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The effect of wall temperature fluctuations on the heat transfer and fluid flow occurring in a liquid enclosure

E. Semma ^a, V. Timchenko ^b, M. El Ganaoui ^{a,*}, E. Leonardi ^b

^a SPCTS, UMR 6638 CNRS-Université de Limoges, Faculté des Sciences et Techniques 123, Albert Thomas 87060, Limoges, France b School of Mechanical and Manufacturing Engineering, The University of New South Wales, Sydney NSW 2052, Australia

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Abstract

A numerical study of the effect of thermal fluctuations, similar to those encountered during directional solidification in Vertical Bridgman configuration (VB), on the heat transfer and fluid flow in a liquid enclosure has been undertaken. The VB when heated from the top is characterized by a stable flow regime maintained for a larger range of Rayleigh numbers than can be obtained with an Inverted Vertical Bridgman configuration (IVB) heated from below. In order to qualify the effect of thermal fluctuations on the heat and flow transfers, investigations are conducted for the range of Rayleigh numbers maintaining a stable flow ($Ra \in [10^4, 10^6]$). The results show that the thermal oscillations at low frequency can destabilize the flow regime. A characteristic frequency at which the average heat transfer rate reaches a minimum value is identified. This minimum value is dependent on the amplitude of thermal fluctuation. The critical frequency increases linearly with the intensity of the convection (Rayleigh number).

Keywords: Thermal fluctuation; Computational heat transfer; Vertical Bridgman configuration

1. Introduction

The Bridgman configuration is often used for growing semiconductor crystals by directional solidification. It offers simultaneously an industrially efficient process and an ideal academic configuration for fundamental studies (Garandet and Alboussière, 1999). For the Vertical Bridgman configuration (VB), the classical Rayleigh–Bénard problem gives a first approach to understand the complexity of flow development during the transition from conductive to convective regimes and its effect on the coupling with solid/liquid transition. Stable flows are of interest in practical applications because of their impact on the redistribution of species. For example, in the crystal growth for electronic applications, convection in the liquid phase strongly affects

dopant segregation and influences the interface shape. In this type of configuration, fluctuations of the interface velocity can lead to microsegregation. This phenomenon can introduce undesirable effects on the physical properties of grown crystals as was underlined by Hurle et al. (1974) and Muller (1996).

During directional solidification, the oscillation of the phase change front can result from several factors such as fluctuations of the pulling velocity, the non-stationary flows developing for strong thermal or solutal gradients or the fluctuations recorded in the imposed temperature gradient. The effect of the temperature fluctuations on the interface velocity in the vertical Bridgman configuration was studied numerically by Stelian et al. (2002) for a fluid with Pr = 0.07 in a 2D configuration by using a commercial CFD package. The effect of the period of oscillation on the interface velocity has been investigated for a duration ranging between 5 and 3000 s. As a cut-off period for the velocity amplitude was observed it was

^{*} Corresponding author. Fax: +33 5 55 45 72 11.

E-mail address: ganaoui@unilim.fr (M. El Ganaoui).

Nomenclature AR aspect ratio, =W/Hmodulation amplitude Hampoule height dynamic viscosity μ time kinematic viscosity Ttemperature density ρ \boldsymbol{U} velocity vector stream function velocity component in x direction и velocity component in y direction Subscripts vintegration volume h hot P pressure cold kthermal conductivity internal PrPrandtl number, $=v/\alpha$ max maximum Ra Rayleigh number, $= \rho g \beta \Delta T H^3 / \alpha \mu$ min minimum f dimensionless frequency reference dimensionless coordinates x, ygravity acceleration Superscript temperature difference Nusselt number, = $\int_0^1 \frac{\partial T}{\partial y}(x, 0) dx$ ΔT dimensional variable ' NuWampoule width Greeks thermal diffusivity α $\beta_{\rm T}$ thermal expansion coefficient

concluded that temperature oscillations with periods lower than the cut-off period have no harmful effect on the growth process.

