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CFD ANALYSIS OF SMART SEMICONDUCTOR ELECTRO-CONDUCTIVE MARANGONI MELT CAVITY FLOW

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1.INTRODUCTION

- When *free surfaces* are present in natural convection flows it has been shown that motion is induced in the fluid via surface tension at the free surface. This so-called *Marangoni* convection or *thermocapillary convection* plays a crucial role in various aspects of crystal growth technology, semiconductor melts, laser melting thermofluid dynamics etc and as such has stimulated widespread attention [1,2]. A number of Marangoni convection cavity flow problems in the presence of magnetic fields have also appeared. Magnetic fields have been shown to effectively regulate the heat transfer rates and stabilize flows in semiconductor crystal growth. Oscillatory instability can have a damaging influence on crystal development and magnetic fields have been shown to enhance compositional uniformity and minimize defect density. A further damping mechanism for Marangoni magnetic convection is offered by deploying porous media. In this work, we present a mathematical and numerical study of the transient thermo-convection flow of an electrically conducting fluid in an isotropic non-Darcy porous rectangular semiconductor melt enclosure with buoyancy and internal heat generation effects, in an (x, y) coordinate system. The governing equations comprising the mass conservation, x-direction momentum, y-direction momentum and energy equation are formulated subject to a quartet of boundary conditions at the four walls of the enclosure. The magnetic field is applied at an angle of ϕ with the horizontal (x-direction) axis. The upper enclosure wall is assumed to be free with an appropriate dynamic boundary condition. A series of transformations are implemented to render the mathematical model, dimensionless and into a vorticity form. The governing thermophysical parameters are shown to be the Marangoni number for surface tension (thermocapillary) effects (Ma), Prandtl number (Pr), Grashof number for buoyancy effects (Gr), aspect ratio (A), Hartmann hydromagnetic number (Ha), Darcy number for bulk porous resistance (Da), Forchheimer number (Fs) and the internal heat generation parameter (Γ) the latter being a function of the internal (Ra_I) and global Rayleigh numbers (Ra). A marker-and cell (MAC) method is employed to solve the boundary value problem numerically. Isotherms and isovels (streamlines) are computed. Solutions for the case of *Pr = 0.054* (semiconductor melt) are compared with earlier studies showing excellent correlation. The model finds applications in the bulk crystal growth of semiconductors, electromagnetic control of materials processing

