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Melting and solidification: processes and models/Flows in solidification

Secondary and oscillatory gravitational instabilities in canonical three-dimensional models of crystal growth from the melt. Part 2: lateral heating and the Hadley circulation

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Abstract

The focused discussion limited in Part 1 (C. R. Mecanique, this issue) to systems heated from below is now extended to the case of laterally heated configurations and the related problem of the Hadley flow stability. ***To cite this article: M. Lappa, C. R. Mecanique 335 (2007).***

Résumé

Instabilités secondaires et oscillatoires dans des modèles 3D canoniques pour la croissance cristalline. 2ème partie : des configurations latéralement chauffées et la circulation de Hadley. La première partie 1 (C. R. Mecanique, ce numéro) de cette discussion restreinte aux systèmes de chauffage est ici étendue aux cas des configurations chauffées latéralement et au problème de la stabilité de l'écoulement de Hadley. ***Pour citer cet article : M. Lappa, C. R. Mecanique 335 (2007).***

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Mots-clés : Mécanique des fluides numérique ; Transitions ; Convection thermique

1. Horizontal temperature gradients: lateral heating

The simplest geometry, among several crystal growth technologies, has the horizontal configuration of the Bridgman method (see, e.g., [1,2] and Semma et al. [3]), where the convective flow is induced by the horizontal component of the temperature gradient (in an industrial setting, the crucible containing the molten crystal is withdrawn horizontally from a furnace, resulting in a horizontal temperature difference). This configuration has gained considerable academic interest because of its relative simplicity which allows progress to be made using analytical and numerical models of the flows.

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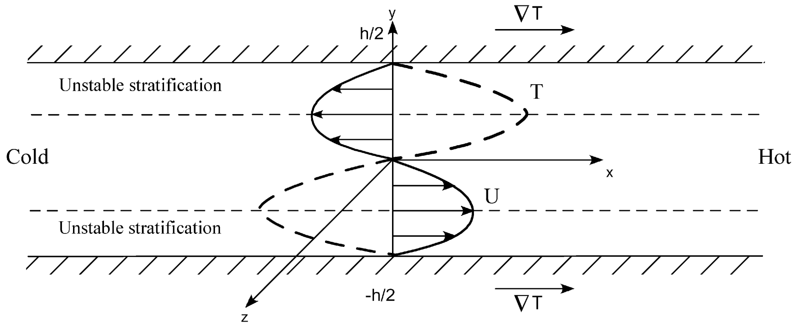

Fig. 1. Basic-state velocity and temperature profiles for an infinite horizontal liquid layer confined by two rigid walls with a linear temperature distribution along them.

Fig. 1. Profils de base de vitesse et de température pour une couche liquide horizontale infinie confinée par deux murs rigides soumis à une distribution linéaire de la température.

A synthesis of available stability analysis results concerning the simplified case of horizontal fluid layers of infinite extent limited from below and from above by parallel planes (with temperature changing linearly as a function of the horizontal coordinate) obtained by different research groups, is given in the article of Gershuni et al. [4]. It is shown therein that, if a velocity profile with an inflection point in the center of the layer section is assumed as representative of the basic flow in this configuration (Fig. 1, known as the Hadley circulation), three perturbing mechanisms (two-dimensional hydrodynamic, three-dimensional oscillatory helical wave and two-dimensional Rayleigh modes) are possible: The hydrodynamic mode (also referred to as 'transverse' mode) corresponds to a shear instability and is related to the formation of vortices on the frontier (i.e. close to the midsection of the layer) of the two opposing flows characterizing the basic state (i.e. close to the aforementioned inflection point); the Rayleigh mode follows from the presence of zones of potentially unstable stratification near the upper and lower horizontal boundaries (induced by the aforementioned basic flow) that makes possible the onset of instability of the Rayleigh–Bénard type therein (steady longitudinal rolls (SLR): in practice, this flow exhibits strong analogies with the convective case already discussed in Part 1, elsewhere in this issue, in the case of uniform heating from below); finally, the helical wave mode is due to the onset of a pair of gravitational traveling waves perpendicular to the basic flow, i.e. along the z axis in Fig. 1 (this instability appears in the form of oscillating longitudinal rolls (OLR) and is basically a three-dimensional phenomenon).