In order to investigate flow instabilities occurring in the liquid during directional solidification process under full or low gravity conditions, fluid phase models in 2D configuration have been largely used by number of authors including Larroudé et al. (1994), El Ganaoui and Bontoux (1998), Semma et al. (2003) and Kaenton et al. (2004). Flow and thresholds of unsteadiness are further enhanced when thermal boundary conditions vary with time. Such situations are encountered for example in periodically energized electronic components, which induce unsteady heat generation.

During the past decade, the effects of time-periodic thermal boundary conditions on the evolution of the flow and thermal transfer have been considered for various geometrical configurations. Kazmierczak and Chinoda (1992), studied numerically natural convection of water, Pr = 7.0, $Ra = 1.5 \times 10^5$, in a cavity heated from the side with a time-periodic temperature. It was concluded that although the instantaneous heat flux through the hot wall fluctuates greatly in time, the time-averaged heat transfer across the enclosure is rather insensitive to the time-dependent boundary condition. Lage and Bejan (1993) investigated numerically and analytically natural convection in a configuration heated by a pulsating heat flux. They showed that the amplitude of oscillation of the heat flux through a vertical surface

reaches maximum values for a given value of the angular frequency. Antohe and Lage (1996) investigated the effects of heating amplitude and frequency on the transport phenomena considering clear fluid and fully saturated porous medium enclosures under time periodic square wave heating in the horizontal direction for a fluid (Pr = 0.7). It was observed that the response of the system to changes in the heating amplitude is essentially linear and that the flow resonance appears as the heating frequency matches the natural frequency of the flow inside the enclosure. The resonance frequency was shown to be independent of the heating amplitude for both clear fluid and porous medium configurations.

Kwak et al. (1998) studied numerically the effects of the amplitude and frequency of the hot side sinusoidal wall oscillation on the enhancement of heat transfer in a square cavity with fixed $Ra = 10^7$ and Pr = 0.7 for the configuration similar to the one used by Antohe and Lage (1996). Once more it was observed that the maximum increase of the time-averaged heat transfer rate occurs at the resonance frequency between natural frequency of the flow and the modulation frequency and therefore by implying external proper frequency it is possible to achieve a resonant enhancement of heat transfer in the cavity. The resonance phenomenon in natural convection was described by Abourida et al. (1998), Barletta and Zanchini (2003) and recently by Barlletta and Rossi di Schio (2004) for an external thermal oscillation. Iwatsu et al. (1992) and Kim et al. (2002) considered

the resonance in natural convection for the case of an external mechanical oscillation. Such behaviour can be used for possible control of industrial processes such as encountered during crystal growth from the melt.

From the studies listed above, only Stelian et al. (2002) applied thermal modulation to a realistic situation occurring in the VB configuration with focusing on the oscillation of the growth velocity. Although this study provides information on the effects of the thermal oscillations on the interface it does not give any insight into the heat transfer which is occurring.

In this paper we study liquid enclosure analogous to the fluid phase of a Vertical Bridgman configuration heated from the top similar to the one considered by Stelian et al. (2002). Previous investigation of the authors for the full VB configuration showed a strong effect of time dependent convection on the solid/liquid interface (Kaenton et al., 2004). In this work we have restricted our study to the liquid domain only in order to evaluate separately the effects of thermal fluctuations on the instability of the flows for solidification phenomena. Oscillatory convection is studied numerically for different aspect ratios of the cavity, sizes of adiabatic zone and Ra numbers. The present study considers the effects of the amplitude and the frequency of an imposed sinusoidal oscillation on the hot wall. Results are compared to available accurate solutions without temperature fluctuations. We show that external thermal modulation can permit a control strategy of the flow oscillations to be developed in order to minimize effects of instability on the solid/liquid interface.

