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Hydrodynamic boundary conditions derived from Onsager's variational principle

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Abstract

In addition to hydrodynamic equations in the bulk region, proper hydrodynamic boundary conditions are essential to theoretically understanding and numerically simulating the hydrodynamics of many soft matter systems, e.g. two-phase flows on solid surfaces and viscoelastic fluids on solid surfaces. In this work, we show that Onsager's variational principle, first proposed by Lars Onsager in his seminal work in 1931, provides a convenient instrument for deriving not only hydrodynamic equations in the bulk region but also thermodynamically consistent hydrodynamic boundary conditions. To demonstrate its applications, we consider one-component liquid-vapor flows and immiscible two-phase flows on solid surfaces where moving contact line is involved.

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Keywords: Hydrodynamic boundary conditions; Onsager's variational principle; two-phase flows; moving contact line

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1. Introduction

What happens at the fluid-solid interface has been a classical problem of particular relevance to the study of multiphase fluid flows. The moving contact line (MCL) problem has been a classical problem in continuum hydrodynamics for decades. The contact line denotes the intersection of the fluid-fluid interface with a solid wall. When one fluid displaces the other, the contact line moves along the wall. It has been well known that the MCL is incompatible with the no-slip boundary condition — the latter leads to a non-integrable singularity in viscous dissipation[6]. The heart of the MCL problem lies in the boundary conditions at the fluid-solid interface. In fact, there has been a lasting debate over the boundary conditions for a fluid flowing past a solid surface. Recently the Newtonian flows in confined geometries have received much attention, and numerous experimental efforts have shown that fluid slip occurs at the solid boundary in many circumstances[7,8,9].

Molecular dynamics (MD) simulations have proven to be instrumental in investigating the fluid dynamics of the MCL. Through analysis of extensive MD data, it was found that the fluid slip measured in nanoscale MD simulations is governed by the generalized Navier boundary condition (GNBC)[11]. The GNBC states that the relative slip velocity between the fluid and the solid wall is proportional to the total tangential stress — the sum of the viscous stress and the uncompensated Young stress which arises from the deviation of the fluid-fluid interface from its static configuration.

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By combining the GNBC with the Cahn-Hilliard hydrodynamic formulation for immiscible two-phase flows[11], a continuum model for MCL hydrodynamics has been obtained with continuum solutions in quantitative agreement with MD results[11].

In general, boundary conditions are essential to a mathematical description of two-phase flows on solid walls. It is worth pointing out that the physics associated with boundary conditions can not be simply deduced from that associated with hydrodynamic equations in the bulk region — the boundary conditions can not be regarded as simply a routine or conventional mathematical hypothesis associated with the partial differential equations in the bulk region. Physically, they should be derived from an understanding of the dissipative processes at the fluid-solid interface.

The coexistence of different dissipative processes is a common phenomenon in soft matter with multiple components and/or internal degrees of freedom. To describe coupled irreversible processes in the linear response regime, Onsager formulated a variational principle that is of fundamental importance to macroscopic thermodynamics[1,2,3,4,5]. This variational principle is based on a general class of reciprocal relations and provides a reliable and unified approach to deriving dynamic equations for soft matter[12,13,14]. Applying this principle, we present a variational approach to the derivation of hydrodynamic boundary conditions for two-phase flows on solid surfaces where MCL is involved.

The paper is organized as follows. In section 2 there is a brief review of Onsager's variational principle. As a simple demonstration, hydrodynamic boundary conditions are derived for single phase flows on solid surfaces in section 3. We then turn to one-component liquid-vapor flows in section 4 and immiscible two-phase flows in section 5. It is seen that thermodynamically consistent boundary conditions are derived together with hydrodynamic equations in the bulk region. The paper is concluded in section 6 with a few remarks.

2. Onsager's variational principle

For a closed system, consider the fluctuations of a set of (macroscopic) variables $\alpha_i\,(i = 1, ..., n)$ with respect to their most probable (equilibrium) values[1,2,3,4,5]. The entropy of the system S has a maximum S_e at equilibrium so that $\Delta S = S - S_e$ can be written in the quadratic form

$$\Delta S\,(\alpha_1, ..., \alpha_n) = -\frac{1}{2}\beta_{ij}\alpha_i\alpha_j, \tag{1}$$

where β is symmetric and positive definite. Here the Einstein summation convention is used. The probability density is given by $f\,(\alpha_1, ..., \alpha_n) = f\,(0, ..., 0)\,e^{\Delta S/k_B}$, where k_B is the Boltzmann constant. The thermodynamic forces conjugate to α_i are defined by

$$X_i = \frac{\partial \Delta S}{\partial \alpha_i} = -\beta_{ij}\alpha_j, \tag{2}$$

which are linear combinations of α_i not far from equilibrium.

For small deviation from equilibrium, the system is in the linear response regime, where the state variables $\alpha_i\,(i = 1, ..., n)$ evolve according to the linear kinetic equations

$$\dot{\alpha}_i = L_{ij}X_j, \tag{3}$$

or equivalently

$$X_i = R_{ij}\dot{\alpha}_j, \tag{4}$$

where the kinetic coefficients L_{ij} form a symmetric and positive definite matrix, and so do the coefficients R_{ij}, with $L_{ij}R_{jk} = \delta_{ik}$. Off-diagonal entries L_{ij} and R_{ij} are referred to as cross-coupling coefficients between different irreversible processes labeled by i and j. Under the condition that the variables α are even, i.e., their signs remain invariant under time reversal operation, Onsager derived the reciprocal relations

$$L_{ij} = L_{ji}, \tag{5}$$

and consequently $R_{ij} = R_{ji}$, from the microscopic reversibility[1,3], which does not require detailed knowledge of the irreversible processes.