Exploring the Teapot Effect: Microscale Investigations and Mechanistic Analysis

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摘要

In this work, we construct a microscopic model to study the fluid dynamics when moving over the teapot surface, which is also called "teapot effect". This question has been extensively studied via the Navier-Stokes equations and effective models in the past decades. As it is very difficult to solve hydrodynamic equations with a complicated boundary conditions, we developed a new microscopic model, which treat water as many fluid cells. These fluid cells interact with other surrounding fluid cells and also the teapot solid surface due to the adhesive forces. The complex evolution of the fluid is simulated by programming the motion of these droplets. We calculate the viscosity of the fluid via the microscopic model, and also calculate the trajectotries of the fluid cells when water moving over the teapot surface.

We conducted a thorough examination of the interaction strength within the water, particularly focusing on the attractive forces between water droplets and the teapot surface. We analyzed how these forces are influenced by the velocity of the water flow and the shape of the teapot. Detailed investigations were carried out to understand the effects of these factors on the behavior of the water on the teapot surface, including its movement on the broken areas of the teapot.

The novel microscopic model developed in this research enables us to delve into the intricate interactions occurring within the fluid system. We were able to explore forces acting between individual water droplets, as well as the intermolecular forces at play. This level of microscopic analysis surpasses the capabilities of traditional macroscopic fluid mechanics. Notably, although our microscale particle collision model was originally designed for the study of incompressible flows, it also exhibits innate potential for simulating compressible fluids. Given the well-known challenges associated with solving problems involving compressible fluids, our microscale particle collision model holds significant promise for a wider range of applications.

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I. INTRODUCTION

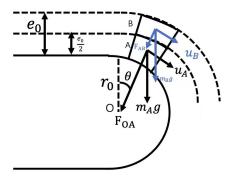
how to write this part (1-2 pages):

explain water flow over many solid surface, explain what is teapot effect why teapot effect is important? (for hydrodynamics, for physics.....) some models to explain teapot effect: momentum balance model, Navier-Stockes model

finally, explain microscopic model

explain that even the strong coupling system can be simulated with the microscopic model, so we can build this model to simulate water flow.

one photo here to show the teapot effect



 \boxtimes 1: Schematic figure to show a drop of fluid moving with a velocity \vec{u} . The liquid is treated as two-layer system to study the the layer-sepration phenomenon in the teapot effect. The mass of the layer-A and the layer-B are the same, $m_A = m_B = m$.

In the field of science and engineering, fluid flow is an extremely important and widely studied area. Understanding fluid flow plays a crucial role in the development of fields such as aerodynamics, ocean and atmospheric science, biology, chemical engineering, and aerospace technology. Simulation and understanding of fluid flow are essential in these fields. However, different shapes of containers and complex internal structures often give rise to a series of peculiar effects on fluid flow. One significant effect is known as the "Teapot Effect" [1 3]. The Teapot Effect refers to a phenomenon where the fluid flowing out of a curved and tilted container exhibits a peculiar behavior, seemingly flowing against the tilt. Although this phenomenon has been widely observed, the underlying mechanisms of fluid flow behind it have remained a challenging scientific problem. To explain and predict the Teapot Effect, researchers have proposed various models and theories. Early theories attempted to describe fluid motion using complicated mathematical models. However, due to the involvement of fluid-container surface contact and interaction, these models were excessively complex and difficult to solve. With the rapid development of computer science and numerical simulation, researchers have begun using Computational Fluid Dynamics (CFD) methods [4-7] to simulate the Teapot Effect. In the current field, several models and simulation results regarding the Teapot Effect have been developed. Some of these models are based on fundamental principles such as the Navier-Stokes equations [8-11], turbulence models [12-14], and boundary conditions involving surface contact [15, 16]. Since the 1950s [17], the teapot effect has been extensively studied by different groups. It can be treated as a purely hydrodynamic process [18, 19]. It can also be investigated via the principles of conservation of mass and momentum balances [20], taking into consideration the influence of inertia. This approach proved to be effective and provided a simplified yet semi-quantitative method for studying the phenomenon. More recently, the group led by E. Jambon-Puillet employed the momentum balance method to explore the formation of liquid helixes resulting from the teapot effect [21]. Additional research, such as that conducted by the Duez Group, has indicated that capillary effects and surface wettability play significant roles in the teapot effect [22]. These models focus on analyzing the mechanical characteristics of the flow and attempt to simulate the generation and evolution of the Teapot Effect using numerical methods. Other studies approach the topic from an experimental standpoint, using extensive observation and measurement data to validate the accuracy of the models. These models and experiments provide important references and foundations for our understanding of the Teapot Effect in fluid flow. Nevertheless, despite the existing models and experimental research on the teapot Effect, many unresolved issues remain. For example, the causes and mechanisms of the teapot Effect have not been fully explained. Additionally, the current models and experiments have not sufficiently accounted for the microscale interaction between the fluid and the container surface. In this work, we try to analyze the teapot effect via another aspect by building a toy model focusing on the interactions between the layers of the fluid and the interactions between the fluid and the teapot surface. This will help to reveal the connections between the teapot effect and the interaction strength between the fluid and the teapot surface. In this study, we explore various forces, including the adhesive forces between the fluid and the solid surface, the internal coupling strength within the fluid, the influence of gravity, and the impact of teapot thickness on the motion of liquid pouring out of a container. While our investigation does not encompass a comprehensive analysis of the teapot effect, we aim to approach the phenomenon using fundamental principles from college physics. We examine the effects of different force magnitudes on the fluid and discuss how the fluid behaves under various initial velocities. We also calculate the conditions under which the teapot effect can be observed. Additionally, we investigate the occurrence of layer separation within the fluid, where certain layers move along the outer wall of the container while others are ejected due to centrifugal force [23].

II. THEORETICAL METHODS TO ANALYSE THE TEAPOT EFFECT

A. Physical quantity

1. Mean free path

The "certain value" at this time is called the molecular effective diameter d. Define the molecular collision cross section σ , that is, the molecules injected outside the range of this circular cross section

will not deviate from the direction of velocity. For this section, the following equations are given:

$$\sigma = \pi d^2 \tag{1}$$

The number of collisions of gas molecules per unit time is called the average collision frequency, which represented by the following equation:

$$\overline{Z} = n\sigma \overline{v_{rel}} \tag{2}$$

We can use the average relative velocity \mathbf{v}_{rel} between particles to drive the mean free path.

$$\mathbf{v}_{rel} = \mathbf{v}_1 - \mathbf{v}_2 \tag{3}$$

$$\mathbf{v}_{rel} = \sqrt{\mathbf{v}_{rel} \cdot \mathbf{v}_{rel}} \tag{4}$$

$$\mathbf{v}_{rel} = \sqrt{(\mathbf{v}_1 - \mathbf{v}_2) \cdot (\mathbf{v}_1 - \mathbf{v}_2)} = \sqrt{\mathbf{v}_1 \cdot \mathbf{v}_1 - 2\mathbf{v}_1 \cdot \mathbf{v}_2 + \mathbf{v}_2 \cdot \mathbf{v}_2}$$
(5)

the average of the terms leads to

$$\overline{\mathbf{v}_{rel}} = \sqrt{\overline{\mathbf{v}_1 \cdot \mathbf{v}_1} - 2\overline{\mathbf{v}_1 \cdot \mathbf{v}_2} + \overline{\mathbf{v}_2 \cdot \mathbf{v}_2}} \tag{6}$$

Since \mathbf{v}_1 and \mathbf{v}_2 are random and uncorrelated,

$$2\overline{\mathbf{v}_1 \cdot \mathbf{v}_2} = 0 \tag{7}$$

Thus, the expression of relative velocity is

$$\overline{\mathbf{v}_{rel}} = \sqrt{\overline{v_1^2 + \overline{v_2^2}}} = \sqrt{2}\overline{\mathbf{v}} \Rightarrow \overline{v_{rel}} = \sqrt{2}\overline{v}$$
(8)

Let the average molecular velocity be \overline{v} , the mean free path is:

$$\overline{\lambda} = \frac{\overline{v}t}{\overline{Z}t} = \frac{\overline{v}}{n\sigma\overline{v_{rel}}} = \frac{1}{\sqrt{2}n\pi d^2}$$
(9)

Where d is the molecular effective diameter, as we mentioned above.

