

Dynamic van der Waals Theory

A Phase Field Model of Fluids

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In usual theories of phase transitions, the fluctuations of the temperature T are assumed to be small and are neglected. However, there can be situations in which phase transitions occur in inhomogeneous T . For example, wetting properties near the gas-liquid critical point are very sensitive to applied heat flux and boiling processes remain largely unexplored [A. Onuki, *Phase Transition Dynamics* (Cambridge, 2002)]. To treat such problems we propose to start with a coarse-grained entropy rather than a Ginzburg-Landau free energy. For one-component fluids, let an entropy functional \mathcal{S} be determined by the local number density $n = n(\mathbf{r}, t)$ and the local internal energy density $e = e(\mathbf{r}, t)$ as

$$\mathcal{S} = \int d\mathbf{r} \left[ns - \frac{1}{2} C |\nabla n|^2 \right] \quad (1)$$

We assume that $s = s(n, e)$ is the entropy per particle defined as a function of n and e . The gradient term represents a decrease of the entropy due to inhomogeneity of n . We introduce the local temperature $T = T(n, e)$ by

$$\frac{1}{T} = \frac{\delta}{\delta e} \mathcal{S} \quad (2)$$

where n is fixed in the derivative. For the special form of Eq.1 we simply obtain $1/T = n(\partial s / \partial e)_n$. Maximization of \mathcal{S} under a fixed total particle number $\int dr n$ and a fixed total energy $\int dre$ leads to the equilibrium conditions $T = \text{const.}$ and $h/T \equiv \delta \mathcal{S} / \delta n = \text{const.}$ As first derived by van der Waals, the equilibrium interface density profile $n = n(x)$ is determined by $h = \mu(n, T) - CT d^2 n / dx^2 = \text{const.}$ [J.S. Rowlinson, *J. Stat. Phys.* **20**, 197 (1979)]. In the van der Waals theory $s = s(n, e)$ is given by

$$s = k_B \ln[(e/n + \epsilon v_0 n)^{d/2} (1/v_0 n - 1)] + \text{const.} \quad (3)$$

where v_0 and ϵ are positive constants representing the molecular volume and the magnitude of the attractive potential, respectively, and d is the space dimensionality.

The reversible part of the stress tensor reads

$$\Pi_{ij} = p \delta_{ij} + CT \left[\nabla_i n \nabla_j n - (n \nabla^2 n + |\nabla n|^2 / 2) \delta_{ij} \right] \quad (4)$$

where $p = n(\mu + sT) - e$ is the van der Waals pressure. The mass density $\rho = mn$ obeys the continuity equation. The momentum density $\mathbf{J} = \rho \mathbf{v}$ and the energy density obey appropriate dynamic equations

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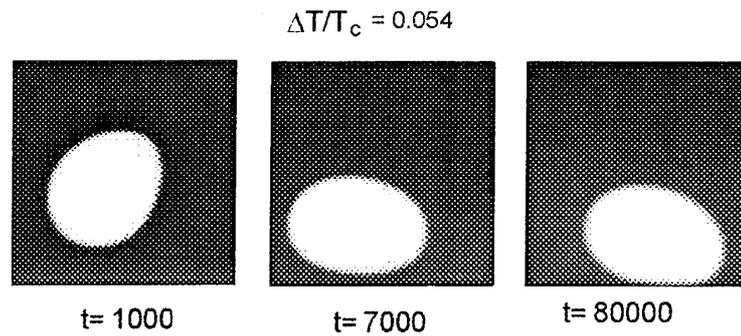


FIG. 1: Migration of a gas droplet towards the heated boundary (bottom) in zero gravity.

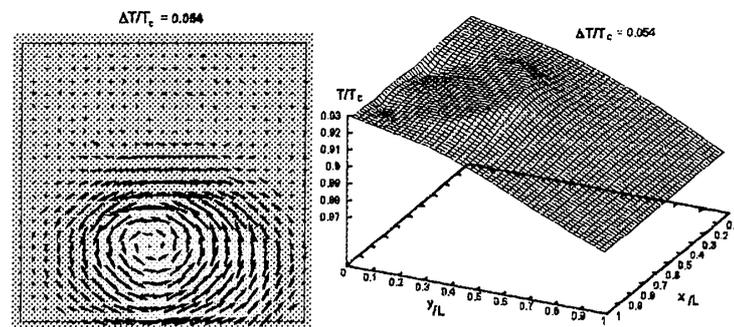


FIG. 2: The velocity field (left) and the temperature (right) in the nearly steady state at $t = 80000$ in Fig.1. There is a velocity component through the interface. The latent heat transport makes ∇T vanish inside the droplet.

including the gradient part of the stress tensor. The entropy production rate dS/dt within the fluid is non-negative-definite if there is no heat flow from outside.

We give a numerical solution of our phase field model imposing a wetting boundary condition on all the boundaries. At $t = 0$ we placed a gas droplet at the center of the cell in equilibrium at $T' = 0.875T'_c$. The bottom boundary was then increased by a constant $\Delta T = 0.054T'_c$ for $t > 0$, while the top boundary was held at the initial temperature. There is no gravity, while we use "bottom" and "top". Fig.1 shows droplet migration toward the bottom, caused by a Marangoni effect. See a first report: N. O. Young *et al.*, J. Fluid Mech. **6**, 350 (1959) (where bubbles and liquid were different fluids and there was no first-order transition at the interface). Fig.2 displays the velocity and the temperature in the steady state. It is a new finding that the velocity component through the interface is nonvanishing, leading to **latent heat transport**. Because it is highly efficient, a flat temperature or **no temperature gradient** appears inside the droplet. In the steady state the gas droplet apparently wets the bottom partially, while a very thin liquid layer is sandwiched between the bottom boundary and the droplet. We can define an apparent contact angle θ_{eff} , which is a decreasing function of $\Delta T'$. Garrabos *et al.* observed in space that gas spreads on a heated wall initially wetted by liquid and exhibits an apparent contact angle even larger than $\pi/2$ [Phys. Rev. E **64**, 051602 (2001)]. With further increasing $\Delta T'$ the heated wall is completely covered by gas, eventually leading to film boiling in gravity.