Using Onsager principle as an approximation tool for complicated two-phase flow problems

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Abstract

We review some recent work on using the Onsager principle as an approximation tool in model reduction for some complicated two-phase flow problems. We introduce the basic idea of the method and also give some examples. The examples show that the method be used to derive some reduced model for a set of carefully chosen slow variables. The reduces model is much easier to solve than the standard two-phase flow equations, while it can also generate reasonable results which are consistent with physical experiments.

1 Introduction

Two-phase flow is common in nature and our daily life. It is also widely used in many industrial applications [1, 2, 3]. For example, the oil-water flow in porous media is a fundamental problem in oil industry. Two-phase flow is also a basic problem in coating, painting, printing and many other industrial processes. Therefore the quantitative study for two-phase flow is of critical importance for these real applications.

The two-phase flow problem is very complicated due to the existence of a free boundary and moving contact lines [4]. In general, it can be described by a two-phase Navier-Stokes equation with some interface and

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boundary conditions. If there exists a contact line, which is the line where the two-phase interface intersects with the solid boundary, the boundary condition will be very complicated. The standard no-slip boundary condition for viscous fluid leads to infinite energy dissipations[5]. This is so called moving contact line paradox. Many models have been developed to cure the paradox[5, 6, 7, 8, 9, 10, 11, 12]. But there still are many problems in this field[13, 4]. For example, it is not clear how to choose a proper boundary condition in real simulations to quantitatively compare with the experiments.

From mathematical point of view, the two-phase Navier-Stokes equation with complicated interface and boundary conditions is very difficult. Beside the analysis for the well-posedness, numerical simulations for the problem are very challenging. One needs not only to handle the motion of the interfaces, but also to capture the motion of the moving contact lines. In principle, the moving contact line is a muli-scale problem where the slipness of fluid in nanoscale is necessary in a macroscopic model. This implies that one needs extremely fine meshes near the contact line to fully capture the physical law its motion. This makes numerical simulations for two-phase flow problems with moving contact lines extremely difficult to fit physical experiments.

Recently the Onsager Principle is used as an approximation tool to study many problems in two-phase flow[14, 15, 16, 17, 18, 19, 20, 21]. It is a new and powerful method to do model reduction in these nonlinear dynamic problems. In principle, the method is to use the fundamental Onsager Principle for a restricted set of slow variables in the system so that to derive some reduced model for the slow variables. In this paper, we will introduce the basic idea and the main steps of the method. We review some examples previously studied in [16, 17] to show how the method works. We can see that the method can lead to accurate results for slow variables by solving some simple reduced models.

The structure of the paper is as follows. In section 2, we introduce the Onsager variational principle in physics and show how they can be used to derive a partial differential equation model for viscous fluid. In section 3, we introduce the basic idea of using the Onsager Principle as an approximation tool. In section 4, we give two examples on how to apply the method to some complicated two-phase flow problems. In the last section, we give some conclusion remarks.

2 The Onsager Principle

The Onsager Principle is a variational principle used widely in soft matter science [22, 23]. Suppose a system is described by a complete set of parameters $\{u_i\}_{i=1}^n$, in the sense that all other parameters can be determined solely by them. Denote $u = (u_1, \cdots, u_n)$. Suppose that the total free energy is given as $E(u)$. The Rayleigh dissipation function is given by $\Phi(\dot{u})$, which is defined as the half of the total energy dissipation rate. If the system is over-damped, the evolution of the parameters u are obtained by minimizing the total Rayleighian in the system, which is defined as

$$R(u, \dot{u}) = \Phi(\dot{u}) + \frac{dE(u)}{dt}. \tag{1}$$

In other words, the dynamic equation for u is given by

$$\min_{\dot{u}} R(u, \dot{u}) \tag{2}$$

This corresponding Euler-Lagrange equation is

$$\frac{\delta \Phi}{\delta \dot{u}} + \frac{\delta E}{\delta u} = 0. \tag{3}$$

This is basically a force balance equation for the generalized friction force $\frac{\delta \Phi}{\delta \dot{u}}$ and the generalized driven force $-\frac{\delta E}{\delta u}$.

