Chapter 2
Numerical Modelling of Hydrodynamic Instabilities in Supercritical Fluids

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ABSTRACT

The case of a supercritical fluid heated from below (Rayleigh-Bénard) in a rectangular cavity is first presented. The stability of the two boundary layers (hot and cold) is analyzed by numerically solving the Navier-Stokes equations with a van der Waals gas and stability diagrams are derived. The very large compressibility and the very low heat diffusivity of near critical pure fluids induce very large density gradients which lead to a Rayleigh–Taylor-like gravitational instability of the heat diffusion layer and results in terms of growth rates and wave numbers are presented. Depending on the relative direction of the interface or the boundary layer with respect to vibration, vibrational forces can destabilize a thermal boundary layer, resulting in parametric/Rayleigh vibrational instabilities. This has recently been achieved by using a numerical model which does not require any equation of state and directly calculates properties from NIST data base, for instance.

INTRODUCTION

Hydrodynamics of near-critical fluids have gained considerable interest since the identification of the thermo-acoustic effect which is responsible for the fast thermal equilibration of a cell heated on one boundary (Zappoli *et al.*, 2015). Transport coefficients exhibit strong deviations near the critical point (Zappoli *et al.*, 2015; Stanley, 1971). Near-critical fluids are characterised by a large density like a liquid and a low viscosity and a high compressibility like a gas. Their thermal diffusivity goes to zero whereas the isothermal compressibility (and on the same way the heat capacity at constant pressure and thermal expansion) diverge.

Over the past several decades, there has been a growing demand for supercritical fluids in industrial applications as varied as alternative eco-friendly refrigerants, cold energy storage of Liquefied Natu-

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ral Gas (LNG) (Nakano & Shiraishi, 2004), superconducting magnet cooling (Dobashi *et al.*, 1998), chemical extraction/separation processes (Peter *et al.*, 2007), supercritical chromatography, drying and catalysis. In space, in the absence of gravity effects, the behaviour of fluids is markedly different than on earth. The management of fluids in such conditions (flow control, heat exchange, etc.) is often a challenge and "artificial" gravity can be looked for. It happens that fluids submitted to vibrations of "high" frequency, e.g. frequency larger than the inverse hydrodynamics times (typically thermal diffusion and viscous dissipation times) and "low" amplitude (e.g. amplitudes smaller than the sample size) exhibit convective flows that are similar to buoyancy flows under earth gravity. The interest of studying fluids in such conditions is manifold. Firstly, supercritical oxygen, hydrogen, and helium are already used by the space industry. Secondly, their high compressibility and slow dynamics (critical slowing down) emphasize the behavior encountered in regular fluids. Thirdly, fluids in such conditions obey universal, scaled power laws, valid for all fluids.

We present here an overview of thermal Rayleigh-Bénard (Amiroudine *et al.*, 2001; Chiwata&Onuki, 2001; Meyer&Kogan, 2002), Rayleigh-Taylor (Amiroudine *et al.*, 2005; Boutrouft *et al.*, 2006) and thermo-vibrational (parametric, Rayleigh-vibrational (Amiroudine&Beysens, 2008; Gandikota *et al.*, 2013)) instabilities in near-critical fluids. The cases of Rayleigh-Bénard and Rayleigh-Taylor instabilities will be briefly presented and more emphasis will be considered on Rayleigh-vibrational instabilities.

The case of a supercritical fluid heated from below (Rayleigh-Bénard configuration) in a rectangular cavity is first presented. Owing to the homogeneous thermo-acoustic heating (piston effect), the thermal field exhibits a very specific structure in the vertical direction. A very thin hot thermal boundary layer is formed at the bottom, then a homogeneously heated bulk settles in the core at a lower temperature; at the top, a cooler boundary layer forms in order to continuously match the bulk temperature with the colder temperature of the upper wall. We analyze the stability of the two boundary layers (hot and cold) by numerically solving the Navier-Stokes equations with a van der Waals gas and slightly above its critical point. A Finite-Volume method is used together with an acoustic filtering procedure. The onset of the instabilities in the two different layers is discussed with respect to the results of the theoretical stability analyses available in the literature and stability diagrams are derived.

The stability analysis of a two-layer fluid system (Rayleigh-Taylor like instabilities) is then developed. The very large compressibility and the very low heat diffusivity of near critical pure fluids induce very large density gradients which lead to a Rayleigh–Taylor-like (RTL) gravitational instability of the heat diffusion layer when the top layer temperature is some milli-Kelvin cooler than the bottom one. This instability in a one-phase fluid seems to be similar to that which occurs in between two miscible liquids where the species diffusion is replaced by the heat diffusion coefficient. We find that this RTL configuration becomes stable when the heat diffusion length, on the time scale of the faster unstable mode, becomes larger than the bottom hot layer thickness.

Finally thermovibrational instabilities will be presented at the end with a new approach for the calculation of the density. It was indeed surprisingly observed in several terrestrial and weightless experiments that a destabilization of thermal boundary layers occurred when the fluid was vibrated. The interaction of a thermal boundary layer (TBL) with vibration is a stimulating problem of fluid physics. Depending on the relative direction of the interface or the boundary layer with respect to vibration, vibrational forces can destabilize a TBL, resulting in parametric / Rayleigh vibrational instabilities. Till now, the mathematical model has assumed a van der Waals state equation or a linear equation of state being valid near the critical point. This poses limitations on the quench (or heating) conditions and a more sophisticated numerical and mathematical model is further detailed. The evaluation of the effect