International Journal of Frontiers in Engineering Technology
ISSN 2706-655X Vol.4, Issue 6: 76-81, DOI: 10.25236/IJFET.2022.040612

Physical and Mechanical Analysis of Moving Contact Line

Qinyi Zhou

Hebei Normal University, Shijiazhuang, Hebei, China

Abstract: *As a typical moving contact line problem, the industrial coating and coating problem has a very important application. The purpose of this paper is to study the physico-mechanical analysis of moving contact lines. The research background and significance of the moving contact line problem are given, the research progress of the plate pull-up coating is reviewed, and the research status of the moving contact line problem on the chemically uneven surface is given. The tilt-pulling problem of chemically inhomogeneous surfaces with horizontal fringe distribution is studied. Numerical simulations investigate the effects of different strip widths on the dynamic behavior of the contact line and the evolution of the liquid film morphology. The effects of the plate width and the angle between the plate edge and the pulling direction on the critical state of the wetting transition, the dynamic process of the inclined contact line and the evolution of the liquid film morphology were investigated. When the widths of the hydrophilic and hydrophobic strips are sufficiently small, both the critical velocity of the wetting transition and the dynamic evolution process of the contact line and the liquid film are the same as the uniform surface results with the equilibrium contact angle being the predicted value of Cassie theory.*

Keywords: *Moving Contact Line, Physical Mechanics, Precursor Film Model, Wetting Theory*

1. Introduction

In industrial production and daily life, fluid flows are generally diverse and complex. These are not caused by single-phase fluid motion, but are the result of the coupled motion of gas, liquid and solid [1]. The wetting behavior of solid surfaces also has high economic value in industry, and the flow mechanism and physical mechanism of moving contact lines on rough surfaces can give guidance and optimization solutions to industrial problems [2]. Although the motion of the contact line is controlled by the molecular force between the two-phase fluid and the solid, it has a significant impact on the macroscopic motion of the fluid, that is, the change of the moving contact line will bring about different flow mechanisms [3-4]. In addition, all substrate surfaces in nature have rough textures at the microscopic scale, and in practical engineering applications and industrial production, roughness is an important factor that has to be considered. It is of great significance to explore the influence of these rough textures on flow characteristics [5].

At the capillary scale, especially in flows dominated by surface tension, the magnitude of the contact angle and the motion of the contact line have important effects on multiphase hydrodynamics. Some scholars have used molecular dynamics to study the electrowetting of water and electrolytes in three anti-skid coordination stages. In the case of using static electricity, the friction of the contact wire is reduced [6]. Yang J studied the synthesis mechanism and physical and mechanical properties of hydraulic lime from loess. The composition of loess dolls before and after calcination was studied by X-ray fluorescence spectrometer and X-ray diffractometer. The physical and mechanical properties of the mortar specimens were studied by the white light DSCM (Digital Speckle Correlation Method) deformation field detection system [7]. Various multiphase flow problems with moving contact lines are often involved in industrial applications, such as dropper tips to reduce drug residues, special surfaces to accelerate liquid film dehumidification, etc. Because of the multi-scale nature of the flow, it is difficult to accurately measure experimentally. Numerical research It has more scientific significance [8].

Based on the lubrication theory under different conditions, the motion law of the contact line and the liquid film on the solid wall is studied by the method of theoretical analysis combined with numerical calculation. We generalize the moving contact line asymptotic theory and apply it to the problem of dip coating on flat plates and the spreading and retraction of droplets; we study the wetting transition in dip coating on flat plates, and give the critical speed of wetting transition in general cases Formula; focuses on the gravity-driven receding liquid film on the inclined plate, and gives the effect of the plate inclination and inertia on the contact linear velocity; explores the evolution of the liquid film on the plate, and gives the liquid film morphology and evolution in different stages and regions law.

