Manipulation of a droplet in a planar channel by periodic thermocapillary actuation

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Received 8 November 2007, in final form 28 January 2008
Published 14 March 2008
Online at stacks.iop.org/JMM/18/045027

Abstract
Thermocapillary manipulation of a droplet in a planar microchannel with periodic actuations has been demonstrated by both theoretical simulation and experimental characterization. The driving temperature gradients are provided by four micro heaters embedded in the boundaries of the planar channel. The temperature distributions corresponding to the periodic actuations are calculated, and are coupled to the droplet through the surface tensions which drive the droplet. The results show that the droplet will be driven to move along closed loops whose patterns can be designed and controlled by the periodic heating schemes and actuation frequencies. Qualitative agreement between the simulation and experimental observation, in terms of the temperature distributions and droplet moving tracks, has been obtained.

1. Introduction
Biological science research in the micro-scale has grown in importance in recent decades, and droplet-based microfluidics has emerged as an alternative for bio-chemical analysis. A microdroplet is a good option to be the carrier for reactant transport in a microchannel, which provides a platform for chemical reactions. The emerging field of droplet-based microfluidics leads to the need for effective manipulation of an individual droplet in the micro-scale [1]. Most bio-chips use continuous-flow platforms based on microchannels and the active control of microdroplets can be achieved by pressure differences [2], thermocapillary forces [3] and so on. Comparing to one-dimensional (1D) droplet-based microfluidic devices, a two-dimensional (2D) droplet-based microfluidic device handles droplets individually with more flexibility. The actuation may be achieved by chemical or thermal gradients [4], surface acoustic waves [5] and electric fields [6]. Manipulation of a droplet by thermal gradient actuation was reported by Darhuber et al [7, 8]. They designed a microfluidic device for the actuation of liquid droplets or continuous streams on a solid surface by means of integrated micro-heater arrays. The micro-heaters provided the control of the surface temperature distribution with high spatial resolutions. In combination with chemical surface patterning, the device can be used as a logistic platform for parallel and automated routing, mixing and reacting of a multitude of liquid samples. In their work, a complex programmable multi-heater array design was used to achieve motion control of the droplet. Similar control can be obtained by using boundary heaters with programmable heating schemes [9–12]. In these studies, 1D simulations and experiments were conducted on the dynamics of a liquid plug actuated between two heaters in a capillary. The actuation concept allowed both transient and reciprocating motions. In the present study, the 1D model for the periodic thermocapillary actuation in capillary tubes is extended to a 2D planar microchannel with heating at the boundaries, which is different from the work by Darhuber et al [7, 8]. A liquid droplet is positioned inside the planar channel formed between a square substrate and a top layer with four heaters aligned at the edges. The square area is considered to be much larger compared to the droplet size. Temperature distributions in the square region are realized spatially with four controllable heating boundary conditions. Through the coupling between the temperature field and the surface tension, the droplet motion and position are under control. It is to demonstrate that a complete manipulation of the droplet in a region can be achieved by various heating schemes at the boundaries, which may be simple in design and fabrication compared to conventional digital microfluidics based on electrowetting. However, the temperature effect in thermocapillary actuation should be taken into account in applications, especially in biomedical engineering, where some biological samples may be sensitive to the temperature variations.
2. Theoretical modeling

2.1. Temperature distributions

Figure 1 shows the schematic concept of thermocapillary actuation of an individual droplet in a planar channel. In order to simplify the model, a square region has been considered in this study. The temperature distribution inside the channel can be described by the following governing equation

$$\frac{\partial \theta}{\partial t} = \alpha \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} \right) - \frac{h}{\rho c} \theta,$$

where $\theta$ is the temperature difference relative to the environmental temperature, $H$ is the thickness of the substrate plane, $\alpha$, $\rho$, $h$, and $c$ are the thermal diffusivity, density, convection coefficient and specific heat capacity of the substrate material, respectively. Heat radiation is neglected in this model because of the relatively low temperature of the substrate surface. The boundary conditions are

