MINISTRY OF EDUCATION AND TRAINING

VIETNAM ACADEMY OF SCIENCE AND TECHNOLOGY

GRADUATE UNIVERSITY OF SCIENCE AND TECHNOLOGY

Nguyen Dinh Hoe

A NUMERICAL STUDY OF A DROPLET INTERACTING WITH A SUBSTRATE UNDERGOING THERNAL CONVECTION

SUMMARY OF DISSERTATION ON
FLUID MECHANICS
Code: 9 44 01 08

Ha Noi - 2024

The dissertation is completed at: Graduate University of Science and Technology, Vietnam Academy Science and Technology

Supervisor
Supervisor 1: Prof., Dr. Vu Van Truong
Supervisor 2: Dr. Nguyen Hong Phan

Referee 1: Assoc. Prof. Ha Ngoc Hien

Referee 2: Assoc. Prof. Tran Ngoc Doan

Referee 3: Assoc. Prof. Hoang Thi Kim Dung

The dissertation will be examined by Examination Board of Graduate University of Science and Technology, Vietnam Academy of Science and Technology at: 09 am, May 14, 2024

The dissertation can be found at:
1. Graduate University of Science and Technology Library
2. National Library of Vietnam

INTRODUCTION

1. The necessity of the dissertation

The microfluidic chip is a small device that integrates the processes in a sample analysis. It was born in the 70s of the previous century. The operation of this device relies on the investigation of flow in a microfluidic device. The fluid moves in a small channel (from a few hundred μm to a few mm). To actuate the fluid, we can use external sources, i.e., electricity, magneticity, thermocapillary, and so on. The investigation of the motion of droplets attached to the surface of the chip is important to develop a more complicated, effective chip. Thus, the topic of the dissertation is "A numerical study of a droplet interacting with a solid surface undergoing thermal convection". The main part of the dissertation is the investigation of the migration of a droplet attached to a substrate undergoing the Marangoni effect.

This topic was investigated for the case of a single droplet. However, in many practical applications i.e., medicine, food technology, materials, and so on, the compound droplet is more often used. Thus, the dissertation focuses on the compound droplet. There are two type of interaction: the obstructed interaction (for example, droplet moving in a constricted channel) and the direct interaction (it mean, the droplet directly in contact with the wall).

2. The aim of the dissertation.

The dissertation provides the numerical studies of droplets interacting with a substrate undergoing the Marangoni effect.

3. The main content of the dissertation

The main contents of the dissertation include: Introduction, Conclusion, and five chapters:

Chapter 1: An overview of research topic

This chapter provides some basic concepts such as thermocapillary, substrate, compound droplet, and so on. In addition, this chapter also presents some past studies of the obstructed interaction and direct interaction.
Chapter 2: Mathematical equations and numerical methods

This chapter provides the mathematical equations and the numerical method to solve the given problem of the dissertation.

Chapter 3: A numerical study of a compound droplet interacting with a constricted channel under isothermal conditions.

This chapter presents a numerical study of a compound droplet migrating in a constricted channel (obstructed interaction).

Chapter 4: A numerical study of a compound droplet interact with a non-wetting surface with the presence of a thermal gradient.

This chapter presents a numerical study of the impact of a compound droplet on a solid wall undergoing the Marangoni effect (direct interaction). The thermocapillary force is generated from a vertical temperature gradient. The hotter temperature is located above the compound droplet and the colder one is embedded on the substrate. The thermocapillary force supports the compound droplet detaching from the wall.

Chapter 5: A numerical study of the thermal migration of a compound droplet attached on a wetting substrate.

This chapter presents a numerical study of the thermal migration of a compound droplet on a substrate. The hotter temperature is located on the domain right and the colder temperature is on the left side. Depending on the static contact angle and the size of the inner droplet, the compound droplet can migrate toward the colder or hotter side.

Chapter 1: AN OVERVIEW OF RESEARCH TOPIC

In this chapter, some basic concepts such as a droplet, microfluidic chip, compound droplet, droplet formation, and thermocapillary force … This chapter also provides past studies of a droplet interacting with a substrate and migration of a droplet on a wetting wall undergoing thermal convection.

