Three-dimensional Rayleigh-Bénard instability in a supercritical fluid
by direct numerical simulation

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An experimental observation by Nitsche & Straub in 1987 initially showed a fast thermal equilibrium in the absence of convection in supercritical fluids (SCF). This phenomenon termed as the ‘piston effect’ (PE), was predicted theoretically in 1990 by Boukari et al., Onuki et al., and Zappoli et al. In the past ten years, most of the attention was devoted to the interaction between the PE and natural convection. Experimental investigations in the Rayleigh-Bénard configuration revealed the development of a convective instability near critical conditions. Direct numerical simulations (DNS) of 2D Navier-Stokes equations contributed to the understanding of the hydrodynamic behaviour of such complex flows. The continuation of previous works led us to extend DNS to fully three-dimensional cases [1].

A SCF is enclosed in a cubic shape box, heated from below, and subjected to the earth vertical gravitational field $g$ (Fig. 1). Initially, the fluid is in thermodynamic equilibrium at constant temperature $T_i$ slightly above its critical temperature $T_c$ such that: $T_i = (1+\varepsilon)T_c$, where $\varepsilon < 1$. The fluid is stratified in pressure and density, with a mean density equal to its critical value $\rho_c$. Numerical simulation starts with the application of a progressive weak heating ($\Delta T \sim$ few mK) to the bottom box wall, while maintaining the upper one at its initial temperature $T_i$. The mathematical model for a SCF flow is described by the Navier-Stokes and energy equations written for a van der Waals fluid. We consider the $CO_2$ critical coordinates ($T_c=304.13K$, $\rho_c=467.8Kg.m^{-3}$) and transport properties, and the simulations were carried out for $T_i - T_c = 1K$. The governing equations are solved using a finite-volume method, second order accurate in space and third order in time.

![Figure 1. SCF in the Rayleigh-Bénard configuration, with no-slip walls and insulated vertical ones.](image)

Bottom heating induces a wall temperature gradient and the development of a thin thermal boundary layer along the hot wall. This boundary layer expands upward, compressing adiabatically the rest of the fluid, and leading to a fast and homogeneous heating of the cavity bulk by thermoacoustic effects (PE). Since the top wall temperature is maintained at its initial value, a cold boundary layer settles near the top wall. In this PE-dominated phase, the flow is divided into three distinct zones: two thermal boundary layers along the horizontal walls and the cavity bulk.

As long as the flow in the boundary layers is dominated by the diffusion, the thermal boundary layers grow in time at heat diffusion speed. This thermal expansion is hindered by the density stratification of the fluid, leading to a well-known situation ending with a convective instability when the local Rayleigh number exceeds a critical value. Owing to the divergence of the isothermal compressibility of the SCF, the classical Rayleigh criterion includes a stabilizing contribution, the Schwarzschild criterion
usually encountered in atmospheric sciences for large air columns. We recently showed that this stabilizing effect can lead to a reverse transition towards a stable state [2].

Figure 2-a illustrates the convection onset: convective plumes rise from both thermal boundary layers; the space distribution of these structures in the (x,y) plane seems to match the squared geometric shape. In figure 2-b, temperature field is subjected to radical changes: on the top wall, a circular distribution of the thermal plumes is observed, while on the bottom wall, some convective structures take vertical fin shapes. In figure 2-c, these new shapes are more localized on the bottom wall and spread on the insulated walls leaving flat zones where convective plumes rise, are pinched off, and release thermal balls floating upwards, leaving horn-like shafts. The convective improvement of the heat transfer between the isothermal walls and the cavity bulk leads to the faster temperature equilibrium in the whole cavity.

![Figure 2](image2.png)

Figure 2. Instantaneous temperature fields for $\Delta T=1mK$, exhibiting the three-dimensionality of the flow. From (a) to (c), $t = 22.6s, 36.9s, 63.1s$, and the shaded isotherms of $(T-T_i)$ in $mK$ are respectively: (0.4,0.6), (0.44,0.6), (0.37,0.65).

Figure 3 shows a comparison of the temperature patterns obtained for three values of heating $\Delta T=0.5mK, 2.5mK$, and $5.0mK$. A stronger heating increases the number of the convective plumes while reducing their space scales. As the heating increases, the convective instability is released earlier, starting always with an organized space distribution in the horizontal plan that matches the squared geometric shape.

![Figure 3](image3.png)

Figure 3. Heating effects on the instantaneous temperature field. From left to right, $\Delta T=0.5mK, 2.5mK, 5.0mK$; $t=45.3s, 16.7s, 11.4s$; and the shaded isotherms of $(T-T_i)$ in $mK$ are respectively: (0.2,0.3), (1.0,1.5), (2.2,3.2).