With the formula of the mean free path in the form Eq.(48), one can calculate the "mean-free-path" of the fluid cells, even though this concept was first defined for the case of gas. As we treat the fluid as a "dense gas" with a large cross-section and strong interaction. The mean-free-path will also be used to calculate the viscosity in the next pages.

add a figure here to illustrate the cencept of fluid cell: consisting of many water molecules

In the teapot effect, we divide the water into N cells, where \bar{v} is the mean velocity of the fluid cells. n is the density of the fluid cells, while σ is the cross-section between two fluid cells. The value

of σ will be estimated according to the formula of Van der Waals interaction in the next section.

2. Viscosity Coefficient

As a preliminary theory, assume that the velocities of all molecules are of magnitude \bar{v} (average speed) and are uniformly distributed in the six possible directions. Consider a surface element ΔS on $z=z_0$. Thus, the number of particle that pass through the surface ΔS within time Δt is 1/6 of the total particle number in volume $n\bar{v}\Delta S\Delta t$ where n is the numerical density of the particle in the space. Thus,

$$N_{pass} = \frac{1}{6} n\bar{v}\Delta S\Delta t \tag{10}$$

Each molecule passing through the plane carries some physical quantity from one side to the other side. Since we are studying viscosity, consider the momentum mu. Since the system is not uniform along the z direction, the physical quantity Q pass through surface element is

$$\Delta Q = \left(\frac{1}{6}n\bar{v}\Delta S\Delta tQ\right)_A - \left(\frac{1}{6}n\bar{v}\Delta S\Delta tQ\right)_B \tag{11}$$

And the flow should be

$$\mathcal{F} = \frac{\Delta \mathcal{Q}}{\Delta t} = \frac{\bar{v}}{6} \left[(n\mathcal{Q})_A - (n\mathcal{Q})_B \right] \Delta S \tag{12}$$

Where A and B respectively represent where $z=z_0\mp\bar{\lambda}$ and $\bar{\lambda}=\bar{v}\Delta t$ is the mean free path of gas. It should be emphasized that the thermal equilibrium distribution is achieved by frequent collisions between molecules. Then, we can make another simplifying assumption that alien molecules are assimilated through a single collision. Thus,

$$\mathcal{F} = \frac{\Delta \mathcal{Q}}{\Delta t} = \frac{\bar{v}}{6} \left[(n\mathcal{Q})_A - (n\mathcal{Q})_B \right] \Delta S$$
$$\sim -\frac{\bar{v}}{6} \left[\frac{\mathrm{d}}{\mathrm{d}z} (n\mathcal{Q}) \right]_{z=z_0} \cdot 2\bar{\lambda} \cdot \Delta S$$
$$= -\frac{1}{3} \left[\frac{\mathrm{d}}{\mathrm{d}z} (n\mathcal{Q}) \right]_{z=z_0} \cdot \bar{v} \cdot \bar{\lambda} \cdot \Delta S$$

Then we make the substitution that Q = P = mu; $\mathcal{F} = f$, then

$$f = \frac{\Delta P}{\Delta t} = -\frac{1}{3} \left[\frac{\mathrm{d}}{\mathrm{d}z} (nmu) \right]_{z=z_0} \bar{v}\bar{\lambda}\Delta S \tag{13}$$

$$= -\frac{1}{3}\rho\bar{v}\bar{\lambda}\left(\frac{\mathrm{d}u}{\mathrm{d}z}\right)\Delta S \tag{14}$$

Notice that the Newton's viscosity law is

$$f = -\mu A \frac{\partial u}{\partial z} \tag{15}$$

Thus, the viscosity coefficient is

$$\mu = \frac{1}{3}\rho\bar{v}\bar{\lambda} \tag{16}$$

where ρ is the mass density and $\bar{\lambda}$ is the mean free path.

B. Model-1: Navier-Stokes equation

1. Continuity Equation

According to the law of conservation of mass, the mass of a fluid remains constant during the flow process. Thus, consider a substance composed of randomly selected mass points in a fluid, with a volume of V and a mass of M, we have that

$$M = \int_{V} \rho dV \tag{17}$$

Where ρ is the mass density of the fluid. The conservation of mass suggest that

$$\frac{\partial M}{\partial t} = \frac{\partial}{\partial t} \int_{V} \rho dV = -\oint_{S} \rho \mathbf{v} \cdot d\mathbf{S}$$
 (18)

Consider the mass derivative of the volume integral,

$$\int_{V} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right) dV = 0 \Rightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$
(19)

This is the Continuity Equation, and for incompressible fluid, ρ is a constant. Thus,

$$\nabla \cdot \mathbf{v} = 0 \tag{20}$$

2. Momentum Balance Equation

The mass forces and surface forces acting on the fluid volume V and the surface S, respectively, are as follows:

$$\int_{V} \rho \mathbf{F} dV \tag{21}$$

$$-\oint_{S} p d\mathbf{S} = -\int_{V} \nabla \cdot p dV \tag{22}$$

The viscous force should be expressed by Newton's law of viscosity:

$$\tau = \mu \nabla \mathbf{v} \tag{23}$$

Consider the incompressible fluid, the change of momentum should be

$$\frac{\mathbf{D}\rho\mathbf{v}}{\mathbf{D}t} = \rho \left(\frac{\partial\mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla\mathbf{v}\right) \tag{24}$$

assume the mass force is gravity and there exist a pressure as the active force. We can also take viscosity into consideration. Thus, the momentum balance equation can be written as

$$\int_{V} \rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) dV = - \oint_{S} p d\mathbf{S} + \int_{V} \rho g dV + \oint_{S} \mu \nabla \mathbf{v} d\mathbf{S}$$
 (25)

Use Guass' law to eliminate integral

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v} + g \tag{26}$$

This is the vector form of the momentum equations in Navier-Stokes Equations, where ρ is the mass density of the fluid, $\nu = \mu/\rho$ is the kinetic viscosity coefficient, \mathbf{v} is the velocity of fluid, g is the gravitational acceleration, p is the pressure.

Consider the ideal fluid without viscosity. The momentum equations in Navier-Stokes Equations will degenerates into Euler's equation:

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + g \tag{27}$$

3. Boundary Conditions

In order to find the solution that suitable to teapot effect, we can add some boundary conditions to the equations. The methods of adding boundary conditions is easy. First of all, the fluid cannot enter the solid surface, while considering the interaction between the solid-liquid interface. We can assume that the flow is non-slip, which means

$$v_{S-L} = 0 (28)$$

Similarly, we can limit the maximum value of the flow velocity, that is, the flow velocity at the gas-liquid interface.

$$v_{L-G} = U (29)$$

Simultaneously, we can consider that the flow velocity of the flow in the flat plate part is only related to the viscosity in the y direction and is linearly distributed along the y-axis.

Although finding the numerical solution of Navier-Stokes Equations is a universal methods to solve fluid mechanic problem, it is not easy to apply in teapot effect. That is because the teapot effect is the result of coupling of various factors such as surface tension and viscous force. Surface tension play a significant role in this phenomenon. However, it is hard to consider the affect of surface tension in Navier-Stokes equations, and the fluid mechanics equations is challenging to solve. Thus, the Navier-Stokes Equation is not useful in this problem.

