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On the oscillatory hydrodynamic modes in liquid metal layers with an obstruction located on the bottom

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ABSTRACT

Hydrodynamic disturbances represent the preferred mode of instability of thermogravitational flow for a relatively wide range of substances and conditions (essentially pure or compound semiconductor and superconductor materials in liquid state). As nowadays almost all modern technologies rely greatly on such crystallized materials, targeting an improved understanding of the convective phenomena which occur in the melt has become a subject of great importance. Here an “ad hoc” model is developed to inquire specifically about the role played in such a context by geometrical “irregularities” affecting the melt container. More precisely, results are presented for the case of a fluid with $\mathrm{Pr} = 0.01$ (silicon) filling an open cavity with a single backward-facing or forward-facing step on the bottom wall or with an obstruction located in the centre. It is shown that the presence of sudden changes in the considered geometry can lead to a variety of scenarios with a significant departure from classical situations examined in the past. These configurations have different spatial symmetries and show different dynamics, including rhythmic roll expansions and contractions along the vertical and horizontal directions at different locations, roll nucleation, deformation, transport and merging phenomena. In some circumstances a travelling wave with front perpendicular to the imposed temperature gradient emerges, which has never been reported in the literature. A frequency spectrum analysis is used to support the identification of the multiple convective phenomena enabled by the new geometric features.

1. Introduction

Over the past thirty or forty years, the industrial world has witnessed the rapid development of new technologies based on a variety of pure or compound semiconductor and superconductor crystals. Such crystals constitute the basis for microprocessors and computer memories and play an important role in several related advanced applications.

Most remarkably, although much effort has been directed to the technological development of such materials, current attempts towards further “improvements” (in terms of “product” quality and production costs) seem to show no obvious sign of reaching a stop. Indeed, with the growing deployment of such crystalline substances in new fields and for innovative industrial exploitations, researchers continue to keep concentrated on these subjects. In particular, as the manufacturing technology becomes increasingly more mature and standardized, and few uncertainties are left in the physical and chemical “overarching” factors which determine the performances of such materials in the solid state, “optimization” of related production techniques from a “fluid-dynamic” perspective is becoming a topic of considerable interest.

Industrial methods for which such an optimization is being actively sought include the horizontal Bridgman (HB), the Floating zone (FZ) or the Czochralski (CZ) technique (see, e.g., [1,2]). A feature common to all such processes is the presence of thermal (or compositional) gradients in the melt, which, in general, provide driving forces for natural convection. The melt is, therefore, subject to non-uniform heat- and mass-transfer conditions, which often result in strongly undesired effects.

Of special interest in such a context is the so-called “Hadley flow”, namely buoyancy convection driven by *horizontal* temperature gradients in elongated cavities or shallow geometries (Dupret and Van der Bogaert [3]; Monberg [4]). Since the pioneering work of Hadley [5] (who originally introduced this flow model as a simplified representation of the circulation developing in our atmosphere), such regimes of fluid motion have been largely studied due to their relevance to the industrial processes mentioned above.

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In particular, Hurle [6] was the first to show that *oscillatory buoyancy convection* of this type could be responsible for the emergence of undesired "imperfections" in crystallized materials.

The nature and spatio-temporal structure of the fluid-dynamic disturbances responsible for such oscillations were clarified in ensuing studies such as those by Hart [7,8] and Gill [9]. These authors identified two main categories of disturbances according to their spatial structure (transverse or longitudinal orientation in space). They also disclosed that the so-called transversal instability is driven by the mean shear stress (this is the reason why it is often referred to as "shear instability" and the related disturbances as *hydrodynamic* ones), whereas the longitudinal instability arises as a consequence of a dynamical coupling between the mean shear stress and the thermal buoyancy force.

In the first case, the instability manifests itself in the form of two-dimensional (2D) vortices appearing on the frontier of the two opposing (primary and return) horizontal currents characterizing the basic Hadley flow. For open cavities (upper free surface exposed to an ambient gas) such disturbances are in general oscillatory (the first instability is a *Hopf bifurcation*, Laure and Roux [10]; Wang and Korpela [11]; Okada and Ozoe [12]; Gelfgat et al. [13]), whereas for closed cavities the Hopf bifurcation is generally preceded by a *stationary* instability. Regardless of their stationary or oscillatory nature, these vortices have axis perpendicular to the imposed temperature gradient (the general outcome of this instability is the replacement of the initial "unicellular" Hadley flow with a two-dimensional *multicellular* convective structure). The other mode of convection due to longitudinal disturbances consists essentially of a pair of gravitational or "helical" waves travelling in the spanwise direction, i.e. with front parallel to the temperature gradient.