Based on past studies of a droplet interacting on a solid surface undergoing thermal convection on the world, there are some remark conclusions as follows:

For numerical studies:

- A droplet interacting with a wall have great attention to researchers. However, they only focused on the simple droplet. There is no investigation of the compound droplet.
- There were almost two-dimensional studies.
- In experiments, there were a small amount of liquids existing on the substrate as the droplet moved. However, the numerical studies could not simulate this phenomenon.

For theoretical studies:

- The theoretical studies were accurate at the small static contact angle (less than 45°). There was no theoretical study of the compound droplet.

For the experiments:

- The experimental studies were not diverse. The number of experiments was limited and no experiments of the compound droplet.

Based on the literature, there was no study on the thermal migration of a compound droplet attached to a substrate. The inner droplet may have a great influence on the outer interface. The interaction of the compound droplet and the wall undergoing thermal convection is difficult to anticipate. The results may be different from the simple droplet. Therefore, the dissertation will provide in details of the dynamic behaviors of the attached compound droplet undergoing the Marangoni effect. The topic has not been investigated so far. The results will provide important knowledge in development of the lab-on-a-chip devices, particularly, in applications related to the development of drug (compound droplet is used).

Chapter 2: THE MATHMATICAL EQUATION AND NUMERICAL METHOD

In this chapter, the mathematical equations include the Navier-Stokes equation, the continuity equation, the energy equation, and the other equations. The derivative terms in the governed equations are discretized using the finite difference method. The fluids are distinguished using the front-tracking method. The simulation is implemented in FORTRAN language.

The momentum equation is (Navier-Stokes equation):

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \rho\nabla.(\mathbf{uu}) = -\nabla p + \nabla.\left[\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\right] + \mathbf{f} + \rho\mathbf{g} \tag{2.1}$$

The mass conservation equation is:

$$\nabla.\mathbf{u} = 0 \tag{2.2}$$

The energy equation is:

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla.\left(\rho c_p T \mathbf{u}\right) = \nabla.(k \nabla T) \tag{2.3}$$

The surface tension is assumed to be a linear function of the temperature:

$$\sigma = \sigma_0 + \sigma_T (T - T_0) \tag{2.4}$$

Fluids are distinguished by constructing interfaces between them. An interface is formed by connecting the marker points following a certain direction. The material properties of fluids (ρ, μ, c_p, k) are computed by the following functions:

$$\varphi = I\varphi_1 + (1 - I)\varphi_2 \tag{2.5}$$

The interfaces are then moved by the following equation:

$$x_f{}^{n+1} = x^n{}_f + \Delta t V_f \mathbf{n} \tag{2.6}$$

The surface tension of a front element is computed as following:

$$\delta \mathbf{f}_\sigma = \int_{\Delta s} \sigma \kappa \mathbf{n} ds = \int_{\Delta s} \frac{\partial \sigma t}{\partial s} ds = (\sigma \mathbf{t})_2 - (\sigma \mathbf{t})_1 \tag{2.7}$$

The interaction of the droplet and the substrate is handled by utilizing the dynamic contact angle model proposed by Muradoglu and Tasoglu. The dynamic contact angle θ_D is computed based on the value of the apparent contact angle θ_{Di}:

$$\theta_{Di} = f_{Hoff}(Ca_{clm} + f_{Hoff}{}^{-1}(\theta_e)) \tag{2.8}$$

The Hoffman function f_{Hoff} is defined as:

$$f_{Hoff} = \cos^{-1}(1 - 2\tanh\left[5{,}16\left(\frac{x}{1+1{,}31x^{0{,}99}}\right)^{0{,}706}\right]) \tag{2.9}$$

The dynamic contact angle then is computed as:

$$\theta_D = \begin{cases} \theta_{Di} & khi\ V_{cl} \geq 0 \\ 2\theta_e - \theta_{Di} & khi\ V_{cl} < 0 \end{cases} \tag{2.10}$$

Firstly, the momentum equation (eq. (2.1)) is solved by the projection method. Discretizing this equation using the forward scheme we have:

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\mathbf{A}^n{}_h + \frac{1}{\rho^n}\left(-\nabla_h p + \mathbf{D}^n{}_h + \mathbf{f}^n\right) + \mathbf{g}^n \tag{2.11}$$

Omitting the pressure term we have:

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\mathbf{A}^n{}_h + \frac{1}{\rho^n}\left(\mathbf{D}_h{}^n + \mathbf{f}^n\right) + \mathbf{g}^n \tag{2.12}$$

The pressure term then is included:

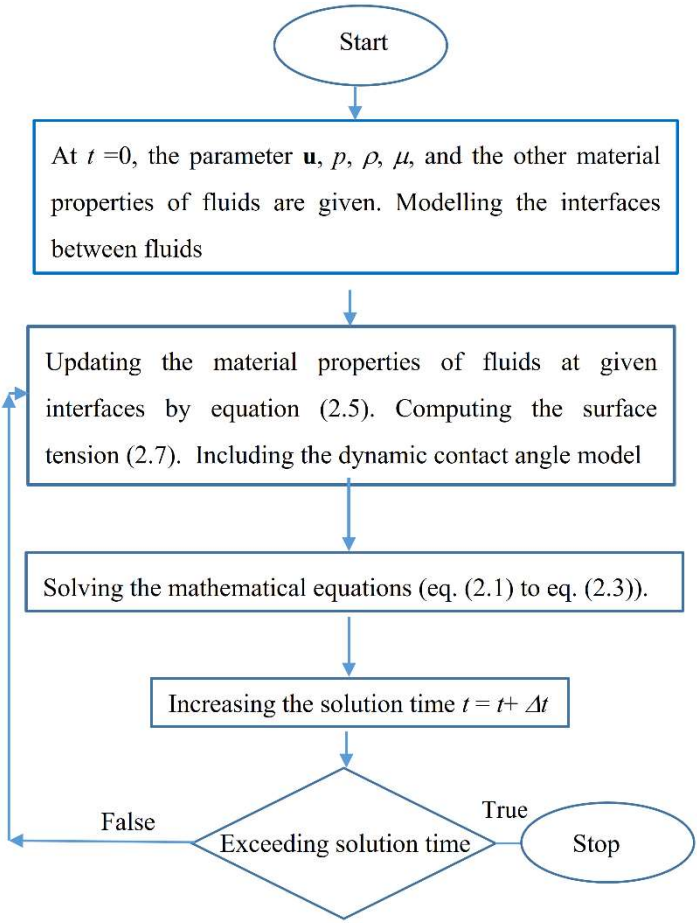
$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} = -\frac{1}{\rho_h}\nabla_h p \tag{2.13}$$

Adding the equation (2.13) and (2.12) we have equation (2.11). To find the pressure, we take diverge both side of equation (2.13) and the continuity equation ($\nabla_h.\mathbf{u}^{n+1}$) to cancel out $\mathbf{u}^{n+1}$ we have:

$$\frac{\nabla_h.\mathbf{u}^*}{\Delta t} = \nabla_h.\left(\frac{1}{\rho^n}\nabla_h p\right) \tag{2.14}$$

Solving the equation (2.14) we have the pressure at step *n*. Using the pressure solved in the equation (2.14) to find the velocity at the step *n*+1 by solving equation (2.13).

The energy equation is solved by the finite difference method. The derivative terms are discretized by the forward and center schemes. The flowchart of the solution is then given in *Figure 2.1*

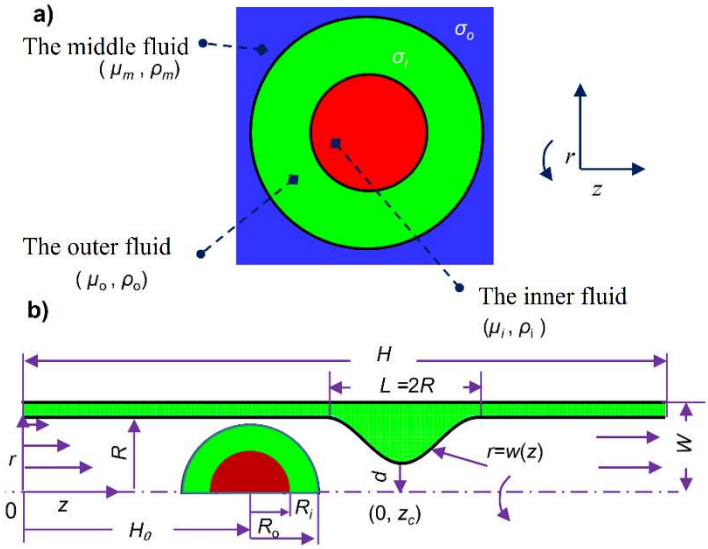


Hình 2.1 The flowchart

Chapter 3: A NUMERICAL STUDY OF A DROPLET MIGRATING IN A CONSTRICTED CHANNEL UNDER ISOTHERMAL CONDITIONS.