$$\left. \frac{\partial \theta}{\partial x} \right|_{x=0} = f_1(t) \frac{q''_0}{k}, \quad \left. \frac{\partial \theta}{\partial y} \right|_{y=0} = -f_3(t) \frac{q''_0}{k},$$

$$\left. \frac{\partial \theta}{\partial x} \right|_{x=a} = f_2(t) \frac{q''_0}{k}, \quad \left. \frac{\partial \theta}{\partial y} \right|_{y=a} = f_4(t) \frac{q''_0}{k},$$

where $q''_0$ is the maximum heat flux that can be supplied by an individual heater and $k$ is the conductivity of the substrate material. $f_1(t)$, $f_2(t)$, $f_3(t)$, and $f_4(t)$ are time-dependent factors controlling the four heaters, respectively. In the periodic actuation, we assume that all heaters are activated periodically with the same period, $T_h$. By introducing the dimensionless variables $\theta^* = \theta k/q''_0 a$, $x^* = x/a$, $t^* = t/T_h$, we have the dimensionless heat transfer equation and boundary conditions

$$\eta \frac{\partial \theta^*}{\partial t^*} = \alpha \left( \frac{\partial^2 \theta^*}{\partial x^{*2}} + \frac{\partial^2 \theta^*}{\partial y^{*2}} \right) - \xi \theta^*,$$

where $\eta = a^2/(\alpha T_h)$ and $\xi = ha^2/Hk$. In order to homogenize the time-dependent boundary conditions, we set

$$f(x^*, y^*, t^*) = x^* f_1(t^*) + \frac{x^2}{2} [f_2(t^*) - f_1(t^*)]$$

$$+ y^* f_3(t^*) + \frac{y^2}{2} [f_4(t^*) - f_3(t^*)],$$

where $x^*$ and $y^*$ are the dimensionless coordinates, and $f_1(t^*)$, $f_2(t^*)$, $f_3(t^*)$, and $f_4(t^*)$ are the time-dependent factors controlling the four heaters, respectively.
such that
\[
\begin{align*}
\left. \frac{\partial f}{\partial x^*} \right|_{x^*=0} &= f_1(t^*) \\
\left. \frac{\partial f}{\partial x^*} \right|_{x^*=1} &= f_2(t^*) \quad \left(5\right) \\
\left. \frac{\partial f}{\partial y^*} \right|_{y^*=0} &= f_3(t^*) \\
\left. \frac{\partial f}{\partial y^*} \right|_{y^*=1} &= f_4(t^*) \quad \left(6\right)
\end{align*}
\]

By setting
\[
\theta^*(x^*, y^*, t^*) = g(x^*, y^*, t^*) + f_1(x^*, y^*, t^*) + f_2(x^*, y^*, t^*) + f_3(x^*, y^*, t^*) + f_4(x^*, y^*, t^*) \quad \left(7\right)
\]
and substituting equations (5) and (7) into equation (3), we have
Figure 5. Different periodic heating schemes and the corresponding droplet tracks.

\[
\frac{\partial g}{\partial t^*} = \alpha \left( \frac{\partial^2 g}{\partial x^{*2}} + \frac{\partial^2 g}{\partial y^{*2}} \right) - \xi g + [f_2(t^*) - f_1(t^*) + f_3(t^*)] \right] - \xi f
\]

\[
\left\{ \begin{array}{l}
\frac{\partial g}{\partial x^{*}} |_{x^{*}=0} = 0 \\
\frac{\partial g}{\partial x^{*}} |_{x^{*}=1} = 0 \\
\frac{\partial g}{\partial y^{*}} |_{y^{*}=0} = 0 \\
\frac{\partial g}{\partial y^{*}} |_{y^{*}=1} = 0.
\end{array} \right.
\]

