STUDY ON DROPLET DEFORMATION IN CONTRACTION MICROCHANNEL

NGHIÊN CỨU VỀ SỰ BIẾN DẠNG CỦA GIỌT NHỎ TRONG KÊNH THU LẠI

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Abstract - Microfluidics systems based on two-phase fluid dynamics have been widely applied from industrial machinery to the aerospace and automotive applications. The systems are designed to handle small volumes of liquids, often in the microliter or even nanoliter range. Droplet-based microfluidics is used for biochemical analysis or materials synthesis as well. The effectiveness of the interactive manipulation between two fluidic phases was significantly impacted by the droplet dynamics of deformation. This research aims to describe the droplet deformation for a wide range of parameters such as capillary number, viscosity ratio, and entry angle in a contraction microchannel. The results show that, droplet deformation is significantly influenced by the parameter mentioned above.

Key words - Droplet dynamics; Contraction microchannel; droplet-based microfluidics; numerical simulation; capillary number

Tóm tắt - Các hệ thống vi chất lỏng dựa trên động lực học chất lỏng hai pha đã được áp dụng rộng rãi từ máy móc công nghiệp đến các ứng dụng hàng không vũ trụ và ô tô. Các hệ thống này được thiết kế để xử lý một lượng nhỏ chất lỏng, thường ở mức microlit hoặc thậm chí nanolit. Hệ thống vi chất lỏng dựa trên giọt nhỏ cũng được sử dụng để phân tích mẫu hoặc tổng hợp vật liệu. Hiệu quả của thao tác tương tác giữa hai pha chất lỏng bị ảnh hưởng đáng kể bởi động lực biến dạng của giọt nước. Nghiên cứu này nhằm mục đích mô tả biến dạng giọt cho các tham số như hệ số mao dẫn, hệ số tỷ lệ độ nhớt giữa hai pha và góc vào kênh trong một vi kênh thu lại. Kết quả cho thấy, biến dạng giọt bị ảnh hưởng đáng kể bởi những tham số nêu trên.

Từ khóa - Động lực học giọt; vi kênh thu lại; hệ thống vi lỏng giọt; phân tích số; hệ số mao dẫn

1. Introduction

Over the past few decades, microfluidic systems applied widely and developed strongly, which play a vital role in the in Lab-on-a-Chip (LoC) and micro TAS systems in predominantly fields like biomedical, environmental and pharmaceutical domains [1]. These systems have many highlight advantages such as low-volume specimens and reagent expending, short-time analysis. It can allow manipulation ability of tiny particles, droplets and cells, with low-manufacturing cost. Additionally, microfluidic technologies based on droplets had a strong development in chemical and biological fields [2]. The deformation of droplets in microfluidic systems was attended to recently. To increase the control and handling of reagents and chemical substances more precisely in digital devices, these systems will create droplets by using two or more fluid substances which cannot be mixed together [3], [4].

Contraction microchannels are quite widely used in much microfluidic equipment which are based on droplets for different purposes such as to create emulsification [5]–[7] or to detect and analyze genes optically [8]. Pipe and McKinley measured the rheological properties of polymeric materials in the contraction microchannel [9].

By using numerical simulation and experiment, the droplets' dynamics in the contraction microchannel were studied in quite a detail. Most previous literature using numerical simulation techniques was done in two-dimensional models. For instance, the boundary element method (BEM) is adopted to describe the droplets' deformation in the contraction entry geometry and rheology. Chung et al. presented the influences of viscoelasticity to the deformation of droplets in a planar contraction-expansion microchannel following the scale 5:1:5 [10]–[12]. Moreover, Christafakis and Tsangaris studied the effects of the fluid parameters in a two-dimensional model like capillary number (Ca), Reynolds number (Re), Weber number (We), and viscosity ratio on the deformation of droplets [13]. The examination of dynamics of droplets in an axisymmetric contraction microchannel caused by the Reynolds number, viscosity ratios and capillary number [14]–[16]. The deformation of droplets in a three-dimensional model of contraction microchannels has not been investigated in many papers of the literature. In a contraction channel, the conduction of typical three-dimensions studies to describe the deformation of droplets under different microchannels and control droplets, cells and particles deformation presented [17]–[19]. Imani et al. explored the droplet deformation caused by capillarity and wettability through a channel having capillary number is constricted [20]. Patlazhan et al. investigated the elongation deformation of droplets as an equation of the ratio through entry droplet diameter and cross-sectional area of the channel having a narrow part [21].

