RAYLEIGH-TAYLOR LIKE INSTABILITY

IN NEAR CRITICAL PURE FLUIDS[1]

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[1] Paper presented at the Thirteenth Symposium on Thermophysical Properties, June 22-27, Boulder, Colorado, U.S.A.

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ABSTRACT

The hydrodynamic stability of a thermodiffusive interface in near supercritical fluid is studied. The Navier Stokes equations written for a van der Waals gas set above its critical point are solved by the means of a finite volume numerical method. The growth rate of the fluctuations shows that it exists a cutoff wave number beyond which the short wave lengths are stabilized by diffusion. The good agreement between the obtained values and the recent theories for miscible fluids confirms that a near critical fluid subjected to a thermal gradient may develop a gravitational instability for which the density gradient is driven by thermal diffusion and high compressibility.

KEY WORDS: supercritical fluids, Rayleigh-Taylor instability, numerical hydrodynamics, finite volume methods.

1. INTRODUCTION

The week diffusivity of near critical pure fluids and their large compressibility lead to very specific mechanisms of thermal homogenization. The Piston Effect which is of thermoacoustic nature allows for a very fast thermal homogenization under zero gravity conditions although the thermal diffusivity is very small. [1], [2], [3],[4],. Under normal gravity conditions and for a side heated square-shaped cavity we have recently shown that this mechanism is still responsible for heat equilibration [5]. We are interested here to a different situation although it is also linked with the storage of cryogen's and more generally to the stability of diffusion fronts in miscible fluids. When one performs the numerical modeling of a bottom-heated cavity filled with a supercritical fluid (Rayleigh-Benard configuration), the lateral walls of which are insulated, while the top wall is thermostated at the initial temperature, thermal plumes are forming over the bottom wall. As the bulk is homogeneously heated by the Piston Effect, a cooling thermal boundary layer forms along the upper wall [6]. This layer of fluid is heavier than the fluid located below and gives thus birth to droplets as shown in Fig. 1. The mechanism of formation of these droplets looks like a Rayleigh-Taylor instability. We thus oriented our investigations towards a diffusion front instability, analogous to the one encountered in miscible fluids [7], [8], [9], [10],. We have considered a simpler situation (see Fig. 2) in which the upper half part of a square-shaped isobaric cavity of infinite extension filled with a near supercritical fluid at rest is some mK cooler than the bottom half part. The top and bottom walls are at constant initial temperature. This work aims to perform the numerical stability study of the thermal diffusion interface which is present

between the two half parts of the cavity. To this end we use the technique which consists in studying the dynamics of growth of fluctuations of a fluid property at the interface.

2. MATHEMATICAL MODEL

The model is identical to the one used in [5], and is merely repeated here. The Navier Stokes equations are those describing a Newtonian, viscous and hypercompressible pure fluid. The equation of state is the van der Waals equation. Pressure is normalized with respect to the one that would exist for an ideal gas at critical conditions. The other variables are referred to their critical value. The characteristic time is taken as the Piston Effect characteristic time (which is between the acoustic and the diffusion times) (see ref. [5]). The governing equations thus write under the following form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad (1)$$

$$\frac{D(\rho \mathbf{v})}{Dt} = -\gamma^{-1} \nabla P + \varepsilon \left[\nabla^2 \mathbf{v} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{v}) \right] + \frac{1}{F_r} \rho \mathbf{g} \qquad (2)$$

$$\frac{D(\rho T)}{Dt} = -(\gamma - 1)(P + a\rho^2)(\nabla \cdot v) \frac{\varepsilon \gamma}{P_r} \nabla \cdot [\lambda \nabla T] + \Phi \qquad (3)$$

Where $\Phi = \varepsilon \gamma (\gamma - 1) \left[v_{i,j} v_{j,i} + v_{i,j} v_{i,j} - \frac{2}{3} v_{i,i} v_{j,j} \right]$ is the viscous dissipation rate, ε is a small parameter defined by $\varepsilon = P_r t_a^{'} / t_d^{'}$ where $t_d^{'}$ is the characteristic heat diffusion time for the ideal gas and $t_a^{'}$ the characteristic time of acoustic phenomena. The quantity P_r is the Prandtl number for an ideal gas and F_r the acoustic Froude number. The following transport coefficient are considered:

$$\lambda = 1 + \Lambda (T - 1)^{-0.5}; \quad C_v = 1; \quad \tilde{\mu} = 1$$

where λ, C_v et $\tilde{\mu}$ are respectively the heat conductivity, the specific heat at constant volume and the dynamical viscosity reported to their ideal gas value. Those expression of course do not describe the real critical behavior of a critical fluid but correspond to a mean field theory which is correct enough to study phenomenology and not to perform quantitative comparisons with experimental results.