2. Research on Physical Mechanics of Moving Contact Line

2.1 Precursor Membrane Model

In addition to the stress singularities near the contact line, the moving boundary problem is another difficulty for numerical calculations with moving contact lines. For the solution of the lubrication equation, if the slip model is used, the method of transforming the independent variables can be used to convert the moving boundary problem into a fixed boundary problem; while the precursor film model can make the liquid film near the contact line have a limited thickness, so that the contact line is connected to a balanced precursor film, thereby avoiding the moving boundary problem. At this point, the boundary condition of the equation is on the equilibrium precursor film, not at the contact line. Therefore, the information related to the contact line is added to the equation in the form of separation pressure [9]. At this time, in the case of ignoring the body force, the pressure P in the liquid contains both the contribution of the interface curvature K and the contribution of the separation pressure $\overline{\Pi}$:

$$p = p_0 - \sigma k - \overline{\Pi}, \tag{1}$$

Where p0 is the atmospheric pressure and σ is the surface tension coefficient. The separation pressure mainly acts in the vicinity of the contact line and at the precursor membrane, and has little effect on the macroscopic region far from the contact line. For the vicinity of the contact line, the solid wall can be considered to be flat. Under the lubrication approximation, the curvature K can be estimated as the spatial second derivative of the interface, $k \approx h''(x)$, where x is the spatial coordinate along the tangent to the solid wall.

2.2 Surface Properties and Static Wetting

The exploration of knowledge is from the shallow to the deep, from the simple to the complex. Young's equation is only suitable for ideal rigid, smooth and chemically uniform surfaces, not for rough surfaces [10]. The deviation of the apparent contact angle presented by the liquid on the rough solid surface is not only related to the surface physical and chemical properties of the matrix, but also has a great relationship with the surface structure. Both Wenzel and Cassie theories recognize that there is a large difference between the actual solid surface situation and the ideal surface, resulting in the variation of the contact angle [11]. Wenzel's theory attributes this difference to the irregular texture of the actual surface, and proposes the concept of roughness, which relates the contact angle on the actual surface to the intrinsic contact angle of the ideal surface; Cassie's theory attributes this difference to the surface structure The difference in surface free energy caused by the inhomogeneity of the surface can be used to construct two different surfaces, and the concept of composite contact angle is proposed, which is related to the intrinsic contact angle of the ideal surface [12].

Cassie and Baxter proposed the concept of composite contact angle by considering the deviation of apparent contact angle and static contact angle of actual rough surfaces from the viewpoint of surface diversity (surfaces with many different wetting characteristics), and droplets do not It will infiltrate into the ravine, but the gas will be trapped in it. At this time, the interface situation is much more complicated, and the total surface free energy is composed of the free energy of each component. Also in the model, a virtual displacement dz is given to the contact line, then the change of surface free energy per unit length is:

$$dE = f_1(\sigma_{ls} - \sigma_{sg}) \cdot dz + (1 - f_1)\sigma_{ls} + \sigma_{ls} dz \cdot \cos\theta^* \tag{2}$$

Where f1 is the fraction of the solid surface wetted by the liquid, and the composite interface formula of the two phases can be extended to the N-phase composite interface to obtain the following composite contact angle.

3. Investigation and Research on the Physical Mechanics of Moving Contact Lines

3.1 Multiphase Flow Problem

The problem of multiphase flow is a common problem in life and productivity, and one of the most important problems in multiphase flow is the existence of contact lines. On optically and chemically coherent surfaces, the vertical edges of vertical water droplets are determined by the surface tension coefficient between the water and the solid wall and the surface tension coefficient between the two types of water, while the roughness and chemical inhomogeneity of the upper wall affects the surface.

3.2 Numerical Simulation

In this paper, a precursor film model is used to eliminate the stress singularity problem at the contact line, with a thin liquid film at the nanoscale. The contact line is defined at the maximum value of the second derivative of the liquid film thickness, and the distance from the contact line to the horizontal plane along the plate pulling direction is denoted as Xcl. The dimensionless characteristic height, characteristic length and characteristic time are h_e、$l=\sqrt{3/5}h_e/\theta_2$ and $\tau=27\mu h_e/25\gamma\theta_2^4$ respectively, and the form as follows:

$$\partial_t h+\partial_x(h^3\partial_x(\partial_x^2 h+\Pi(h))-Gh^3\partial_x h)+3G\alpha h^2\partial_x h-U\partial_x h=0, \quad (3)$$

