

VARIATIONAL THEORY FOR VAN DER WAAL FLUID*

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Статья посвящена некоторым обратным задачам вариационного исчисления. Ряд вариационных принципов для жидкостей Ван-дер-Ваальса получены непосредственно из начально-краевой задачи для соответствующей системы уравнений, начальных и краевых условий с помощью полуобратного метода, предложенного автором. Результаты работы могут усилить теоретические основы метода конечных элементов и других прямых вариационных методов, таких, как методы Ритца, Треффтца и Канторовича.

Introduction

Variational model for fluid mechanics is the theoretical basis for the finite element techniques and other direct variational methods such as Ritz's, Trefftz's and Kantorovitch's methods [1]. Most recently, a new and very effective numerical technique called meshless method or element-free method [2] is developing. In contrast to the finite element methods, the meshless methods requires no elements but a set of scattered nodes in the solution domain without recourse to any elements or zones. Accordingly the meshless methods do not have a rigid connectivity provided a priori, making them ideal in applications where finite element methods have the most difficulties. And the variational model is also the theoretical basis for the variational-based meshless method [3]. Furthermore, variational principles can also easily deal with the free or moving faces in fluid mechanics and hybrid problems [4–6] of determining unknown shape in design or modification of channels, bladings and dams etc., where some part of the wall is unknown but the pressure distribution is described. So the importance of searching for a variational representation of fluid mechanics must not be demonstrated in detail in this paper, however, it is very difficult to search for a variational representation directly from the field equations and boundary and initial conditions. In this paper, we apply the semi-inverse method [7–11] to establish various variational principles for Van der Waal fluid.

1. Mathematical model

Let's consider the one-dimensional fluid, the governing equations are [8–10]

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0, \quad (1)$$

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$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial P}{\partial x} = 0, \quad (2)$$

where P , ρ and u are pressure, density and velocity respectively. For Van der Waal fluid, we have the following pressure-density relation [12]

$$P = \frac{RT\rho}{1 - b\rho} - a\rho^2, \quad (3)$$

where a , b , R and T are considered constants in this paper.

Using (3), equation (2) can be rewrite in the following conservative form

$$\frac{\partial u}{\partial t} + \frac{\partial H}{\partial x} = 0, \quad (4)$$

where H is defined as

$$H = \frac{1}{2}u^2 + RT \ln \rho - RT \ln(1 - b\rho) + \frac{RT}{1 - b\rho} - 2a\rho.$$

We introduce two general functions: path function Ψ and potential function Φ , which are defined respectively as

$$\frac{\partial \Psi}{\partial t} = -\rho u, \quad (5)$$

$$\frac{\partial \Psi}{\partial x} = \rho, \quad (6)$$

and

$$\frac{\partial \Phi}{\partial t} = -H, \quad (7)$$

$$\frac{\partial \Phi}{\partial x} = u. \quad (8)$$

The boundary and initial-value conditions (BC and IC) can be expressed as follows

(A) for Φ :

at inlet C_1

$$\rho u(0, t) = f_0(t),$$

at outlet C_3

$$\rho u(L, t) = f_1(t),$$

at initial time (on C_2)

$$\Phi(x, t_0) = f_2(t),$$

and

$$\rho(x, t_0) = f_3(t),$$

(B) for Ψ :

at inlet C_1

$$H(0, t) = g_0(t),$$

at outlet C_3

$$H(L, t) = g_1(t),$$

at initial time (on C_2)

$$\Psi(x, t_0) = g_2(t),$$

and

$$u(x, t_0) = g_3(t).$$

2. Generalized variational principles

The variational principle for 1-D unsteady flow in a flexible tubes in turbomachinery aerodynamics has been studied extensively in Refs. [9, 13]. In this paper, we will extend the results in Refs. [9, 10] to Van der Waal fluid.

The traditional way to arrive at a generalized variational principle is the Lagrange multiplier method, which uses Lagrange multipliers to remove its constraints in a known variational principle under constraints. But here we have no known variational principles, so the method isn't valid herein.

The basic idea of the proposed method is to construct a trial-functional with an unknown variable F like this

$$J(\Phi, \rho, u) = \iiint \left\{ \rho \frac{\partial \rho}{\partial t} + \rho u \frac{\partial(\rho u)}{\partial x} + F(\rho, u) \right\} dt dx, \quad (9)$$

where Φ , ρ and u are all independent variables, F is an unknown function of ρ and u .

The trial-functional can be constructed by various ways, details can be found in Refs. [7]. We search for such F so that the stationary conditions of the trial-functional (9) satisfy the field equations (1), (7) and (8).

