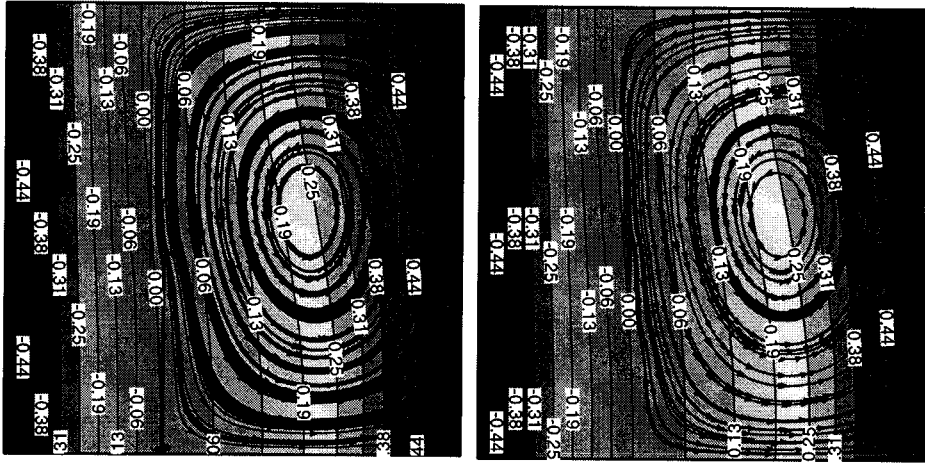
thermal boundary conditions: left wall at T_c , right wall at T_h , and top and bottom walls thermally insulated. Gravity was assumed to act vertically downwards. Physical properties of molten and solid silicon (Table 1) were used in these two example test cases. **T1**

The physical properties of the liquid phase from Table 1 were adopted as the reference properties. For $\Delta T_r = T_h - T_c = 10 \text{ K}$, and $Re = 1000$, the resulting non-dimensional parameters are given in Table 2 for two different sizes of solidification containers, it should be noted out that these test cases used the physical properties for silicon with one exception. The magnetic Prandtl number that was used was three orders of magnitude larger than its physical value. This was done because the realistic extremely small values of P_m caused the explicit numerical integration algorithm used in the MHD analysis to diverge. **T2**

Figures 1 and 2 present the results for both test cases without magnetic field applied ($Ht = 0.0$) using two different grid sizes. **F1 F2**

In both test cases, the results for the coarser grid (50×50 grid cells) are very similar to the results with a refined grid (80×80 grid cells). The coarser grid was used for the MHD solidification simulations during the optimization process. Figure 3 shows the convergence history for containers of both sizes when using a grid size of 50×50 grid cells. **F3**

236
237
238
239
240
241
242
243
244
245
246
247
248
249
250

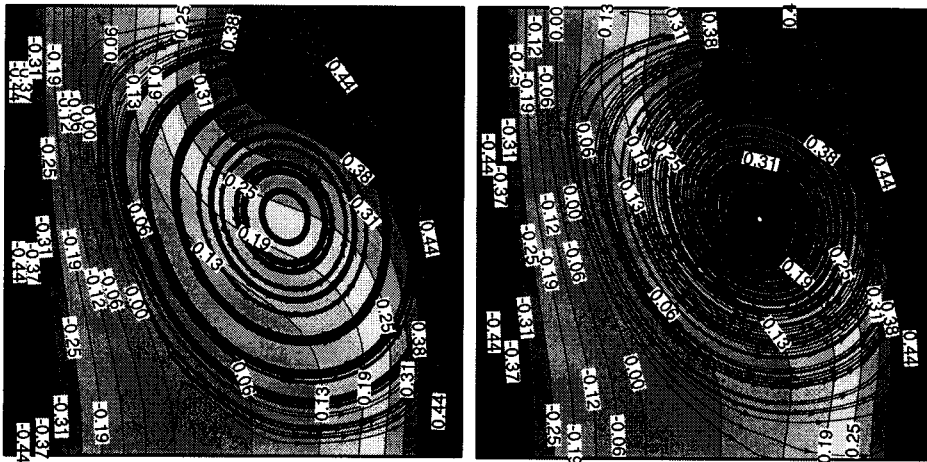


(a) 50 x 50 grid cells

(b) 80 x 80 grid cells

251
252
253
254 **Figure 1.** Temperature field and streamlines for smaller container using two grid sizes
255 (Ht = 0.0).
256

257
258
259
260
261
262
263
264
265
266
267
268
269
270
271
272



(a) 50 x 50 grid cells

(b) 80 x 80 grid cells

273
274
275 **Figure 2.** Temperature field and streamlines for larger container using two grid sizes
276 (Ht = 0.0).
277

278
279 **OPTIMIZATION OBJECTIVES AND ALGORITHMS**

280
281 A variety of optimization algorithms have been developed and used for
282 problems from many different disciplines. Various optimization algorithms have