The dimensionless numbers $\alpha=\frac{l}{h_e}\tilde{\alpha}$, $U=\frac{\tau}{l}u$ and $G=\frac{3pgh_e^2}{5\gamma\theta_2^2}$ in equation (1) are the dimensionless plate inclination angle, the plate pulling speed and the gravitational constant, respectively. Its $\tilde{\alpha}$ and u are the physical real plate inclination angle and plate pulling speed, respectively. The influence of the plate inclination angle is not discussed in this paper, so the plate inclination angle a=1 is a fixed value. Equation (1) is the separation pressure, and its form is:

$$\Pi(h)=\begin{cases}-\frac{1}{h^3}+\frac{1}{h^6}, & \text{A more hydrophilic surface with a contact angle of } \theta_2,\\ \frac{\theta_1^2}{\theta_2^2}\left(-\frac{1}{h^3}+\frac{1}{h^6}\right), & \text{A more hydrophobic surface with a contact angle of } \theta_1,\end{cases} \quad (2)$$

θ_1/θ_2 characterizes the difference in wettability of hydrophilic and hydrophobic bands. It should be noted that, in the process of pulling the flat plate, the surfaces with different contact angles will move upward continuously.

4. Analysis and Research on Physical Mechanics of Moving Contact Line

4.1 Critical Speed of Wetting Transition

The influence of the width of the hydrophilic and hydrophobic strips on the critical speed of wetting transition is shown in Figure 1. Here, only the case where the widths of the hydrophilic and hydrophobic strips are equal, that is, L1=L2, is considered. When the width of the hydrophilic and hydrophobic strips is much smaller than the capillary length, such non-uniform surfaces have chemical patterns distributed on the microscopic scale, but can be regarded as a uniform surface with an equivalent equilibrium contact angle on the macroscopic scale. The effective contact angle is the equilibrium contact angle predicted by Cassie theory, namely $\cos(\theta_c)=f_1\cos(\theta_1)+f_2\cos(\theta_2)$, where f1=L1/(L1+L2), f2=L1/(L1+L2). The dotted line in the figure represents the critical speed of wetting transition for a uniform surface with an equilibrium contact angle of θ_c, and the dots represent the critical speed of the chemically inhomogeneous flat plate pulling out the liquid film at different strip widths. It can be seen that when the chemical inhomogeneity scale of the surface is sufficiently small $(L1\le 1)$, the critical speed of wetting transition on the non-uniform surface is in good agreement with the results of the uniform surface. With the increase of the strip width, the critical speed of wetting transition gradually deviates from the result predicted by Cassie theory and decreases gradually.

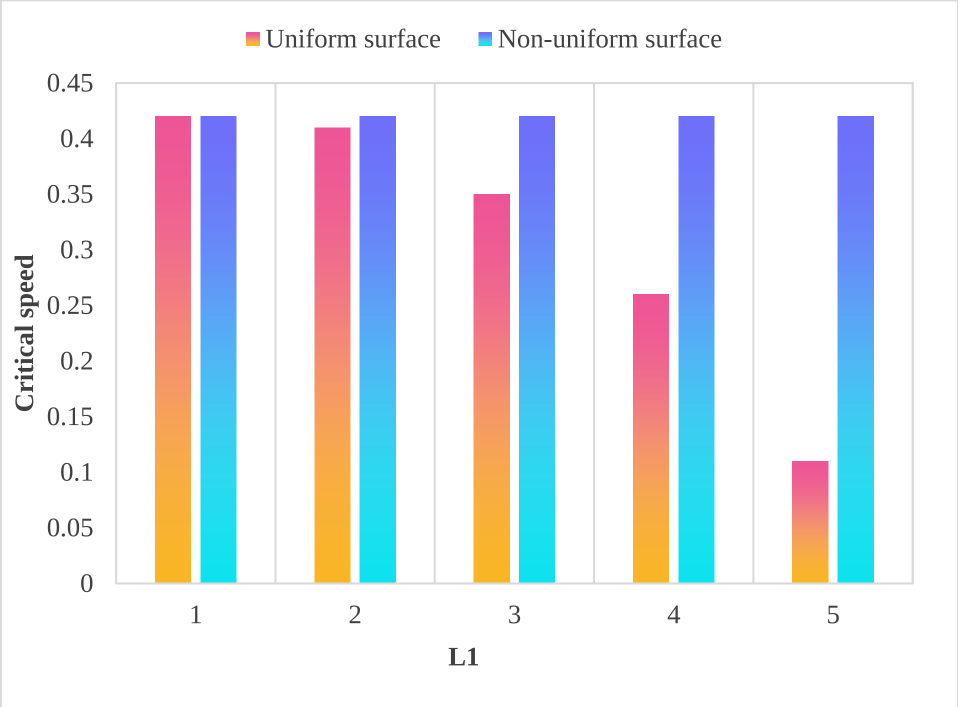

Figure 1: The critical velocity of wetting transition as a function of strip width, considering only the case where the hydrophilic and hydrophobic strip widths are the same and smaller than the capillary scale