Function \( g(x^*, y^*, t^*) \) can be expanded by the Fourier series method according to the homogeneous boundary conditions (9) and the periodic characteristic, and can be solved from equation (8). The final temperature distribution is obtained as

\[
\theta^*(x^*, y^*, t^*) = g(x^*, y^*, t^*) + f(x^*, y^*, t^*)
\]

\[
= \sum_{n=1}^{\infty} \sum_{N=\infty}^{\infty} g_{00n} e^{i2\pi N t^*} + \sum_{n=1}^{\infty} \sum_{N=\infty}^{\infty} g_{m0N} \cos(m\pi x^*) e^{i2\pi N t^*}
\]

\[
+ \sum_{n=1}^{\infty} \sum_{N=\infty}^{\infty} g_{m0N} \cos(n\pi y^*) e^{i2\pi N t^*}
\]

\[
+ \frac{x^*}{2} [f_4(t^*) - f_3(t^*)] + \frac{y^*}{2} [f_4(t^*) - f_3(t^*)].
\]

where

\[
\begin{align*}
g_{00N} &= \frac{d_{00N} - (i2\eta\pi N + \xi) f_{00N}}{i2\eta\pi N + \xi} \\
g_{m0N} &= \frac{-i2\eta\pi N + \xi f_{m0N}}{i2\eta\pi N + \xi + m^2\pi^2} \\
g_{m0N} &= \frac{-i2\eta\pi N + \xi f_{m0N}}{i2\eta\pi N + \xi + N^2\pi^2}
\end{align*}
\]

and

\[
\begin{align*}
d_{00N} &= \int_0^1 \int_0^1 \int_0^1 f e^{-i2\pi N t^*} dx^* dy^* dt^* \\
f_{00N} &= \int_0^1 \int_0^1 \int_0^1 f \cos(m\pi x^*) e^{-i2\pi N t^*} dx^* dt^* \\
f_{m0N} &= \int_0^1 \int_0^1 \int_0^1 f \cos(n\pi y^*) e^{-i2\pi N t^*} dy^* dt^*.
\end{align*}
\]

2.2. Coupling of temperature with droplet motion

The temperature distributions in the channel are coupled to the droplet through surface tensions. The unbalanced surface tensions on the droplet, due to the temperature gradients, drive the droplet moving inside the channel. The surface tension \( \sigma_{lg} \) of the liquid depends on the temperature. For a small temperature range, a linear relation can be assumed:

\[
\sigma_{lg}(\theta) = \sigma_{lg0} - \epsilon(\theta - \theta_0),
\]

where \( \sigma_{lg0} \) is the liquid–gas surface tension at the reference relative temperature \( \theta_0 \) and \( \epsilon \) is the temperature coefficient of surface tension. The temperature field resulting from equation (1) is in turn a function of time and position \( (x, y, t) \). Assuming a weak thermal interaction between the droplet and the substrate surface, the surface tension can be described as a function of time and position \( (t, x, y) \) through the temperature distributions:

\[
\sigma_{lg}(\theta) = f[\theta(x, y, t)] = \sigma_{lg}(x, y, t).
\]

Since the droplet diameter \( 2R \) is normally less than the Laplace length \( \kappa^{-1} = \rho g/\sigma_{lg} \), the droplet profile can be assumed to be circular, the curvature radius constant and the dynamic contact angle uniform along the contact line. For flat structures the dominant viscous dissipation occurs in the bulk, and the dissipation at the solid–liquid–gas contact line
is negligible. With the lubrication approximation, the viscous drag force generated within the liquid is [13]

\[
\begin{align*}
F_{vx} &= 3 \mu u \int_{M}^{N} \frac{dx}{\lambda(x)} = \frac{6 \mu R}{h_g}, \\
F_{vy} &= 3 \mu v \int_{M}^{N} \frac{dy}{\lambda(y)} = \frac{6 \mu R}{h_g},
\end{align*}
\]

(15)

where \( \lambda(x) \) is the droplet height profile function, \( u, v \) are the velocity magnitudes in \( x \) and \( y \) directions respectively, \( \mu \) is the liquid viscosity, \( R \) is the droplet base radius and \( h_g \) is the channel height. The liquid viscosity, based on the previous work of Yarin, is dependent on temperature at the droplet center [14],

\[
\mu = \mu_0 \exp \left[ 3.87h_b \left( \frac{1}{T_{\text{center}}} - \frac{1}{T_0} \right) \right].
\]