2. Model and numerical approximations

2.1. Problem definition

A Vertical Bridgman (VB) growth configuration is shown schematically in Fig. 1a. It consists of a vertical ampoule heated from a top at temperature T'_h and cooled from below at T'_{c} . The lateral walls in the hot zone (at T'_{h}), and the cold zone (at T'_{c}) are separated by an adiabatic zone of length $H_{\Lambda T}$. In this paper we consider only the liquid part of the VB with a flat interface maintained at $T = T'_{c}$ (Fig. 1b). A prime denotes a dimensional variable. The problem can be non-dimensionalized using H, the height of the cavity, as the scale factor for length; H^2/α and $\rho \alpha^2/H^2$ as the scaling factors for time and pressure respectively. The non-dimensional temperature is $T = (T' - T'_c)/(T'_h - T'_c)$. The problem is solved in the domain $D = [0, AR] \times [0, 1]$, where AR = W/H is the aspect ratio of the physical domain. The cavity is filled with a fluid with a low Prandtl number (Pr = 0.01) and heated periodically. The bottom wall is set to be isothermal and maintained at the cold temperature $T_{\rm c}'$. The sinusoidal hot temperature is characterized by its modulation amplitude ε and frequency f as $T_h = 1 + \varepsilon \sin(2\pi f t)$. The modulation amplitude and frequency in non-dimensional form are given by

$$\varepsilon = \frac{\varepsilon'}{\Lambda T}, \quad f = H^2 \frac{f'}{\alpha}$$
 (1)

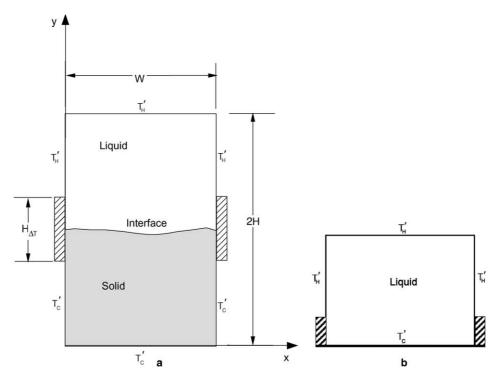


Fig. 1. Geometric configuration (a) full cavity, (b) the restricted fluid domain.

2.2. Mathematical model

The flow is Newtonian, incompressible and laminar. The fluid considered is assumed to satisfy the Boussinesq approximation, that is all properties are constant except for the density in the buoyancy term of the equation of motion; where it is assumed to be a linear function of temperature, i.e., $\rho = \rho_0(1 - \beta_T(T' - T'_0))$ and T'_0 is the reference temperature.

The governing equations are the continuity, Navier–Stokes and energy conservation Partial Differential Equations, written in Cartesian coordinates in non-dimensional form as following:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{2}$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + Pr \nabla^2 u \tag{3}$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{\partial p}{\partial y} + Pr \nabla^2 v + Ra Pr T \frac{g}{\|g\|}$$
(4)

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \nabla^2 T \tag{5}$$

The associated Boundary Conditions (BCs) are:

$$T = 0, \quad u = v = 0$$
 at $y = 0$
 $T_h = 1 + \varepsilon \sin(2\pi f t), \quad u = v = 0$
at $x = 0, \ y > H_{\Delta T}/2; \ x = 1, \ y > H_{\Delta T}/2;$
 $0 < x < AR, \ y = 1$

$$\frac{\partial T}{\partial x} = 0$$
, $u = v = 0$ at $x = 0$ and $0.0 < y < H_{\Delta T}/2$

and
$$x = 1$$
 and $0.0 < y < H_{\Delta T}/2$

(6)

In order to study the effect of the wall temperature oscillation on the heat transfer characteristics, the following quantities are introduced in the manner described by Kwak et al. (1998):

$$G(Nu) = \frac{Nu(\varepsilon) - Nu(0)}{Nu(0)} \tag{7}$$

$$A(Nu) = \frac{Nu_{\max}(\varepsilon) - Nu_{\min}(\varepsilon)}{Nu(0)}$$
(8)

where Nusselt number, $Nu = \int_0^1 \frac{\partial T}{\partial y}(x,0) dx$, is defined along the solid/liquid interface (here the cold wall), Nu(0) refers to the case without fluctuations and $Nu(\varepsilon)$ is a Nusselt number averaged over the period of oscillation. G(Nu) represents the relative difference for a Nusselt number with and without temperature fluctuation while A(Nu) corresponds to the non-dimensional amplitude of heat transfer oscillation.