The van der Waals equation write under the following non dimensional form:

$$P = \frac{\rho T}{1 - b\rho} - a\rho^2 \qquad (4)$$

where a=9/8 et b=1/3 are given by the expression of the critical coordinates.

The fluids is initially at rest and stratification is neglected since the distance to the critical point is not smaller than 1 K. The initial conditions for the upper layer are:

$$\begin{cases} \rho_1 = 1; \quad T_1 = 1 + \Delta T,\ P_1 = b(1 + \Delta T) - a \\ \qquad\qquad u = v = 0 \end{cases} \qquad for \quad y \in [0.5,1]$$

where $\frac{T_1^{'} - T_c^{'}}{T_c^{'}} = \Delta T << 1$, $T_1^{'}$ et $T_c^{'}$ are respectively the initial and critical temperatures, while the variables with prime are dimensional ones. For the lower layer the initial conditions are such that density is given while temperature is determined in such a way pressure is homogeneous within the whole cavity:

$$\begin{cases} \rho_2 = 1 - \Delta\tilde{\varepsilon}; \quad T_2 = \left[\frac{\rho_1 T_1}{1 - b\rho_1} + a\left(\rho_2^2 - \rho_1^2\right)\right]\frac{(1 - b\rho_2)}{\rho_2}; \quad P_2 = P_1 \\ \qquad\qquad u = v = 0 \end{cases} \qquad pour \quad y \in [0,0.5]$$ whe

re $\Delta\tilde{\varepsilon}$ corresponds to the given density difference between the two layers. On the horizontal wall, the following boundary conditions are considered:

$$\begin{cases} u = 0; \quad v(x,0,t) = v(x,1,t) = 0 \\ T(x,0,t) = T_2; \quad T(x,1,t) = T_1 \end{cases}$$

For the lateral walls, periodic boundary conditions are considered, i.e. for any field variable ϕ (Temperature, velocity) the following relation still holds at any times:

$$\phi(0, y, t) = \phi(\tilde{\lambda}, y, t)$$

where $\tilde{\lambda}$ represents the wave length of the initial perturbation the dynamics of which is aimed to be studied. When the thermal constraint is suppressed, thermal diffusion which is the driving force of the evolution begins to operate. As density is related to temperature via the equation of state, a diffusive interface forms which is similar to the one which would form between two miscible liquids. The fluctuations the dynamics of which is to be studied are introduced under the form of an initial non zero velocity written as:

$$v(x, y = 0.5, t = 0) = A\cos\left(\frac{2\pi}{\tilde{\lambda}} x\right)$$

Where A is the amplitude of the perturbation (A= 10^{-2}).

3. THE NUMERICAL METHOD

the governing equations are discretized by a finite volume method and a SIMPLER type algorithm [11], [12] is used to solve the obtained system. The numerical scheme is of first order in time and the discretisation in space uses Patankar's power lower scheme. A non uniform staggered grid is used to take into account the presence of huge initial gradients at the interface. The grid is uniform in the x direction. The acoustic filtering procedure is used to reduce computational cost [5], [12], because the calculations are performed on the Piston Effect time scale : on that time scale, the pressure can be separated into two parts [13], one which is homogeneous plus a small non homogeneous acoustic perturbation which can be filtered at first order. The dynamic of growth of the fluctuations, that is to say the determination of rate of growth $\sigma(k)$, where k is the wave number of the initial perturbation, is determined in the following way: after sampling two values of a field variable (the velocity for instance) at a grid

point for two different times t_1 et t_2, one determine $\sigma(k)$ in writing that the velocity depends exponentially on time that is to say that:

$$\begin{cases} v_1 = A_1 e^{\sigma t_1} \\ v_2 = A_2 e^{\sigma t_2} \end{cases}$$

from which one can extract $\sigma(t, k)$ from:

$$\sigma = \frac{Ln\left(A_1 / A_2\right)}{t_1 - t_2}$$

The value of $\sigma(k)$ which corresponds to the linear regime under study is considered to be the one corresponding to the plateau zone of the time history of $\sigma(t)$ for which A_1 and A_2 do not depend on time.