It can be seen that contraction microchannel plays an important impact in droplet-based microfluidics system. As far as the contraction microchannel is concerned, there are very few studies mentioning the effect of entrance geometry on droplet deformation. This research provides an insight of droplet dynamics in micro contraction channel depending on capillary number, viscosity ratio, contraction ratio, and entry angle.

2. Problem statement

The geometrical shape of the contraction microchannel is shown in Figure 1. The initial location of a droplet with radius R and the origin of the coordinate system are shown in the figure by a red sphere. Because the microchannel in this work is $5R$ deep, the top and bottom surfaces have a minimal impact on the droplet's behavior [22]–[24]. The greater microchannel has a length of L_i and a width of $4R$, whereas the contraction microchannel has $30R$ and W, respectively.

With no outlet boundary effect, a contraction microchannel length of $15D$ was selected to fully capture the droplet movements. The non-dimensional number $C = D/W$ is used to define the contraction level. Because the contraction C in this investigation was selected as 1.25, the microchannel width is consistently smaller than the initial droplet diameter. As shown in Figure 1, a symmetric model representing a fourth of the entire three-dimensional model is used in this work to reduce processing costs.

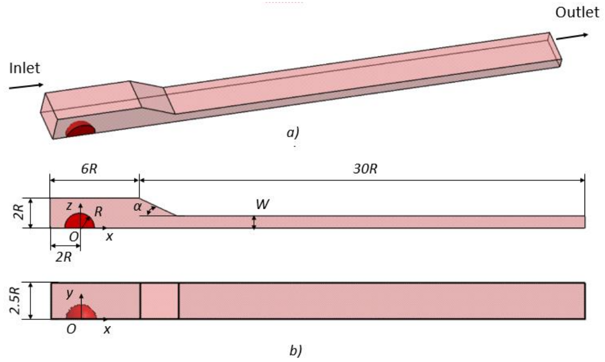

Figure 1. *Geometrical description*
a) 3D model; b) 2D model

3. Computational Model

A commercial program called ANSYS Fluent is used to run the simulation. The computational methods used in this work are the Geo-Reconstruct scheme for interface interpolation, the PRESTO! strategy for pressure interpolation, the PISO scheme for pressure-velocity coupling, a second order upwind scheme for the momentum conservation equation, and the momentum conservation equation [25]. It is fine enough for the current inquiry that the hexahedral elements utilized to evenly discretize the computing domain have a size of $W/30$ [25]. Using a variable time stepping method, the time discretization is done with a Courant number of 0.25.

The practical results of the droplet generation problem given in earlier works were used to validate the computational model [25], [26]. It should also be mentioned that similar computational models have been widely accepted in numerous studies of droplet dynamics in two-phase microfluidic devices [17], [18], [27]–[29].

The formula for the capillary number (Ca), which is defined as Eq. (1), includes the characteristic velocity V, the medium phase's viscosity (μ_m), and the coefficient of surface tension (σ) between the droplet phase and the medium phase. Two different capillary numbers will be used in the discussion that follows depending on where the droplet is in the microchannel. In the larger microchannel, the capillary number is denoted as "Ca_1" and is determined by the entrance velocity, which serves as the characteristic velocity V_i; in contrast, the capillary number in the contraction microchannel is determined by the average velocity in the contraction microchannel, which serves as V_c.

$$Ca = \frac{\mu_m V}{\sigma} \tag{1}$$

4. Results and Discussion

The term "trap" indicates that a droplet does not pass through the entrance contraction position, whereas the term "squeeze" represents a phenomenon in which a droplet is moving in the contraction microchannel. Figure 2 plots the transition from trap to squeeze for a wide range of capillary numbers and entry angles. The entry angle ranges from 15° to 75°, and it is dependable to be trapped or squeezed as capillary change ranges from 0.001 to 0.0018. It can be seen that when increasing the entry angle, a droplet tends to be trapped at a high capillary. Although at high capillary number but droplet still trap, this can rely that increase in entry angle will obstruct movement of droplet at contraction position.