Optimization of Intensities and Orientations

283
 284
 285
 286
 287
 288
 289
 290
 291
 292
 293
 294
 295
 296
 297
 298
 299
 300
 301
 302
 303
 304
 305
 306
 307
 308
 309
 310
 311
 312
 313
 314
 315
 316
 317
 318
 319
 320
 321
 322
 323
 324
 325
 326
 327
 328
 329

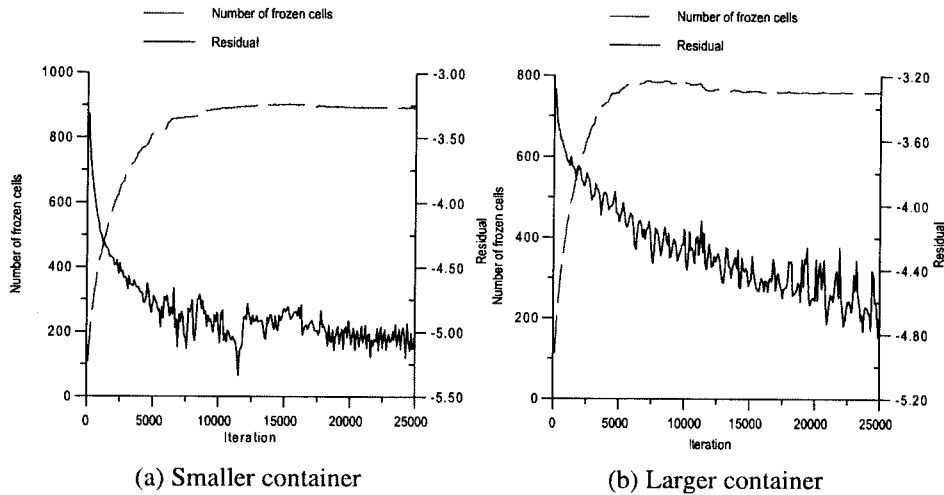


Figure 3. Convergence history for solidification in both containers ($H_t=0$; grid 50×50 cells).

been known to provide different rates of convergence depending on the size and shape of the mathematical design space, the nature of the constraints, and where they are during the optimization process. This is why we created a hybrid constrained optimization computer program^[10] that incorporates several of the most popular optimization modules: the Davidon-Fletcher-Powell (DFP) gradient search method, a genetic algorithm (GA), the Nelder-Mead (NM) simplex method, quasi-Newton algorithm of Pshenichny-Danilin (LM), differential evolution (DE), and sequential quadratic programming (SQP). The original package did not have the DE, SQP, and LM methods. A set of analytic rules were coded into the program to automatically switch among the different optimization algorithms to avoid local minima and to accelerate the overall convergence. Different versions of this hybrid optimization package have been successfully applied during the optimization of various multi-disciplinary problems.^[11] Another conceptually different optimizer, known as IOSO, was also used in this work. It is based on semi-stochastic methods and self-adaptive response surface methodology.^[11,12] Different numerical analysis methods (finite volume and finite element methods) and different optimization algorithms (a hybrid optimizer and a IOSO optimizer) were used to demonstrate and compare their respective accuracies, robustness, and versatility.

MINIMIZATION OF THE NATURAL CONVECTION
 USING MHD AND A HYBRID OPTIMIZER

It is well known that application of a magnetic field to a solidifying flow-field of an electrically conducting fluid will create additional body forces that are

330 capable of significantly altering the flow-field and heat transfer.^[13-16] It has also been
 331 demonstrated that it is possible to optimize the boundary values of the magnetic field
 332 with the objective of achieving certain desired features of the flow-field.^[17,18] Let us
 333 now try to optimize the magnetic field applied on each of the four walls of the square
 334 container of test case 1 (smaller container) described in the previous section. The
 335 objective is to minimize the effects of the thermally induced natural convection
 336 in case of solidification from a sidewall. To satisfy magnetic flux conservation
 337 (Eq. 12), we consider the simple case of periodic boundary conditions.

338
 339
$$B_1(0, y) = B_2(1, y) \tag{17}$$

340
 341
 342
$$B_3(x, 0) = B_4(x, 1) \tag{18}$$

343 The unknown boundary values of the magnetic field were parameterized as
 344 follows:

345
 346
 347
$$B(x_k) = \sum_{i=1}^M P_i C_i(x_k) \tag{19}$$

348 where P_i is unknown parameter and the function $C_i(x_k)$ is given as

AQ3

350
 351
 352
$$C_i(x_k) = \cos\left[(i-1)\frac{\pi}{2}x_k\right] \text{ for } i = 1, 3, 5, \dots \tag{20}$$

353
 354
 355
$$C_i(x_k) = \cos\left[i\frac{\pi}{2}x_k\right] \text{ for } i = 2, 4, 6, \dots \tag{21}$$

356
 357 The objective function for this optimization problem was to minimize the sum of all
 358 vertical temperature gradient magnitudes in the entire liquid region that should
 359 minimize thermally induced buoyancy flow-field in the melt. Thus, our problem is to
 360 minimize the objective function, F , defined as

361
 362
 363
$$F = \left[\frac{1}{\#\text{liquid cells}} \sum_{i=1}^{\#\text{liquid cells}} \left(\frac{\partial T}{\partial y} \right)^2 \right]^{1/2} \tag{22}$$

364
 365
 366 In all test cases, the initial guess for the parameters was zero, while the number
 367 of optimization population members was equal to three times the number of
 368 parameters. The hybrid optimizer started with the DE method in all test cases and
 369 the initial population was randomly generated around the initial guess.