These three mechanisms occur in delimited intervals of Prandtl number: For small Prandtl numbers ($0 < Pr < 0.14$) the most dangerous is the plane (2D) hydrodynamic mode (this instability is initially stationary but onset of oscillatory convection is possible for large values of the temperature gradient); in a narrow range of Prandtl numbers ($0.14 < Pr < 0.44$) instability is caused by the OLR mode; for $Pr > 0.44$ the instability source is transferred to the Rayleigh mode which remains the most dangerous up to extremely large Pr. Naturally this mode does not exist in the case of absence of unstable stratification zones, like the case of a layer with horizontal insulated boundaries (see Kuo and Korpela [5]) where only hydrodynamic and OLR modes occur in the range of small Pr. Hart [6,7] determined the sensitivity the Hadley circulation to both these transverse (shear) and longitudinal disturbances (corresponding, as explained before, to perturbation rolls with axis perpendicular and parallel to the temperature gradient, respectively), whereas Gill [8] focused specifically on the longitudinal disturbances. These results were refined by Laure [9] and Kuo and Korpela [5] who found that for finite size enclosures with adiabatic horizontal boundaries, the first transition is to steady rolls for $Pr < 0.033$, and to OLR for $0.033 < Pr < 0.2$ (see also Roux et al. [10]).

These authors also showed that the stationary transversal instability is driven by the mean shear stress (this is the reason why it is often referred to as 'shear instability') while the oscillatory longitudinal instability arises as a consequence of a dynamical coupling between the mean shear stress and the buoyancy force (a dynamical balance between the inertial and gravitational forces).

A quite exhaustive parametric numerical study of multiple steady states, their stability, onset of oscillatory instability, and some supercritical unsteady regimes of convective flow pertaining to the hydrodynamic mode in two-dimensional laterally heated rectangular containers of finite extent with adiabatic upper and lower boundaries has been carried out recently by Gelfgat et al. [11,12] for $Pr = 0.015$.

Many possible distinct branches of steady-state flows were found for this configuration. A complete study of stability of each branch was performed for the aspect ratio of the rectangular container varying continuously from 1 to 11. The results were represented as stability diagrams showing the critical parameters (critical Grashof number and the frequency at the onset of the oscillatory instability) corresponding to transitions from steady to oscillatory states, appearance of multiroll states, merging of multiple states and backwards transitions from multiroll to single-roll states.

These hydrodynamic and OLR instabilities (typical of liquid metals) disappear when other types of fluids are considered.

For $Pr \geqslant O(1)$, in fact, the scenarios dramatically change. Within this context it is worth citing the recent work of Delgado-Buscalioni [13] who has investigated the problem from both theoretical and numerical points of view.

Such a study is focused on the characterization of the convection patterns arising at the core of the basic steady unicellular Hadley flow and covers the whole range of Prandtl numbers ($0 < Pr < \infty$). It has been shown therein that the onset of the flow instabilities basically depends on the core Rayleigh number, defined in terms of the local streamwise temperature gradient and that the effect of confinement can decisively change the stability properties of the core.

As the Rayleigh number increases the unicellular flow evolves from a diffusive regime to a boundary layer regime in which almost all the temperature drop and the vorticity production are localized in thin layers adjacent to the end walls.

As a consequence, a stagnant region is formed at the center part of the layer and the flow at the core occurs only as a result of the entrainment of mass from the vertical boundary layers being confined in thin intruding flowing layers near the horizontal walls.

If the steady unicell reaches such a boundary layer regime the local temperature gradient vanishes at the core leaving a completely stable core region. As confirmed by numerical calculations and in agreement with the studies previously carried out for the infinite Hadley parallel flow, in the case of adiabatic horizontal walls, Delgado-Buscalioni [13] has shown that the core-flow instabilities can only develop for $Pr < O(1)$ whereas, at larger Pr the core region remains stable and the instabilities may only develop at the boundary layers arising close to the side-walls.

In practice, there is a sudden increase of stability for $Pr > O(10^{-1})$, owing to the presence of the aforementioned completely stable cross-stream stratification and for $Pr > 0.2$ (where the OLR instability is no longer possible), the breakdown of the steady unicell takes place inside the boundary layers developed at large values of Ra.

It is known that for $Pr > O(1)$, oscillations (affecting the time history of the Nusselt number) can be generated during the transient phase approaching the steady state; this behavior has been investigated by Patterson and Imberger [14], Patterson and Armfield [15] and Schladow [16]; for large enough Rayleigh values, the transients are dominated by internal waves and the approach to steady state is achieved in an oscillatory manner by decay of internal wave motion.