C. Model-2: Momentum balance method

1. Balance State

Take vertically downwards as the positive direction of y-axis. The force balance equation is

y - direction:
$$\pi(p_{up} - p_{down})R^2\cos\psi + mg + F\cos\psi = 0$$
 (30)

x - direction:
$$\pi(p_{uv} - p_{down})R^2 \sin \psi + F \sin \psi = 0$$
 (31)

Where the first term represent the affect of surface tension, while the second term is the gravitational force. γ_{LG} is the coefficient of surface tension between liquid-gas surface, θ is the contact angle between liquid and solid surface, m is the mass of the liquid and g is the gravitational acceleration. The term F is the normal force and other force that may exist to affect the balance.

2. Unbalance State

In order to simplify the model, we assume the viscosity is negligible. Consider the direction \hat{n} of the vertical streamline, due to the centripetal acceleration

$$a_n = \frac{U^2}{R}$$

So the net force on the fluid cell is:

$$\sum \delta F_n = a_n \delta m = \frac{\rho U^2}{R} \delta V$$

According to the Bernoulli's Law, the equation of motion in the direction of the vertical streamline is

$$\left(-\rho g \frac{\mathrm{d}h}{\mathrm{d}n} - \frac{\partial P}{\partial n}\right) = \frac{\rho U^2}{R} \tag{32}$$

Where ρ is the density of the fluid, h is the vertical length, $R = r + \Delta n/2$ is the radius of curvature of the streamline, P is the pressure caused by surface tension, and the volume of the flow cell we consider is $V = \delta s \delta n \delta y$. This equation can be rewrite as

$$-\rho g \Delta h - \Delta P \sim \frac{\rho U^2 \Delta n}{R} \tag{33}$$

In the calculation, we can assume $\cos \psi_0 = \frac{dh}{dn} \sim \frac{\Delta h}{\Delta n}$. The difference on pressure should be caused by the adhesion force, or surface tension. Thus, according to the Yang-Laplace Equation

$$\Delta P = \frac{\gamma_{LG}}{C^{-1}} \tag{34}$$

The definition of Weber number is the ratio of inertia and surface tension

$$We = \frac{\rho U^2 \Delta n}{\gamma_{LG}} \tag{35}$$

Where C is the curvature of the capillary effect half-moon area, from the Eq.33 and Eq.34 we can drive to the expression of the curvature

$$C = \frac{\rho(U^2 \Delta n + g\Delta hR)}{R\gamma_{LG}} \tag{36}$$

Since the equation of motion Eq.32 and Eq. 33 is a equation of the surface distribution of force, and the surface that surface tension have signefacent effect on is the wetted area $A_{wet} = r \times \psi_{wet}$

$$|F_{total}| = \frac{\rho U^2 \Delta n}{R} \times A_{wet} = \frac{\rho U^2 \Delta n}{R} r \psi_{wet}$$
(37)

From the geometry relationship, we can get the expression of the change of momentum flux

$$D = \rho U^2 \Delta n (1 - \sin \psi_0) \tag{38}$$

$$= \frac{\gamma_{LG}}{C^{-1}} r(\psi_0 + \psi_{menisc}) + \rho gr \Delta h(\psi_0 + \psi_{menisc})$$
(39)

$$= |F_{total}| \tag{40}$$

substitute the expression of Weber number

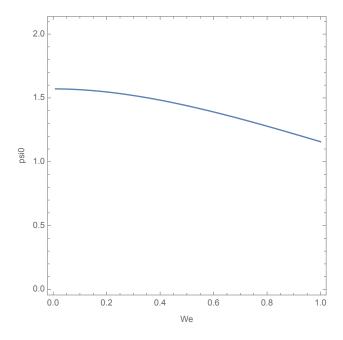
$$\frac{1 - \sin \psi_0}{\psi_0 + \psi_{menisc}} \text{We} = \frac{r}{C^{-1}} \text{We} + 2r \frac{\rho g h}{\gamma}$$
(41)

If we assume the capillary effect half-moon area is part of a circle, the expression of ψ_{men} is availble to get

$$\psi_{menisc} = \left\lceil \frac{2C^{-1}(1+\cos\theta)}{r} \right\rceil^{1/2} \tag{42}$$

$$= \left[\frac{R}{r} \frac{2\gamma_{LG}(1 + \cos \theta)}{\rho(U^2 \Delta n + g\Delta hR)} \right]^{1/2}$$
(43)

These equation show that the teapot effect do rely on the geometry properties that represented by the factor r/R in the expression of ψ_{mensic} and the surface wettability of the solid surface which is rely on the contact angle θ .



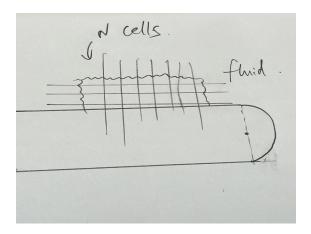
 \boxtimes 2: This is the numerical result of the momentum balance equation Eq.41, which shows that the ejection angle ψ_0 will decrease when the Weber number We increasing.

III. NEW APPROACH: MICROSCOPIC MODEL (ORIGINAL WORK)

A. Model construction

Studying fluid dynamics on a solid surface has been one of the difficult physical problems in the past decades. Usually, the general variables to describe the fluid dynamics are the pressure p, density ρ , fluid velocity \vec{u} , viscosity μ , etc. These macroscopic variables satisfy the hydrodynamic equations with specific boundary conditions. For the teapot effect we care about here, the boundary conditions of water on the teapot solid surface is needed, where the adhesive forces between the fluid and the teapot surface must be given as one of conditions. One typical hydrodynamic equation is the famous Navier-Stockes equation. This equation is too complicated for realistic problems due to the complicated boundary conditions. The finite-element method has been applied to study the numerical solutions of Navier-Stokes equation. These have been extensively studied in many previous references.

From statistical physics, we know that these macroscopic variables can be expressed as a summation of small fluid cells. In other words, one can divide the fluid into many small cells. The dynamical evolution of the fluid can be regarded as a **collective motion** of a large number of fluid cells. When the fluid is a strongly coupled system, instead of a weakly coupled medium, then the interaction forces between the fluid cells are large. It means that how the fluid cells move depends on the forces from surrounding fluid cells. The macroscopic variables, like the **density** ρ , **pressure** p, etc can be expressed as an integration of the fluid cells' velocity and momentum. This relation will be given in the later section of this manuscript. Further, the other important physical variables, like **viscosity** μ , **Reynolds number** Re, etc, can also be written as a function of the small fluid cells' positions and momenta. In the following parts, we will treat the fluid cells as a kind of particle. The fluid consists of these particles. Please see the schematic diagram in Fig.3.



 \boxtimes 3: schematic diagram: the water flows over the solid surface (teapot). 2-dimensional case is considered to simplify the question. The fluid is separated into N parts (consisting of N "particles"). The edge of the teapot mouse is simplified as a semicircle. The fluid moves in the right direction with an initial velocity u_0 .

As we know, the fluid is strongly coupled together. Therefore, the fluid cells will also interact with the surrounding cells. The interaction force between each cell (or particle) is connected with the coupling strength of the fluid.