The Onsager Principle is very useful to derive some partial differential equation model for problems in soft matter. Here we give a simple example. It is to derive the well-known Stokes equation. Suppose the viscous fluid occupies a domain Ω. We would like to derive an equation for its velocity $\mathbf{u}$ by using the Onsager Principle. The total potential energy is the gravitational energy,

$$E = \int_\Omega \rho g x_3 dx. \tag{4}$$

The time derivative of E is written as

$$\frac{dE}{dt} = \int_\Omega \rho g u_3 dx. \tag{5}$$

where u_3 is the component of $\mathbf{u}$ in z direction.

The energy dissipation function is given by

$$\Phi = \frac{\eta}{4} \int_\Omega |\partial_i u_j + \partial_j u_i|^2 dx. \tag{6}$$

Here we use the Einstein summation convention. Then the Rayleighian is written as

$$R(\mathbf{u}) = \Phi(\mathbf{u}) + \frac{dE}{dt}.$$

By the Onsager Principle, the equation of $\mathbf{u}$ is determined by

$$\begin{aligned} &\min_{\mathbf{u}} \; R(\mathbf{u}) \\ &s.t. \; \mathrm{div}\mathbf{u} = 0 \end{aligned} \tag{7}$$

The Euler-Lagrange equation leads to the standard Stokes equation

$$\begin{aligned} -\eta\Delta\mathbf{u} + \nabla p &= -\rho g \mathbf{e}_3, \\ \mathrm{div}\mathbf{u} &= 0. \end{aligned}$$

This is the standard Stokes equation and p is a Lagrange multiplier.

3 The main idea

Consider a two-phase flow which includes some interfaces (interface between fluid and solid or fluid and fluid). If the interfaces are moving driven by certain potential forces (gravity, surface tension, etc), the evolution of the system is determined by the Onsager Principle. If we use the variational principle to obtain the evolution of the droplet shape in the entire parameter space, we obtain the same set of equations that have been used in previous theories[23]. Here we use the variational principle in a restricted parameter space. This gives us a new way of solving the problems approximately.

Let $a(t) = \{a_1(t), a_2(t), ...a_N(t)\}$ be the set of the parameters which specify the position of the interfaces approximately. The time evolution of the system, i.e., the time derivative $\dot{a}(t) = \{\dot{a}_1(t), \dot{a}_2(t), ...\dot{a}_N(t)\}$ is determined by the minimum condition for the following function of $\dot{a}$

$$R(\dot{a}, a) = \Phi(\dot{a}, a) + \sum_i \frac{\partial A}{\partial a_i}\dot{a}_i \tag{8}$$

where $A(a)$ is the potential energy of the system, and $\Phi(\dot{a}, a)$ is the energy dissipation function which is defined as the half of the minimum of the energy dissipated per unit time in the fluid when the boundary is changing at rate $\dot{a}$. Suppose the fluid obeys Stokesian dynamics, $\Phi(\dot{a}, a)$ is always written as a quadratic function of $\dot{a}$.

$$\Phi(\dot{a}, a) = \frac{1}{2}\sum_{i,j} \zeta_{ij}(a)\dot{a}_i\dot{a}_j \tag{9}$$

The minimum condition of eq.(8)

$$\frac{\partial \Phi}{\partial \dot{a}_i} + \frac{\partial A}{\partial a_i} = 0 \quad \text{or} \quad \sum_j \zeta_{ij}(a)\dot{a}_j = -\frac{\partial A}{\partial a_i} \tag{10}$$

represents the force balance of two kinds of forces, the hydrodynamic frictional force $\partial\Phi/\partial\dot{a}_i$, and the potential force $-\partial A/\partial a_i$ in the generalized coordinate.