Such instabilities can be controlled and/or related effects "mitigated" via the application of magnetic fields (Ben Hadid et al. [14]; Kaddeche et al. [15–17]) or imposed vibrations (Lappa [18]). By contrast, the flow becomes increasingly more complex if the configuration is "inclined" with respect to vertical gravity (Delgado-Buscalioni et al. [19]) or if solid/liquid phase change is taking place (El Ganaoui et al. [20]; Le Quéré and Gobin [21]). Such past findings have been obtained essentially for very simple geometrical models such as layers of infinite extent or bounded shallow rectangular cavities (these simplified and "easy to handle" configurations have been expressly used by researchers, on the one hand, to get important fundamental information on these phenomena and, on the other hand, to introduce well-defined benchmark cases for model validation and comparison).

While for the companion case of buoyancy convection in gases, some effort has been devoted to consider (both experimentally and numerically) flows over vertical or horizontal backward- and forward-facing steps (Hong et al. [22]; Abu-Mulaweh et al. [23]; Abu-Mulaweh [24–26]; Meskini et al. [27]; Dihmani et al. [28]; Mahrouche et al. [29]), there seems to be a disappointing lack of equivalent knowledge relating to liquid metals or semiconductor melts.

For these substances, experimental works are rather rare, this being due in large part to the well-known difficulties of setting up suitable laboratory test cases that would be at the same time well-controllable and allow exploration of an extended range of dynamical regimes (a key observation regarding such a lack of results is that, in general, semiconductor materials are opaque and very reactive in the liquid state). Past geometrical models used for flow stability analyses usually contained a number of symmetries. The present investigation proceeds one step further with the express aim to devise a more general mathematical and numerical framework in which such simplifications are somehow removed and the results carefully diagnosed (a kind of "modelling hierarchy"). In this context, CFD has the potential to offer valuable insights. As a valid alternative to past analysis strategies based on difficult expensive experiments, recent improvements in numerical techniques as well as computing hardware make sophisticated computer-based modelling and simulations possible.

The layout of this paper is as follows. In Sect 2, a brief summary of existing theory for the considered class of fluid-dynamic disturbances is given. In this section we also lay the general foundation of our theoretical and mathematical treatment. The related numerical method is presented together with a mesh sensitivity analysis and a validation study. Section 3 is entirely devoted to the discussion of the structure and spatio-temporal behaviour of the emerging disturbances in connection with the specific geometrical details considered (geometries with varying cross-section, i.e. a topography in the bottom wall). Section 4 is used for a critical discussion of the present results in the light of past work devoted to flow instabilities in constrained geometries. In Section 5, this framework is further extended by examining the response of the system to the presence of surface-tension-driven (Marangoni) effects introduced as "a weak perturbation" of the buoyancy flow (this subject complements that of pure hydrodynamic gravitational disturbances by addressing the case of "hybrid" convection, which so much attention has also received in the literature devoted to crystal growth from the melt in configuration with a free liquid-gas interface).

2. Mathematical model and numerical method

2.1. The system

Following earlier studies, we concentrate on a two-dimensional shallow cavity with free liquid-gas interface parallel to the x axis and characteristic depth d, laterally delimited by solid walls at different temperatures (one cooled, the other heated).

This classical geometry (the so-called R-F system, Laure and Roux [10], see Fig. 1) is varied by incorporating in it a backward-facing or a forward-facing step. In order to characterize the resulting geometrical model, we introduce relevant nondimensional parameters, namely: the overall system aspect ratio (A), defined as its length-to-depth ratio (L/d), $\Gamma = L_s/L$ to account for the horizontal extension of the region with reduced cross-sectional area and $\Lambda = d_s/d$, i.e. the nondimensional height or depth of the step (hereafter, simply referred to as the "expansion ratio" or "compression ratio" depending on the specific case considered). Combination of the two geometrical models with the backward-facing and forward-facing steps results in a third configuration with an "obstruction" located in the centre (Fig. 1c) for which we introduce the additional parameter $\Gamma_1 = L_1/L$ to account for the distance of the obstruction from the (cold) wall.

2.2. The considered fluid

The aspect ratio of the cavity is fixed to $A = 20$. The choice of a relevant work liquid to be considered accordingly is not as straightforward as one would expect.

Indeed, both the nature of the fluid and the kinematic and thermal boundary conditions can play a significant role in determining the nature of the first instability (bifurcation) affecting the Hadley flow in such systems.

Some useful information along these lines (for the case of infinite or very elongated cavities such as that considered in the present work) can be extracted from the literature. As an example, in the case of top and bottom solid boundaries with adiabatic conditions, Hart [8] found transverse *stationary* hydrodynamic modes to be the most unstable if $Pr < 0.015$ (where Pr is the well-known Prandtl number: ν/α, ν being the fluid kinematic viscosity