We study the dynamic evolutions of the fluid on the solid surface, like the case of water flowing out of the teapot. To simplify the question, we focus on the two-dimensional case, shown as Fig.3. The fluid move above the solid surface, where the edge of the teapot mouse is treated as a semicircle with the radius $r_0 = 2$ cm. The thickness of the water is taken as $e_0 = 3$ cm according to the realistic estimation. How the water flows over the edge of the teapot mouse, i.e., whether the teapot can be observed or not, depends sensitively on the following factors:

- · initial velocity of the fluid
- coupling strength between the fluid and teapot
- coupling strength inside the fluid
- shape of the teapot mouse
- other external forces (like gravity)

In the following sections, I will study how these factors affect the dynamical evolutions of the fluid, i.e., the teapot effect.

B. Parameters and setups

If we study the dynamic evolution of the water on the teapot surface, the boundary conditions like the adhesive force between the water and the teapot, the flow velocity, and the pressure gradient p, must be considered. The Navier-Stokes equation with these complicated boundary conditions is difficult to solve. There has been a comprehensive study on this part [?]. It turns out to be difficult for readers.

In this study, we will develop a new method to study fluid dynamics. The above factors controlling the flow dynamics will be considered via the forces between particles, which consist of the fluid. Furthermore, this method developed to study the non-compressible fluid, can be easily extended to the case of compressible fluid.

After treating the fluid as a large set of particles (fluid cells), the particles' motion is connected with the forces coming from the surrounding object. In Fig.4, the particle suffers the forces including gravity mg with the mass m, the supporting force from the teapot surface, and also the adhesive forces.

The force between two particles is written as $F_{p-p}(r)$ here, which depends on the distance r between two particles. The force $F_{p-p}(r)$ becomes an attractive force when the distance is large, and the repulsive force when the distance r is small. The repulsive force indicates that the fluid (water) is close to non-compressible. The internal attraction of water, also known as water's cohesion, is caused by intermolecular forces between water molecules. This attraction is primarily due to hydrogen bonding, which is caused by the electronegativity difference between water molecules. Water molecules are composed of one oxygen atom and two hydrogen atoms, with the oxygen atom being more electronegative than the hydrogen atoms. This results in the oxygen atom carrying a partial negative charge, while

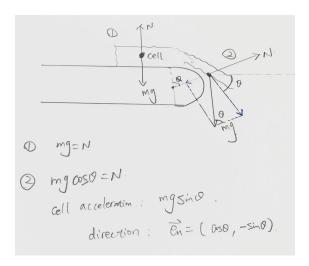


图 4: The forces acting on the fluid cell (particle). For a particle next to the teapot surface, it includes gravity (external force), the (adhesive and supporting) force from the teapot surface, and the interaction force from surrounding particles.

the hydrogen atoms carry a partial positive charge. Due to this charge difference, hydrogen bonds can form between water molecules. In water, hydrogen bonds can form a network structure, allowing water molecules to come close to each other and tightly connect. This hydrogen bonding leads to strong attractive forces between water molecules, enabling them to closely aggregate together. The interaction force between different particles is illustrated in Fig.5.

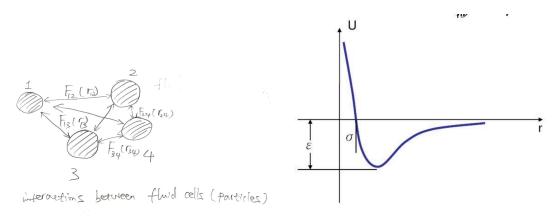


图 5: The interactions between different fluid cells (particles).

Short-range forces: Inspired by the formula of the van der Waals force between water molecules, we approximate the forces between particles to be,

$$f_{p-p}(r) = \begin{cases} -C_1 \times mg, & \text{if } 0 < r \le L_0 \\ C_2 \times mg, & \text{if } L_0 < r \le L_1 \\ 0, & \text{if } r > L_1 \end{cases}$$
(44)

where m is the mass of the fluid cell (particles), this can be fixed by the fluid density (given latter). L_0 and L_1 is the interaction length.

When the distance is smaller than L_0 , the forces between two particles are repulsive, represented by the minus before C_1 . When the distance is between $L_0 \sim L_1$, the force becomes an attractive force. f_{p-p} is close to zero when the distance is too large. To get a better estimation about the magnitude of the particle-particle interaction, we use the gravity of the fluid cell mg as a measurement. Therefore, the forces between fluid cells can be regarded as a several times of its gravity. The value of the parameter C_1 and C_2 is closely connected with the coupling strength of the fluid. Different values of the C_1 and C_2 will be employed to calculate different kinds of fluid moving on the teapot surface. The corresponding macroscopic variables like viscosity will be calculated.

There is also adhesive force f_{p-S} between the fluid and also the teapot surface. We also employ a similar formula,

$$f_{p-S}(r) = \begin{cases} -C_3 \times mg, & \text{if } 0 < r \le L_0 \\ C_4 \times mg, & \text{if } L_0 < r \le L_1 \\ 0, & \text{if } L_1 < r \end{cases}$$
 (45)

This equation means the fluid cells can not "move into" the teapot surface due to the repulsive force. Also, there is adhesive force that "pull" the fluid cell toward the teapot surface. This force becomes important for Hydrophilic materials, while becomes zero for Hydrophobic materials.

Now, the fluid is separated into N=3000 parts. Each part is represented with a particle in the figure. As we know the density of the fluid ρ , the length of the fluid over the teapot surface (see fig.3), then the mass of each particle (fluid cell) is,

$$m = \rho \times e_0 l_f / N \tag{46}$$

To get a better numerical simulation of a large set of particles moving on the teapot surface, instead of taking all the initial velocities (u_x^i, u_y^i) of the particles as the same value, we initialize the value of u_x^i with the normal distribution, where the mean value is taken as $\langle u_x \rangle = 5$ cm/s, and the width as $0.01 \ (cm/s)^2$. While for the velocity along the y-direction, u_y^i satisfies the mean value $\langle u_y \rangle = 0$ and the same width. With this setup, a large number of particles move collectively to the right with the velocity $\langle u_x \rangle$, while simultaneously exhibiting a certain degree of random and chaotic motion internally.

Long-range forces: In order to simulate fluid dynamics, introducing short-range forces between fluid cells is not enough. This can be reflected in the numerical simulations between particles. We introduce an additional long-range-force mode, which can give a more realistic simulation of fluid dynamics with the microscopic model. The Long-range force is set to be a weak force, which simulates the collective motion of the fluid. The magnitude of the long-range force inside the particles is set to be on the order of 10^{-1} of the short-range forces between particles (Eq.(44). With this longe range interaction, the system consisting of particles can better simulate the motion of the fluid.

In future studies, we will employ a more realistic form similar to the Van der Waals force to describe the interactions between adjacent particles (fluid cells). Including the London force (which contributes repulsive force when r is small) and the Column force (which contributes attractive force

when r is large), the combined force between two fluid cells is written as,

$$F_{p-p}^{real}(r) = -A/r^6 + B/r^2 (47)$$

This more realistic interaction force will be included in the future work.