Calculating variation with respect to Φ

$$\delta_\Phi J(\Phi, \rho, u) = \iiint \left\{ -\frac{\partial \rho}{\partial t} - \frac{\partial(\rho u)}{\partial x} \right\} \delta \Phi dt dx = 0,$$

we obtain the equation (1) as stationary condition (Euler equation).

The other two stationary conditions with respect to u and ρ can be written respectively in the following forms:

$$\text{for } \delta u \quad \rho \frac{\partial \Phi}{\partial x} + \frac{\partial F}{\partial u} = 0,$$

and

$$\text{for } \delta \rho \quad \frac{\partial \Phi}{\partial t} + u \frac{\partial \Phi}{\partial x} + \frac{\partial F}{\partial \rho} = 0.$$

The above equations with unknown variable F is called trial-Euler equations, which should satisfy the other two field equations (7) and (8). Accordingly we set

$$\frac{\partial F}{\partial u} = -\rho \frac{\partial \Phi}{\partial x} = -\rho u, \quad (10)$$

and

$$\frac{\partial F}{\partial \rho} = -\frac{\partial \Phi}{\partial t} - u \frac{\partial \Phi}{\partial x} = -\frac{1}{2}u^2 + RT \ln \rho - RT \ln(1 - b\rho) + \frac{RT}{1 - b\rho} - 2a\rho. \quad (11)$$

From (10) and (11), the unknown F can be readily identified

$$\begin{aligned} F &= -\frac{1}{2}\rho u^2 + RT\rho(\ln \rho - 1) + \frac{RT(1-b\rho)}{b}[\ln(1-b\rho) + 1] - \frac{RT}{b}\ln(1-b\rho) - a\rho^2 = \\ &= -\frac{1}{2}\rho u^2 + \frac{RT}{b} + RT\rho \ln \frac{\rho}{1-b\rho} - a\rho^2. \end{aligned}$$

We, therefore, obtain the following functional

$$J(\Phi, \rho, u) = \iint L_1 dt dx, \quad (12a)$$

where

$$L_1 = \rho \frac{\partial \Phi}{\partial t} + \rho u \frac{\partial \Phi}{\partial x} - \frac{1}{2}\rho u^2 + \frac{RT}{b} + RT\rho \ln \frac{\rho}{1-b\rho} - a\rho^2. \quad (12b)$$

Now we remove the boundary/initial constraints by using the semi-inverse method. Supposing a generalized variational principle without any constraints has the following form:

$$J^*(\Phi, \rho, u) = J(\Phi, \rho, u) + \int_{C_1} F_1 ds + \int_{C_2} F_2 dt + \int_{C_3} F_3 ds, \quad (13)$$

where F_i ($i = 1, 2, 3$) are unknowns, and $J(\Phi, \rho, u)$ is defined by (12).

Making the above trial-functional (13) stationary, and using the Green's theory, at the boundary (C_1), the following trial-Euler equation can be obtained:

$$\text{for } \delta\Phi \quad \rho u(\mathbf{i}_x \cdot \mathbf{n}) + \frac{\partial F_1}{\partial \Phi} = 0,$$

which should satisfy the condition at C_1 , therefore, we set

$$\frac{\partial F_1}{\partial \Phi} = -f_0(\mathbf{i}_x \cdot \mathbf{n}).$$

The unknown F_1 can be identified as follows

$$F_1 = -f_0\Phi(\mathbf{i}_x \cdot \mathbf{n}).$$

The other unknowns in (13) can be identified by the same way, as a result, we have the following functional:

$$J^*(\Phi, \rho, u) = J(\Phi, \rho, u) + L_\Phi, \quad (14a)$$

where $J(\Phi, \rho, u)$ is defined by (12), and L_Φ is expressed as

$$L_\Phi = - \int_{C_1} f_0(\mathbf{i}_x \cdot \mathbf{n})\Phi ds - \int_{C_2} f_1(\mathbf{i}_x \cdot \mathbf{n})\Phi dt - \int_{C_3} f_2(\mathbf{i}_x \cdot \mathbf{n})\Phi ds. \quad (14b)$$

It is very easy to deduce various variational principles from a known generalized variational principle. Constraining the functional (14) by selectively enforcing field equations or boundary conditions yields various sub-generalized variational principles. For example, substituting equation (8) into the functional (14) yields the following functional:

$$J(\Phi, \rho) = \iint L_2 dt dx + L_\Phi, \quad (15a)$$

where

$$L_2 = \rho \frac{\partial \Phi}{\partial t} + \rho \left(\frac{\partial \Phi}{\partial x} \right)^2 - \frac{1}{2} \rho u^2 + \frac{RT}{b} + RT \rho \ln \frac{\rho}{1 - b\rho} - a\rho^2, \quad (15b)$$

which is subject to equation (8).