The configuration of the problem is presented in *Figure 3.1*. The cross section of the channel is a circle with the radius is R. The length of the channel is H. The maximum constriction depth is located in the middle of the channel $(0,z_c)$. The constriction depth is denoted as d. The length of the constricted portion is $L = 2R$. The radii of the outer droplet and inner droplet are R_o, R_i, respectively. The mathematical equations are similar to equation (2.1) and (2.2). The constricted section has a given equation:

$$\begin{cases} r = w(z) = R\{1\text{-}0{,}5\dfrac{d}{R}[1{,}0+\cos(\pi(z-z_c)/L)]\} & khi \ \ |z-z_c| \le L/2 \\ R & khi \ \ |z-z_c| > L/2 \end{cases} \tag{3.1}$$



Hình 3.1 The configuration of the problem

The inlet velocity is:

$$v = -2U_{ave}(1 - r^2 / R^2) \tag{3.2}$$

The dimensionless parameters are listed in bellows:

$$\begin{aligned} &Re = \frac{\rho_m U_{ave}(2R)}{\mu_m}, Ca = \frac{\mu_m U_{ave}}{\sigma_o}, \sigma_{io} = \frac{\sigma_i}{\sigma_o} \\ &R_{or} = \frac{R_o}{R}, R_{io} = \frac{R_i}{R_o}, d_R = \frac{d}{R}, \mu_{om} = \frac{\mu_o}{\mu_m}, \mu_{im} = \frac{\mu_i}{\mu_m} \end{aligned} \tag{3.3}$$

Here, the value of μ_{om}, μ_{im}, and Re is constant during the simulation course. The capillary number Ca is varied in the range of 0,01 to 1,0. R_{io} is varied from 0,2 to 0,9. R_{or} is varied in the range of 0,0 to 0,8.

The computational domain is $W \times H = 1{,}2R \times H = 1{,}2R \times R$. The grid resolution is 096×960. The investigated parameters are the indentation at the rear of the droplets computed at the upstream (*IH*) and in the whole channel (*IF*).

Conclusions of chapter 3

This chapter presents the dynamic behaviors of a compound droplet moving in a constricted channel, the constriction section has a sinusoidal shape. The investigated parameter is the indentation at the rear of the droplets. The effect of the capillary number, the radius ratio of the inner and outer droplet, the ratio of the radius of the outer droplet and the radius of the channel, the surface tension coefficient of the inner and outer droplet, and the maximum constriction depth are presented. The main results are summarized as follows:

As the compound droplet migrates inside the channel, the rear of the droplets can have the following states:

- No indentation.
- Indentation occurred only at the downstream of the channel.
- Indentation occurred both upstream and downstream of the channel.

Increasing the value of Ca, d_R, and R_{or} increases the indentation of both inner and outer droplets.

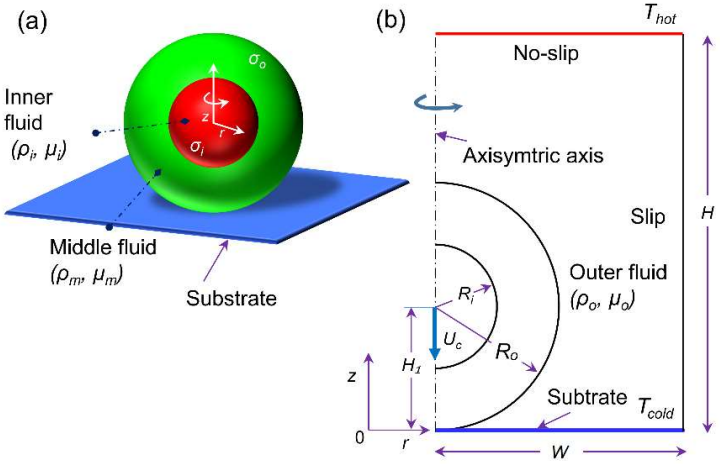
- Increasing the value of R_{io}, the outer droplet is less indented. However, the indentation of the inner droplet increases.
- Increasing the value of σ_{io} does not change the maximum indentation of the outer droplet. However, the indentation of the inner droplet significantly decreases and soon approaches to zero (no indentation).