In summary, the key steps to use Onsager principle as an approximation tool in two-phase flow problems are as follows. First, we make sure that the two-phase flow problem is in Stokesian regime in the sense that the viscous effect dominate and the inertial effect can be ignored. We choose some slow variables to characterize the motion of the fluid. Then we calculate the free energy in the system approximately. The energy is a function of these slow variables. Meanwhile, we also compute the dissipation function in the system approximately. The dissipation function is usually a quadratic function of the time derivative of these parameters. In the third step, we use the Onsager principle to derive a simplified model for these parameters. The model can be solve easily by numerical or analytic methods. Then the model is used to study some phenomena we are interested in.

4 Some examples

We will introduce two examples on how we use the Onsager Principle to study the complicated fluid problems with free interfaces. The first example is a sliding droplet problem take from [17] and the second one is a capillary rising problem between an elastic film and a substrate[16].

4.1 Sliding droplet on an inclined surface

We consider a droplet which slides downward from an inclined surface under gravity. The motion of the droplet depends on the inclined angle. When the inclined angle increases, the sliding velocity increases and the shape of the droplet also changes. To characterize the shape changes of the droplet, usually one needs to solve the a Navier-Stokes equation in a domain with a free boundary. It is a difficult problem due to the existence of the moving contact line.

Here we use the Onsager principle as an approximation tool to study this problem. Motivated by the previous studies[24], we assume the profile of the droplet is approximately represented by

$$h(x,y,t) = H(x,t)\left[1 - \left(\frac{y}{Y(x,t)}\right)^2\right]. \tag{11}$$

where $H(x,t)$ and $Y(x,t)$ are the functions to be determined. According to Equation (11), the contact line of the droplet is given by the function $y = Y(x,t)$. The side view of the droplet is specified by the function $z = H(x,t)$.

Ansatz. If we use Onsager principle for the functions $H(x,t)$ and $Y(x,t)$, we will obtain a one-dimensional partial differential system for them. To make the problem simpler, we further assume that $H(x,t)$ and $Y(x,t)$ have the following form:

$$H(x,t) = (x - a_1(t))(a_2(t) - x)(a_3(t) + a_4(t)x), \tag{12}$$

$$Y(x,t) = (x - a_1(t))^{\frac{1}{2}}(a_2(t) - x)^{\frac{1}{2}}(a_5(t) + a_6(t)x). \tag{13}$$

where $a_i(t)$ $(i = 1, 2, ...6)$ are the parameters dependent only time. These parameters have the following meaning : a_1 and a_2 represent the x-coordinates of the tail and the front of the contact line. The other parameters a_3, a_4, a_5 and a_6 represent the deformation of the droplet from the equilibrium shape. The fractional power law dependence of $Y(x,t)$ at $x = a_1$ and at $x = a_2$ indicates that the top view of the droplet is round at the front and at the tail, but the tail can have a cusp if $-a_5/a_6$ becomes equal to a_1. The volume of the droplet VOL is given by

$$VOL = \int_{a_1}^{a_2}\int_{-Y}^{Y} h(x,y,t)dydx \tag{14}$$

Since VOL is constant, only five in $\{a_1(t), \ldots, a_6(t)\}$ are independent. We will use the Onsager variation principle to determine these parameters.

The free energy. The potential energy of the system include the gravitational potential energy and the interface energies. It is given by

$$\begin{aligned} A(a) \quad &= \textstyle\int_{a_1}^{a_2}\int_{-Y}^{Y}\left[\frac{1}{2}\gamma\theta_e^2 + \frac{1}{2}\gamma[(\partial_x h)^2 + (\partial_y h)^2]\right. \\ &\quad \left. + \frac{1}{2}\rho g h^2 \sin\alpha - \rho g x h \cos\alpha\right] dydx \end{aligned} \tag{15}$$

It can be expressed as a function of $a = (a_1, a_2, ...a_6)$ by using the equations (11)-(13).