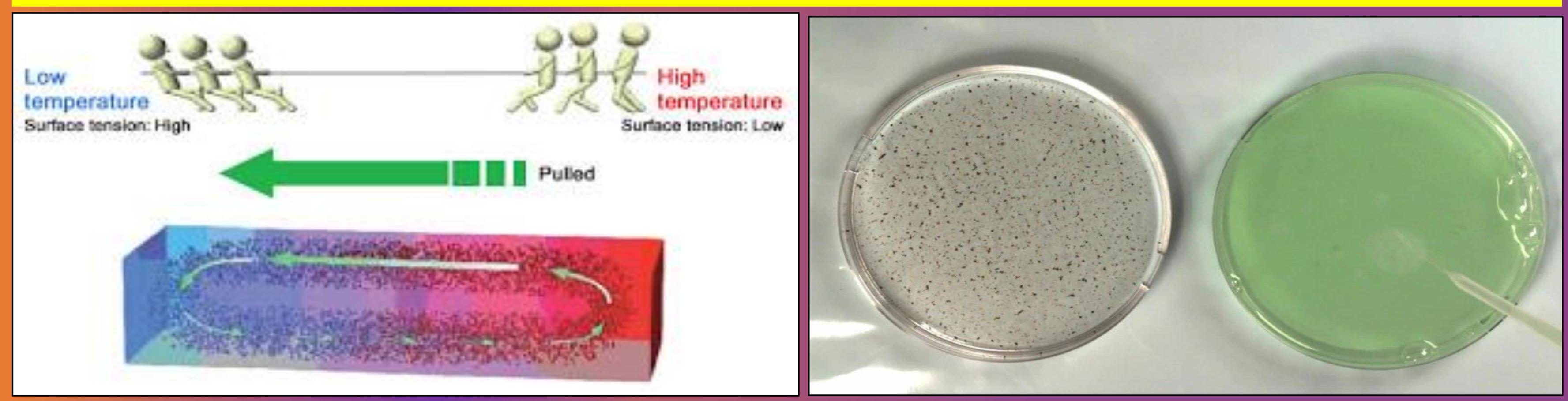


Fig 1: Marangoni convection phenomena

2. MATHEMATICAL MODEL AND DATA

Marangoni convection cavity flow problems in the presence of magnetic fields have been studied extensively due to semiconductor and fuel cell applications. Magnetic fields have been shown to effectively regulate the heat transfer rates and stabilize flows in semiconductor crystal growth. Oscillatory instability can have a damaging influence on crystal development and magnetic fields have been shown to enhance compositional uniformity and minimize defect density. Magnetic field dampens hydrodynamic oscillations and can increase the purity of crystals. Heat generation effects in the circulating fluid are also important in the context of laser melts and also chemical energy systems. However porous media can also be utilized for semiconductor growth systems. In the present study we therefore consider the combined effects of buoyancy, Forchheimer inertia, Darcian bulk retardation, internal heat generation and magnetic field on Maragonic convection flow in a rectangular porous medium enclosure. Additionally, we present MAC finite difference solutions for the flow regime isotherms and stream-function patterns. Such a study constitutes an important extension to the literature on semiconductor melt convection in porous enclosures and has not been communicated thus far in the technical literature. It is also important in chemical engineering control technologies and hybrid green fuel cell applications.

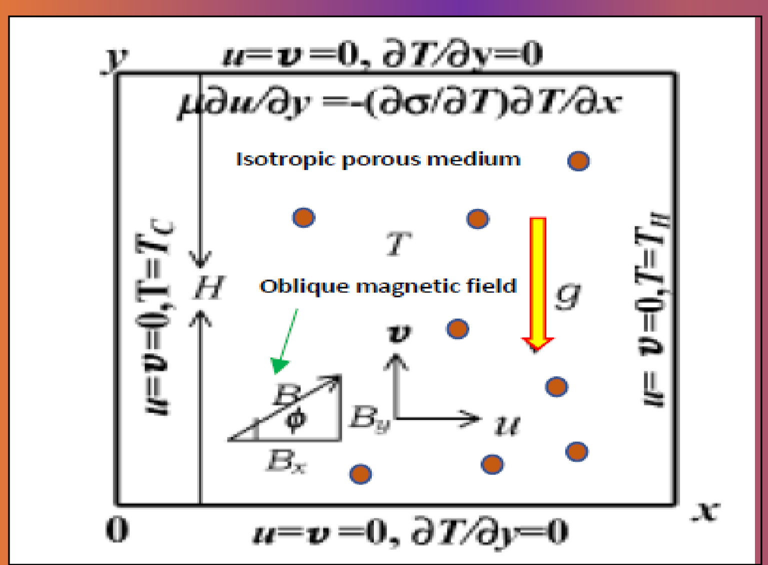


Fig 2: Model for Marangoni semiconductor melt enclosure

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

$$\rho\left[\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right]=-p_x+\mu\nabla^2 u-\frac{\mu}{K}u+\sigma B_0^2\left(v\sin\varphi\cos\phi-u\sin^2\varphi\right)$$

$$\rho\left[\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right]=-p_y+\mu\nabla^2 v-\frac{\mu}{K}v+\sigma B_0^2\left(u\sin\varphi\cos\phi-v\cos^2\varphi\right)+\rho g\beta\left(T-T_c\right)$$

$$\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}=\alpha\nabla^2 T+\frac{q'''}{\rho C_p}$$

The field equations are given above. All material data, membrane and boundary conditions are :

$$At\ \ t=0: u=v=T=0$$

$$u=v=0, T=T_H\ \ for\ 0\le y\le H\ \ at\ \ x=L\ (right\ \ wall)$$

$$u=v=0, T=T_C\ \ for\ 0\le y\le H\ \ at\ \ x=0\ (left\ wall)$$

$$u=v=0, \frac{\partial T}{\partial y}=0\ \ for\ 0\le x\le H\ \ at\ y=0\ (base\ wall)$$

