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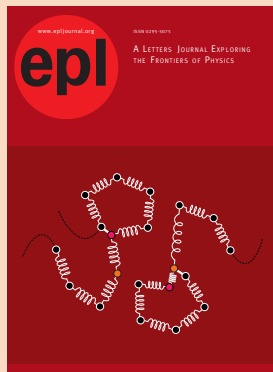
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## Focus Article

# Equilibrium states of the ice-water front in a differentially heated rectangular cell<sup>(a)</sup>

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**Abstract** – We study the conductive and convective states of phase change of pure water in a rectangular container where two opposite walls are kept respectively at temperatures below and above the freezing point and all the other boundaries are thermally insulating. The global ice content at the equilibrium and the corresponding shape of the ice-water interface are examined, extending the available experimental measurements and numerical simulations. We first address the effect of the initial condition, either fully liquid or fully frozen, on the system evolution. Secondly, we explore the influence of the aspect ratio of the cell, both in the configurations where the background thermal gradient is parallel to the gravity, namely the Rayleigh-Bénard (RB) setting, and when they are perpendicular, *i.e.*, vertical convection (VC). We find that for a set of well-identified conditions the system in the RB configuration displays multiple equilibrium states, either conductive rather than convective, or convective but with different ice front patterns. The shape of the ice front appears to be always determined by the large scale circulation in the system. In RB, the precise shape depends on the degree of lateral confinement. In the VC case the ice front morphology is more robust, due to the presence of two vertically stacked counter-rotating convective rolls for all the studied cell aspect ratios.

focus article

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**Introduction.** – Convective liquids undergoing melting or freezing give rise to a rich phenomenology of flow patterns and solid-phase morphologies. This bears great relevance in the geophysical domain, *e.g.*, in volcanology for the understanding of the solidification of magma chambers [1–3], in planetology for the study of magma oceans [4], or in geomorphology and glaciology for glacier dynamics and their induced erosion [5], and in marine sciences for the prediction of arctic sea ice annual cycles [6]. In the technological context, convection-driven phase change has a key role in metallurgy [7], in the purification of substances [8] and in the storage of thermal energy through phase change materials [9]. Depending on the application, the fluid can be either very complex in composition and rheology like a heterogenous molten rock magma, or simpler like muddy water or sea water, or

nearly ideal as for purified materials employed in chemical industrial processes. However, probably the most common instance is the one where the fluid is relatively clean water. This is a rather intriguing case due to the peculiar non-monotonous buoyancy force intensity in water above the freezing point. A large variety of situations of thermal or mechanical driving mechanisms are encountered. The fluid motion can be the result of natural convection due to a cooling process, as in the case of volcanic magma, or it can be steadily driven by localized heat sources, such as a hot/cold boundary, or by distributed ones, as in the case of internal heating by radioactive decay (common in rock formation) or by absorption of solar radiation as it happens for water in glaciers or in the oceans [10,11]. Finally, the thermal convection can also be maintained by a mechanical driving of the fluid, as it happens below the sea ice and around icebergs [12]. From a physicist's perspective, a relevant question is how the convecting fluid flow, which can be either laminar or turbulent depending on the driving intensity, can determine the overall shape of ice.

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Table 1: Four regimes of water-freezing RB system for increasing temperature differences (left to right) as identified in [26]: in the second line, the first two letters of the acronyms specify the stratification type, either stably stratified (SS, with temperature ranging from  $T_0$  to  $T_c$ ) or unstably stratified (US, with temperature ranging from  $T_c$  to  $T_b$ ); the third letter specifies the mode of heat transport, either diffusion (D) or convection (C); top and bottom denote the positions of the layers in the RB system.

Regime	1	2	3	4
Stratification type	SSD	SSD(top) + USD(bottom)	SSD(top) + USC(bottom)	SSD(top) + USC(bottom)
Equilibrium state	diffusive	diffusive	convective	convective
Ice front shape	flat	flat	flat	deformed

Is there just a single general mechanism? Can one envisage a phenomenological model, *i.e.*, a predictive argument for the shape of the ice-water front that does not need to take into account the exceptional complexity of the thermodynamics and fluid dynamics equations involved in its description?