The dissipation function. To determine the time evolution of a_i, we need to know the energy dissipation function expressed as a function $\dot{a}_i$. In the lubrication approximation, the energy dissipation in the droplet can be generally written as a functional of the average velocity fields $\mathbf{v} = \{v_1(x,y), v_2(x,y)\}$

$$\Phi[v_1, v_2] = \frac{1}{2}\int_{a_1}^{a_2}\int_{-Y}^{Y}\frac{3\eta}{h}(v_1^2+v_2^2)dydx \tag{16}$$

In calculations, a cut-off of the integral is needed and that will generate a logarithm term. In addition, we do not include the dissipation term due to the contact line friction, which is small related to the viscous dissipations. If the droplet profile is changing with the rate $\dot{h}$, the velocity field has to satisfy the volume conservation equation

$$\dot{h} = -\partial_x(v_1 h) - \partial_y(v_2 h) \tag{17}$$

The variational principle states that the proper energy dissipation function $\Phi(\dot{a})$ are the minimum of $\Phi[v_1, v_2]$ for the velocity field (v_1, v_2) that satisfies the constraint (17). It is not easy to compute (v_1, v_2) accurately. We compute the velocity in an approximate way.

For equation (11), the equation (17) is rewritten as

$$\left(1-\frac{y^2}{Y^2}\right)\left(\dot{H}+\partial_x(v_1 H)+H\partial_y v_2\right)+\frac{2Hy}{Y^3}(y\dot{Y}+yv_1\partial_x Y - Yv_2) = 0 \tag{18}$$

This constraint is satisfied if v_1 and v_2 satisfy

$$\dot{H}+\partial_x(v_1 H)+H\partial_y v_2 = 0, \tag{19}$$

$$y\dot{Y}+yv_1\partial_x Y - Yv_2 = 0. \tag{20}$$

A simple velocity field which satisfies the above equations is

$$v_1(x,y,t) = V(x,t), \quad v_2(x,y,t) = W(x,t)y \tag{21}$$

where $V(x,t)$ and $W(x,t)$ are given by

$$V(x,t) = -\frac{1}{HY}\int_{a_1}^{x}(\dot{H}Y+H\dot{Y})dx, \tag{22}$$

$$W = \frac{1}{Y}\left(\dot{Y}+V\partial_x Y\right). \tag{23}$$

Since $\dot{H}$ and $\dot{Y}$ are expressed as a linear combination of $\dot{a}_i$, eqs.(21),(22) and (23) give the energy dissipation function $\Phi(\dot{a})$

$$\Phi(\dot{a}) = \frac{1}{2}\sum_{i,j}\zeta_{ij}\dot{a}_i\dot{a}_j, \tag{24}$$

which is a quadratic function of $\dot{a}$. Here the coefficients ζ_{ij} are some functions of $a = (a_1, a_2, ..a_6)$.

The reduced model. Using the above expressions for the free energy $A(a)$ and the energy dissipation function $\Phi(\dot{a})$, the time evolution equation for a_i is obtained as

$$\sum_{j=1}^{6} \zeta_{ij}\dot{a}_j + \frac{\partial A}{\partial a_i} = 0 \tag{25}$$

All quantities in eq.(25) are expressed as function of a_i, and can be evaluated numerically.

The equation (25) can be solved numerically. We consider a droplet of silicone oil sliding down a glass plate coated with fluoro-polymers. The parameters used in the calculation are from [24] and given as: $\eta = 104\text{cP}$, $\rho = 964\text{kgm}^{-3}$, $\gamma = 20.9\text{mNm}^{-1}$ and $\theta_e = 53^o$(the advancing angle in [24]). The volume of the droplet is 6.3mm^3. An example of the results of such calculations is shown in Figure 1. We could see that the shape of the droplet changes with time for different inclined angle α. When α is small, the shape of the droplet(top view) is slightly changed. When α becomes larger, the length of the droplet increases and the shape changes a lot. Specifically, there is a cusp at the tail of the droplet when $\alpha = 45^o$. The observations are consistent with the physical experiments [24]. More results and discussions are given in [17].

4.2 Capillary rising between a flexible surface and substrate

The second example is taken from [16]. We consider the capillary rise problem between two vertical plates of width $2w_m$ and height h_m, separated along the vertical edges by a pair of spacers of thickness e_m (Figure 2). One of the plates is a thick rigid glass plate, while the other one is a flexible polymer film that is simply supported on the spacers. The lower part of the imbibition cell is put in contact with a bath of wetting liquid.We investigate the liquid front that rises owing to capillary forces.