370
 371 Figures 4a and b show the results for the test case 1 without an applied magnetic
 372 field and with an optimized magnetic field applied. One can see that the buoyancy
 373 effects are reduced. In this test case, three parameters were used for $B_1(0, y)$
 374 and three parameters were used for $B_3(x, 0)$. Figure 5 shows the optimized boundary
 375 conditions, where one can see that the magnetic field is constant at the boundaries
 376 $y = 0.0$ and $y = 1.0$.

F4

F5

Optimization of Intensities and Orientations

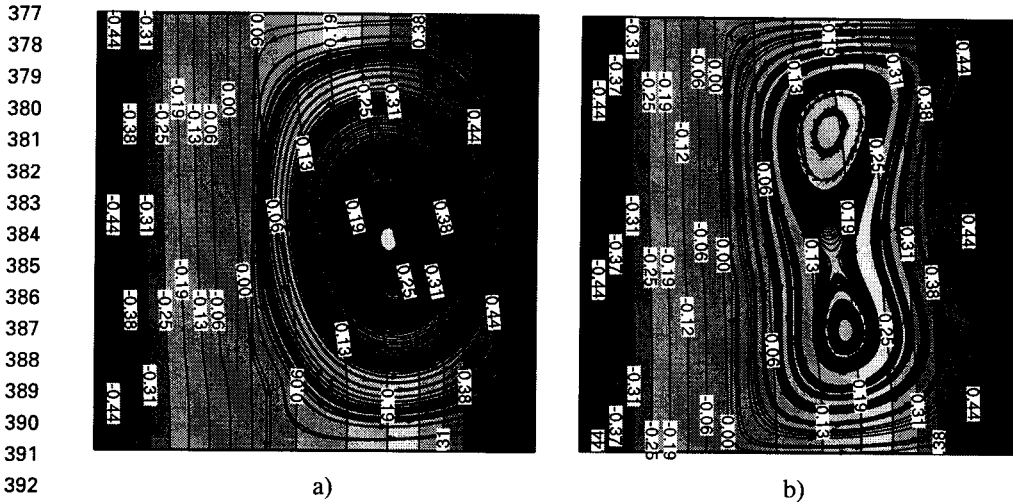


Figure 4. Isotherms and streamlines without: (a) and with (b) an optimized applied magnetic field (test case 1: smaller container).

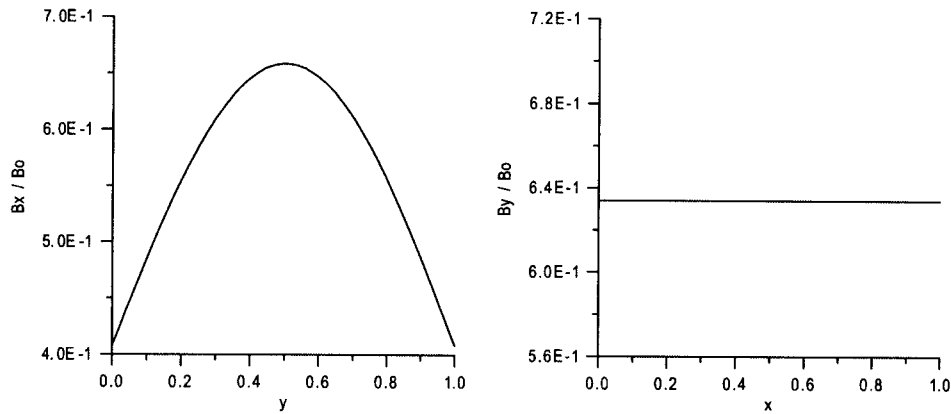


Figure 5. Optimized magnetic field boundary conditions (test case 1: smaller container).

Figure 6 shows the convergence history for the hybrid optimizer in this case F6
where the DE and NM optimization modules were automatically used most often. F6