4. RESULTS AND DISCUSSION.

The calculations are performed for a cavity filled with CO_2 at critical density the temperature of the upper part of which is 1K above the critical temperature. This value determines the value of the transport coefficients, the other variations being only perturbations. The density difference between the upper and the lower parts of the cavity is directly related to the temperature difference and compressibility. Two non dimensional density differences are studied, 10^{-2} and 10^{-3}, that correspond respectively to temperature differences of 15.2 and 1.49 mK. The values of the kinematic viscosity and thermal diffusivity at 1 K above the critical point are respectively $\nu = 4{,}48\ 10^{-4}$ cm²/s and $\kappa = 0.86\ 10^{-4}$ cm²/s.

The values of $\sigma(k)$ are reported on Fig. 3. One can point out first that it exists a cutoff wave number beyond which the small wave lengths are damped by diffusion. This

is agreement with the conclusions of recent works [7], [9], [14], following which taking into account both viscosity and diffusion make it necessary for a cutoff wave number to be put in evidence which is equal to:

$$\tilde{\lambda}_c = 2\pi\left(\frac{16\,\nu\,D}{3\,g\,R}\right)^{1/3} \quad \text{from [9]}$$

where D is the interdiffusion coefficient for miscible fluids (which is replaced in our case by the thermal diffusion coefficient), g the gravity value and $R = \dfrac{\rho_1 - \rho_2}{\rho_1 + \rho_2}$.

Table 1 compares the cutoff values obtained by the present numerical simulations with the one deduced from the abovementioned formulas.

Fig. 4 shows the temperature field at a given time (t'= 1 s) for an initial perturbation wavelength $\tilde{\lambda}$=0.1 that gives a high growth rate. It must be emphasized here that the values of the Schmidt number for the critical fluid is of order 10 whereas it is of order 10^3 for usual miscible liquids. This is due to the strong decrease of the kinematic viscosity, the thermal diffusivity of the critical fluid, although weak for a gas, being two orders of magnitude higher that mass diffusion in miscible liquids. The length scale associated with the micro-drops formed by the instability is thus small and it appears that the thermal homogenization process of a supercritical fluid on ground may undergo a micro mixing phase: micro-drops are formed that then relax by diffusion. The measured homogenization time may thus appear much smaller than the one calculated on the cell length scale. The present calculations have to be completed now by a systematic study as a function of the distance to the critical point as well as by a linear stability analysis.[15]

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FIGURE CAPTIONS.

Table 1 : Cutoff wavelength as a function of the density difference.

Figure 1 : Temperature difference ($T'-T'_0$) in K for a square-shaped cavity heated from below initially at 1K from the critical point and 8.3 s after a 10 mK increase in temperature, from Ref. [6].

Figure 2 : The 2-D Model.

Figure 3 : Instability growth rate as a function of the wave number for $\Delta\rho$= 0.01 (4.678 Kg/m^3) and $\Delta\rho$ = 0.01. (the initial temperature is 1K above the critical point).

Figure 4 : Temperature difference 1 s after the thermal constrainst has been suppressed (the wave length of the initial perturbation is $\tilde{\lambda}'$=1 mm).