At the free surface (upper boundary), dynamic boundary conditions are required. A balance is needed between the surface tension gradient and shear stress at the free surface essential for generating thermo-capillary (Marangoni) convection in the enclosure. These are defined as follows:

$$u=v=0, \frac{\partial T}{\partial y}=0, -\frac{\partial\sigma}{\partial T}\frac{\partial T}{\partial x}=\mu\frac{\partial u}{\partial y}\ \ for\ 0\le x\le H\ \ at\ y=H\ (upper\ free\ surface)$$

3. VORTICITY FORMULATION

Transforming the boundary value problem with appropriate dimensionless numbers and the vorticity formulation, we have the new model:

$$\nabla^2\psi=-\Omega$$

$$\frac{\partial\Omega}{\partial\tau}+\frac{\partial(U\Omega)}{\partial X}+\frac{\partial(V\Omega)}{\partial Y}=\nabla^2\Omega+\frac{Gr}{2}\frac{\partial\theta}{\partial X}+Ha^2[\sin\phi\cos\phi(\frac{\partial U}{\partial X}-\frac{\partial V}{\partial Y})$$
$$+(\sin^2\phi\frac{\partial U}{\partial Y}-\cos^2\phi\frac{\partial V}{\partial X})]-\frac{1}{Da}\left(\frac{\partial V}{\partial X}-\frac{\partial U}{\partial Y}\right)$$

$$\frac{\partial\theta}{\partial\tau}+\frac{\partial(U\theta)}{\partial X}+\frac{\partial(V\theta)}{\partial Y}=\frac{1}{\Pr}\nabla^2\theta+\frac{\Gamma}{\Pr}$$

$$At\ \ \tau=0: U=V=\psi=\theta=0$$

$$U=V=\psi=0, \theta=-1\ for\ 0\le Y\le 1\ \ at\ X=0$$

$$U=V=\psi=0, \theta=1\ for\ 0\le Y\le 1\ \ at\ X=A$$

$$U=V=\psi=0, \frac{\partial\theta}{\partial Y}=0, \Omega=\frac{\partial U}{\partial Y}=-\frac{Ma}{2\Pr}\frac{\partial\theta}{\partial X}\ for\ 0\le X\le 1\ \ at\ Y=1$$

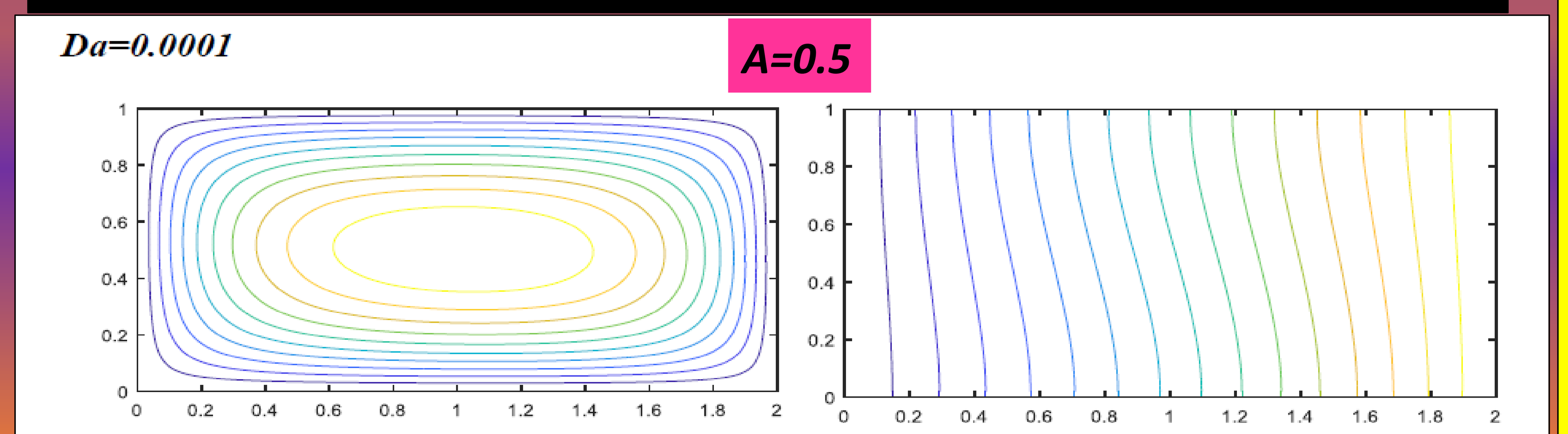
$$X=\frac{x}{H}\qquad Y=\frac{y}{H}\qquad U=\frac{\partial\psi}{\partial Y}=\frac{uH}{\nu}\qquad V=-\frac{\partial\psi}{\partial X}=\frac{vH}{\nu}\qquad \Omega=-\nabla^2\psi$$