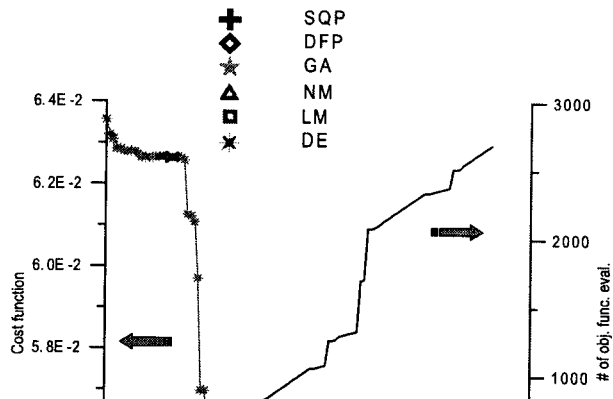
Figure 7 shows the results for test case 2 (a larger container) without an applied F7
magnetic field and with an optimized magnetic field applied. One can see that the F7
buoyancy effects are reduced, but not eliminated. Again, three parameters were used F7
for $B_1(0, y)$ and three parameters for $B_3(x, 0)$, while periodic boundary conditions F7
were enforced on the opposite boundaries. Figure 8 shows the optimized boundary F8
conditions, where, again, the variation of the magnetic field along the boundaries F8
 $x=0.0$ and $x=1.0$ is greater than at the boundaries $y=0.0$ and $y=1.0$. F8

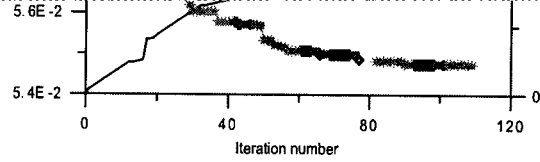
200031887_LMMP19_04_R1_081204

10

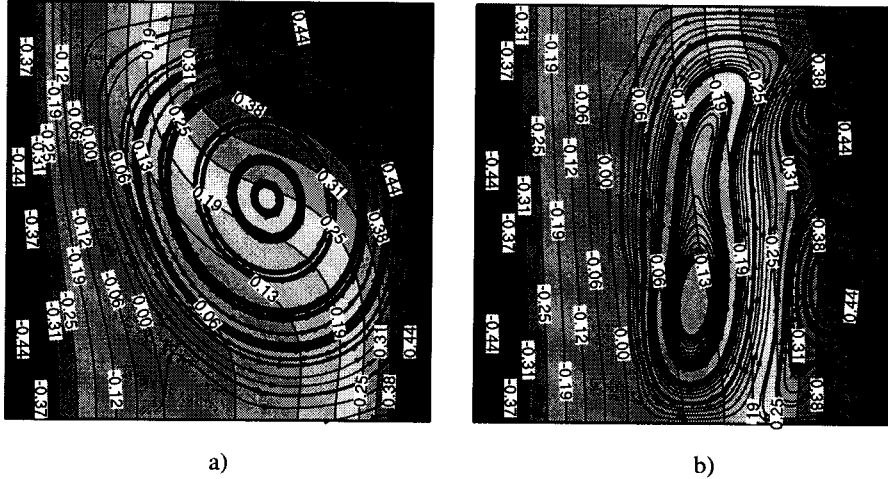
S. Dulikravich et al.

424
425
426
427
428
429
430
431
432
433
434
435
436





438
439
440
441
442
443 **Figure 6.** Convergence history for the hybrid optimizer (test case 1: smaller container).
444
445



462 **Figure 7.** Isotherms and streamlines without: (a) and with (b) an optimized applied magnetic field (test case 2: larger container).
463
464
465

466 Figure 9 shows the convergence history for the hybrid optimizer in this test case where only the DE, GA, and NM optimization modules were automatically applied.
467
468

469 Figures 10 through 12 show the results for test case 2, but using six parameters for $B_1(0, y)$ and six parameters for $B_3(x, 0)$, instead of the three parameters used
470

F9

F10–F12

Optimization of Intensities and Orientations

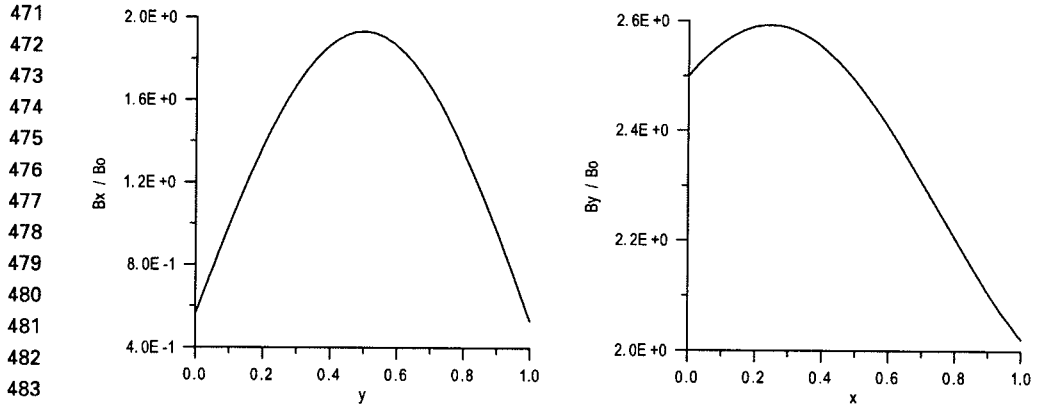


Figure 8. Optimized magnetic field boundary conditions (test case 2: larger container).