4.2 Dynamic Evolution Process of Contact Line and Liquid Film

The evolution law of the moving contact line with time when the width of the hydrophilic and hydrophobic strips is much smaller than the capillary length, where L1=L2=1, as shown in Figure 2. The solid lines and dots in the figure represent the change process of the contact line position with time during the pulling process of the non-uniform surface and the uniform surface. The results show that the dynamic behavior of the contact line on the chemically inhomogeneous surface is the same as that of the uniform contact line, whether it is in the equilibrium state (U=0.20) or when the contact line continues to climb up after the wetting transition (U=0.50). The behavior of the surfaces is consistent, and the small local vibration of the contact line does not affect the macroscopic uniformity, as shown in Table 1.

Table 1: Dynamic evolution process of contact line and liquid film

T	Uneven surface(U=0.20)	Uniform surface(U=0.20)	Uneven surface(U=0.50)	Uniform surface(U=0.50)
100	21	21	67	67
400	25	25	83	83
800	28	28	92	92
1200	29	29	100	100

The evolution of the liquid film structure over time when the width of the hydrophilic and hydrophobic strips is much smaller than the capillary length shows that the dynamic liquid film structure pulled out after the wetting transition occurs is consistent with the results on a homogeneous surface. Comparing the evolution results of the contact line and the liquid film, we find that for the surface with chemical inhomogeneity in the microstructure, the dynamic behavior of the moving contact line in the macroscopic and the dynamic evolution process of the pulled liquid film are both the same as those of the uniform surface. The results are the same, and the equilibrium contact angle of this uniform surface can be equivalently given by the Cassie theory that characterizes the wetting properties of chemically inhomogeneous surfaces. In fact, the variation of the contact line velocity decreases with the decrease of the width of the hydrophilic and hydrophobic strips, that is, the pinning and slipping processes of the contact line are suppressed when the width of the hydrophilic and hydrophobic strips decreases, while the gas-liquid The speed of the interface deformation is much slower than that of the contact line moving on the solid wall, so the liquid film structure does not change much when it continuously crosses the junction of the hydrophilic and hydrophobic strips.