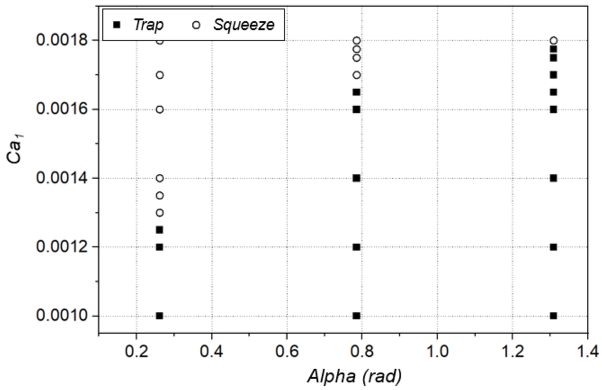

Figure 2. *Transition from trap to squeeze in contraction microchannel*

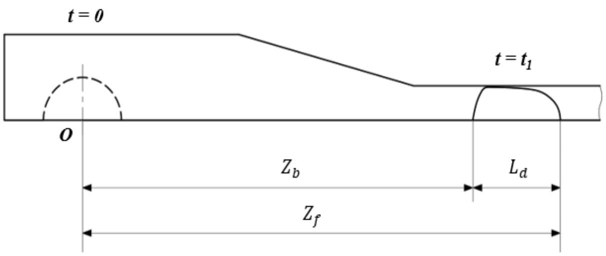

Figure 3. *Droplet description in contraction microchannel*

In order to evaluate droplet dynamics, Figure 3 is used to define droplet deformation in the contraction microchannel. The droplet deformation is defined as L_d, which is measured at the back interface and the front interface. In addition, droplet position is compared with the original coordinator and is expressed by Z_d as shown in Eq. (2), where Z_b and Z_f are the back interface and front interface positions, respectively.

$$Z_d = \frac{Z_b + Z_f}{2} \tag{2}$$

Droplet dynamics as a function of position in the microchannel for a wide range of viscosity ratio is depicted in Figure 4. In general, droplet deformation increases with the viscosity ratios [30]. One can observe that droplet deformation position at changed entry angle area does not depend on viscosity ratio and over deformation phenomenon has not been found at a higher viscosity ratio.

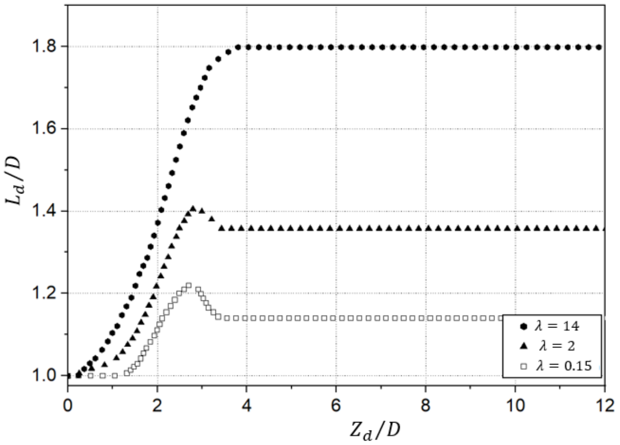

Figure 4. *Droplet deformation as a function of position in microchannel*

The entry angle used to estimate droplet deformation is shown in Figure 5. Generally, droplet deformation at steady state is independent of the entry angles. However, the amount of deformation and position at changed entrance angle area largely depend on the entry angle. A larger entry angle leads to a longer deformation at the entrance contraction position. Large entry angles tend to create large shear stresses at the entrance position.

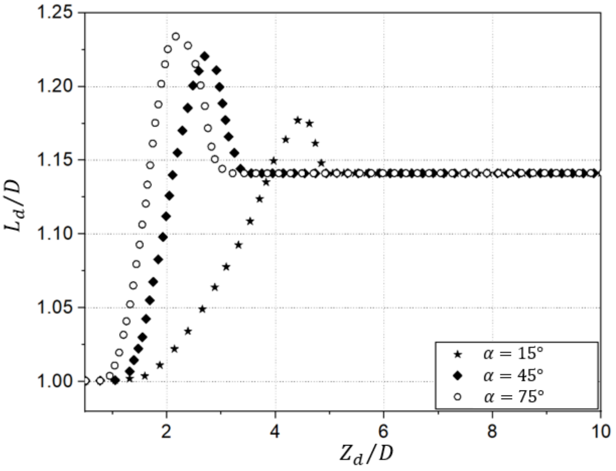

Figure 5. *Droplet deformation as a function of position*

5. Conclusion

This research presents droplet dynamics of deformation under consideration of geometrical contraction shape and flow conditions. There are some findings, as follows: first, when increasing entry angle, droplets tend to be trapped at higher capillary number, vice versa. Second, entry angle does not depend on droplet deformation at steady state in a contraction microchannel. Third, droplet is likely to be trapped even at a large capillary number when contraction entry angle increases. Finally, over-deformation phenomena have not been found when the viscosity ratio is high. These investigations would yield helpful knowledge for designing and fabricating droplet-based microfluidic systems with contraction microchannels.

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