The dynamic of the compound droplet moving in a constricted channel can be affected by many other parameters. The fluids are considered to be Newton, the compound droplet only has one inner droplet. However, this study is important in the many practical fields, i.e., drug development, and drug carrier.

The results of chapter 3 were published in an international journal in the SCIE (Q2) categories, paper 1 in: ″**List of author's scientific works relating to the content of the dissertation**″.

Chapter 4: A NUMERICAL STUDY OF A COMPOUND DROPLET IMPACT A NON-WETTING SURFACE UNDERGOING MARANGONI EFFECT

The configuration of the problem is shown in *Figure 4.1*. The compound droplet is initially spherical and the inner and outer interfaces coincide. The radii of the outer and inner droplets are R_o and R_i, respectively. The droplets are subjected to the initial velocity and the Marangoni effect induced by the temperature gradient. The colder temperature is placed at the



Hình 4.1 The configuration of the problem

wall and the hotter temperature is placed at the domain top. The mathematical equations are presented in Chapter 2 (equation (2.1), (2.2), and (2.3)). The wall is perfectly non-wetting. Thus, in the simulation, the horizontal velocity of the front elements that in contact with the wall is set to zero.

The computational domain is $W \times H = 4R_o \times 4R_o$. The grid resolution is 256×256. The investigated parameters are the maximum (H_m), and steady rebound height (H_s) of the compound droplet. The contact time of the compound droplet and the wall (t_r), and the deformation of the inner and outer droplet is T_i and T_o. The dimensionless parameters are given bellow:

$$Re = \frac{\rho_m U_c D_o}{\mu_m}, We = \frac{\rho_m U^2{}_c D_o}{\sigma_o}, Ma = \frac{\sigma_T D^2{}_o}{\mu_m \alpha_m}, \quad (4.1)$$

$$Bo = \frac{\rho_m g D^2_o}{\sigma_o}, \frac{\rho_o}{\rho_m}, \frac{\rho_i}{\rho_m}, \frac{\mu_o}{\mu_m}, \frac{\mu_i}{\mu_m}, \frac{k_o}{k_m}, \frac{k_i}{k_m}, \frac{c_o}{c_m}, \frac{c_i}{c_m}, \sigma_{io} = \frac{\sigma_i}{\sigma_o}, V_{io} = \frac{V_i}{V_o} \quad (4.2)$$

Here, the Reynolds number *Re* varies in the range of 10-40, the Weber number *We* varies from 0,32 to 1,4, the Marangoni number *Ma* varies from 50-350, the bond number *Bo* varies from 0,1 to 5,6, the value of V_{io} varies droplet 0,064 to 0,512, and the surface tension coefficient σ_{io} varies from 0,6 to 4,8. The other parameters are constant.

Conclusions of chapter 4

This chapter presents the impact of a compound droplet on a non-wetting surface undergoing thermal convection. The influence of some dimensionless parameters such as *Ma*, *Bo*, *Re*, *We*, V_{io}, and σ_{io} are evaluated. The main results are summarized as follows:

+ Undergoing the Marangoni effect, the compound droplet can have the following state:

- The compound droplet rebounds and stabilizes above the wall.
- The compound droplet cannot rebound.
- The compound droplet rebounds. However, it falls and lies on the wall.

+ The rebound heights (H_m, H_s) strongly depend on the value of the Marangoni number. As the value of $Ma < 150$, the compound droplet cannot rebound. As the value of *Ma* is between 150 and 250, the compound droplet rebounds. However, it then falls and lies on the wall. As the value of $Ma >$ 250, the compound droplet rebounds and balances above the wall.

+ Increasing the radius of the inner droplet, the rebound height of the compound droplet decreases. As the value of V_{io} > 0,216 (R_{io} > 2,16), the compound droplet rebound. However, it then falls and lies on the wall.

+ The variation of the value of σ_{io} significantly affects the deformation of the inner droplet. However, it does not influence the rebound height and the contact time of the compound droplet.

+ Increasing the value of *Bo* decreases the rebound height of the compound droplet. As the value of *Bo* > 1,0, the compound droplet lies on the wall.

+ As the value of *We* > 0,64, the rebound height of the compound droplet increases.

+ Decreasing the value of *Re*, the compound droplet rebound more easily.