A way to reply to these questions is to envisage a sufficiently simplified and well-controllable system that retains part of the physical complexity and rich phenomenology observed in nature. A well studied and commonly used convective setup in fluid dynamics is the Rayleigh-Bénard (RB) system, a fluid filled container heated at the bottom surface (of temperature  $T_b$ ) and cooled at the top (of temperature  $T_t$ ) and thermally insulated on the lateral sides. The thermal instability, the onset of convection, the flow bifurcations, the self-organization of the system in distinct parts, the turbulent regime and its scaling laws, have been analyzed in great detail [13–18]. This makes RB an ideal system on top of which the complexity of phase change phenomena and its coupling with fluid convection can be added. Previous studies of melting in RB have highlighted the complexity of the solid-liquid interface topography, and its dependencies on the strength of convection (parametrized by the Rayleigh number), on material properties (Stefan and Prandtl numbers), on the system dimensionality and geometry [19–23]. Furthermore, an intriguing phenomenon of bistability depending on whether the system has been initialized as fully liquid or fully frozen has been identified [22,24]. However, most of the above-mentioned studies have focused on the case of pure materials and small thermal gaps so that the resulting buoyancy is linear with respect to temperature (Boussinesq approximation). For water, the density anomaly, *i.e.*, the local mass density maximum at around  $T_c \sim 4^\circ\text{C}$  at atmospheric pressure, leads to a non-linear buoyancy force, which plays a great role in the icing dynamics. Recently, [25] combined experiments and numerical simulations to understand the hydrodynamical mechanisms that control the global extent and the shape of the ice in a freezing RB rectangular quasi-two-dimensional cell. They identified four distinct regimes of coupling between thermal stratification, buoyancy forces, and phase change [25] (see table 1 for a brief summary). Other research efforts have explored the effect of the RB system inclination on the overall icing process [26].

In this work, we aim at extending further the available experimental measurements and numerical simulations of

water melting and icing in an RB cell, in particular by testing the existence of the bistability in a water-filled RB cell and at exploring the container aspect ratio dependence and its role with respect to the system inclination, either straight or rotated by  $90^\circ$ .

### Experimental setup and numerical methods.

– The experiments are conducted in a battery of standard RB cells with four different geometrical proportions of the container. The details of the setup are documented in the Supplementary Material `Supplementarymaterial.pdf` (SM). Here we only give a brief description. The cell aspect ratio,  $\Gamma = l_x/h$ , is here defined as the quotient between the largest width of the isothermal plates ( $l_x$ ) and the distance between the isothermal plates (also called height)  $h$ . We choose  $l_x = 24$  cm and  $h = 12, 24, 48, 96$  cm leading to  $\Gamma = 0.5, 1, 2, 4$  respectively. The third spatial dimension,  $l_z = 6$  cm, is kept fixed and it is smaller than the others, a fact that allows to designate the system as quasi-two-dimensional. We note that  $h$  stands for the vertical direction, parallel to the gravitational acceleration, in the RB configuration, while it is horizontal in the vertical convection (VC) setting, when the same experimental cells are tilted by 90 degrees. In the present study, we only perform solidification experiments, *i.e.*, experiments whose initial condition is liquid water with uniform initial temperature same as the hot plate temperature  $T_b$ . Given the difficulty of manufacturing a cell-sized homogeneous ice block, we could not perform (well controlled) melting experiments. For this reason, in the present study we also rely on the results of numerical simulations. We employ the CH4-PROJECT code [27] which is based on a Lattice-Boltzmann equation algorithm for the description of fluid and temperature dynamics, and on the enthalpy method for phase change. Both the numerical methods and the specific algorithm implementation have been extensively validated, particularly against RB water freezing experiments in [25,26]. We use the non-monotonic relationship of the water density as a function of the temperature,  $\rho = \rho_c(1 - \alpha^*|T_b - T_c|^q)$ , with  $\rho_c = 999.972$  kg/m<sup>3</sup> the maximum density corresponding to  $T_c \approx 4^\circ\text{C}$ ,  $\alpha^* = 9.30 \times 10^{-6}(K^{-q})$ , and  $q = 1.895$  [28]. We conduct two-dimensional simulations, which have been proved to match well the experiments for the present quasi-2D cells [25,26]. The initial conditions encompass both the fully liquid and fully frozen cases, *i.e.*, freezing and melting numerical