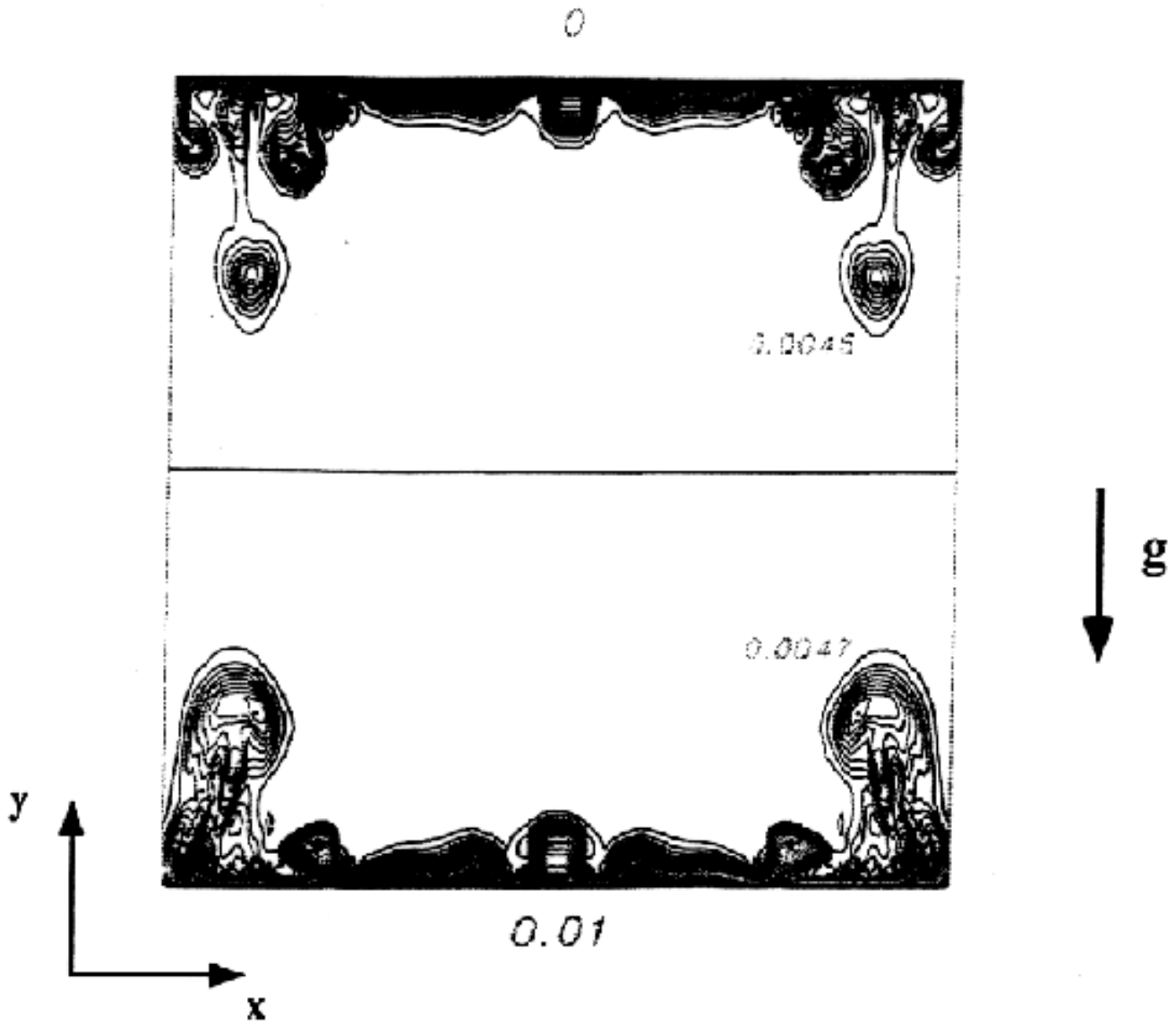

Figure 1 :