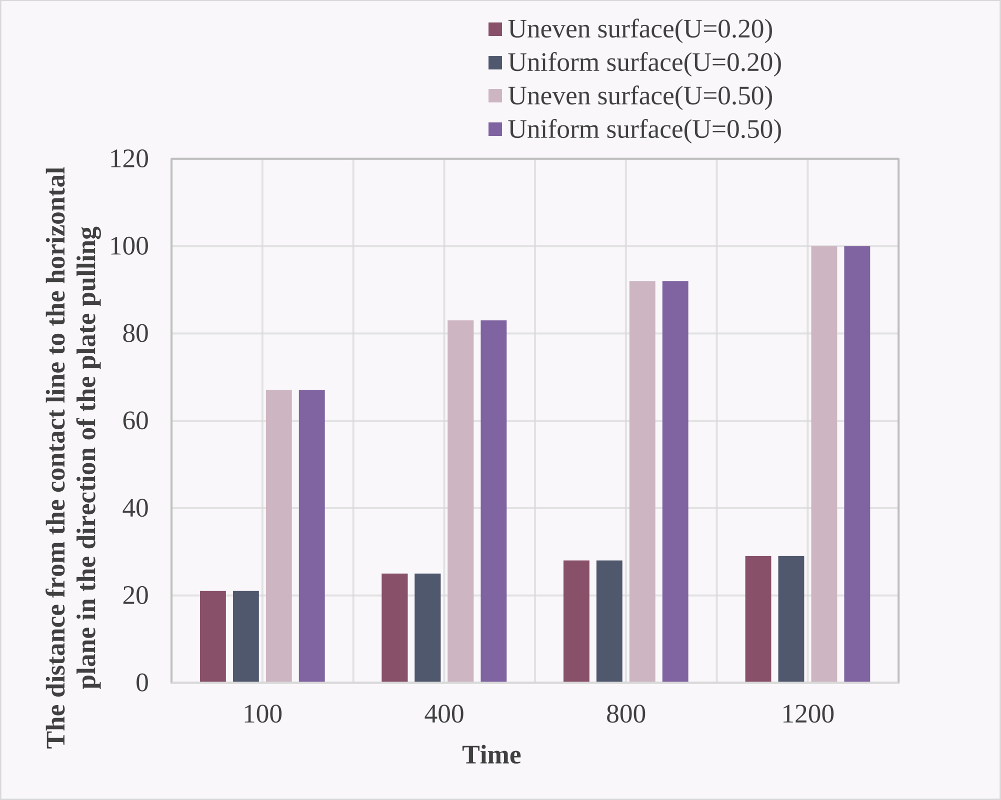

Figure 2: The time evolution curve of the moving contact line position, the strip width is much smaller than the capillary length, where L1=L2=1.

5. Conclusions

At present, there are still few numerical studies on the two-phase flow with moving contact lines on solid materials, especially considering the contact angle hysteresis effect on the material surface. With the in-depth development of computer technology, people's research on complex fluids has also entered the micro-scale stage, and the continuum model is gradually unable to meet the research needs. In this paper, the phase field method is used to explore the multiphase flow problem on rough walls with various morphologies. Based on the existing research progress, in-depth research can also be done in the following aspects. In evaluating the influence of rough surfaces, the focus Concentrating on specific geometric parameters, it is necessary to broaden the geometric parameters or further quantitatively compare whether an equivalent relationship can be established under different geometric rough models; there are differences between experiments and lubrication theory or numerical simulation due to the three-dimensional effect, how to describe the three-dimensional effect in the contact line motion The impact is a major difficulty and hot spot.

References

[1] Ambrozy M, M Lokaj ěk, Valo M. CLASSICAL MECHANICS AND CONTEMPORARY FUNDAMENTAL PHYSICAL RESEARCH. Philosophia (Philippines), 2019, 20(2):212-237.*

[2] Brata K C, Hidayatulloh S. An idea of intuitive mobile diopter calculator for myopia patient. TELKOMNIKA Indonesian Journal of Electrical Engineering, 2019, 17(1):307-313.

[3] Anyanwu M U, Okpala C, Chah K F, et al. Prevalence and Traits of Mobile Colistin Resistance Gene Harbouring Isolates from Different Ecosystems in Africa. BioMed Research International, 2021, 2021(12):1-20.

[4] Morozov V A, Bogatko V I, Yakovlev A B. On the Mathematical Modeling of Loading High-Speed Material at the Department of Physical Mechanics, St. Petersburg State University. Vestnik St.

Petersburg University, Mathematics, 2020, 53(4):450-458.

[5] Ahmad Q A, Wu G. A rock physical approach to understand geo-mechanics of cracked porous media having three fluid phases. Geomechanics and Engineering, 2020, 23(4):327-338.

[6] Hartner N T, Raddatz C R, Thoben C, et al. On-Line Coupling of Chip-Electrochromatography and Ion Mobility Spectrometry. Analytical Chemistry, 2020, 92(22):15129-15136.

[7] Yang J, Song W, Wang L, et al. Research on the synthesis and physical-mechanical properties of hydraulic lime prepared from loess-doll. Yanshilixue Yu Gongcheng Xuebao/Chinese Journal of Rock Mechanics and Engineering, 2018, 37(7):1766-1775.

[8] Maudlin T. Foundations of Quantum Mechanics: An Exploration of the Physical Meaning of Quantum Theory. American Journal of Physics, 2018, 86(12):953-955.

[9] Shibata S, Hirabuki K, Hata N, et al. Pivotal Role of Heart for Orthostasis: Left Ventricular Untwisting Mechanics and Physical Fitness. Exercise and Sport Sciences Reviews, 2021, 49(2):88-98.

[10] Malkin A I, Klyuev V A, Popov D A, et al. Physical and Chemical Mechanics of the Synthesis of Boron-Containing Composite Powders. Russian Journal of Physical Chemistry, 2020, 94(3):490-495.

[11] Ferreira R M, Brando-Rangel M, Reis A S, et al. The Practice of Physical Activity Protects the Lung Function And Mechanics In Hypertensive Elderly: 1225 Board #351 May 27 1:30 PM - 3:00 PM. Medicine & Science in Sports & Exercise, 2020, 52(7S):327-327.

[12] Zhang L, Han J, Wang H, et al. Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. Physical Review Letters, 2018, 120(14):143001.1-143001.6.