471
472
473
474
475
476
477
478
479
480
481
482
483
484
485
486
487
488
489
490
491
492
493
494
495
496
497
498
499
500
501
502
503
504
505
506
507
508

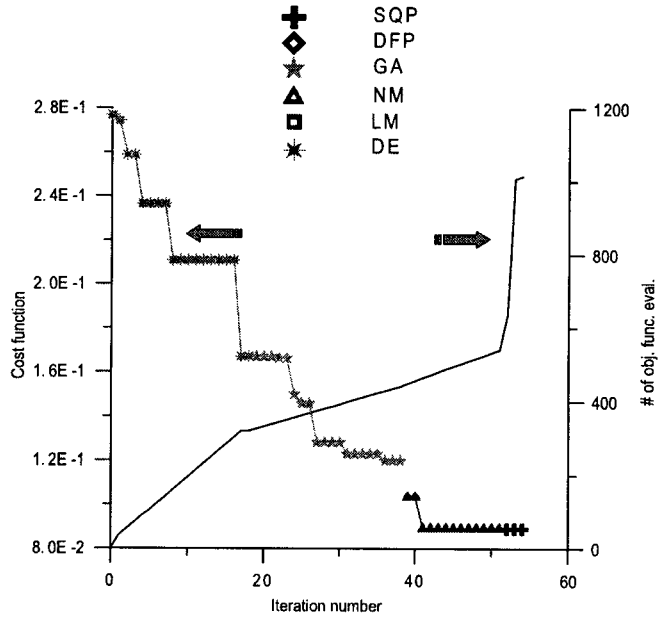


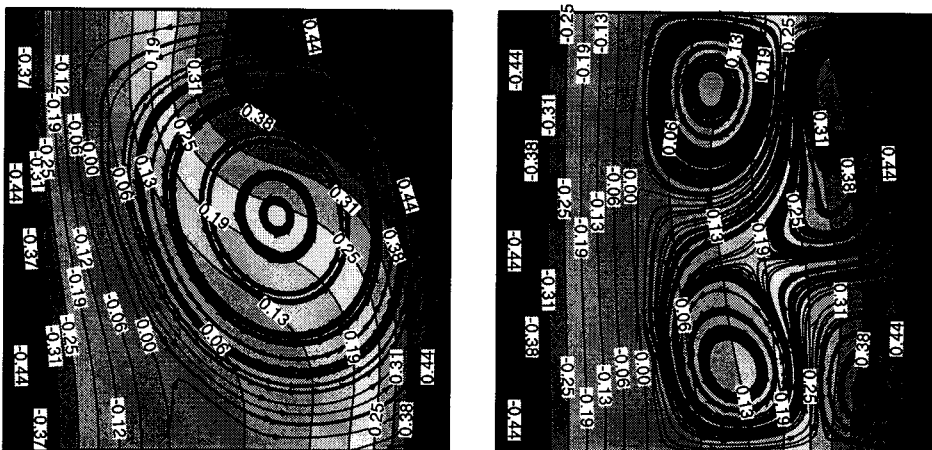
Figure 9. Convergence history for the hybrid optimizer (test case 2: larger container).

509
510
511
512
513
514
515
516
517

before. One can see that the natural convection effects are further reduced in this case. It is interesting to note that the variation of the applied magnetic field is greater at the boundaries $y=0.0$ and $y=1.0$.

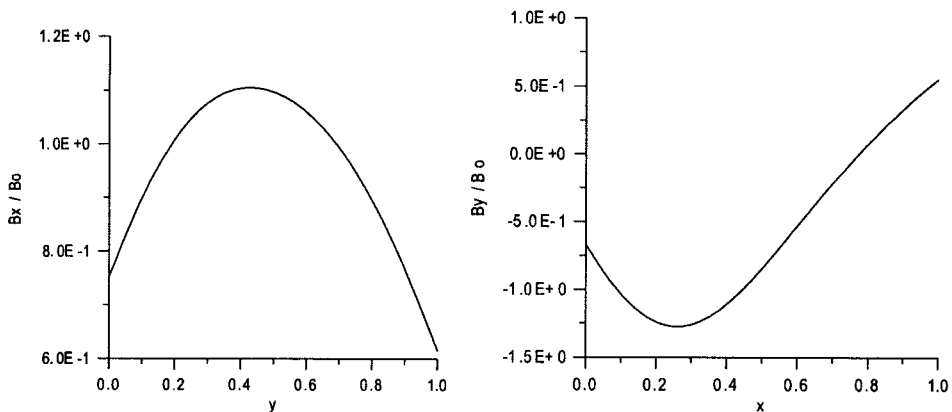
Figure 12 shows the convergence history, where, again, we applied the DE and GA modules. In fact, the GA module did the entire job in this test case.