2.3. Numerical approximations

For numerical approximations of the problem a finite volume method has been used. The approach is summa-

rized in the following section which outlines the numerical schemes chosen followed by validations.

2.3.1. Numerical method

We consider a two-dimensional convection diffusion equation for a general variable φ coupled with the continuity equation

$$\frac{\partial \varphi}{\partial t} + \nabla(F(\varphi)) = f \tag{9}$$

$$\nabla \cdot u = 0 \tag{10}$$

Here, $F(\varphi) = u\varphi - \gamma_{\varphi}\nabla\varphi$ is the advection–diffusion tensor with the convective part $F^{c} = u\varphi$ and the diffusive part $F^{d} = -\gamma_{\varphi}\nabla\varphi$.

As Eq. (9) gives the expression for the conservation of φ in an infinitesimal domain, it is equivalent to write in any subdomain V and for all time t and t'

$$\int_{V} \varphi(x,t') d\mathbf{x} - \int_{V} \varphi(x,t) d\mathbf{x} + \int_{t}^{t'} \int_{\partial V} F \cdot \tau_{V}(\mathbf{x}) d\sigma(\mathbf{x}) d\mathbf{x} dt$$

$$= \int_{V} \int_{t}^{t'} f(\mathbf{x}, t) d\mathbf{x} dt \tag{11}$$

where $\tau_V(x)$ is the normal vector to the boundary ∂V at point x, outward to V.

In order to define a finite volume scheme, the time derivative is approximated by a finite difference scheme with an increasing sequence of time $(t_n)_{n\in IN}$ with $t_0=0$. The discrete unknowns of φ at time $t_n=n\delta t$, are approximated in the cell V around the point $M_{i,j}$ and denoted by φ_{ij}^n . Eq. (11) is integrated over each cell V using the Gauss divergence theorem

$$\int_{V} \left(\frac{\partial \varphi}{\partial t} \right)^{n} d\mathbf{x} + \int_{\partial V} F^{n} . \tau_{V} d\sigma(\mathbf{x}) d\mathbf{x} = \int_{V} f(\mathbf{x}, t_{n}) d\mathbf{x}$$
 (12)

where $(\partial \varphi/\partial t)^n$ is given by the time scheme at the time step $t_n = n\delta t$ in the control volume V. The next step of the method is the approximation of the convective part $F^c \cdot \tau_V$ and the diffusive part $F^d \cdot \tau_V$ of the projected flux $F \cdot \tau_V$ over the boundary ∂V of each control volume.

2.3.2. Discretization schemes

To discretize the convective fluxes various schemes can be adopted. For example, the central differences scheme uses a symmetric interpolation for $\varphi_{i+1/2}$, the upwind scheme utilizes an one side interpolation. Leonard and Mokhtari (1990) introduced the Quick and other schemes as a combination between the two kinds of interpolation to produce more accurate results for complex problems. In the present work, the conductive terms are discretized using the central differences scheme while the convective terms are approximated by using the Quick scheme subjected to a flux limiter Ultimate Leonard (1991). To resolve the velocity-pressure coupling the Simplec algorithm (Van Doormal and

Raithby, 1984) is used. The temporal discretization was done using a second order Euler scheme.

2.3.3. Validation

Extensive validation of the present code to describe complex behaviour occurring in the melt with and without phase change have been presented in Semma et al. (2003). A particular verification of the Ultimate scheme is performed here by comparison with well-established benchmark problem of Roux (1990). We consider a rectangular cavity (Fig. 2a) of an aspect ratio AR = 4, filled with a low Prandtl number liquid (Pr = 0.015) and submitted to a temperature difference between the vertical walls while horizontal walls are kept adiabatic.