Ansatz. We study the evolution of the capillary rise system at long times. Therefore, we ignore the tip part of the liquid. Far from the tip, we assume that the width w of the wet domain is almost constant along the vertical axis and independent of time. Only bending, no stretching is considered here for the flexible film, which leads to that the thickness of liquid between walls $e(t)$ is independent of position. Let $h(t)$ be the height as shown in Figure 2. These two functions are the slow variables in the present system to be determined.

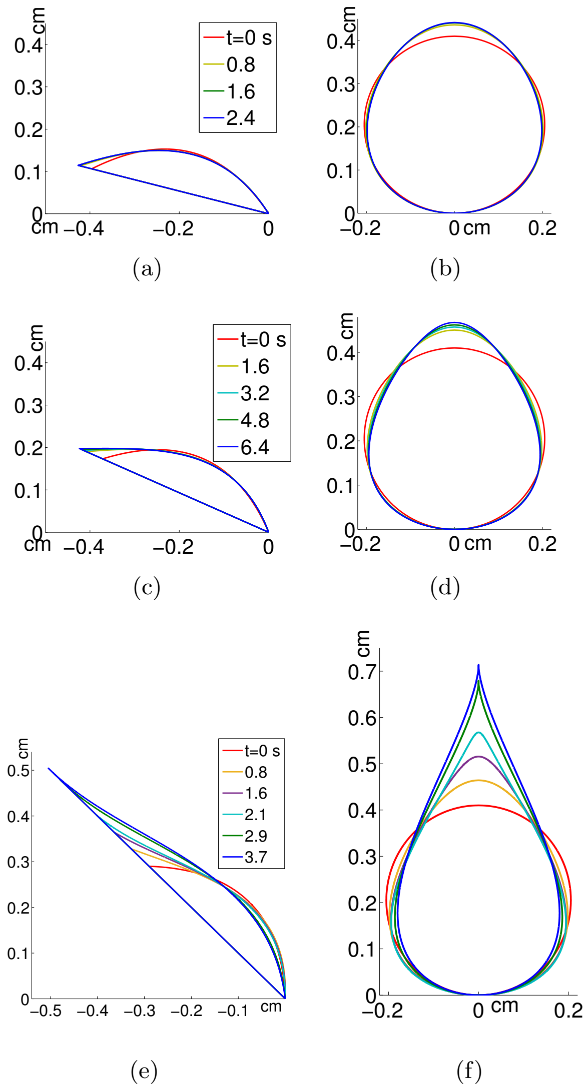

Figure 1: Shape change of a droplet sliding down on an inclined surface with different inclined angle α [17]. Left column: side view, right column: top view. (a),(b): $\alpha = 15^o$, (c),(d): $\alpha = 25^o$, (e),(f): $\alpha = 45^o$.

The free energy. We first calculate the elastic energy in the flexible film. Initially the liquid rising between the plates exerts a negative pressure on the walls which tends to collapse. Capillary forces tend to bring the walls in contact and compete with the stiffness of the sheet. Only simple deformation

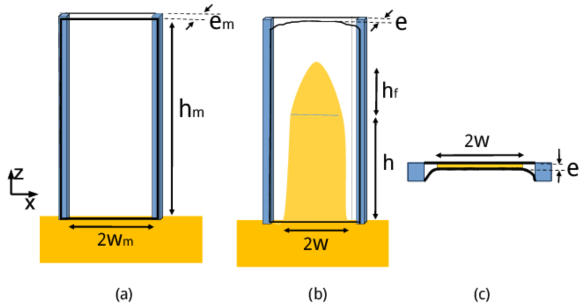

Figure 2: A flexible polymer membrane(white) is separated from a rigid plate of width $2w_m$ by spacers of thickness e_m. The flexible wall is simply supported on the spacers [16].