IV. RESULTS AND ANALYSIS

A. Calculation of mean-free-path λ , viscosity μ

mean-free-path:

To treat fluid as a large set of fluid cells like "dense gas", we divide the fluid with the area S into N cells (see the schematic figure above). In the **two-dimensional case** discussed here, the cross-section between fluid cells has been a typical interaction length instead of a area, i.e. $\sigma \approx \times L_1$, where C and L_1 are the parameters given in above sections representing the interaction strength between fluid cells. (Dimension analyse: n is in m^{-2} , C is dimensionless, L_1 is in m^1 , then $\bar{\lambda}$ is in m^1).

$$\overline{\lambda} = \frac{1}{\sqrt{2}n\pi d^2} = \frac{1}{\sqrt{2}\frac{N}{S}(L_1)}$$
(48)

In this microscopic simulation of the water following over the teapot surface, we take N=3000, where the "volume" (in 2-dimension, it is "area") of the water piece is $S=e_0\times L=0.03\times0.08$ (m^2). The typical interaction distance is estimated via the relation $L_1\sim 2\times \sqrt{S/N}$. With this system we build, the mean free path is calculated to be $\bar{\lambda}\approx 0.00032$ m= 0.32 mm. This value is reasonable for the water system. Note that the value of $\bar{\lambda}$ can be adjusted by taking different values of L_1 or N, to study different dynamical systems with different coupling strengths (such as water, oil, etc).

viscosity of the fluid-cell system:

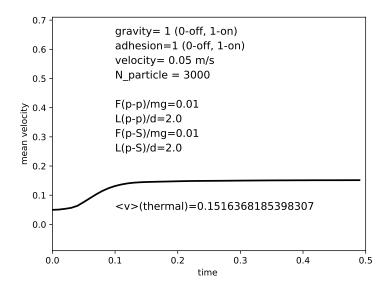
The formula of the viscosity has also been presented in above section. We now calculate the viscosity of our "fluid-cell" system, which use fluid cells to simulate the dynamical evolution of water.

Based on the formula of viscosity given in Section II, the viscosity in 2-dimensional system is

$$\mu_{2d} = \frac{1}{2} \rho \bar{v} \bar{\lambda} \tag{49}$$

where ρ is the mass density and $\bar{\lambda}$ is the mean free path. \bar{v} is the average speed of the random heat motion of the gas molecules (which are fluid cells in our case). The value of \bar{v} can be given by the textbook if the distribution of particle velocity satisfying a Boltzmann distribution. In our case, as we already specify the interaction and density of fluid cells, the average speed of the random motion of fluid cells should be calculated via our model. We simulate the random motion of N=3000 fluid cells with the above parameters. The time evolution of the average speed is plotted. The initial mean velocity of those fluid cells are set to be $u_0 = 0.05$ m/s. With the cell-cell interactions, the thermal velocity after reaching equilibrium is around $\bar{v} = 0.15$ m/s. With the interactions, the average velocity

of fluid cells change with time, plotted in Fig.6.



⊠ 6: time evolution of the mean velocity of a large number of fluid cells. This is calculated based on our "Microscopic scattering model". The interactions between fluid cells are taken as previous sections. The density of the fluid cells is same as the value used in the mean-free-path.

Other relevant parameters in the model are,

$$\rho = 1 \ kg/m^2 \tag{50}$$

$$\bar{\lambda} = 0.32 \ mm \tag{51}$$

One can calculate the dynamical viscosity of the 2-dimensional "fluid" to be $\mu_{2d}=2.4\times 10^{-5}~(\text{kg/s})=2.4\times 10^{-2}~[(\text{mPa}\cdot\text{s})\cdot\text{m}]$. As we consider the 2-dimensional system, there is additional 'm' (length unit) in the μ_{2d} . Note that in the realistic case with 3 dimensions, the dynamical viscosity of the water is around $0.1\sim 1~(\text{mPa}\cdot\text{s})$ at different temperatures.

(Dimension units:
$$1Pa = 1N/m^2 = 1(kg \cdot m/s^2)/m^2 = 1kg/(m \cdot s^2)$$
)

B. Probe microscale force with gravity

How does gravity play the role in fluid dynamics?

When simulating the movement of fluid on the surface of a teapot, the dynamic behavior of the flow is highly sensitive to the coupling strength or the interactions between fluid elements. The key question is: What is the magnitude of the microscopic interactions between fluid elements (or water droplets)?

<u>在模拟流体在茶壶表面移动时,流动的动态行为对耦合强度(或流体单元之间的相互作用)非常敏感。关键问题是</u>

Due to the interaction forces within the fluid (equations (44)-(45)), controlling the evolution of the fluid, we can gauge the magnitude of microscopic forces within the fluid by using gravity as a reference. To gain a more intuitive sense of these forces, we use gravity as a benchmark for studying their magnitude. For instance, the forces between fluid cells include repulsion and attraction, and their magnitudes are taken as multiples of the gravitational force on a fluid cell, as specified by the parameters in equations (44)-(45): $C_1 = C_2 = C_3 = C_4 = 0.01$. In other words, the attractive and repulsive forces between fluid cells are assumed to be only 10^{-2} times their own gravitational forces.

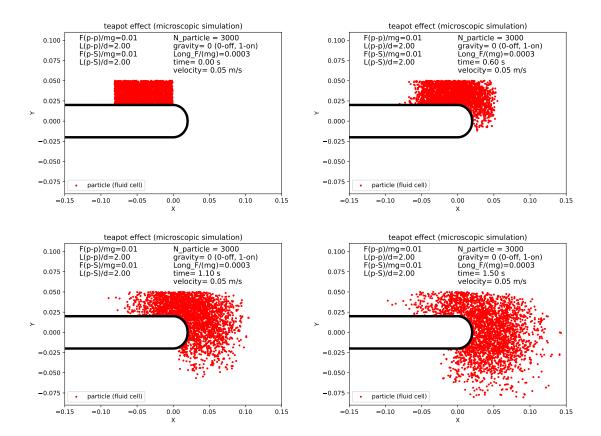
So, what does the evolution of the fluid look like when the forces between fluid cells, whether attractive or repulsive, are only 10^{-2} times their own gravity? The numerical simulations presented below provide the answer. Furthermore, considering that water is an incompressible fluid, we generally assume the following: 1. When the distance between two fluid cells is less than half of the original distance, there is strong repulsion, indicating incompressibility. 2. When the distance between two fluid cells is greater than twice the originally set distance, there is strong attraction, implying that water is incompressible.

Therefore, in the equations governing the interaction forces, the distance parameters are set as follows: $L_0 = 0.5 \times D$, $L_1 = 2 \times D$. Here, $D = \sqrt{S/N}$ represents the average distance (typical distance) between any two fluid cells when N fluid cells are placed within an area of S. 由于流体内部的相互作用力(方程(44)-(45))控制着流体的演化,我们发现可以用重力来检测流体内部微观力的力那么流体的演化是什么样的呢?以下的数值模拟给出了答案。同样,考虑到水流是一个不可压缩流体,所以,我们- $L_1 = 2 \times D$ 。这里的 $D = \sqrt{S/N}$ 是在面积 S 区域内放置 N 个流元时每两个流元之间的平均距离(typical distance)。

If the microscopic forces between adjacent fluid cells within the fluid are much smaller than their own gravitational forces, gravity can be considered an external force that has the potential to significantly influence the collective motion of a large number of fluid cells. Conversely, when the interaction forces between fluid cells are substantial, gravity, acting as a perturbation, may not cause significant changes in the overall motion of a large number of fluid cells. For example, if there is strong attraction and repulsion between a large number of fluid cells, adding gravity may not lead to noticeable alterations in the motion of these fluid cells. This hypothesis is demonstrated in the following model simulations. 如果流体内部,相邻两个流元之间的相互作用力 microscopic force,比其自身的重力小很多的时候,则重力作为一个外力,应该可以极大的改变大量流元的集体运动。

The following two sets of figures depict the collective motion of a large number of fluid cells. We define N=3000 particles representing water droplets, with their initial positions distributed as shown in the figures. The initial velocity is horizontal to the right, denoted as u_0 . The interaction forces between different particles are described by equations Eq.(44-45). When gravity is not considered, the motion of a large number of particles appears as shown in Fig.7, with four panels representing the distribution of the fluid at times t=0, 0.5, 1.0, and 1.5 seconds. 以下两组图,给出了大量粒子(fluid cells)的集体运动行为。我们定义 N=3000 个粒子代表水滴,这些粒子的初始位置分布在如图所示的位置,初始的不同粒子之间的相互作用力也在方程 Eq.(44-45) 给出了,当没有考虑重力的时候,大量粒子的运动如 Fig.7所示。0.5, 1.0, 1.5 s 的分布。