After this transient phase the flow can undergo transition to permanent oscillatory states, but, as explained above, this is strictly related to instabilities of the boundary layers (see, e.g., Daniels and Patterson [17,18]) whereas, as mentioned above, the core flow tends to be stable.

All these studies were mainly devoted to horizontally elongated cavities and/or enclosures with $A = O(1)$, where A is the aspect ratio.

Some analyses have also appeared where the problem was considered in the opposite limit in which the aspect ratio is very small or tends to zero ($A \to 0$), i.e. vertically elongated (also referred to as 'tall') geometries. In such a case the core flow in the horizontal direction is no longer a feature of the system, but a similar behavior (a parallel flow) can be observed along the vertical direction.

In 1954 Batchelor [19] investigated the flow in a fluid-filled container with one opposing pair of vertical walls at different temperatures. His attention was restricted to the limiting case of infinite spanwise aspect ratio (i.e. an infinite vertical differentially heated fluid layer). He realized that if the cavity was narrow enough; i.e. small enough A, a fully developed region might exist in which a one-dimensional solution would apply (that is the temperature would vary linearly between the hot and cold walls and the purely vertical velocity would have an odd-symmetric cubic profile; this solution is often referred to as the 'conduction regime').

Many works of different authors have been devoted to the study of the instabilities associated with this regime. It was shown that the type of instability is determined by the value of the Prandtl number. The critical disturbance modes are hydrodynamically driven and stationary when $Pr < 12.45$ (Birikh [20]), but they are thermally driven and oscillatory when $Pr > 12.45$ (Birikh et al. [21], Korpela et al. [22]). Non-linear analysis has shown that former disturbances evolve into a multicellular pattern of steady transverse rolls (a regular cellular pattern becomes superimposed on the basic flow to produce a 'cats-eye' pattern of streamlines, Gershuni et al. [23]), and the latter ones cause the convection in the form of two counter-propagating waves, one of which travels up on the warm side of the layer and another travels down on the cold side (Fujimura and Mizushima [24]).

A recent linear stability analysis providing the critical Grashof number for this problem in the whole range $0 \leqslant Pr \leqslant \infty$ (first bifurcation) has been carried out by McBain and Armfield [25].

It is worth noting that one of the most interesting aspects of this type of convection, however, is the occurrence of secondary, tertiary and other bifurcations in the evolutionary process from laminar to turbulent fluid flow. The subsequent oscillatory modes of convection which the steady transverse rolls undergo transition to (when the temperature gradient is further increased) have been investigated, e.g., by Clever and Busse [26] and Gelfgat [27]. The evolution of the travelling-wave structures (that occur at $Pr > 12.45$) has been recently considered by Bratsun et al. [28]. They have disclosed that, when the Grashof number is increased, a tertiary three-dimensional flow occurs in the form of wavy travelling waves (longitudinal rolls modulated along their axes).

Interestingly, these authors [28] have pointed out that, in many effective circumstances (a moderately high cavity and $Pr > \mathrm{O}(1)$), when Gr is increased, in practice, the flow evolves towards a boundary layer regime before the conduction state becomes unstable with respect to oscillatory disturbances of the travelling-wave type. In these cases, steep velocity and temperature gradients confined to boundary layers on the vertical side walls are usually observed.

In practice, as the Prandtl number is increased and the heat advection in such fluids becomes more effective in comparison with thermal conduction, the probability for boundary layer regime to take place becomes higher; hence it is expected that in such circumstances the first flow bifurcation will be again related to an instability of the boundary layers as discussed before for $A \geqslant \mathrm{O}(1)$ and $Pr \geqslant \mathrm{O}(1)$.

As an additional variant of the classical problem related to the stability of systems heated from the side, some recent studies have also focused on the case of inclined (horizontally elongated) rectangular boxes (e.g., Delgado-Buscalioni et al. [29], Delgado-Buscalioni and Crespo del Arco [30] and Delgado-Buscalioni [13]).

In a tilted configuration the fluid is stably stratified along the cross-stream direction whereas unstably stratified in the perpendicular (streamwise) direction; the analyses (mentioned above) of the instability mechanisms in such a case have revealed several stabilizing or destabilizing couplings between the momentum and temperature fields that are not possible in the horizontal ($\alpha = 90°$) or vertical ($\alpha = 0°$, fluid heated from below) limits.