(16)

where \( \mu_0 \) is the viscosity at some reference temperature \( T_0 \) (normally 293 K), and \( T_b \) is the liquid boiling temperature. In order to make the droplet evaporate with an imperceptible amount and make hysteretic effects not prominent, silicone oil was chosen to be the droplet liquid. In this case, the capillary number \( Ca = \frac{\mu U}{\sigma} \ll 1 \times 10^{-3} \) when the velocity is less than 1 mm s\(^{-1}\). The low capillary number ensures that the moving droplet has a nearly constant circular profile, and the dynamic contact angles are assumed to be constant for simplification. The circular profile is divided into \( n \) sectors, the resultant force on both \( x \) and \( y \) directions can be calculated by combining all the surface tension forces acting on the individual sector,

\[
\begin{align*}
F_x &= 2 \sum_{i=1}^{n} \frac{2\pi R}{n} \cos \left[ \frac{(2i + 1)\pi}{n} \right] \sigma_b(x_i, y_i, t) \\
F_y &= 2 \sum_{i=1}^{n} \frac{2\pi R}{n} \sin \left[ \frac{(2i + 1)\pi}{n} \right] \sigma_b(x_i, y_i, t),
\end{align*}
\]

(17)

where \( \sigma_b(x_i, y_i, t) = \sigma_b(x_0 + R \cos \frac{(2i+1)\pi}{n}, y_0 + R \sin \frac{(2i+1)\pi}{n}, t) \), \((x_0, y_0)\) is the droplet initial position. A larger \( n \) leads to a more accurate result, and we set \( n = 8 \) in the present study. The velocity \( U = u\hat{x} + u\hat{y} \) can be determined by the forces balance between the inertia, friction and thermocapillary force, i.e.,

\[
\begin{align*}
\rho V \frac{du}{dt} &= -6 \frac{\mu R}{h_g} u + F_x, \\
\rho V \frac{dv}{dt} &= -6 \frac{\mu R}{h_g} v + F_y.
\end{align*}
\]

(18)

Here \( u \) and \( v \) are the velocity components in the \( x \)-axis and \( y \)-axis directions, respectively. \( V \) is the volume of the droplet \( (V \approx \pi R^2 h_b) \). The dynamic contact angle along the contact line is assumed to be the same as the static contact angle, about 10°. By setting \( A = \frac{6\mu R}{\rho V^2}, B_x = -\frac{F_x}{\rho V}, B_y = -\frac{F_y}{\rho V} \), the velocity of the droplet can be solved as

\[
\begin{align*}
u &= -\frac{B_x}{A} + \frac{B_y}{A} e^{-At} \\
v &= -\frac{B_x}{A} + \frac{B_y}{A} e^{-At}.
\end{align*}
\]

(19)
3. Experiment setup and materials

The experimental setup is illustrated in figure 2. The planar channel was formed between a glass wafer as the bottom plate and a glass plate on top. The height of the channel was 0.5 mm. Four micro heaters, made of titanium and platinum, were fabricated on the glass wafer along four sides of a 10 mm × 10 mm square region. The droplet was actuated within this square region. Square wave signals from a power supply were used for controlling the heating process. These signals can also be used to trigger a CCD camera for capturing the droplet motion images. The CCD camera was operated at the rate of two frames per second throughout the experiments. The resolution of the camera was 640 pixels × 480 pixels. A thermal tracer camera (NEC TH9100PMVI) was used for the temperature distribution measurement. In the experiments, the maximum heating power was kept at 0.5 W for all heaters. An in-house-made controller was used to control the individual heater according to a required heating scheme. Silicone oils PDMS (polydimethylsiloxane, Sigma Aldrich) of viscosity 10 cSt was used in the experiments as the working liquid for the droplets, and the droplet radius was controlled at 0.5–0.7 mm. The droplet was injected into the planar channel by a precise syringe. The physical properties of silicone oil are listed in table 1.
4. Results and discussions

The simulation results are presented and discussed first, and part of them are then verified and compared with the experimental characterizations.