From Fig.7, it is evident that due to the initial velocity to the right, these red points representing



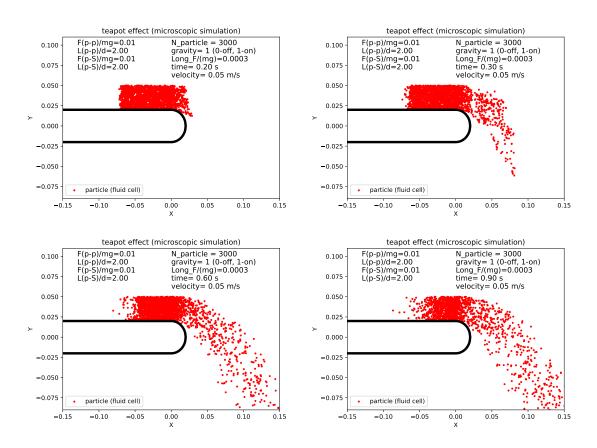
 \boxtimes 7: Using the microscopic model we built to simulate the dynamical evolution of fluids over the teapot solid surface. There are repulsive and attractive forces between fluid cells. Besides, there are adhesive forces between the fluid and the solid surface (plotted with black solid lines). These microscopic forces between water droplets are taken as 10^{-2} of their gravity, i.e. $F/(mg) = 10^{-2}$. For figures represent the fluid distributions at different times. The water droplets are plotted with red points, which move in the right direction with an initial velocity $u_0 = 0.05$ m/s. Gravity is not included yet.

water droplets move to the right. Since the interaction between water droplets and the solid surface accounts for viscosity (Eq.45), you can clearly see that some water droplets become adsorbed on the solid surface, as shown in the 2nd, 3rd, and 4th sub-figures. These red points on the curved surface of the teaport represent water droplets that do not continue moving in a straight line to the right but instead adhere to the vicinity of the curved surface of the solid.

These water droplets near the teapot's solid surface experience forces from both the solid surface and other liquid droplets. The interplay of these forces governs the trajectory of each water droplet, ultimately resulting in the teapot phenomenon. 从 Fig.7中可以看出,由于流体具有一个向右的初速度,这些红色的点(水滴)往右运动,由于水滴与固体表面之间能够明显的看到一些水滴会被吸附在固体表面(如第 2, 3, 4 子图所示),在水壶弯曲的表面吸附着一些红色的点

在 Fig.7中,在流体演化的后期(比如 t=1.0, 1.5s 的两个子图),我们能看到,水滴弥散在更大的空间中,这是由于我们采取的相互作用力 Eq.44的形式导致的。在真实生活中,水流从高处流下的时候,会出现分叉扩散的现象,比如瀑布。在没有重力的时候,不同水滴之间不会被拉着往下走,而是容易出现扩散的现象。如果我们采用更加真实的水滴相互作用,而不是 Eq.44形式,我们应该可以看到更加真实的流体演化图。但这会有新的挑战,所以目前我们将基于当前的模型来研究 teapot effect。

当考虑重力贡献之后,每一个水滴(fluid cells)都会受到重力加速度的影响,而往右下方运动。不同时刻,大量水滴的运动轨迹在 Fig.8展示出来。这个图分别画出了大量水滴在 t=0.2, 0.3, 0.5, 1.0 s 时刻的流体情况。可以看出,重力作为外加的一个力,使得所有粒子往右下方跑。这已经明显的改变了粒子的运动行为。Fig.8 is very different from Fig.7 after considering the contribution of gravity. 这说明了重力的影响非常大。

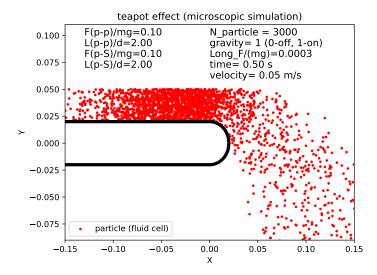


🛚 8: Water dynamics at different times. Red points represent water droplets (fluid cells). All the parameters are the same with Fig.7, but considering gravity.

但如何用重力来探测水滴之间的相互作用力的大致 magnitude 呢? 当我们假设流体之间的耦合非常强,即手动把水滴之间的相互作用力(Eq.44-45)增大 10 倍,即满足 $F/(mg)=10^{-1}$. 这里的 mg 是水滴(或者流元)的重力。可以发现,当流体内部的排斥力和吸引力非常大的时候,重力也就像微扰项一样作用到流元的运动轨迹上,重力对流元的运动就不会起到明显的影响,如图 Fig.9所示。

由于图 Fig.8和 Fig.9都考虑了重力的影响,唯一不同的就是,流体流动时的扩散形式。可以发现,如果重力相对于流体内部相互作用来说很大且不可忽略时,则重力可以明显的改变流体的运动形式。但反之,如果微观相互作用力(包括流体内流元之间的相互作用力、流体与茶壶固体表面的相互作用力)很强,则流体的运动形式不会倍重力明显的影响到。

这种有趣的现象,实际可以被我们用来粗略的估计微观相互作用力的大致量级。从我们的模型计算可以发现,流体内部水滴之间的相互作用力,大概只有其自身重力的 10^{-2} 左右,而不是同等数量级。这对于微观层面理解流体力学有参考意义。



 \boxtimes 9: The dynamical evolution of fluids over the teapot surface. A stronger coupling strength in the fluid is considered, where the interaction forces F_{c-c} , F_{c-s} are taken as 10^{-1} of the fluid gravity, i.e., $F/(mg) = 10^{-1}$, see Eq.(44-45).

C. Ejection angle in the teapot effect

当大量粒子从弧度表面向右下方运动时,类似水流的流动。这些水滴的平均位置,可以采用以下方式来计算。如图.??所示,在每一个区域,流体的位置可以被认为是这个区域中例子的平均位置,比如在一个扇形区域 $\theta_j \sim \theta_j + \Delta \theta$,里面的粒子(水滴的总数是 N_j ,每个粒子的位置是 $\vec{r}_i(\theta_j)$. 则这个区域内,流体距离圆心(坐标原点的位置)为,

$$\langle r(\theta_j) \rangle = \frac{1}{N_j(\theta_j)} \sum_i |\vec{r}_i(\theta_j)|$$
 (52)

这样在每一个区域内,我们都可以计算出它的"平均位置"。当没有水壶固体表面的吸引力时,我们可以计算出水流的平均位置(也就是所有 $\langle r(\theta_i) \rangle$ 点的连线)。这些点的示意图如图 10所示。

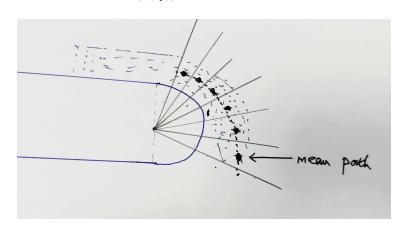
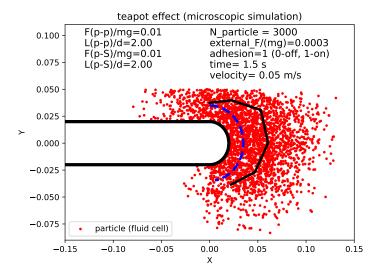


图 10: When the fluid moves along the teapot surface, the fluid flows over the curved surface. We separate the fluid over the curved surface into many pieces, where the center of each piece can be calculated, shown as in the figure.