Results of computations are summarized in the bifurcation diagram describing transition from stationary mode to time-dependent flow regime (Fig. 2b). It can be seen that for low Grashof numbers, the flow is composed of the single convective cell. By increasing Ra (Gr = RalPr is used here for comparison with published data), the cell changes towards three counter rotating cells. When Gr exceeds a threshold value $Gr_c = 35,500$, the flow becomes non-stationary and very sensitive to the value of Gr. The transition obtained around Gr = 35,500 is in agreement with the values of 38,095 given by Winters (1989) and 33,500 published by Pulli-

cani et al. (1990) and therefore the bifurcation diagram obtained using the ULTIMATE scheme shows good agreement for mono to multi cellular transition.

For the following results, simulations have been conducted using a mesh of 64×64 . Grid convergence tests have been carried out by increasing number of mesh points from 32×32 to 128×128 ; the computed results obtained for these meshes differed by less than 0.2%. The convergence is declared for a relative maximal residual value between two successive iterations being lower than 10^{-6} .

3. Results and discussion

The vertical Bridgman cavity heated from the top is characterized by a stable flow regime for large values of the Rayleigh number (Larroudé et al., 1994). Thus, in order to qualify the effect of the thermal modulation on the heat transfer, most of the calculations in this study are performed for $Ra = 4 \times 10^5$ corresponding to a stable flow regime. Some trends are obtained for other Rayleigh numbers so as to confirm the existence of critical thresholds.

The forcing frequency and temperature were varied between 0 < f < 200 and $0 < \varepsilon < 1$. In the real case, if

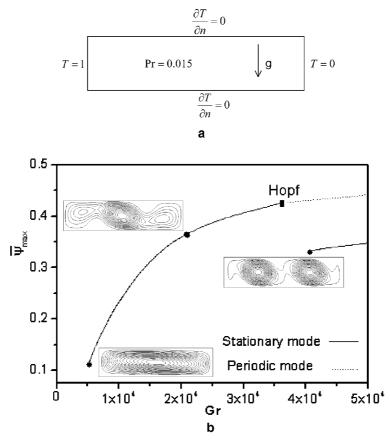


Fig. 2. Test case: (a) Geometry configuration, (b) bifurcation diagram for rigid adiabatic upper and lower boundaries, 5000 < Gr < 50000.

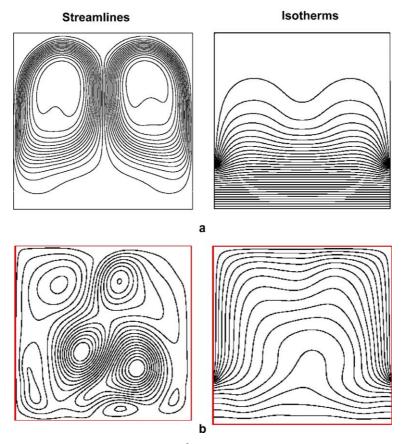


Fig. 3. Symmetry breaking of the flow structure ($Ra = 4 \times 10^5$), (a) without modulation ($\varepsilon = 0$), (b) with modulation ($\varepsilon = 1$, f = 10).

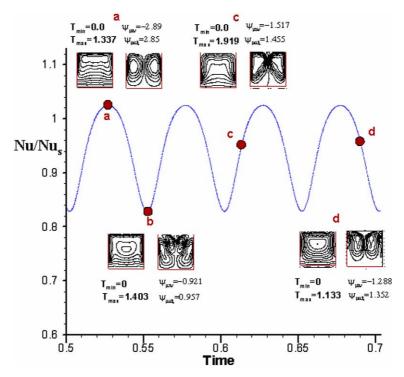


Fig. 4. Time history of Nusselt number on the cold wall together with instantaneous flow patterns and thermal fields $(Nu_s = Nu(\varepsilon = 0))$.

we consider a cavity height H = 12 mm filled with the Gallium (Ga), the maximum dimensionless frequency

is f = 200 corresponds to a real frequency f' = 65 Hz which is close to the frequency of the electric supply