of the flexible walls is considered. The bending energy per unit area stored in this process is of order $B\kappa^2$, where B and κ are the bending modulus and curvature of the elastic membrane. The elastic energy ϵ_B stored per unit height of the cell reads

$$\epsilon_B = \frac{3}{2}\frac{Be_m^2}{(w_m - w)^3}. \tag{26}$$

The total energy stored in the collapsed film is finally given by

$$\epsilon = \epsilon_B + \epsilon_\gamma = \frac{3}{2}\frac{Be_m^2}{(w_m - w)^3} + 2\gamma(w_m - w). \tag{27}$$

To minimize ϵ, w is selected as

$$w_m - w = \left(\frac{9Be_m^2}{4\gamma}\right)^{1/4} = \sqrt{1.5}\sqrt{L_{ec}e_m}, \tag{28}$$

where $L_{ec} = \sqrt{B/\gamma}$ be the elastocapillary length of the system,

The total free energy can be finally calculated by

$$A = -2\gamma hw + \frac{1}{2}\rho geh^2 w + \frac{3B}{2}\frac{(e_m - e)^2}{(w_m - w)^3}h_m, \tag{29}$$

where γ and ρ stand for the surface tension and the density of the liquid and g for the gravitational acceleration. Straight forward calculation gives the following result,

$$\dot{A} = -2\gamma\dot{h}w + \rho gehw\dot{h} + \frac{1}{2}\rho g\dot{e}h^2 w - 3B\frac{(e_m - e)}{(w_m - w)^3}h_m\dot{e}. \quad (30)$$

The dissipation function. Introduce $\mathbf{v}(z,t) = (0,0,v_3)$ as the thickness-averaged velocity of the liquid at position z and time t, which is connected to the slow variables by

$$v_3(z,t) = \frac{z}{h}\dot{h} + \left(1 - \frac{z}{h}\right)V_0, \quad (31)$$

where V_0 is the velocity of the bulk of the bath liquid. The volume conservation of the fluid, i.e.,

$$e(t)v_3(z,t) = -\frac{d}{dt}\int_0^z e(t)dz \quad (32)$$

indicates that V_0 can be expressed in terms of $\dot{e}$ and $\dot{h}$,

$$V_0 = \frac{h}{e}\dot{e} + \dot{h}. \quad (33)$$

In the lubrication approximation, the energy dissipation function can be written down

$$\begin{aligned} \Phi &= \frac{1}{2}\int_0^h\int_0^w \frac{12\eta}{e}v_3^2 dxdz \\ &= \frac{2\eta hw}{e}\left(\dot{h}^2 + V_0\dot{h} + V_0^2\right), \end{aligned} \quad (34)$$

where η is the viscosity of the fluid.

The reduced model. The Onsager principle indicates that

$$\frac{\delta(\Phi + \dot{A})}{\delta\dot{h}} = 0, \quad \frac{\delta(\Phi + \dot{A})}{\delta\dot{e}} = 0. \quad (35)$$

Using equation (34) and (29), we can derive a nonlinear ordinary differential system for the variables $h(t)$ and $e(t)$,

$$\begin{bmatrix} 6 & \frac{3h}{e} \\ \frac{3h}{e} & \frac{2h^2}{e^2} \end{bmatrix}\begin{bmatrix} \dot{h} \\ \dot{e} \end{bmatrix} = \begin{bmatrix} b_2 \\ b_3 \end{bmatrix}, \quad (36)$$

where

$$\begin{bmatrix} b_2 \\ b_3 \end{bmatrix} = \frac{e}{2\eta wh} \begin{bmatrix} 2\gamma w - \rho gehw \\ -\frac{1}{2}\rho gh^2 w + 3B\frac{(e_m - e)}{(w_m - w)^3} h_m \end{bmatrix}. \tag{37}$$

The solutions of the equations (36) give the evolution equations for the height $h(t)$ and the thickness $e(t)$ as follows

$$\begin{bmatrix} \dot{h} \\ \dot{e} \end{bmatrix} = \begin{bmatrix} \frac{2}{3}b_2 - \frac{e}{h}b_3 \\ -\frac{e}{h}b_2 + \frac{2e^2}{h^2}b_3 \end{bmatrix} \tag{38}$$