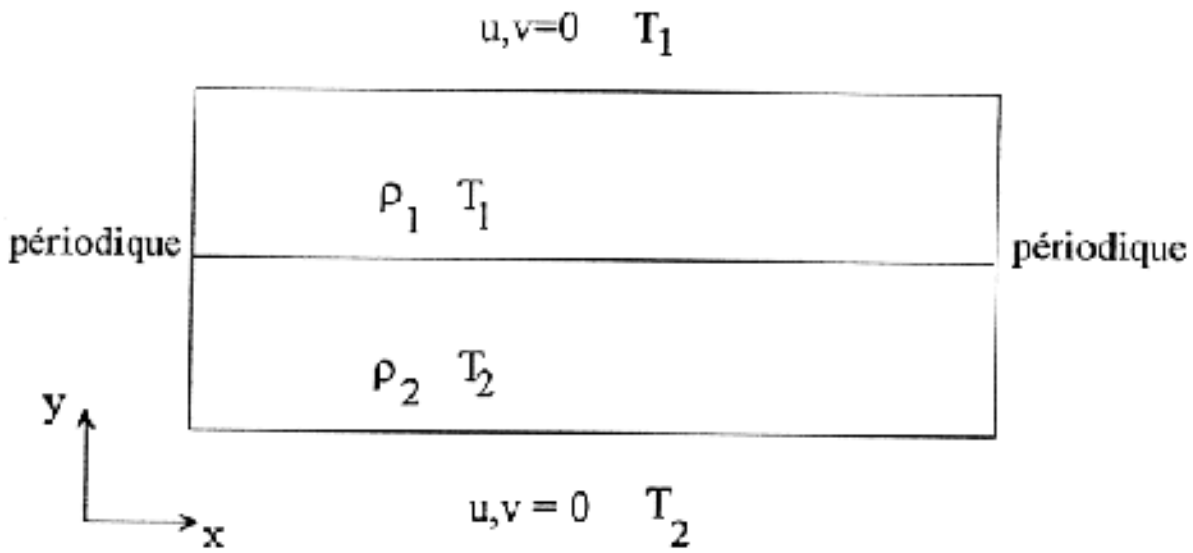

Figure 2

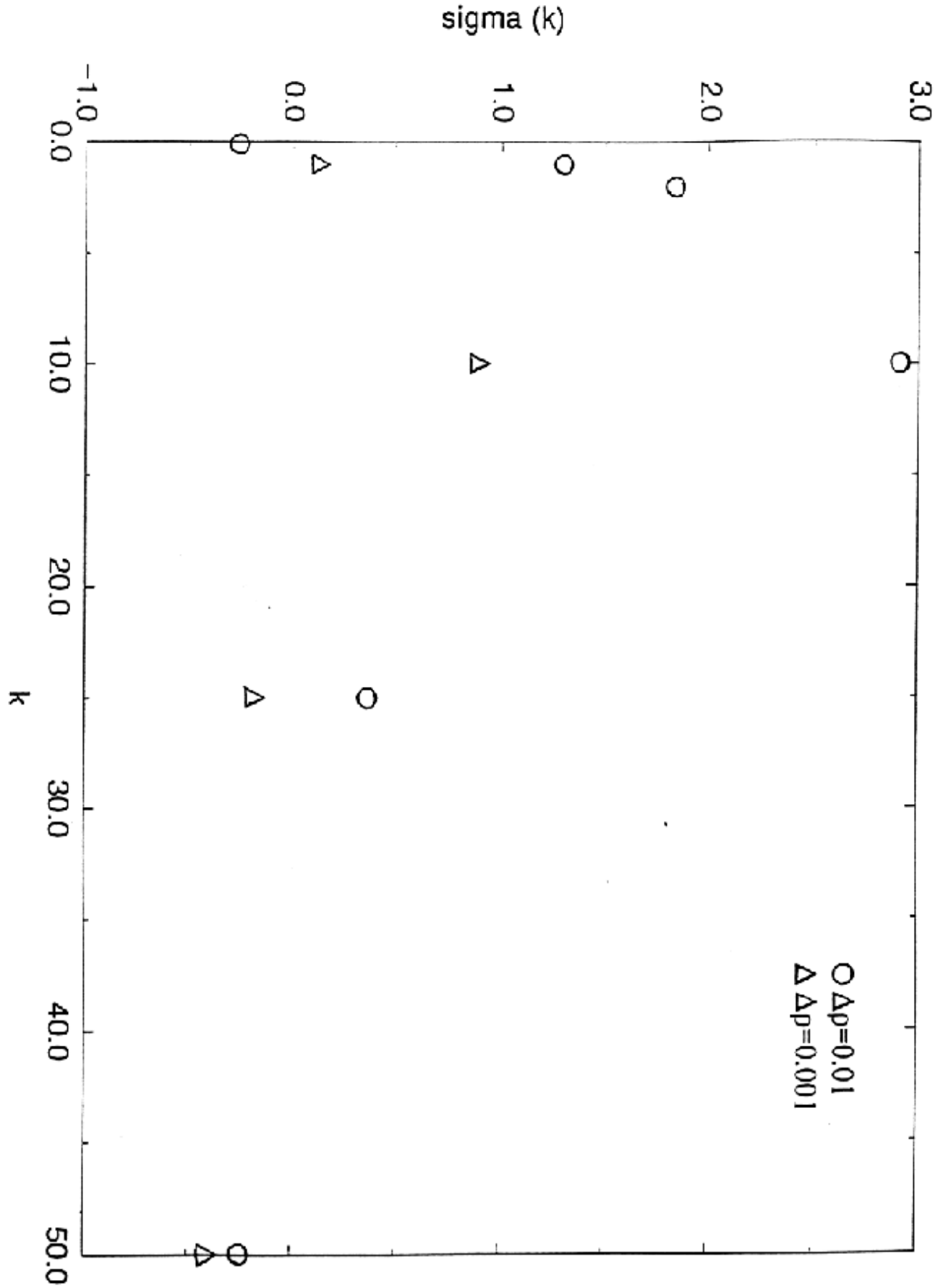