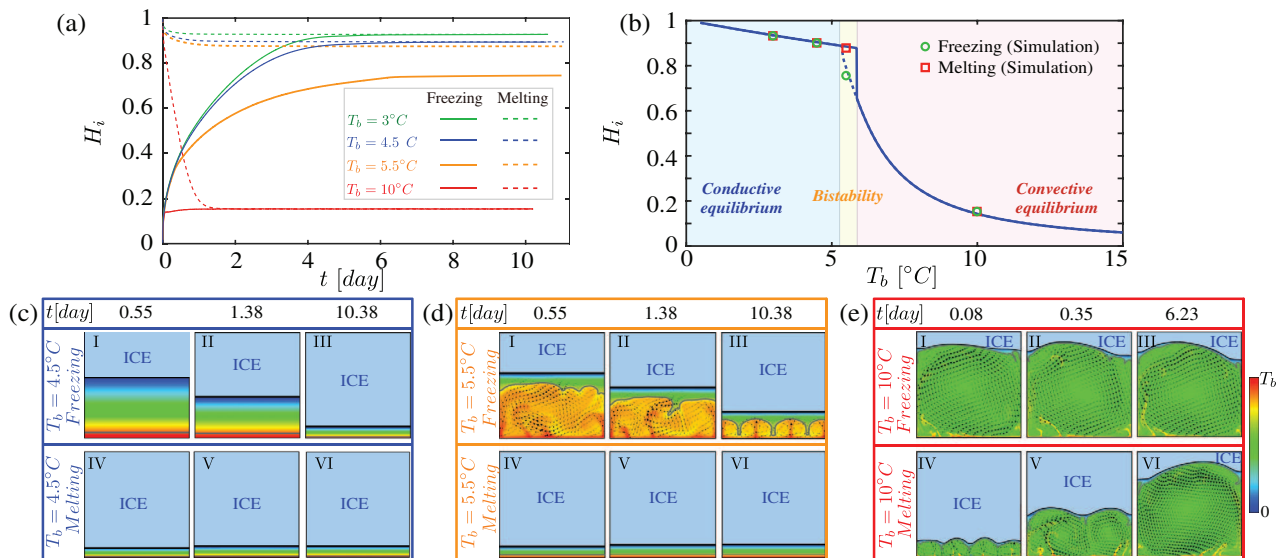


Fig. 1: Bistability phenomenon. (a) Temporal evolution of the ice thickness,  $H_i$ , of the freezing process (thick line) and the melting process (dashed line). (b) Comparison of the simulation (symbols) and the theoretical model (dashed and solid lines):  $H_i$  as a function of  $T_b$ . The blue, yellow, and red shaded areas correspond to the conductive, bistable and convective equilibrium regimes, respectively. The dashed line denotes one of the two branches in the bistable regime which predicts the convective equilibrium state. (c), (d) and (e): panels I-III display the evolution of the instantaneous temperature field of the freezing process, with the bottom plate temperature  $T_b = 4.5, 5.5, 10^\circ\text{C}$ , respectively; panels IV-VI display the evolution of the instantaneous temperature field of the melting process, for the same bottom plate temperatures. The visualizations of the temperature field in the water region are with colors and  $T_0$  (black line) and  $T_c$  (gray line) isotherms, along with the velocity vectors when fluid convection occurs.

experiments. Throughout the investigation, the cold plate is fixed both in the experiments and the simulations at temperature  $T_t = -10^\circ\text{C}$ . The effects of changing  $T_t$  are qualitatively predictable (more details on  $T_t$  effects can be found in the SM). Both in the experiments and in the simulations we monitor the evolution of the ice-water interface  $h_i(x, t)$  ( $i$  stands for ice), and its mean instantaneous value profile  $\bar{h}_i(t) = l_x^{-1} \int_0^{l_x} h_i(x, t) dx$ . Such quantities are more conveniently analyzed in dimensionless terms, hence  $H_i = \bar{h}_i/h$  represents the fraction of the cell that is occupied by the ice ( $H_i = 1$  means complete solidification).

**Results: bistability.** – We first study whether the melting and freezing system configurations evolve into the same equilibrium state. Given the fact that the system in the RB arrangement can display different regimes as the intensity of the thermal driving increases (table 1), we choose four typical cases of the thermal driving condition from each of the existing four different regimes, *i.e.*,  $T_b = 3, 4.5, 5.5, 10^\circ\text{C}$ , and perform long-term numerical simulations for melting (initial condition is  $H_i = 1$ ) and freezing (initial condition is  $H_i = 0$ ). Note that the duration of the simulations is of the order of 10 days in physical units. Figure 1(a) shows the normalized global ice thickness,  $H_i$ , as a function of time under different conditions of thermal driving in the RB setup. The thick (dashed) lines represent the freezing (melting) case. It is