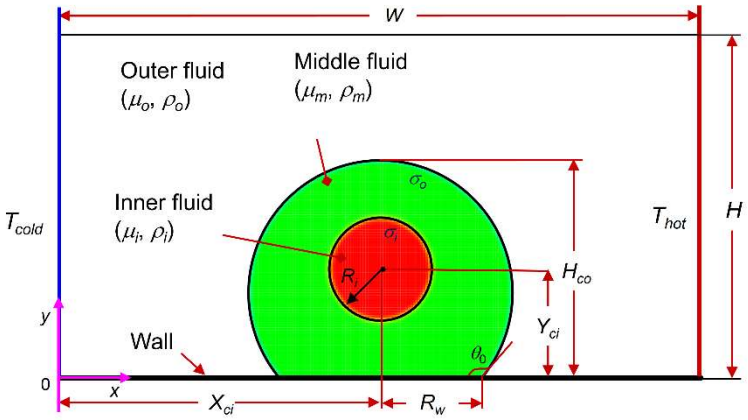
This chapter presents the impact of a compound droplet on a non-wetting surface undergoing thermal convection. It is important in many practical fields such as self-cleaning technology, and the chemical industry. In addition, it provides a new method to transport droplets in a microfluidic chip.

The results of chapter 4 were published in an international journal in the SCIE (Q2) categories, paper 2 in: *"**List of author's scientific works relating to the content of the dissertation**"*.

CHAPTER 5: A NUMERICAL STUDY OF THERMAL MIGRATION OF A COMPOUND DROPLET ON A SUBSTRATE

Figure 5.1 presents the configuration of the problem. There is a compound droplet partially wetted on a substrate. The initial contact angle of the outer droplet and the wall is θ_0. The initial wetting radius and the height of the outer droplet are denoted as R_w, and H_{co}, respectively. The outer droplet has a volume that is equal to a spherical droplet with a radius of R_o. The inner droplet has radius of R_i. The value of $\theta_0 = 130°$. The computational domain is $W \times H = 10R_o \times 5R_o$. The dynamic contact model given in Chapter 2 is applied to handle the contact between the outer droplet and the wall. The grid resolution is 250×130. The investigated parameters are the trajectory of centroids of the inner (X_{ci}, Y_{ci}) and outer droplet (X_{co}, Y_{co}). The dimensionless parameters are listed bellows:

$$Ma = \frac{U_c R_o}{\alpha_m}, Oh = \frac{\mu_m}{\sqrt{\rho_m \sigma_o R_o}}, Pr = \frac{\mu_m c_m}{k_m}, \frac{\rho_o}{\rho_m}, \frac{\rho_i}{\rho_m}, \tag{5.1}$$



Hình 5.1 The configuration of the problem

$$\frac{\mu_o}{\mu_m}, \frac{\mu_i}{\mu_m}, \frac{k_o}{k_m}, \frac{k_i}{k_m}, \frac{c_o}{c_m}, \frac{c_i}{c_m}, \sigma_{io} = \frac{\sigma_i}{\sigma_o}, R_{io} = \frac{R_i}{R_o} \tag{5.2}$$

Here, the viscosity ratio μ_o/μ_m is varied from 0,1 to 2,4. The value of R_{io} is varied from 0,2 to 0,7. The static contact angle is varied from 60° to 120°. The other parameters are constant.

Conclusion of chapter 5

This chapter presents the investigation of the motion of a compound droplet on a substrate undergoing thermal convection. The trajectory of the centroid of the compound droplet depending on the value of the static contact angle, R_{io}, and μ_{om} are pointed out. The main results are summarized as follows:

- The compound droplet can move toward the colder regime or hotter regime depending on the value of θ_e, μ_{om}, and R_{io}.
- Increasing the value of μ_{om}, the compound droplet tends to move to the hotter regime.
- Increasing the radius of the inner droplet ($R_{io} \geq 0,6$), the compound droplet tends to move to the hotter regime. The trajectory of the inner droplet is more stable.
- As the value of $\theta_e \geq 115°$, the compound droplet migrate toward the hotter regime.

This chapter shows the migration tendency of the compound droplet attached on a solid wall undergoing thermal convection. The importance of this chapter has been pointed out in the **INTRODUCTION** section.

The results of Chapter 5 are published in an international journal in SCIE (Q2) categories, paper 4 in: *"***List of author's scientific works relating to the content of the dissertation***"*.