518
519
520
521
522
523
524
525
526
527
528
529
530
531
532



533 **Figure 10.** Isotherms and streamlines without and with an optimized applied magnetic field
534 (test case 2 with six parameters).
535

536
537
538
539
540
541
542
543
544
545
546
547
548
549
550
551
552



553 **Figure 11.** Optimized magnetic field boundary conditions (test case 2 with six parameters).
554

555
556
557 **MHD SOLIDIFICATION OPTIMIZATION USING LSFEM AND**
558 **IOSO OPTIMIZER**
559

560 Other possibly more robust and accurate numerical integration methods were
561 explored^[14,15] to allow for physical values of the magnetic Prandtl number and for
562 significantly higher values of viscosity in the solid region. Consequently, we will
563 present a combination of MHD with solidification where the numerical analysis was
564 performed with a least squares spectral finite element method (LSFEM),^[15,18] and

+

[12.8.2004-7:54pm]

[1-24]

[Page No. 13]

K:/Journals/Inpro/MDI/LMMP/LMMP19(4)/200031887.3d

Materials and Manufacturing Processes (LMMP)

200031887_LMMP19_04_R1_081204

565
566
567
568
569
570
571
572
573
574
575
576
577
578
579
580
581
582
583
584
585
586
587
588
589
590
591
592
593
594
595
596
597
598
599
600
601
602
603
604
605
606
607
608
609
610
611

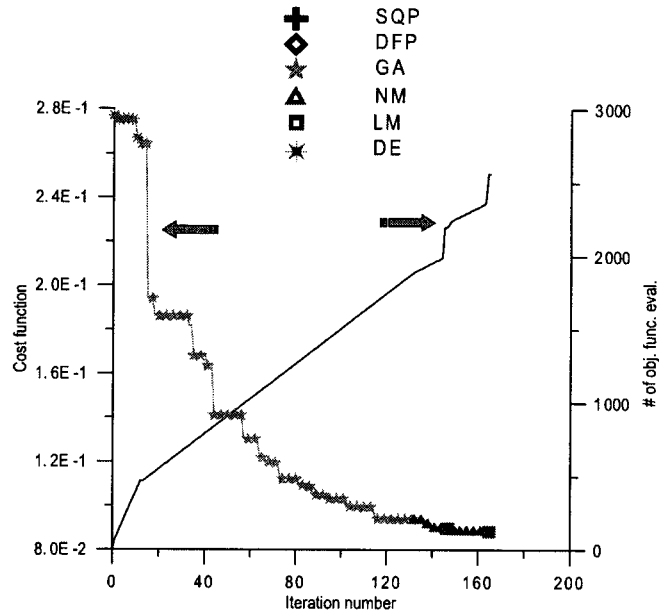


Figure 12. Convergence history for the hybrid optimizer (test case 2 with six sensors).

the optimization was performed using a self-adaptive response surface-based semi-stochastic algorithm^[11,12] called IOSO. Here, the objective of the optimization is to minimize the velocity magnitude of the melt flow near the solid-liquid interface. The optimizer searches for this by changing the orientation and distribution of the sidewall magnets as well as the strength of the applied external uniform vertical magnetic field. The objective function was expressed as the following equation:

AQ4

$$F = \sum_{i=1}^{N_{\text{fluid}}} \sqrt{u_i^2 + v_i^2} \tag{23}$$

Here, N_{fluid} is the total number of grid points located between $y > 0.04 \text{ m}$ and $y < 0.08 \text{ m}$ —that is, only in the flow-field region adjacent to the solid/melt interface. The only constraints considered in this problem were the bounds on the magnitudes of the design variables. In this problem, we considered a container with relatively weak magnets embedded in the sidewalls. The magnetic flux density strength and distribution was parameterized using a B-spline with control variables located at 7 points along the wall ($y = 0.0, 0.02, 0.04, 0.06, 0.08, 0.1 \text{ m}$). These design variables controlled the magnitude, direction, and distribution of the magnetic field.

Two cases were run. For case 1, each control point was allowed to vary from 0.07 Tesla to -0.07 Tesla . In case 2, each control point was allowed to vary from 0.5 Tesla to -0.5 Tesla . This distribution was applied to the right wall. The distribution on the left wall was taken to be of equal magnitude, but opposite sign to that of the right wall. Therefore, the resulting magnetic field was always symmetrical with

612 respect to the y -axis. A vertical magnetic field was also applied so that it could be
613 generated using an electromagnet located on the top and bottom of the container.
614 The optimized magnetic potential produced a uniform vertical field strength varying
615 between 0.0 Tesla to 0.15 Tesla in case 1 and between 0.0 Tesla and 0.5 Tesla in
616 case 2. For this example, the total number of design variables was seven.

617 The optimization procedure was applied to the solidification of a silicon melt in a
618 square container with sides of 0.1 m. A uniform temperature of 1676.0 K was applied
619 to the top wall so that solidification occurred on the top wall of the container.
620 A parabolic temperature profile was applied to the hot bottom of the container
621 to simulate nonuniform heating of the melt. The temperature at the center of the
622 bottom wall was 1688.0 K, and the temperature at the bottom corners was set to
623 1686.0 K. The sidewalls were thermally insulated. A no-slip condition for velocity
624 was enforced on all walls of the container. The magnetic flux density determined
625 from the B-spline parameterization was specified directly on the sidewalls.
626 A constant magnetic potential was specified on the top and bottom of the container.
627 The potentials were determined by calculating the potential required to produce a
628 uniform vertical field of a specified strength. A relatively coarse quadrilateral
629 computational grid with $17 \times 17 = 289$ elements with a p -level of $P = 3$ was used with
630 the LSFEM code (Fig. 13).