observed that melting and freezing reach the same equilibrium state for the cases of  $T_b = 3, 4.5, 10^\circ\text{C}$ ; while for  $T_b = 5.5^\circ\text{C}$ , melting and freezing reach a conductive and a convective equilibrium, respectively. Hence, in the freezing experiments the global amount of ice at the equilibrium is smaller. To better understand this phenomenon, we show the evolution of the temperature field (see fig. 1(c)–(e), we do not show the  $T_b = 3^\circ\text{C}$  case because when  $T_b < T_c$  (Regime-1) the fluid region is trivially stably stratified throughout the entire simulation). At  $T_b = 4.5^\circ\text{C}$  (Regime-2), though the stably and unstably stratified layers coexist, the effective Rayleigh number (which is based on the unstably stratified layer and only defined when  $T_b > T_c$ ),  $Ra_e = \frac{(\Delta\rho/\rho_c)g(h_c)^3}{\nu\kappa} = \frac{g\alpha^*|T_b - T_c|^q(h_c)^3}{\nu\kappa}$  (with  $h_c$  being the averaged height of the  $T_c$  isotherm,  $g$  the gravitational acceleration,  $\nu$  the kinematic viscosity, and  $\kappa$  the thermal diffusivity), decreases from  $Ra_e \sim 10^3$  as the ice thickness increases in the freezing case (fig. 1(c), panels I-III), while increases to  $Ra_e \sim 10$  as the ice thickness decreases in the melting case (fig. 1(c), panels IV-VI). Throughout the process of melting and freezing, the thermal driving remains below the critical Rayleigh number ( $Ra_{cr}$  is  $\sim 2585$  in a laterally closed unit aspect ratio cell [29],  $\sim 1708$  in the laterally infinite RB system [30], and  $\sim 1493$  in a laterally infinite RB with linear buoyancy and melting [22]), and thus conduction holds [31]. Similarly, when the thermal driving

is strong, *i.e.*,  $T_b = 10^\circ\text{C}$ , (Regime-4, see fig. 1(e)), the estimated effective Rayleigh number is  $Ra_e \sim 10^7 \gg Ra_{cr}$  at the final equilibrium state, the turbulent developed convection state prevails both for the freezing and melting numerical experiments. However, freezing and melting behave differently in fig. 1(d) (Regime-3). For the freezing case, as the ice grows, the effective aspect ratio (*i.e.*,  $l_x/(h - h_i)$ ) of the fluid region increases, and thus the convective rolls self-organize into several smaller rolls and the  $Ra_e$  decreases accordingly, but the  $Ra_e$  is still  $\sim 4 \times 10^3 > Ra_{cr}$ , leading to retaining convection. While for the melting case, the system reaches an equilibrium when it is still in the conductive state.

Additionally, we explore the VC configuration in the same conditions. Differently from the RB case, the global ice thickness  $H_i$  always reaches the same final equilibrium independently of the initial conditions or independently of the history of the system (see the SM for the corresponding visualizations). In VC, the temperature gradient is perpendicular to the gravity, making the system thermally unstable for any temperature gap or  $Ra$ . This leads to the immediate breakdown of the stable stratification that is observed in the RB.

The bistability observed in the phase change RB can be quantitatively predicted by means of a one-dimensional heat flux model. This is as follows: We consider the system as the juxtaposition in series of compartments each one characterized by specific thermal properties (we neglect the curvature of the ice-water interface and the interface between the stably and unstably stratified layers). The system reaches an equilibrium state when there is heat flux balance among the conductive heat flux through the ice layer (denoted  $q_i$ ), the conductive heat flux through the stably stratified liquid layer ( $q_s$ ), and the either conductive or convective heat flux (depending on  $Ra_e$ ) of the unstably stratified layer ( $q_u$ ). Note that  $q_u$  exists only when  $T_b > T_c$ . The corresponding thicknesses for each layer are denoted as  $h_i$ ,  $h_s$ , and  $h_u$  (see fig. 2(a)). Depending on whether  $T_b$  is above  $T_c$ , two situations need to be considered: 1)  $T_b \leq T_c$ , the fluid layer is gravitationally stable, so the heat transfers diffusively both in the ice and water, so the definitions of the heat fluxes are  $q_i = k_i \frac{T_0 - T_i}{h_i}$  and  $q_s = k_w \frac{T_b - T_0}{h_s}$ , where  $k_i$  and  $k_w$  are the thermal conductivity of ice and water, respectively; 2)  $T_b > T_c$ , the density gradient takes opposite signs in the layers of temperature ranging from  $T_0$  to  $T_c$  (gravitationally stably stratified) and that ranging from  $T_c$  to  $T_b$  (gravitationally unstably stratified). The heat flux in the gravitationally unstably stratified layer can be predicted based on the relation of the effective Nusselt number,  $Nu_e$  (the dimensionless heat flux normalized by the diffusive heat flux based on the unstably stratified layer), and the  $Ra_e$ . So the definitions of the heat fluxes are  $q_i = k_i \frac{T_0 - T_i}{h_i}$ ,  $q_s = k_w \frac{T_c - T_0}{h_s}$ , and  $q_u = Nu_e k_w \frac{T_b - T_c}{h_u}$ , where  $Nu_e$  as a function of the  $Ra_e$  behaves as in the classical RB convection (as we already studied in [26]). In summary,