$$\tau=\frac{t\nu}{H^2}\qquad \theta=\frac{T-T_0}{T_H-T_0}\qquad A=\frac{L}{H}\qquad Da=\frac{K}{H^2}\qquad Fs=\frac{b}{H}$$

$$Gr=\frac{g\beta(T_H-T_C)H^3}{\nu^2}\qquad \Pr=\frac{\nu}{\alpha}\qquad \Gamma=2\frac{Ra_I}{Ra}\qquad Ra_I=\frac{g\beta q'''H^5}{k\alpha\nu}\qquad Ma=-\frac{\partial\sigma^*}{\partial T}\frac{(T_H-T_C)}{\mu\alpha}\qquad Ha=\frac{B_0H\sqrt{\sigma}}{\sqrt{\mu}}$$

Here the key parameters are: Surface tension (thermocapillary) effect number i.e. Marangoni number (Ma), Prandtl number (Pr), Grashof number for buoyancy effects (Gr), aspect ratio (A), Hartmann hydromagnetic number (Ha), Darcy number for bulk porous resistance (Da), Forcheimmer (second order porous drag) number (Fs), Internal heat generation parameter (Γ) which is a function of the internal (Ra_I) and global Rayleigh numbers (Ra) , orientation of the magnetic field i.e. φ (this is the orientation of the magnetic field with the horizontal axis (such that tan φ = *By/Bx*). The system is solved using a MAC algorithm which is described in Refs. [4-7]. Mesh independence tests are conducted. Validation with earlier non-porous studies is included [8]. Here we present some representative solutions for Darcy number effect (Da) i.e. permeability of the enclosure porous medium. In all these simulations we have constrained Marangoni number (Ma) to be 100. Ma balances thermal transport via flow (convection) due to a gradient in surface tension, with thermal diffusion. When Ma is small thermal diffusion dominates and the there is no flow, but for large Ma, flow (convection) occurs, driven by the gradients in the surface tension. This is called Bénard-Marangoni convection. Isotherms are plotted on the left and streamlines on the right of all subsequent visualizations.