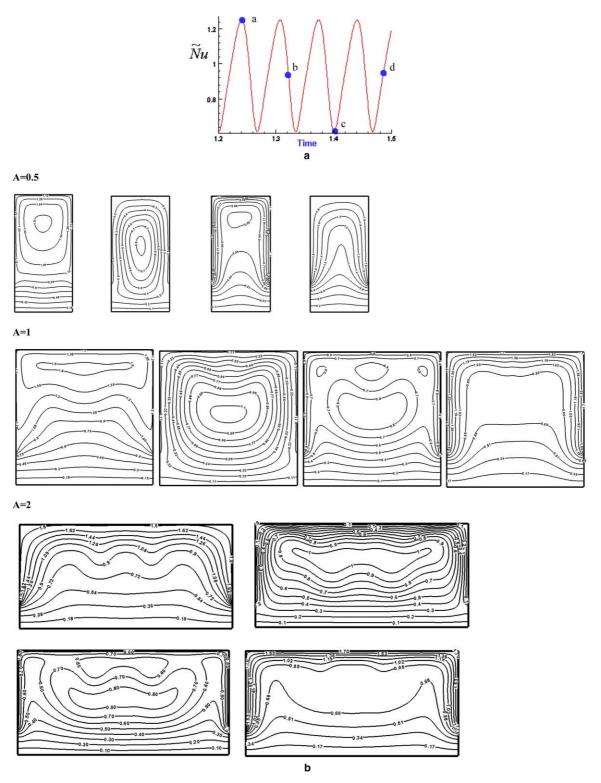


Fig. 5. (a) Time history of Nusselt number, (b) thermal fields and (c) and flow fields for three aspect ratios, AR = 1, AR = 1/2 and AR = 2, at time instants t_a , t_b , t_c and t_d .

signals. As in the study of Larroudé et al. (1994), we wanted to investigate both the fundamental effect of the fluctuations on natural convection and a possibility

of controlling the heat transfer in the cavity using thermal modulation. We have thus used a large range for amplitude of oscillation. This does not necessarily

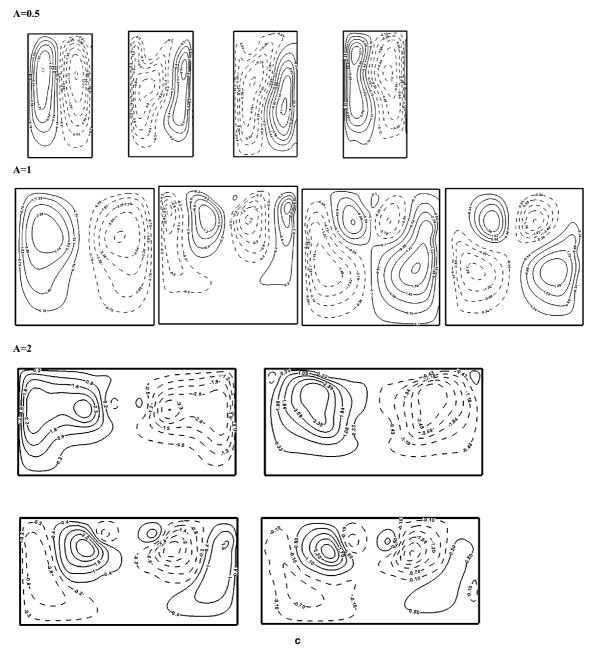


Fig. 5 (continued)

reflects fluctuations in current vertical Bridgman crystal growth.

Applying the thermal modulation with $\varepsilon = 1$ and high frequencies (f > 30), has revealed insignificant effect on the evolution of the flow and thermal fields. Indeed, the oscillation amplitudes of all variables decrease in a logarithmic way with the frequency and the average value of the maximum stream function as well as the heat transfer at the cold wall are practically identical to the values obtained in the regime without modulation. This result is consistent with the concluding remarks of Stelian et al. (2002) who stated that temper-

ature oscillations with periods lower than a cut-off one have no detrimental effect on the VB directional solidification.