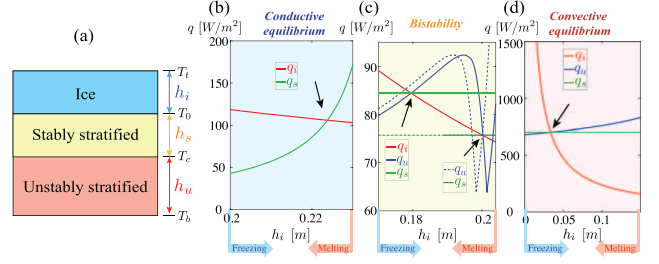


Fig. 2: Mechanism of bistability: (a) sketch of the one-dimensional model: three plane layers are connected in series. Note that if  $T_b < T_c$  the unstably stratified layer is absent; the computed heat fluxes across the cell as a function of the ice thickness,  $h_i$ , in the purely conductive regime (b), the bistable regime (c) and the convective one (d).

depending on the value of  $T_b$  the equilibrium condition reads:

*Case-1:*  $T_b \leq T_c$ . The system is in a conductive state and is independent of the water layer thickness, the heat flux balance reads

$$q_i = q_s. \quad (1)$$

From eq. (1) we obtain  $h_i = \frac{-k_i T_i}{k_w T_b - k_i T_t} h$ .

*Case-2:*  $T_b > T_c$ .

$$q_i = q_s = q_u. \quad (2)$$

From eq. (1) and eq. (2),  $h_i$  can be calculated which is reported in fig. 1(b). The theoretical prediction (dashed and thick lines) agrees well with the numerical simulation results (symbols). As  $T_b$  increases, the system experiences three regimes: 1) the equilibrium state is conduction independently of the freezing or melting initial system configuration (blue shaded area in fig. 1(b)); 2) the freezing case reaches the convective equilibrium state (dashed line in fig. 1(b)), while the melting case reaches the conductive equilibrium state, and this phenomenon is denoted by the bistability (yellow shaded area in fig. 1(b)); 3) the convective equilibrium is reached independently of freezing or melting (red shaded area in fig. 1(b)). This bistable regime which has been recently observed in numerical simulation of fluids with a linear buoyancy force [22], is here verified in the case of freezing pure water.

The one-dimensional model also allows us to understand which equilibrium state is reached depending on the initial conditions. This is illustrated in fig. 2, where we plot the values of the heat fluxes across the layers,  $q_i$ ,  $q_s$ ,  $q_u$  as a function of the ice thickness  $h_i$ . We note that in a freezing experiment  $h_i$  is initially null and shall grow till a matching of the fluxes is reached, and vice-versa, *i.e.*, in melting experiment  $h_i = h$  and decreases over time till the flux matching occurs. While the matching is unique in the Case-1 (fig. 2(b)) and for strongest convection (fig. 2(d)), the freezing front (bottom blue arrow) encounters first an equilibrium position with smaller  $h_i$  than the melting case (bottom red arrow) (fig. 2(c)) in the Case-2 with moderate thermal forcing.