F13

632 The p -version of LSFEM was used to compute all results reported here. The
633 order of the approximation function was increased, or enriched, until the desired
634 level of convergence was obtained. In this case, the size of the grid was fixed and the
635 order of the approximation was increased uniformly across the grid. For problems
636 with smooth solutions, the p -version of the LSFEM converged to the exact solution
637 at an exponential rate as the number of unknowns was increased by the uniform
638 enrichment of the element approximation functions.

639
640
641
642
643
644
645
646
647
648
649
650
651
652
653
654
655
656
657
658

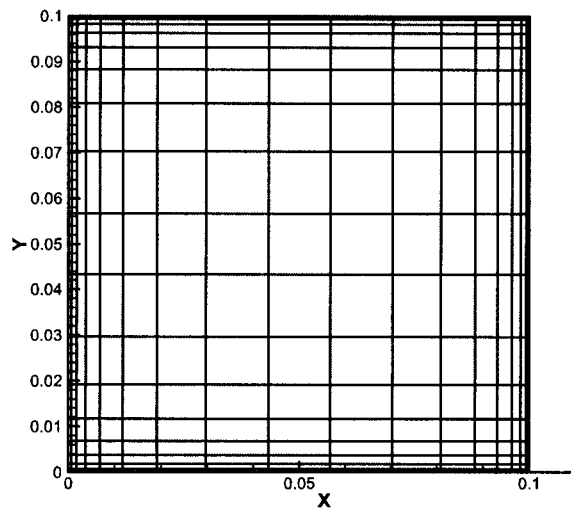


Figure 13. Computational grid for FEM analysis.

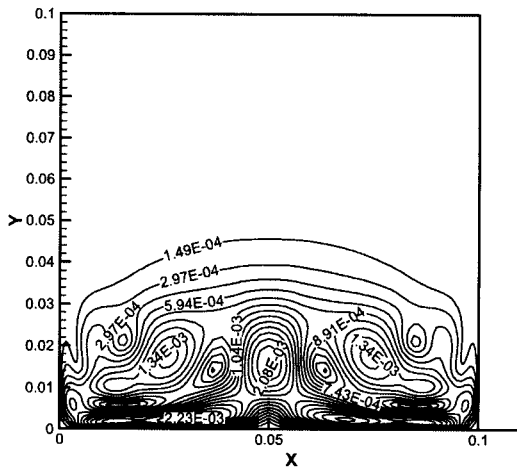
Optimization of Intensities and Orientations

659 In cases where the mushy region was only one grid cell wide, the effective heat
660 capacity including the latent heat release was computed using an enthalpy
661 method.^[15,19]

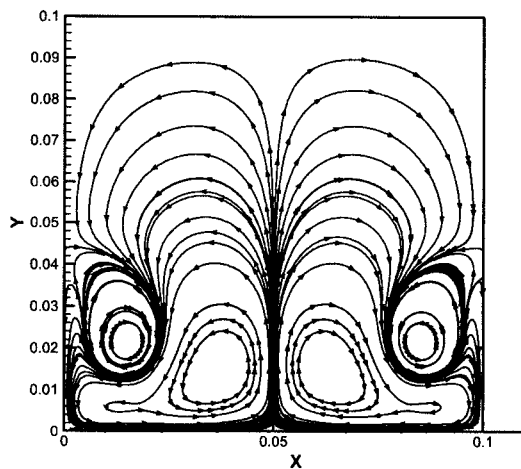
$$\rho C^{eq} = \frac{dH}{dT} \approx \frac{|\nabla H|}{|\nabla T|} \tag{24}$$

666 Using this treatment in the mush region allowed much larger values of the viscosity
667 to be specified in the solid phase. Specifically, LSFEM/MHD solidification with
668 the enthalpy method used seven orders of magnitude higher viscosity in the solid
669 phase than in the liquid phase. Figures 14 and 15 show velocity field and streamlines

F14 F15



687 *Figure 14.* Velocity magnitudes with no applied magnetic field—FEM analysis.



704 *Figure 15.* Streamlines with no applied magnetic field—FEM analysis.

706 computed without the application of a magnetic field. Correct physical value of
 707 the magnetic Prandtl number was used in all simulations based on LSFEM/MHD.

708 The IOSO algorithm was used to optimize the applied magnetic field to this
 709 problem.^[12,11] The optimization code was executed on a commodity component-
 710 based parallel computer with Pentium II processors (400 MHz speed). Twenty
 711 processors were used, and the total execution time was about 16 h. The initial guess
 712 given to the optimizer was that all design variables were set to zero. In other words,
 713 the initial guess was a flow-field without any applied magnetic field. In that case the
 714 normalized value of the objective function is 1.0.