However, when the frequency is decreased, the mean value of the kinetic energy of the system increases above that without modulation. For example, for $Ra = 4 \times 10^5$ modulation with f = 10 and $\varepsilon = 1$, changes the flow from steady (Fig. 3a) to quasi-periodic (Fig. 3b) with a flow structure symmetry breaking as shown in Fig. 3b. Complex multi-cellular flow occupies the domain. The signal corresponding to the ratio of the Nusselt number for the case with modulation to the Nusselt number without

modulation shows that the heat transfer reaches its minimum value when the flow bifurcates from the symmetric two cells solution to a symmetric four cells solution, where the two additional secondary counter rotating cells take place in the bulk of the cavity (see Fig. 4). This situation can be explained by the inversion of the thermal gradient developing between the centre of the cavity and the hot wall, which accelerates the flow in this zone (see time 'b' in Fig. 4). Such observation suggests the importance of the local heat transfer and convection near the interface. For that, at first we investigate local heat transfer and fluid flow for different aspect ratios of the cavity (aspect ratio was changed by modifying the cavity width). Thermal fields and flow patterns for the quasi-periodic flow corresponding to a modulation with f = 15 and $\varepsilon = 1$ for aspect ratios AR equal to 0.5, 1 and 2 are presented in Fig. 5 at the time instants corresponding to t_a —the maximum of the signal, 't_b'—zero value following the maximum, 't_c'—the minimum of the signal and 'td'—zero value following the minimum (see Fig. 5a).

For the narrow cavity, AR = 1/2, the flow is restricted to two main counter rotating cells interacting in the bulk of the cavity without development of secondary convection (Fig. 5c). When the cavity becomes wider (AR = 1 or 2) a thermal boundary layer develops near the vertical walls. The flow varies between a two cells configuration and a four cells configuration. It should be noted that different aspect ratios are considered here only to demonstrate a possible divergence in local behaviour due to the horizontal variation of the cavity width as this variation affects the radial temperature gradient responsible for the convective motion near the solid/liquid interface.

The resultant heat transfer for the three aspect ratios considered is represented by the evolution of the Nusselt number with time as shown in Fig. 6a. The frequency of the signal is the same as the frequency of the thermal modulation. The amplitude of the signal varies with aspect ratio and we can therefore conclude that it is affected by the flow developing for each aspect ratio case (Fig. 6a). The case with AR = 1/2 exhibits a sinusoidal signal as a response to the sinusoidal input. However, for AR = 1 the response seems to be affected by the local secondary convection near the top, the signal is periodic but not sinusoidal. Decrease of the nondimensional amplitude of heat transfer oscillation (A(Nu)) with increasing aspect ratio can be seen on Fig. 6b. This trend can be explained by the response of the flow to the sinusoidal modulation affecting the hot boundary layer. When the aspect ratio is small, the cavity response is global and close to the input signal. Increasing the aspect ratio (i.e., the width of the fluid phase in our case) results in the development of secondary cells in the central region of the cavity, which reduces the amount of heat transported from the hot wall

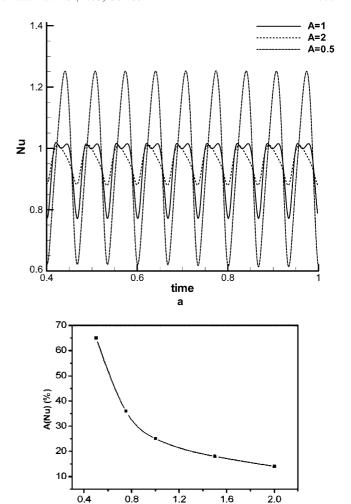


Fig. 6. (a) Evolution of the Nusselt number on the cold wall for three aspect ratios (AR = 1, 1/2 and 2) and $Ra = 4 \times 10^5$, $\varepsilon = 1$, f = 15. (b) Amplitude of oscillation of the Nusselt number on the cold wall according to the aspect ratio ($\varepsilon = 1$, f = 15 and $Ra = 4 \times 10^5$).

AR

to the bulk of the liquid. Consequently, the heat transfer exhibits a more local behaviour.