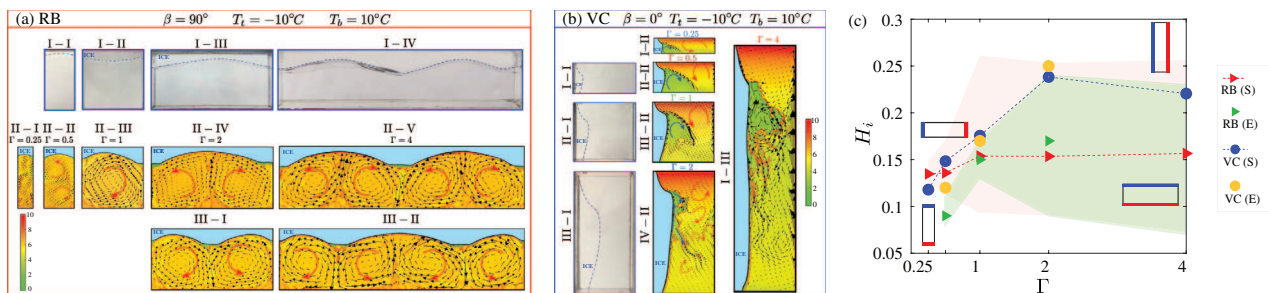


Fig. 3: Aspect ratio dependence. (a) The temperature field at the equilibrium state of the RB case. Panels I-I, I-II, I-III, and I-IV display the experimental results with  $\Gamma = 0.5, 1, 2, 4$ , respectively. Panels II-I, II-II, II-III, II-IV, and II-V display the simulation results, with  $\Gamma = 0.25, 0.5, 1, 2$ , and  $4$ , respectively. Panels III-I and III-II displays the simulation results for  $\Gamma = 2$  and  $4$ , same conditions as II-IV and II-V but with different ice front shapes. (b) The temperature field at the equilibrium state of the VC case. Panels I-I, II-I, and III-I display the experimental results with  $\Gamma = 0.5, 1, 2$ , respectively. Panels I-II, II-II, III-II, IV-II, and I-III display the simulation results, with  $\Gamma = 0.25, 0.5, 1, 2$ , and  $4$ , respectively. The visualizations of the temperature field in (a), (b) display  $T_0$  (black line) and  $T_c$  (red line) isotherms. (c)  $H_i$  as a function of  $\Gamma$  for RB and VC cases from simulations (S) and experiments (E). The shaded area shows the spatial variation of the ice front (from minima to maxima of  $h_i(x, t \rightarrow \infty)/h$ ) in the RB case for experiments (green) and simulations (red).

**Results: aspect ratio dependence.** – We now focus on the case of freezing of an initially liquid-filled cavity with large thermal driving (high  $Ra$ ). We perform both experiments and numerical simulations of the aspect ratio dependence in the RB and VC arrangements. The overall maximal variations of  $H_i$  for different  $\Gamma$  are modest ( $< 20\%$ ) for the RB case, while they can be large (up to  $200\%$ ) for the VC case. For the RB, it is observed that as  $\Gamma \geq 1$ , the global ice content nearly saturates (fig. 3(c)), and the only effect induced by larger  $\Gamma$  is that the number of the corresponding large-circulation convective rolls increases, with each roll of about unit width-to-height ratio (see the one, two, and four convective rolls for  $\Gamma = 1, 2, 4$ , respectively, in the visualizations of the temperature field from simulations in fig. 3(a) panels II-III, II-IV, and II-V). We also remark that the ice is locally flat in between the neighboring convective rolls, in correspondence to the position from which cold plumes detach. The characteristics of the ice front morphology are due to the shield of the stably stratified layer (with temperature ranging from  $T_0$  to  $T_c$ ). Firstly, acting as a buffer layer, the stably stratified layer is able to alleviate the effect of the hot plume impingement, creating a locally cold environment; secondly, at the edge of the two neighboring large scale rolls, the penetration from the unstably stratified layer does not occur, and this creates a locally quiescent region, contributing to the local flattening of the ice (however evident only in the simulations). Another interesting feature is that multiple forms of stable ice profiles can be observed corresponding to different convective states under the same external conditions: different convective roll directions give rise to different ice front shapes (fig. 3(a) panels II-IV *vs.* III-I, and panels II-V *vs.* III-II). This multistability (or bifurcation) of course already exists in the standard RB case where the flow can rotate either in one direction or in the opposite depending on initial tiny perturbations. When coupled with phase change, as the ice front reaches one of the shape forms, the flow is

locked to fit in with this specific shape, leading to a preferred direction of convective rolls. We have not observed large-scale circulation reversals in the system. In the current experiments, we have no control over the convective pattern, *e.g.*, we do not have a system to heat up the liquid locally. While in the simulations we can achieve the multiple equilibrium states by properly preparing the initial condition of the simulation. This interesting feature might be exploited in future experiments for flow control applications. On the other hand, when  $\Gamma < 1$  the system equilibrates at smaller  $H_i$ . In these geometrically confined cases ( $\Gamma = 0.25$  and  $0.5$ ), several convective rolls stacked upon each other penetrate the stably stratified layer and finally affect the ice front (fig. 3(a), panels II-I and II-II). Note that the  $H_i$  from the simulations and the experiments agree well with each other except for very small  $\Gamma$ , which is presumably because of the stronger influence from the external environment in the experiments due to the larger area of the sidewalls.