AQ5

717 **LSFEM: Case 1**

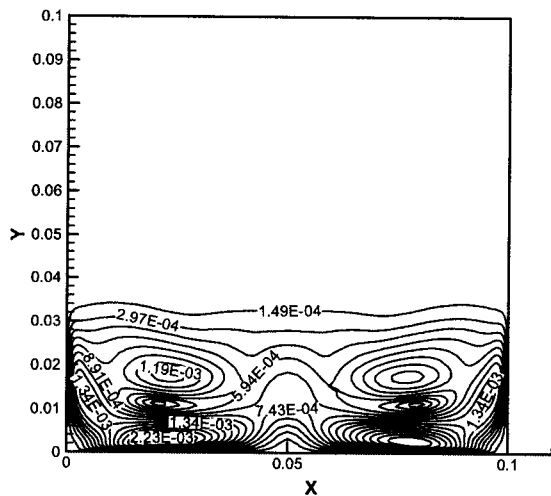
719 In this case, the sidewall magnetic field strengths were very weak. They varied
 720 between 0.07 T and 0.07 T. A maximum strength for uniform vertical field varied
 721 between 0.0 T and 0.15 T. After 12 iterations, the IOSO-based optimizer achieved its
 722 best objective function value of 0.292. In comparison, the objective function for a
 723 simple case of no sidewall magnets and a maximum strength uniform vertical field of
 724 0.15 T achieved a value of 0.771. The optimized magnetic field reduced the average
 725 velocity in the melt region between $y=0.04$ m and $y=0.08$ m by more than a factor
 726 of three. Figures 16 and 17 demonstrate that the magnetic field effectively damped
 727 the flow field circulation, removing the pair of secondary vortices present in the case
 728 with no applied magnetic field. Figure 18 shows the optimized magnetic field lines
 729 of flux density.

F16 F17

F18

730 In the lower half of the sidewall, the magnets were at maximum strength of
 731 0.07 T. Above that, the polarity changed and the strength of the sidewall magnet was
 732 reduced to 0.04 T at the top of the container (Fig. 19). For the top and bottom walls,
 733

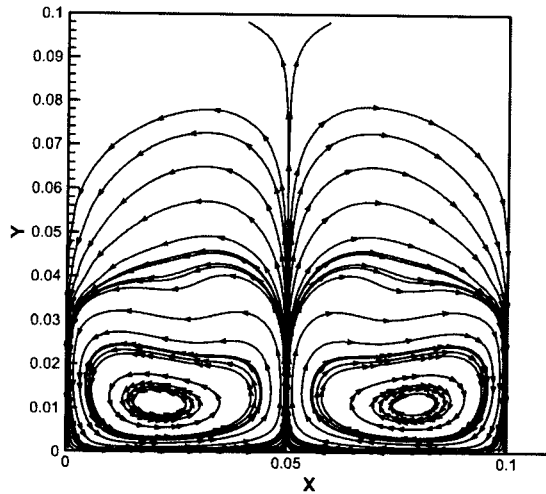
F19



734
735
736
737
738
739
740
741
742
743
744
745
746
747
748
749
750
751
752 **Figure 16.** Velocity magnitudes with optimized applied magnetic field (case 1).

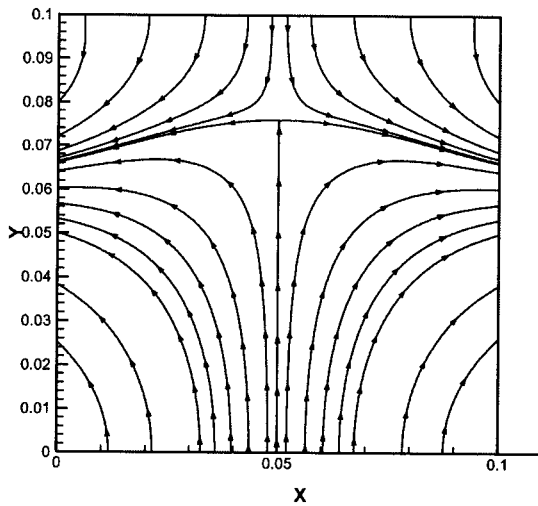
Optimization of Intensities and Orientations

753
754
755
756
757
758
759
760
761
762
763
764
765
766
767
768



769
770 **Figure 17.** Streamlines with optimized applied magnetic field (case 1).

771
772
773
774
775
776
777
778
779
780
781
782
783
784
785
786
787



788
789 **Figure 18.** Lines of magnetic flux for the optimized applied magnetic field (case 1).

793 the optimizer chose a magnetic potential that would produce a uniform vertical field
794 of 0.025 T. This is interesting since the optimizer had the choice of producing up to
795 0.15 T but yet converged to a much smaller value. This indicates that by damping the
796 melt circulation, the shape of the magnetic field was as important as its strong
797 vertical component. Figure 20 compares the temperature distribution between flow
798 with no magnetic field and flow with optimized magnetic field. The optimized field
799 clearly smoothes the temperature contours due to the reduced convection.

F20