Let $U = \gamma/\eta$ represent the characteristic velocity, and $\kappa_e^2 = \rho g/\gamma$ ($1/\kappa_e$ is the capillary length), using the constant width (28), the above equations can be rewritten as

$$\begin{bmatrix} \dot{h} \\ \dot{e} \end{bmatrix} = U \cdot \begin{bmatrix} \frac{2}{3}\frac{e}{h} - \frac{1}{12}\kappa_e^2 e^2 - \sqrt{\frac{2L_{ec}}{3e_m}}\frac{e_m - e}{e_m}\frac{h_m}{w}\frac{e^2}{h^2} \\ -\frac{e^2}{h^2} + \sqrt{\frac{8L_{ec}}{3e_m}}\frac{e_m - e}{e_m}\frac{h_m}{w}\frac{e^3}{h^3} \end{bmatrix}. \tag{39}$$

If we only keep the leading orders in the system (39), we have asymptotically

$$\begin{bmatrix} \dot{h} \\ \dot{e} \end{bmatrix} = U \begin{bmatrix} \frac{2}{3}\frac{e}{h} \\ -\frac{e^2}{h^2} \end{bmatrix}. \tag{40}$$

The system (40) can be solved exactly

$$h(t) = h_0 \left(1 + \frac{7}{3}\frac{e_0 U t}{h_0^2}\right)^{2/7}, \tag{41}$$

$$e(t) = e_0 \left(1 + \frac{7}{3}\frac{e_0 U t}{h_0^2}\right)^{-3/7}, \tag{42}$$

with the initial conditions $h(0) = h_0$ and $e(0) = e_0$.

We will show some numerical results. We choose some typical values of the relevant parameters are as follows, the viscosity $\eta = 15mPas$, density $\rho = 950kgm^{-3}$ and surface tension $\gamma = 21mN/m$ in a cell of thickness $e_m = 1mm$, width $w_m = 10mm$, bending modulus $B = 2.2 \times 10^{-7}mPam^3$. At long times, the prediction (solid lines) for the evolution of the height $h(t)$, equation (41), is in quantitative agreement with the experimental data in [25] (dotted lines) within a wide range of viscosities (different colors) as represented in Figure 3.

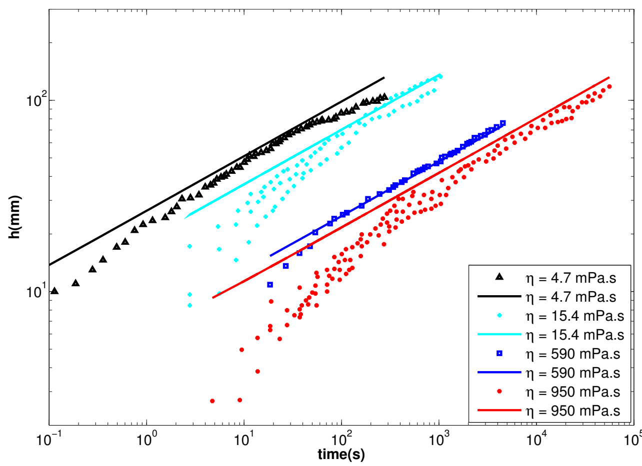

Figure 3: The predictions (solid lines) in equation (41) in comparison with the data (symbols) of the experiments [16].

5 Conclusions

We review some recent work on using the Onsager Principle as an approximation tool in complicated two-phase flow problems. The key steps of the method is as follows. One first carefully chooses some slow variables which can describe the system completely. Then the free energy and the energy dissipation function are computed approximately. Finally, one uses the Onsager Principle to derive a reduced model for the slow variables. It is found that the reduced model can capture the key dynamics of the system even though the model is much simpler than the two-phase Navier-Stokes equation with complicated interface and boundary conditions. The idea of the method can be generalized easily to study other over-damped systems.

There are lots of work to be done in this field. For example, it is an important question how to choose the slow variables. So far, the choice of slow variables is based on some physical intuitions or experimental observations. We need develop some general methods to choose proper slow variables in complicated systems. Secondly, we need do some theoretical studies on the approximation errors between the reduced model and the partial differential equation model.

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