For the VC cases (fig. 3(b)), independently of  $\Gamma$ , the robust ice front morphology due to the ubiquitous presence of two counter-rotating convective rolls is observed, which is unique to the system with density anomaly working fluids [25]. One roll originates from the cold upward convective current along the ice front (visualized by the blue arrow in fig. 3(b)); the other results from the hot plumes detaching from the hot plate (visualized by the red arrow in fig. 3(b)). The competition between these two rolls creates the ice front morphology under different aspect ratios. As  $\Gamma$  increases, the interplay between these two convective rolls intensifies, leading to highly mixing of the colder and warmer fluids, as corroborated by the highly uneven  $T_c$  isotherm in fig. 3(b). At  $\Gamma = 4$ , along the wide extent of the ice front, the penetration of the hot plumes impingement can even modify the local shape of the ice front. The global ice thickness first increases a bit with increasing  $\Gamma$ , and then at large  $\Gamma$ ,  $H_i$  has a much weaker dependence of  $\Gamma$  (fig. 3(c)). Note that we do not perform simulations for



the aspect ratio ranging of  $\Gamma < 0.25$  or  $\Gamma > 4$ , the reasons are 1) for even smaller  $\Gamma$ , multiple modes of convective roll configuration are observed in the classical RB as a consequence of the elliptical instability [32], and 2) for much larger  $\Gamma$ , the simulations are quite expensive to carry out. Future work is required to map out a more comprehensive picture of the aspect ratio dependence, with possible extensions to three-dimensional geometries.

As observed above, the VC cases present robust forms of the ice front morphology due to the presence of two counter-rotating convective rolls. We measure the ice front shape for different aspect ratio cases and we superpose them in a single figure (fig. 4(a)). The ice front morphology is similar particularly at the bottom of the cell. To understand this feature, we use the theoretical model proposed in [25] based on the concept of developing boundary layer (BL). Here we only briefly sketch the model assumptions and its construction. Although phenomenologically, it puts forward the physical mechanism that dominates the form of the ice front. It can be observed that there is a recirculating region induced by the upward convective currents adjacent to the ice (with temperature ranging from  $T_0$  to  $T_c$ , blue arrow in fig. 3(b)). This recirculating region can be separated into the thermal BL along the ice front (orange area in fig. 4(b)) and the main flow region (light red area in fig. 4(b)). When the system reaches an equilibrium, there exists a balance between the heat flux through the BL and that through the ice. A curvilinear coordinate,  $S(x)$ , is introduced to measure the length of the ice front starting from its boundary point at  $x = 0$ , and  $S(x) = \int_0^x \sqrt{1 + \left(\frac{d(h_i(\xi))}{d\xi}\right)^2} d\xi$ . The BL thickness is  $\delta_T(S)$ , which is a function of  $S$ , measured normal to the ice front (see fig. 4(b)). To analyze the heat flux across the ice and the thermal boundary layer, we make the following approximations. For the ice layer, the temperature gradient normal to the ice front in the ice layer can be approximately estimated by  $h_i(x)/\frac{dS(x)}{dx}$  (a detailed explanation for this expression is provided in the SM); for the thermal boundary layer, which is still nested inside the viscous boundary layer ( $Pr \approx 11$ ), the heat transfer normal to the ice front in the BL is mostly conduction [33]. The heat flux balance in the direction normal to the ice surface can be expressed as,  $k_i \frac{(T_0 - T_i)}{h_i(x) \frac{dS(x)}{dx}} = k_w \frac{(T_m - T_0)}{\delta_T(S(x))}$ .  $\delta_T(S)$  is assumed to be  $\delta_T(S) = C_1(S + C_2)^{1/4}$  in which there are two parameters  $C_1 = c \cdot (g[1 - \rho(T_m)/\rho_c]/(\nu\kappa))^{1/4}$  with  $c$  the proportional constant ( $c \approx 5$ ), and the offset  $C_2$  because of non-zero boundary layer thickness at  $x = 0$ , with  $C_2 = (h_i(0)[k_w(T_m - T_0)]/[k_i(T_0 - T_i)]/C_1)^{1/4}$  [34–36]. Figures 4(c)–(g) show the comparison of the ice front morphology from the experiments (blue shaded area), numerical simulations (green line), and the theoretical model (red line). A good qualitative agreement is reached at the bottom of the ice front, indicating that the exact form of the ice front is indeed the thermal boundary layer dominated. The ice front morphology from the numerical simulation and from the experiment is slightly different when the