4.1. Simulation results

In the periodic actuation, we consider the situation that the heaters have been switched on a long time and the periodic temperature distributions have been established inside the
The temperature variations depend on the heating scheme within one period. Figure 3 shows a typical case, in which one period is divided into four quarters and each heater works only in one quarter period, as shown in figure 3(a). The corresponding temperature distributions in each quarter period are plotted in figures 3(b)–(e). In this case, a droplet introduced into the channel will be driven to move in a loop illustrated in figure 4(a). The periodic motion of the droplet is better observed by plotting its displacement and temperature in figures 4(b) and (c), respectively. It is interesting to note that the droplet experiences a quick change from low temperature to high temperature in each period, which is depicted in figure 4(d). This could have potential applications in some biomedical processes. Three different periodic heating schemes and the corresponding droplet moving patterns are illustrated in figure 5. A variety of loop patterns for the droplet moving inside the channel can be generated by different periodic heating schemes.

4.2. Experimental characterization

The experimental characterizations of the droplet under periodic thermocapillary actuation are conducted to verify the simulation results, and also to demonstrate that the periodic manipulation is achievable. Figure 6 shows the measured periodic temperature distributions in four quarters of a single period, captured by the thermal tracer camera. The heating scheme is the same as that used in figure 3(a) with the period $T_h = 80$ s. By comparing the predicted temperature distributions presented in figure 3, it is seen that the experimental results agree well with the modeling, except the low temperatures at four corners. The low temperatures observed at four corners are probably caused by the nonuniform heat flux along the individual micro heater, especially at the corners where two heaters are not really joined as the boundary conditions assumed in the simulation. Under this heating scheme, figure 7 shows the real images of the silicone oil droplet at different time instances, the motion track and the displacements against time based on the recorded images. Comparing figures 4(a) and (b), we can see a qualitative agreement between the simulation and experimental observation in terms of the periodic motion track and displacements. Three more heating schemes, the same ones used in simulations shown in figure 5, were tested in the experiment with the period $T_h = 80$ s, and the results are presented in figure 8. The motion tracks, obtained from the recorded images, are seen similar to those closed loops predicted in figure 5. The effect of the heating period on droplet motions was studied in the experiment by actuating a droplet with the same heating scheme but different periods. The results are shown in figure 9. The main differences are in the loop sizes and corner shapes. The longer period leads to a larger loop with sharp corners, while the shorter period results in a smaller loop without sharp corners, indicating that the actuation period or the frequency is a parameter to affect the loop shapes.

5. Conclusions

The periodic thermocapillary actuation of a droplet inside a planar microchannel has been simulated and experimentally verified. The heaters are located at the channel sides. The results show that, under the periodic actuation, the droplet can be driven to move in a closed loop whose pattern is controlled by the periodic heating schemes and actuation frequencies. Under various heating schemes, the droplet can be manipulated with great flexibility in terms of moving tracks inside the channel. Qualitative agreement has been obtained between the modeling results and experimental characterizations, in terms of temperature distributions and droplet-moving tracks. The actuation concepts reported in this paper may offer an alternative platform for the droplet process and would have potential applications in droplet-based microfluidics, such as concurrent mixing and moving of biological and chemical samples contained in the liquid in planar channels.

Acknowledgment

The authors would like to thank the Academic Research Fund of the Ministry of Education Singapore (grant no RG26/06) for its financial support.

References


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**Table 1. Physical properties of silicone oil.**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Silicone oil</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, $\rho$</td>
<td>930 kg m$^{-3}$</td>
</tr>
<tr>
<td>Surface tension (293 K), $\sigma_{tv}$</td>
<td>20.3 mN m$^{-1}$</td>
</tr>
<tr>
<td>Temperature surface tension coefficient, $\alpha$</td>
<td>0.06 mN mK$^{-1}$</td>
</tr>
<tr>
<td>Viscosity (293 K), $\nu$</td>
<td>10 cSt</td>
</tr>
<tr>
<td>Boiling point, $T_b$</td>
<td>413 K</td>
</tr>
</tbody>
</table>