Further constraining the functional (15) by the equation (7), we have

$$J(u) = \iint L_3 dt dx + L_\Phi, \quad (16a)$$

where

$$\begin{aligned} L_3 &= -\rho H + \rho u^2 - \frac{1}{2} \rho u^2 + \frac{RT}{b} + RT \rho \ln \frac{\rho}{1 - b\rho} - a\rho^2 = \\ &= -\rho \left[\frac{1}{2} u^2 + RT \ln \rho - RT \ln(1 - b\rho) + \frac{RT}{1 - b\rho} - 2a\rho \right] + \\ &+ \rho u^2 - \frac{1}{2} \rho u^2 + \frac{RT}{b} + RT \rho \ln \frac{\rho}{1 - b\rho} - a\rho^2 = -\frac{RT\rho}{1 - b\rho} + a\rho^2 + \frac{RT}{b} = -P + \frac{RT}{b}, \end{aligned} \quad (16b)$$

which is a functional under the constraints of equations (7) and (8). The above functional (16) can be written equivalently in the form

$$J(u) = - \iint P dt dx + L_\Phi,$$

which is very similar with the well-known Bateman's principle [1].

We can also establish a variational principle with independent variables Ψ , ρ and u . The trial-functional can be constructed as follows

$$J(\Psi, \rho, u) = \iint \left\{ u \frac{\partial \Psi}{\partial t} + H \frac{\partial \Psi}{\partial x} + F(\rho, u) \right\} dt dx. \quad (17)$$

We search for such F , so that the stationary conditions of the above trial-functional (17) satisfy the field equations (4), (5) and (6). Taking variation with respect to u and ρ yields the following trial-Euler equations:

$$\text{for } \delta u \quad \frac{\partial \Psi}{\partial t} + u \frac{\partial \Psi}{\partial x} + \frac{\partial F}{\partial u} = 0, \quad (18)$$

and

$$\text{for } \delta \rho \quad \left[\frac{RT}{b} + \frac{RTb}{1 - b\rho} - \frac{RTb}{(1 - b\rho)^2} - 2a \right] \frac{\partial \Psi}{\partial x} + \frac{\partial F}{\partial \rho} = 0. \quad (19)$$

The above trial-Euler equations (18) and (19) should satisfy the equations (5) and (6), we therefore set

$$\frac{\partial F}{\partial u} = \rho u - u\rho = 0,$$

and

$$\frac{\partial F}{\partial \rho} = -RT - \frac{RTb\rho}{1 - b\rho} + \frac{RTb\rho}{(1 - b\rho)^2} + 2a\rho.$$

So the unknown F can be determined as

$$F = \frac{RT}{b(1 - b\rho)} - a\rho^2. \quad (20)$$

Substituting (20) into (17) results in the following functional:

$$J(\Psi, \rho, u) = \iint \left\{ u \frac{\partial \Psi}{\partial t} + H \frac{\partial \Psi}{\partial x} + \frac{RT}{b(1-b\rho)} - a\rho^2 \right\} dt dx.$$

By the same manipulation as before, we can eliminate the “boundary constraints” by the semi-inverse method:

$$J^*(\Psi, \rho, u) = J(\Psi, \rho, u) + L_\Psi,$$

where

$$L_\Psi = - \int_{C_1} g_0 \mathbf{i}_x \cdot \mathbf{n} \Psi ds + \int_{C_2} g_3 \Psi dt - \int_{C_3} g_1 \mathbf{i}_x \cdot \mathbf{n} \Psi ds.$$

It should be specially pointed out that on C_4 it requires a special treatment, for details please see Refs. [9, 10].

It is easy to obtain the following two generalized variational principles with four independent variables (Ψ, ρ, u, P) and (Φ, ρ, u, P) :

$$J^{**}(\Psi, \rho, u, P) = J(\Psi, \rho, u) + \lambda \iint \left\{ P - \frac{RT\rho}{1-b\rho} - a\rho^2 \right\}^2 dt dx + L_\Psi,$$

$$J^{**}(\Phi, \rho, u, P) = J(\Phi, \rho, u) + \lambda \iint \left\{ P - \frac{RT\rho}{1-b\rho} - a\rho^2 \right\}^2 dt dx + L_\Phi,$$

where λ is a nonzero constant.

Conclusions

It is obvious that the semi-inverse method is an effective approach to searching for various variational principles for fluid mechanics without using Lagrange multipliers. Applying variational theory with a variable-domain [4, 5], we can readily obtain the shock relations for Van der Waal fluid.

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