As illustrated by Delgado-Buscalioni [13] (linear stability analysis), in fact, when the cavity is inclined a rich dynamical behavior arises as a consequence of the competition between several instabilities and new types of instabilities can occur, e.g., the 'Stationary Longitudinal long-wavelength instability' (SLL) and the 'Oscillatory Transversal long-wavelength instability' (OTL). The first appears for any $\alpha < 90°$ and has essentially the same origin as the critical mode of an unstable vertical configuration. The latter is a standing wave with a rather long wavelength (typically $9h$ where h is the depth of the box); it only comes up if the cavity is inclined and heated from below ($0° < \alpha < 90°$) (in such a case the perturbation gains the most part of its kinetic energy from the streamwise buoyant force).

The other traditional instabilities for the horizontal configuration ($\alpha = 90°$) are also affected by the inclination.

In particular, for $\alpha < 90°$ and $Pr \geqslant \mathrm{O}(1)$, transversal perturbations can take kinetic energy out from the buoyant excess generated by the cross-stream perturbative advection and as a consequence stationary transversal rolls (the 2D hydrodynamic instability), that for $\alpha = 90°$ can arise only in fluids with $Pr < 0.033$, can become unstable even in gases ($Pr \cong 1$, as also observed by Delgado-Buscalioni and Crespo del Arco [30]).

Moreover, by tilting the cavity with respect to $\alpha = 0°$, the (Rayleigh–Bénard) stationary thermal mode is suppressed in cavities whose depth is smaller than a theoretically predicted cutoff wavelength.

The inclination also alters the properties of the oscillatory longitudinal instability (OLR).

2. Three-dimensional numerical simulations

Since two-dimensional flows cannot be rigorously realized as side walls play an important role in finite flow configurations, i.e., the end wall bias or 'contamination' is unavoidable (see Melnikov and Shevtsova [31]) and the information provided by linear stability analyses is limited to the first flow bifurcation, many numerical studies (mostly based on the solution of the non-linear Navier–Stokes equations) have been recently devoted to the stability of laterally heated configurations for the case of effective horizontal three-dimensional boxes (differentially heated over two opposing vertical walls with adiabatic horizontal and lateral walls).

As an example, Fig. 2 shows the three-dimensional solution for the box with the same aspect ratio already considered in Fig. 2 in Part 1 ($4 \times 1 \times 4$). It is evident that, unlike the steady flow predicted for $Ra = 2 \times 10^3$ by

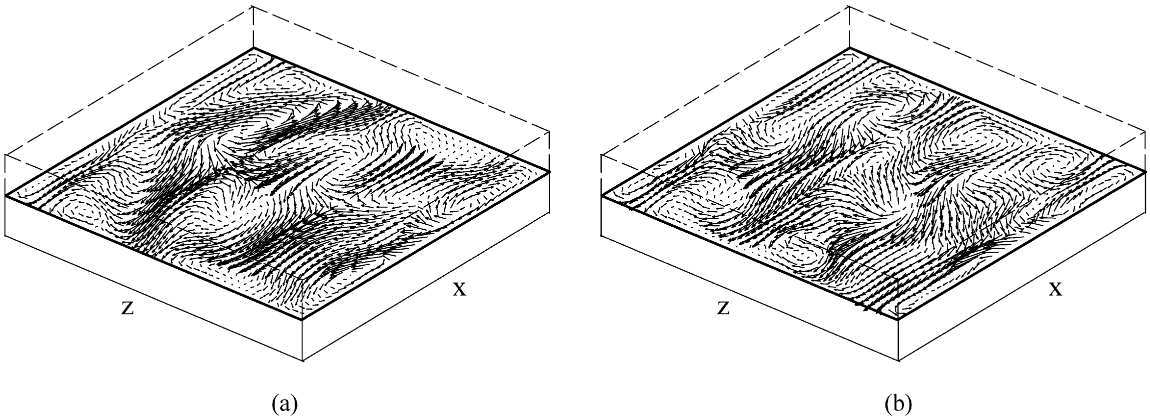

Fig. 2. Snapshots of 3D buoyancy convection (projection of the velocity field in the horizontal midplane) in a laterally heated enclosure with adiabatic horizontal walls and $L_x = 4$, $L_y = 1$, $L_z = 4$ ($Pr = 0.01$, silicon, $Ra = 2 \times 10^3$, oscillatory convection) at two different times during a period of the oscillations.