CONCLUSION

The dissertation has shown the investigation of the interaction of a droplet with a solid substrate undergoing thermal convection. The results of Chapter 3, Chapter 4, and Chapter 5 were published in some reputation journals as papers 1, 2, and 4 in the LIST OF AUTHOR'S SCIENTIFIC WORKS RELATING TO THE CONTENT OF THE DISSERTATION. Expanding the investigation in Chapter 3, the motion of a compound droplet moving in a wavy channel was also published (paper 5). The dissertation achieves the following results:

1. A simulation model for such a problem of a droplet interacting with a substrate undergoing thermal convection. It is important contribution so as to expand the numerical method.
2. The dissertation pointed out the motion of a compound droplet in a constricted channel. The dissertation also shows that a compound droplet can rebound and balance above a non-wetting surface.
3. The dissertation points out the trajectories of an attached compound droplet undergoing thermal convection. The compound droplet moves to the hotter regime as the radius of the inner droplet is sufficiently large. In this case, the outer droplet moves following the inner one. In addition, the dissertation also reveals the other parameters that affect the trajectory of the droplets.

NEW CONTRIBUTIONS OF THE DISSERTATION

So far, the investigation of droplets with the substrate has been considered. However, the presence of another droplet causes the dynamic of the problem to change and there may be many new interesting phenomena. The dissertation has the following new contributions:

- The dissertation provides a simulation program of the droplet interacting with a substrate undergoing thermal convection. The dissertation also pointed out many new behaviors of the compound droplet compared to the single droplet.
- The dissertation provides the effect of the dimensionless parameters on the indentation at the rear of the compound droplet and points out the crucial parameters.
- The dissertation provides a phenomenon that the compound droplet rebounds and stabilizes above the substrate with the presence of thermal convection.
- The dissertation provides the effect of the dimensionless parameters on the indentation at the rear of the compound droplet and points out the crucial parameters.

LIST OF AUTHOR'S SCIENTIFIC WORKS RELATING TO THE CONTENT OF THE DISSERTATION

International Journal SCIE (ISI):

1. **Hoe D. Nguyen**, Truong V. Vu, Phan H. Nguyen, Binh D. Pham, Nang X. Ho, Cuong T. Nguyen & Vinh T. Nguyen, "Numerical study of the indentation formation of a compound droplet in a constriction," *J Mech Sci Technol*, Mar. 2021, https://doi.org/10.1007/s12206-021-0316-7. (**SCIE**, IF2020 = 1.734, Q2).
2. **Hoe D. Nguyen,** Truong V. Vu, Phan H. Nguyen, Binh D. Pham, Vinh T. Nguyen, Hung V. Vu, Cuong T. Nguyen, Duong K. Tran, "A numerical study of an impacting compound droplet undergoing thermocapillary convection" *Acta Mechanica*, 2022, https://doi.org/10.1007/s00707-022-03230-6 (SCIE, IF2020 = 2.698, Q2).
3. **Hoe D. Nguyen**, Truong V. Vu, Nang. Ho Xuan. "Impact of Two Successive Compound Droplets Undergoing Thermal Convection", *Iranian Journal of Science and Technology, Transactions of Mechanical Engineering*, https://doi.org/10.1007/s40997-023-00673-7, (SCIE, IF2021 = 1.53, Q2).
4. **Hoe D. Nguyen,** Truong V. Vu**,** Nang X. Ho**,** Phan H. Nguyen**,** Anh D. Le, "Thermocapillary migration of a compound droplet on a substrate" European Journal of Mechanics/ B fluids, SCI, IF2023 = 2.598, Q2)
5. Hung V. Vu, Truong V. Vu, Binh D. Pham, **Hoe D. Nguyen**, Vinh T. Nguyen, Hoa T. Phan, Cuong T. Nguyen, Deformation of a compound droplet in a wavy constricted channel, J Mech Sci

Technol. 37 (2023) 191–202. https://doi.org/10.1007/s12206-022-1220-5. (SCIE, IF2020 = 1.734, Q2).

National Conference:

1. **Nguyễn Đình Hòe**, Vũ Văn Trường, Nguyễn Hồng Phan, Phạm Duy Bính, Nguyễn Tuấn Vinh, Vũ Văn Hưng, Nguyễn Tiến Cường, Trần Khánh Dương, "*Tương tác của hạt lưu chất đa lớp với bề mặt rắn không thấm ướt dưới tác động của mao dẫn nhiệt*", Hội nghị khoa học Cơ học Thủy khí toàn quốc lần thứ 25