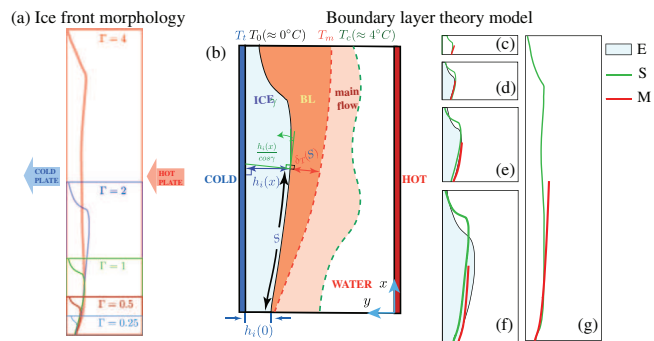


Fig. 4: Ice front shape boundary layer based model. (a) Ice front morphology at the statistical equilibrium in VC as extracted from the numerical simulation with aspect ratio,  $\Gamma = 0.25$  (light blue line),  $0.5$  (red line),  $1$  (green line),  $2$  (dark blue line),  $4$  (orange line). The system is cooled at the left side and heated at the right side. (b) Sketch of the phenomenological BL model: the ice front at  $T_0 = 0^\circ\text{C}$  (black line), the  $T_m$  isotherm which is the outer boundary of the thermal boundary (red dashed line), the  $T_c$  isotherm (green dashed line). The angle between the tangential direction of the ice front and the  $x$ -direction is  $\gamma$ ; the thickness normal to the ice front (the green thick line in the ice) is  $\frac{h_i(x)}{\cos \gamma}$  (with  $\cos \gamma = \frac{dS}{dx}$ ). (c)–(g) Comparison of ice front morphology between experiments (blue shaded area), simulations (green line) and the model (red line) for  $\Gamma = 0.25$  (c);  $0.5$  (d);  $1$  (e);  $2$  (f);  $4$  (g).

aspect ratio is large (fig. 4(f) and (g)), which is possibly because near the large extent of the ice front, the mixing behavior between the colder (with the temperature from  $T_0$  to  $T_c$ ) and the warmer (with the temperature from  $T_c$  to  $T_b$ ) convective rolls intensifies, which is attested by the highly irregular  $T_c$  isotherm in fig. 3(b)IV-II, and I-III.

**Conclusion and perspectives.** – We have explored the equilibria of icing water in a differentially heated cavity by means of laboratory experiments, numerical simulations, and (phenomenologically) theoretical modeling. We showed through simulations that the effect of the initial conditions, either fully liquid or fully solidified, can lead to different equilibria, a phenomenon only observed for the RB arrangement of the system in the moderate thermal stratification case (Regime-3) and not in the VC case. We have also introduced a simple one-dimensional model that in part relies on the known heat flux scaling relation in the RB system without melting, which is capable of predicting the multiplicity of equilibria in the system and their occurrence depending on the initial condition of the numerical experiment. In the VC configuration, the system reaches the same equilibrium state independently of the system's initial condition, and this is due to the intrinsic thermal instability of this configuration, which displays convection for every Rayleigh number different from zero.

Secondly, we have studied experimentally and numerically the dependence of the ice front morphology on the  $\Gamma$  aspect ratio in the freezing case for the RB and VC. It was shown that for  $\Gamma \geq 1$  in the RB case, the global ice thickness is nearly independent of  $\Gamma$ . The ice front

displays large wavelength modulations and presents a local flatness in between neighboring convective rolls. Multiple forms of the ice front morphology can be observed under the same external conditions: different convective roll configurations lead to different ice front shapes. Once the system reaches a specific ice front shape, the convective roll appears locked in a certain direction. This multi-stability behavior provides possibilities for flow control to maintain desirable flow structures or solid-fluid interfacial morphology. For the VC case, despite the major differences in the global ice extension as compared to RB, a robust form of the ice front morphology can be observed at all  $\Gamma$ . Such interfacial form is due to the presence of two counter-rotating convective rolls and is dominated by a developing boundary layer in the upward direction.

We hope that both the methodology of the present study on water melting/freezing in idealized conditions and its findings will stimulate further investigations. More complex natural and industrial phenomena are still challenging because many crucial factors should be considered, *e.g.*, the effect of persistent shear flows [23,37,38] or induced by rotation [39], the concentration gradients of solute components, and the extremely high pressure in deep water body environments, which are of great relevance for the appropriate modeling of geophysical and climatological processes.

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*Data availability statement:* All data that support the findings of this study are included within the article (and any supplementary files).

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