Results presented above certainly show the influence of modulated heating on the heat and flow transfer in the VB configuration. The following part of this study focuses on the effect of modulation for a square domain (AR = 1) which corresponds to the previous study of the melt instability without modulation (Kaenton et al., 2004). Fig. 7a shows the Nusselt number evolution versus frequency for different amplitude modulation with $Ra = 4 \times 10^5$ and confirms the effect of the frequency on the heat transfer. It shows the presence of a critical frequency minimizing such heat transfer independent of the amplitude. As this result can provide useful data for crystal growing processes it needs to be confirmed for a range of Ra. These simulations were extended to include Ra equal to 10⁵ and 10⁶. Fig. 8 represents the variation of the heat transfer rate (Nusselt number) with frequency for various Ra. It is shown that for each Ra a

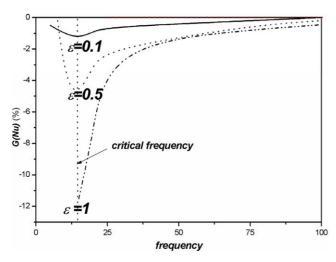


Fig. 7. Relative difference of Nusselt number with and without oscillations on the cold wall as a function of modulation frequency $(Ra = 4 \times 10^5, AR = 1)$.

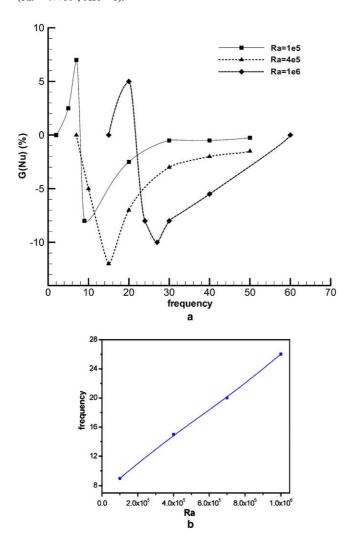


Fig. 8. (a) Relative difference of Nusselt number with and without oscillations on the cold wall versus frequency modulation for three values of Ra ($Ra = 10^5$, 4×10^5 and $Ra = 10^6$), AR = 1. (b) Variation of the critical frequency according to the Rayleigh number (AR = 1, $\varepsilon = 1$).

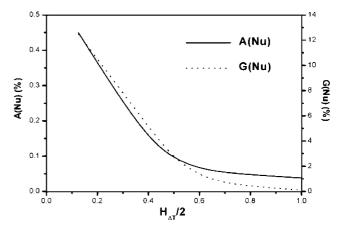


Fig. 9. Variation of the relative difference of Nusselt number with and without temperature fluctuation, G(Nu), and non-dimensional amplitude of heat transfer oscillation, A(Nu) as a function of the size of adiabatic zone (AR = 1, ε = 1, f = 15).

critical frequency exists. Calculations show an almost linear increase of that critical frequency (Fig. 8b). This result is in good agreement with a general correlation given by Antohe and Lage (1996) obtained for a clear liquid and porous media.

It is important to mention that simulations show that the size of the adiabatic zone and the aspect ratio (between 0.5 and 2) do not have a noticeable effect on the critical frequency. However, the amplitude oscillations of the thermal transfer at the cold wall vary with the size of the adiabatic zone. Indeed, for $\varepsilon = 1$ and f = 15, the temperature fluctuation effect is reduced (Fig. 9) when this zone is increased.

4. Conclusion

Because the VB configuration heated from the top maintains stable flows for a large range of Rayleigh numbers, the destabilizating influence of such external factor as temperature modulation is rarely studied.

In the present paper, the effect of the thermal fluctuation on a vertical Bridgman configuration containing a fluid with a low Prandtl number has been analyzed. For high frequency, weak effects on the velocity and the temperature oscillations have been observed. However, it was found that these variables are very sensitive to the hot temperature fluctuations for low frequencies. We also have identified the existence of a critical frequency for which the heat transfer from the cold wall reached a minimum value.

The present work can be considered as the first step in quantifying the response of the interface to the hot wall modulation. In the future it is planned to include the interaction between the shape of the interface and the oscillatory convection.

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Further reading

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