Fig. 2. Instantanés de la convection gravitationnelle 3D (projection du champ de vitesse dans le plan median horizontal) dans une cavité latéralement chauffée à murs horizontaux adiabatiques pour $L_x = 4$, $L_y = 1$, $L_z = 4$ ($Pr = 0{,}01$, silicium, $Ra = 2 \times 10^3$, convection oscillatoire) à deux différents instants pendant une période d'oscillation.

two-dimensional studies [11], the flow is oscillatory. Such a simple argument demonstrates that the presence of constraints along the third direction, like the presence of solid walls along x can play a significant role in the selection of the possible multiple states of convection with respect to the 2D case. In the 3D case for the same value of Ra corresponding to a steady solution in the 2D case, the flow is no longer steady and undergoes transition to an oscillatory behavior (see Figs. 2(a) and (b)); under the constraint of 2D flow (two-roll multicellular structure), transition to time-dependence occurs for larger values of Ra.

Remarkable differences between 2D and 3D studies were also reported by Afrid and Zebib [32]. These investigators considered a zero Prandtl (Pr) number fluid in 4 × 1 × 2 (length to height to width) and 4 × 1 × 1 rectangular boxes. They found that the flow field is steady at relatively low Rayleigh number, and is represented by one cell, unlike the multicellular flow predicted by two-dimensional computations. When Ra reaches a certain threshold Ra_{cr} , the flow becomes oscillatory. The transition to time dependence is a function of the geometry. The extension along z of the enclosure has an important effect on transition to oscillatory convection, for it was found by Afrid and Zebib [32] that reducing this extension from two to one, leads to a much higher Ra_{cr} (see also Pratte and Hart [33]), making the results of two-dimensional numerical simulations somewhat inadequate.

Within this context it is also worth noting that the nature of the oscillatory instability that appears in 3D boxes for a given low Prandtl number is still an open question (the location of the points in the parameter space where the branches pertaining to the different instability mechanisms, transverse or longitudinal, meet is affected by the finite size of the system). It is known that the 2D-hydrodynamic (shear) transversal mode can become oscillatory when Ra is increased, however, according to experimental evidence it seems that the 3D instabilities found in liquid metals (mercury and gallium) could be due to a longitudinal mode (see the discussion in Hung and Andereck [34] and/or to the superposition of a secondary transversal disturbance on a primary longitudinal one (Delgado-Buscalioni et al. [35]). Along these lines there have been many works focusing on regions of the space of parameters where these two different types of bifurcation may intersect (Braunsfurth and Mullin [36]). Around $Pr = 0.025$ rather complex dynamics may arise because the transversal and oscillatory longitudinal rolls are triggered at relatively close values of Ra; along these lines new types Hopf–Hopf interaction were reported in the experiments of Braunsfurth and Mullin [36].

In 2D enclosures (e.g., $A = 4$) at a low Prandtl number, the flow becomes oscillatory after the onset of stationary shear rolls and it gains in complexity by several possible paths (Pulicani et al. [37], Gelfgat et al. [11,12]), which as a matter of fact, do not satisfactory explain the flow oscillations found in the earlier experiments. The transition to time-dependent flow seems to be of different nature in the 2D and 3D situations.

In the light of all these arguments, like the case of Rayleigh–Bénard convection, the presence of lateral solid constraints along the z-coordinate ($L_z/L_x \leqslant \mathrm{O}(1)$) can be thought of as altering the mode selection process and the pattern symmetries.

These studies have been also extended to the case of cylindrical geometries.

Two possible configurations have been considered in the literature: (i) horizontal cylinder with differentially heated end walls; (ii) laterally heated vertical cylinders.

For the first case, in the past, flow predictions have often been made by using an asymptotic analytical approximation in the core, or by assuming a two-dimensional solution for the plane of symmetry. Three-dimensional computations by Bontoux et al. [38] showed, however, that in reality the steady buoyancy flow in this configuration is highly three-dimensional. The subsequent onset of unsteadiness has been investigated more recently by Xin et al. [39] by direct numerical integration and by linear stability analysis. They have shown that the steady 3D state solution can undergo a Hopf bifurcation and that depending on the Prandtl number the most unstable eigenvector may break or keep the symmetry of the base 3D flow. The critical Rayleigh number has been found to achieve an asymptotic value for large enough Prandtl number.

The case of a laterally heated vertical configuration is even more interesting for the aims of the present review, since, like the case of a rectangular container, it has extensive background application in the field of bulk crystal growth.