在我的模型中,大量的水滴的运动,可以通过模型来描述。在某一时刻,我们可以得到这些水滴的位置,如图11所示。在每一个弧面的方位角,我们都可以计算出这个区域的粒子的平均位置,然后把不同方位角 θ_i 的平均位置连线,就得到了水流中心的运动轨迹。在图中,蓝色的虚线,是假设极端情况下,水流紧紧的贴着水壶固体表面运动的轨迹。但由于真实的情况下,水流会犹豫自身的初始速度,而向右侧冲出去。这使得水滴倾向于离开固体表面。但由于固体表面对水滴的吸引力,使得一部分水滴可能沿着固体表面运动。大量水滴的平均位置如实线所示,图11。这个黑色的实现明显有远离固体表面的趋势,但在右下方,又有点被拉回固体表面的趋势,这就是 teapot surface 对水流的吸引力造成的。很显然,如果没有 teapot surface adhesive force,那么水滴会在初始速度 u_0 的作用下,往右侧运动,远离固体表面。在图11,为了简化分析,我们暂时忽略了重力的影响,这样水滴(红色的点表示)的运动,主要受到水滴之间的相互作用,和水滴-固体表面的相互作用的影响。这使得分析更加清晰。

通过以上的方法和方程 Eq.(52),我们可以较为量化的定义水滴何时视为离开固体表面,或者沿着固体表面运动。通过这个定义,我们可以引入一个概念,喷射角度,也就是在这个角度,流体离开固体表面。这在我们的 microspic model 中就可以通过粒子的平均位置的计算体现出来。



🗏 11: The mean path of the fluid moving over the teapot surface. The blue dashed line is the mean path when fluid is most strongly coupled with the teapot's solid surface. The black solid line represents the mean path of the red points. As the red points move in the right direction, they also suffer forces from other red points and the solid surface, their position is shown in the figure. They tend to leave the solid surface. Gravity is not included to simplify the analyse.

D. Factors Influencing the Teapot Effect

水流在茶壶口的固体表面运动时,水流的运动情况依赖于水的耦合强度、水与茶壶材料的粘性大小。这些物理量体现在爱 microscopic model 中,就是粒子-粒子之间的相互作用力的大小和力程,还有 particle-surface 的力大小和力程。这反应了物理过程的规律。但还有另外的几个因素会影响流体的运动,一个是水流的初始速度,另一个是茶壶口的几何形状。

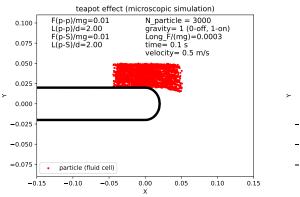
当水流的初始速度不一样的时候,即使水滴在初始时刻(t=0)受到相同的作用力,那么这些水滴在后期(t>0)的运动轨迹也不同,则它们与茶壶表面的距离也不同,这样在后期 t 时刻,这些水滴与茶壶表面的距离也会变的不同。特别是,当水流的初始速度较大时,水流可能直接喷射出去,而几乎不会受到固体表面的力的影响。

1. flow velocity:

如何在微观层面上研究这些因素对 teapot effect 的影响,是本公主的重点之一。

我们可以把粒子的初速度变为之前的 10 倍,也就是现在的粒子的平均初始速度为 $u_0 = 0.5$ m/s, 且水平向右。在我们的模拟中,分别给出在不同时刻,粒子在空间的分布情况。为了真实的考虑粒子的演化,我们把重力也加入进来,如图12. 可以发现,当粒子运动到曲面区域时,由于粒子的速度较大,向右运动趋势很明显,来自 teapot mouse 的 adhesive force 不足以明显的改变流体的运动趋势,这样红色点就继续往右运动。在后期时间中,由于重力的作用,使得这些粒子往右下方坠落。如果没有重力的话,这些粒子可能直接继续往右运动(接近水平运动),而不是像 Fig.7那样流体沿着 teapot mouse 流动。

所以,通过对比这几个图: Fig.12 and Fig.7-8,可以发现,流体的初始速度对流体的后期演化很重要。这也是与我们的日常观察吻合。如果水流的初始速度非常小的话,



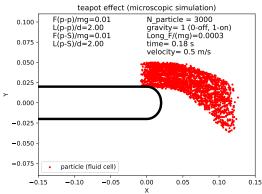


图 12: Fluid with a large initial velocity $u_0 = 0.5$ m/s. Parameters are plotted in the figure. The fluid tend to eject from the teapot surface, without the tendency to flow over the solid surface.

2. Geometry of teapot mouse

在日常生活中,当水壶的口厚度不一样的时候,水流出的情况也不一样。这是因为,当水壶口的形状不同,水流过它的表面,运动轨迹也不同,则水滴与 teapot mouse 的距离也不同,这样水滴受到的 teapot surface adhesive force 也不同。为了研究不同 teapot mouse 对流体演化的影响,我们可以把 teapot mouse 的形状取的不一样。

在图 Fig.13中,水壶口的半径取为原先的 2 倍,也就是水壶口的厚度变为 R=4~cm. 当水壶口变得很厚的时候,部分粒子往右下方运动时,依然会距离户口固体表面较近,进而感受到固体表面的adhesive force。这就会使得一部分的水滴容易沿着固体表面流下来。反之,当固体表面比较薄,这样水滴在离开 teapot mouse 时,就可以很快的远离固体表面,进而感受不到固体表面的adhesive force。通过我们的模拟,可以看出来,当 teapot mouse 厚度较大时,有一部分的水分子容易倍吸附到固体表面。这在 Fig.13里可以看出(teapot mouse with larger radius)。

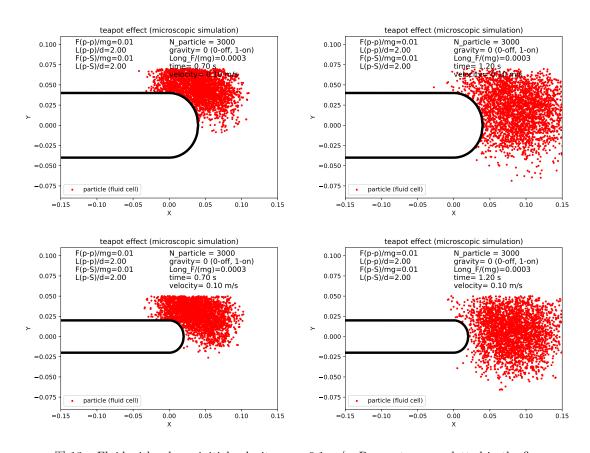


图 13: Fluid with a large initial velocity $u_0 = 0.1$ m/s. Parameters are plotted in the figure.