Figure 3

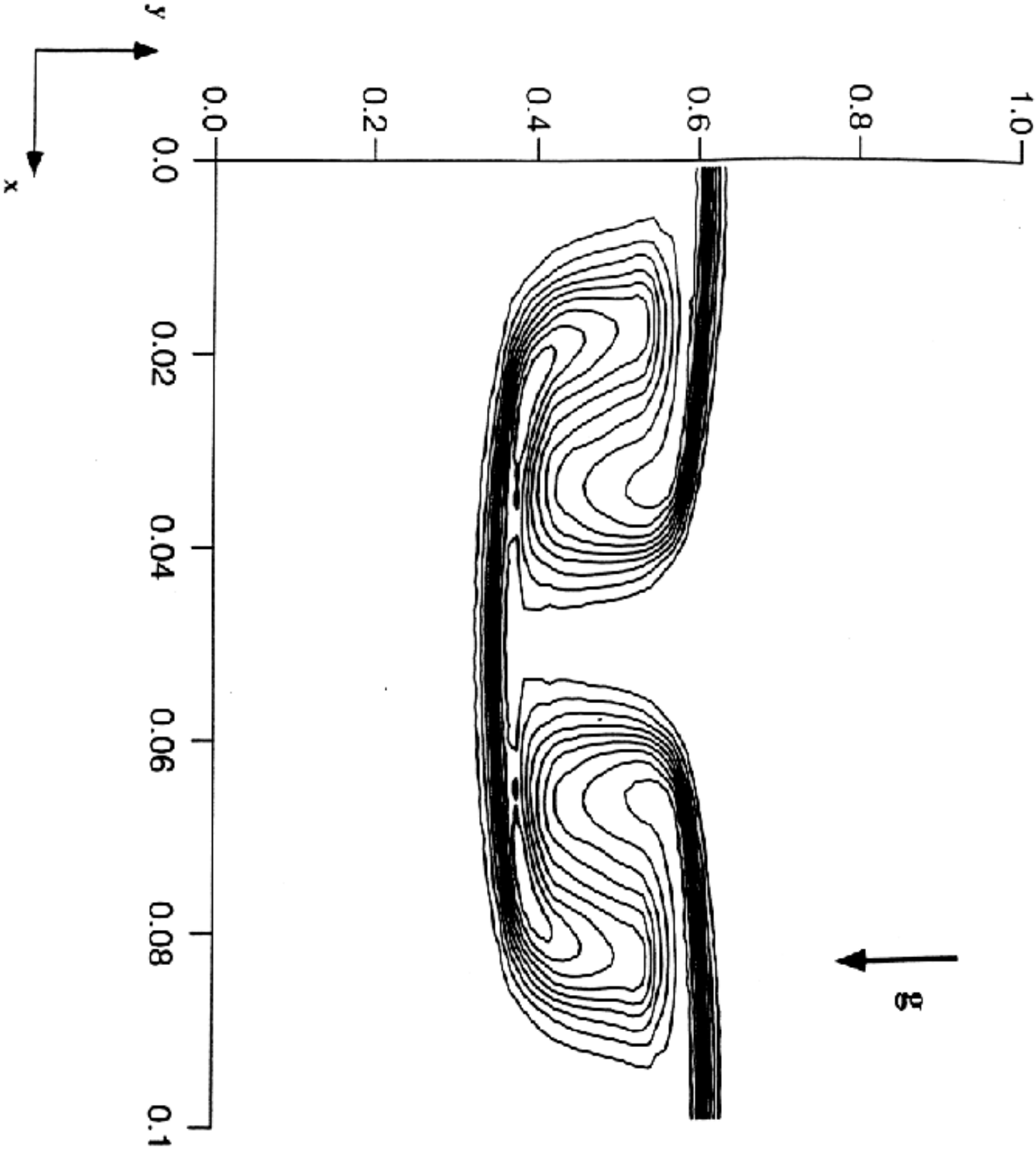

Figure 4 :