4. SELECTED MAC SIMULATIONS



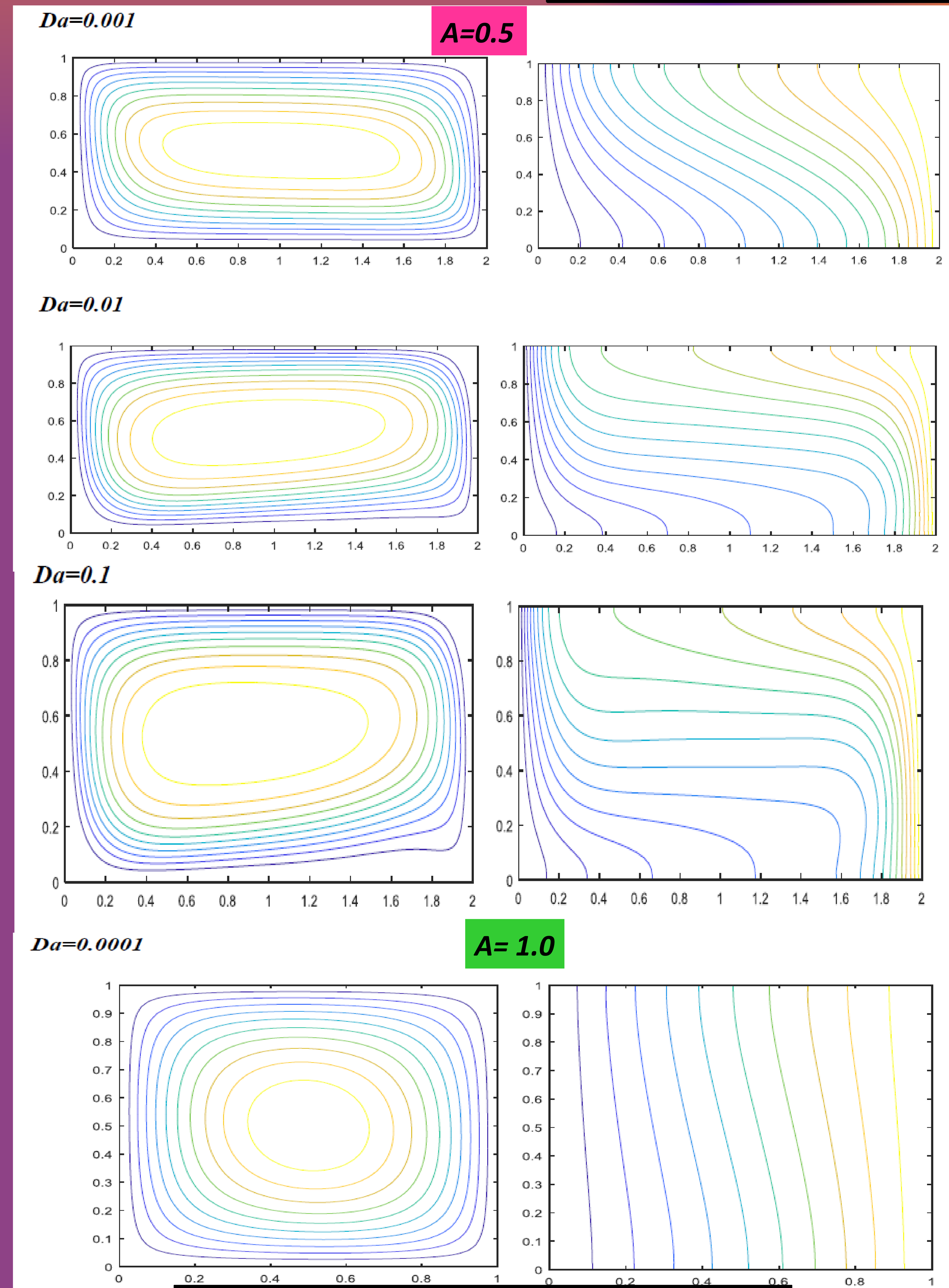


Fig 3: MAC Computations with different Darcy number and/or aspect ratio

REFERENCES

- [1] W. Vielstich, Arnold Lamm, Hubert A. Gasteiger, *Handbook of Fuel Cells: Fundamentals, Technology and*
- *Applications,* Wiley, New York (2003).
- [2] Langlois WE. Buoyancy-driven flows in crystal-growth melts. Annu Rev Fluid Mech. 1985;17:191-215
- [3] A.Y. Gelfgat, P.Z. Bar-Yoseph, Effect of an external magnetic field on oscillatory instability of convective flows in rectangular cavity, Phys. Fluid 13 (2001) 2269–2278.
- [4] K. Venkatadri, O. Anwar Bég, V. R. Prasad, Numerical simulation of thermal radiation influence on natural convection in a trapezoidal enclosure: heat flow visualization through energy flux vectors, *Int. J. Mechanical Sciences (2019*
- [5] K. Venkatadri, S. Abdul Gaffar, V. R. Prasad, B. Md. Hidayathualla Khan and O. Anwar Bég, Simulation of natural convection heat transfer in a 2-D trapezoidal enclosure, *International Journal of Automotive and Mechanical Engineering, 16 (4) 7375-7390 (2019).*
- [6] K. Venkatadri, S. Abdul Gaffar, M. Suryanarayana Reddy, V. Ramachandra Prasad, B. Md. Hidayathulla Khan and O. Anwar Bég, Melting heat transfer analysis on magnetohydrodynamics buoyancy convection in an enclosure: a numerical study, *J. Applied and Computational Mechanics 6(1) 52-62 (2020).*
- [7] T Sarala Devi, C Venkata Lakshmi, K Venkatadri, V. R. Prasad, O. Anwar Bég and M.S. Reddy, Simulation of unsteady natural convection flow of a Casson viscoplastic fluid in a square enclosure utilizing a MAC algorithm, *Heat Transfer-Asian Research (2020). DOI: 10.1002/htj.21690 (19 pages)*
- [B] M. Anwar Hossain, M.Z. Hafiz, D.A.S. Rees, Buoyancy and thermocapillary driven convection flow of an electrically conducting fluid in an enclosure with heat generation, International Journal of Thermal Sciences 44 (2005) 676–684.