Some interesting results concerning the stability of buoyant axisymmetric convection in a vertical cylinder with a parabolic temperature profile at the sidewall (see also Baumgartl et al. [40]) have been recently presented by Gelfgat et al. [41] for $0 \leqslant Pr \leqslant 0.05$ and $0.5 \leqslant A \leqslant 2$ ($A =$ height/diameter). This configuration has been studied as a relevant model of the vertical Bridgman or liquid encapsulated melt zone technique.

It is known that in such a model stratified fluid layers develop near the top and the bottom. The stratification near the bottom (the cold fluid below the hot one) is stable, while stratification near the top (the cold fluid above the hot one) is unstable with respect to the action of buoyancy forces.

The critical parameters corresponding to a transition from the steady axisymmetric (basic state) to the three-dimensional asymmetric (steady or oscillatory) flow pattern have been computed by Gelfgat et al. [41] and it has been elucidated that the instability of the flow is three-dimensional for the whole range of governing parameters studied. In particular, the axisymmetric flow in relatively shallow cylinders tends to be oscillatorily unstable via a hydrodynamic Hopf bifurcation of the circulating flow, while in tall cylinders the instability sets in due to a steady bifurcation of the aforementioned unstably stratified fluid layer caused by the Rayleigh–Bénard mechanism. In the first case the three-dimensional perturbation has the form of a traveling wave; accordingly the oscillatory perturbation patterns (as well as the oscillatory component of the flow) rotate around the axis of the cylinder with the angular velocity $2\pi f/m$ (where f is the frequency of the oscillations).

In the latter case (see, e.g., the experiments of Selver et al. [42] about natural convection in cylinders filled with gallium, localized heating from the circumference and aspect ratio ranging from 2 to 10), the flow is initially three-dimensional and steady, but it can undergo a subsequent transition to time-dependent states if the Rayleigh number is increased.

In qualitative agreement with the study of Gelfgat et al. [41], Selver et al. [42] found that the toroidal flow tends to become non-axisymmetric and oscillatory at the same time beyond a certain Ra when the aspect ratio of the cylinder is smaller than a certain value whereas for larger aspect ratios, the flow becomes non-axisymmetric and then time-dependent, both transitions being the result of pure thermal instabilities as demonstrated by the experimental evidence of oscillations affecting mainly the upper-half of the domain (the zone where thermal unstable stratification occurs).

More recently, Ma et al. [43] have simulated three-dimensional steady and oscillatory flows in a vertical cylinder partially heated from the side (vertical wall heated in a zone at midheight and insulated above and below this middle zone, with both ends of the cylinder cooled; aspect ratio ranging from 1 to 4, fixed Prandtl number, $Pr = 0.021$; fixed length of the heated zone, equal to the cylinder radius). Three-dimensional steady and unsteady simulations as well as mode decomposition techniques and energy transfer analyses have been used to characterize the flows and their transitions. In agreement with the earlier studies they have found that the flows that develop from the steady toroidal pattern beyond the first instability threshold break the axisymmetry. At small A ($1 < A < 1.25$), the flow corresponds to a two-roll rotating pattern, which is triggered by a $m = 2$ azimuthal mode as a result of a hydrodynamic instability. At large A ($1.5 < A < 4$), the flow is steady and corresponds to a main one-roll pattern in the upper part of the cylinder; this flow is triggered by a $m = 1$ mode as a result of buoyancy effects affecting the unstably stratified upper part (Rayleigh–Bénard instability), but shear effects are involved in the instability for the smaller values of A; these steady flows then transit at a higher threshold to a standing-wave oscillatory one-roll pattern. For intermediate values of A ($1.35 < A < 1.45$), the transition is toward an oscillatory pattern, but hysteresis phenomena with multiplicity of steady and oscillatory states occur.

3. Conclusions

In this review (Parts 1 and 2) some effort has been devoted to illustrate the state-of-the-art about possible secondary and oscillatory regimes pertaining to various types of gravitational natural convection (canonical Rayleigh–Bénard, lateral heating and possible mixed states) in geometrical configurations traditionally used as canonical models of crystal growth processes. Differences, analogies as well as some unexpected theoretical links among subjects usually treated separately in the literature have been pointed out.

For reviews and/or very recent results about other types of convection (Marangoni, vibrational, magnetic, etc.) the reader may consider references [44–63].

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