Phase transition induced hydrodynamic instability [*]

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Instabilities leading to oscillations in some particular properties of a system are intimately related to pattern formation. Nontrivial patterns form spontaneously as a result of the occurrence and propagation of the fronts of instability. These spontaneous patterns can be turned into functional structures at the corresponding length scale when the pattern forming processes are properly designed and controlled. In this work, we propose a scenario for mass transfer instability in a one dimensional flow of a one-component fluid near its discontinuous liquid-gas phase transition. Instability leading to density oscillations occurs when the system fails to support steady-state flow due to the absence of mechanically stable uniform state as a consequence of a discontinuous transition. The phenomenon can be useful in patterning thin films and may play a role in the formation of nanoscopic channel during an unstable Langmuir-Blodgett transfer reported in recent experiments [1].

We consider a one-dimensional compressible flow described by the continuity equation and the Navier-Stokes equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0, \tag{1}$$

$$\rho\left(\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x}\right) = -\frac{\partial P}{\partial x} + \eta\frac{\partial v^2}{\partial x^2}, \tag{2}$$

where ρ is the density, v is the velocity and η is the viscosity. The main feature of the system is contained in the quantity P, the local pressure of the inhomogeneous fluid. It is expressed as [2]

$$P = \rho\frac{\delta\Psi[\rho]}{\delta\rho} - \psi(\rho) + \frac{\kappa}{2}\left(\frac{\partial\rho}{\partial x}\right)^2, \tag{3}$$

which is also the equation of state of the fluid. Here, the quantity $\Psi[\rho]$ denotes the Helmholtz free energy density for an inhomogeneous fluid [2] given by,

$$\Psi[\rho] = \int\left\{\frac{\kappa}{2}\left(\frac{\partial\rho}{\partial x}\right)^2 + \psi(\rho)\right\}dx, \tag{4}$$

where $\psi(\rho)$ is the Helmholtz free energy density of the homogeneous system and κ is a phenomenological constant associated to the gradient term with a meaning that is specific to the particular system chosen. For a van der Waals (vdW) fluid, the Helmholtz free energy density of a uniform system is given by

$$\psi(\rho) = 8\rho T\ln\frac{\rho}{3-\rho} - 3\rho^2, \tag{5}$$

where T is the temperature and κ is proportional to the surface tension of the liquid-gas interface. The reason for choosing a vdW fluid for our investigation is that it is one of the simplest descriptions that includes a discontinuous liquid-gas transition and a region in the $P-\rho$ plane where the uniform fluid is unstable (negative compressibility) below the critical temperature $T_c \equiv 1$. We note that the quantities P, ρ and T in Eqs. (3) and (5) have been normalized by their respective values at the critical point for convenience. of a fluid for which the pressure tensor is derived from the equation of state of a inhomogeneous van der Waals fluid [2].

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FIG. 1. Schematics of the flow configurations. The quantities v_i and ρ_i are, respectively, the inlet velocity and density while the outlet velocity is denoted by v_o.

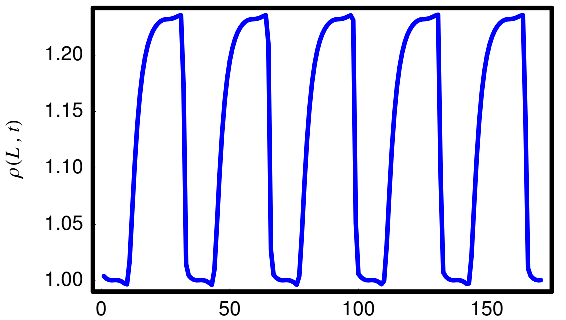

FIG. 2. The density at the outlet $\rho(L,\ t)$ at $v_0 = 0.136$. The other parameters are set to $v_L = 0.100$, $\rho_0 = 0.8$, $T = 0.987$, $\eta = 0.01$, and $\kappa = 0.0001$.

A numerical algorithm has been developed to solve Eqs. (1) and (2) using the forward-time-centered-space approach described in Ref. [3]. We will restrict ourselves to a special case depicted in Fig. 1: a flow in the region $x \in [0, L]$ subject to the following set of boundary conditions

$$v(x < 0,\ t) = v_0, \tag{6}$$
$$v(x > L,\ t) = v_L, \tag{7}$$
$$\rho(x < 0,\ t) = \rho_0, \tag{8}$$
$$\rho(x > L,\ t) = \rho(L,\ t). \tag{9}$$

The fluid velocity has been arbitrarily chosen so that it flows from left to right. The positions $x = 0$ and $x = L$ correspond to, respectively, the inlet and the outlet. The quantities v_0 and v_L are, respectively, the velocities at the inlet and the outlet. The density at the inlet is kept at ρ_0. This set of boundary conditions describes a situation where both the fluid density and velocity are kept fixed at the inlet, and the fluid density at the outlet is allowed to vary with time while keeping the velocity constant. Under this special circumstance, the instability of the flow is necessarily reflected in the time dependence of the density at the outlet and we systematically analyze $\rho(L,\ t)$. Oscillations in fluid density at the outlet ($x = L$) , shown in Fig. 2, have been demonstrated at some appropriately tuned sets of parameters.

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