在某些情况下,如果水壶口不是圆形,而是呈现缺口的形状,那么水流是什么样的呢? 比如极端的情况,就是水壶口被刀切了一下,这样水壶口呈现矩形的形状,很显然,这种情况下,水滴距离固体表面的具体会发生变化,水滴感受到的固体表面的 adhesive force 也会不同。我们采用不同流速的流体,来研究它们在固体表面的流动。可以发现,当流速更小时,突然变化的 teapot mouse,让流体更加容易的离开固体表面,进而让水滴不容易沿着固体表面滴落下来。

3. Broken mouse of the teapot

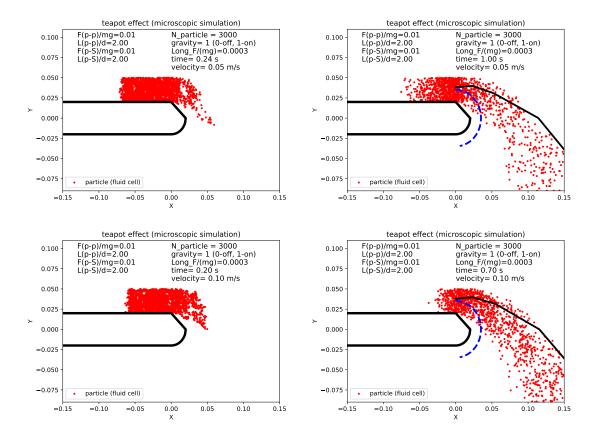
基于这个模型,我们还研究了水壶口破损时的水流运动情况。当水壶的口破损时,水与 teapot mouse 表面的相互作用就会不同,因为水流在自身惯性的作用下,往前运动,这时如果水壶口的形状突然变化,导致固体表面与水流分子的距离发生变化,这样固体表面与水流的相互作用会变化,甚至突然消失,这样,靠近固体表面的那些水滴,在运动到水壶口破损处时,不再受到来自固体表面的 adhesive force,这使得水滴可以被周围其他水滴吸附并继续往前运动,水滴不再沿着水壶固体表面留下来。这意味着 teapot effect 不再容易发生。通过以下 Fig.14显示,可以看到,即使水流的速度很小时,比如流速为 0.05m/s 时,水滴也会明显的往右下方运动(由实现画出它们的运动趋势),当水流增加到 0.1 m/s 时,水流向右下方运动的趋势更加明显(第四个子图所示)。第二个子图和第四个子图中的视线,代表水滴运动的趋势。而虚线代表水流完全贴附在水壶表面时的运动轨迹。

在图中,我们假设水壶口的上半部分缺口为一个规律的切口,这在模型计算上比较方便。当水滴运动到缺口处时,原先的缺口处是圆形,水滴可以接触到固体表面进而受到 teapot mouse 的 adhesive force。当有缺口存在时,在缺口处,水滴受到固体表面的吸附力突然降低,使得水流继续往前方运动。这个图 Fig.14中,水滴往右下方运动,而在茶壶口没有破损的图 (Fig.13),许多水滴由于受到茶壶的adhesive force 而往正下方运动。这是图14与前面图的极大不同之处。

在后期的研究中,我们甚至可以画出每个区域的水滴的速度,即 u(x,y,t),这样可以清晰的展示在不同水流区域,水滴的运动情况,或者研究湍流的运动形式。

V. WEAKNESS OF OUR MODEL

- (1) The interaction force between fluid cells and the fluid-teapot.
- (2) 更多的流体被考虑进来时,在流体的左边末端,那些流元就会受到来自左边的碰撞,这些碰撞代表着从左往右的压力,使得流体尽快的流下去。而在以上的模拟中,采用了 3000 个 fluid cell 进行模拟,这使得流体的右端可以较真实的流动。但为了考虑 3000 个 fluid cell 之间的 two-body interaction,每个时间步长,需要计算的次数是 3000² ~ 10⁷ 次 two-body interaction。这是很耗时的,如果考虑更多的 fluid cell,我们需要借助大型计算机。在流体的最左端的一些 fluid cell,似乎往右流动的趋势变弱,这就是因为这些 fluid cell 受到右边 fluid cells 的碰撞(压强),而左边没有流体,所以使得最左端的 fluid cell 没有较快的往右运动。这些都可以通过采用更大的计算机资源来弥补和提升。



 \boxtimes 14: Water moves above the broken teapot mouse. Assume that the damaged part of the teapot spout is in a regular shape. In the upper sub-figures, fluid moves with a velocity u=0.05 m/s. While in the lower sub-figures, the fluid velocity is u=0.1 m/s. Solid lines represent the moving tendency of the fluid. The dashed line is the moving tendency when the fluid is mostly attached to the solid surface of the teapot mouse.

vi. SUMMARY

In daily life, when water flows out of a teapot, it can either detach from the teapot or flow down along the teapot's spout surface. This phenomenon is commonly referred to as the "teapot effect." Over the past few decades, this phenomenon has been extensively studied, and its underlying principles have been explored through fluid mechanics. However, the teapot effect presents a challenge due to complex boundary conditions and the difficulty of solving fluid dynamics equations, making it a challenging problem.

In this work, we take a different approach by developing a microscopic model inspired by the finite element method, where we divide the fluid into a multitude of discrete water droplets. Each water droplet interacts with its neighboring droplets and interacts with the teapot surface. Consequently, the complex evolution of the fluid can be simulated computationally by tracking the motion of these discrete water droplets. By establishing this mathematical model and implementing it through computer programming, we can effectively study the collective motion of a large number of water droplets. The advantage of this model lies in our ability to investigate interactions at the microscopic level, including the forces between water droplets and even intermolecular forces, which are beyond the reach of macroscopic fluid mechanics.

Furthermore, the microscopic particle collision model we have developed, initially designed for simulating incompressible fluids like water, can naturally be extended to simulate compressible fluids. Considering the significant challenges in solving compressible fluid dynamics equations, our microscopic particle collision model offers a promising avenue for broader applications.

To simplify the problem, we abstract the 3D fluid flow into a 2D scenario. Through the microscopic particle collision model, we investigate the flow of water on the teapot spout surface. We address several aspects:

- 1. By considering the gravitational force on the water droplets as a reference, we study that the interaction forces between the droplets should be significantly smaller than their own gravity, providing valuable insights into the magnitude of forces at the microscopic level.
- 2. Based on the model, we examine how the flow of fluid differs on the teapot spout surface at varying fluid velocities, including scenarios where it jets out or flows downward along the solid surface.
- 3. Given that the flow of water depends on the interaction forces with the teapot spout's solid surface, we investigate the impact of different solid surface shapes on the fluid's evolution. Complex boundary conditions in fluid mechanics are known to pose significant challenges, but our model allows for the inclusion of various boundary conditions through programming. We examine cases with thin, thick, and rectangular teapot spouts. Additionally, we calculate physical quantities such as the average mean free path and viscosity coefficient for the particle system, which can serve as valuable reference points for comparison with real-world fluid properties, verifying the reliability of our model.

It's important to acknowledge that the current framework employs a simplified version of microscopic interactions between particles, which plays a crucial role in the fluid's evolution. In future research, this work can be extended to consider more realistic forms of intermolecular forces to further explore fluid dynamics.

在日常生活中、水流从茶壶中流出来时、水流可能离开水壶、或者沿着水壶口表面流下来。这个现象、一般

effect。这个问题,在过去几十年内,被广泛的研究,内在的规律可以通过流体力学来研究。但在这个问题中,流体在这个工作中,我们通过另一种思路,建立微观模型,借鉴有限元的思路,把流体分为大量的水滴,每个水滴都会surface 之间存在相互作用。这样,流体复杂的演化,可以通过计算机编程模拟大量水滴的运动来求解。通过建立发另一方面,我们建立的微观粒子碰撞模型,虽然是用来研究水流(不可压缩流体),其实,它可以很自然的拓展到可为了简化问题,我们把 3 维的水流抽象成 2 维问题。我们通微观粒子碰撞模型,研究了水流在 teapot mouse 表面流动的情况,(1)通过水滴的重力作为参考,研究了水滴之间的相互作用力应该是比其自身的重力小很 mouse 表面流动的情况不同:喷射出去,或者沿着固体表面流下来。我们的模拟,可以清晰的给出,不同流体速度 mouse 固体表面的相互作用力,所以固体表面的形状对水流的演化很重要。我们知道在流体力学中,复杂的边界条 mouse 很薄、很厚、以及矩形的水壶口的水流情况。此外,我们还计算了粒子体系的平均自由程、粘滞系数等物理但需要承认的是,目前的框架下,我采用的粒子之间的微观相互作用力是简化版的,这对于流体的演化是重要的。

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VII. APPENDIX: CODES

A. codes for momentum balance method

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B. codes for microscopic model

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