Original Paper

A Three-Dimensional Simulation of Thermocapillary Flow in a Circular Thin Liquid Film under Zero Gravity

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Dr. D. Pettit, a NASA Astronaut, carried out a thermocapillary flow experiment in a thin water film on-board the International Space Station (ISS) in 2003. The thin water film containing milk powder tracers was formed in a stainless-steel wire ring. The heating of a section of the ring by a soldering iron induced a thermocapillary flow in the water film. This flow was towards the heated part of the ring (*outward flow*); in the opposite direction (from hot to cold) to the ordinary thermocapillary flows observed in a liquid bridge and a liquid film. To shed light on the discrepancy observed between the space experiment and the ordinary thermocapillary flow, we have carried out a three-dimensional numerical simulation study. In the simulation we have also included the effect of meniscus shape. The simulation results showed that the meniscus shape determines the flow direction. Its consideration in the simulation also led to the prediction of an *outward flow* (from center to the heated part of the ring) in the water film as observed in the space experiment of Dr. D. Pettit.

Key Words: Numerical Simulation, Marangoni Effect, Thermocapillary, Meniscus

Nomenclature

v	: velocity
t	: time
x	: position
p	: pressure
ν	: dynamic viscosity
T	: temperature
α	: thermal diffusivity
μ	: viscosity
σ_T	: surface tension coefficient of temperature
w	: width
h	: height
δ	: film thickness
r	: radius of a liquid film
θ	: angle from heated point
k	: thermal conductivity
q	: heat flux

Subscripts

τ	: tangential direction to the free surface
n	: normal direction to the free surface
m	: meniscus
s	: swelling
0	: initial

1. Introduction

Surface tension along a free surface is a function of temperature and solutal concentration. When the surface tension varies (with a gradient) along the free surface, thermocapillary, solutocapillary, and Marangoni convective flows develop in the liquid. For instance, a thermocapillary flow develops when a temperature difference along the free

surface exists. Pearson¹⁾ investigated the Marangoni instability in a static liquid layer heated from the bottom. In crystal growth, due to their adverse effects on crystal quality, thermocapillary flows in the melts have often been studied, such as in a liquid bridge²⁻⁴⁾, a rectangular liquid layer^{5,6)}, and an annular pool^{7,8)}. (for further reading on thermocapillary effects, see the review articles of Schatz and Neitzel⁹⁾, and Lappa^{10,11)})

On the Earth, temperature differences in fluids give rise to both buoyancy (natural) convection and thermocapillary flow. However, in the microgravity environment, the natural convection becomes negligible, and thermocapillary flow becomes dominant. Thus, a microgravity environment is a very useful platform for studying thermocapillary flows in various systems. In that direction numerous experiments have been conducted using the available platforms on sounding rockets and the International Space Station (ISS)^{2,4,9-11)}. For instance, a series of interesting experiments on thermocapillary effects was conducted by Dr. D. Pettit onboard the ISS¹²⁾ in a program called “Saturday Morning Science”. These experiments were simple and did not require complex systems. Dr. D. Pettit has conducted an experiment in a thin water film sustained in a circular stainless wire ring. The wire diameter was about 0.6 mm and the film thickness was not measured in this experiment. In spite of a large ring diameter, about 50 mm, it was possible to form a water film due to the reduced gravity level of the ISS. The thin water film containing milk powder tracers was held in the wire ring. When a section of the ring was heated by bringing a soldering iron close to the wire, a thermocapillary flow, driven by the surface tension gradient along the free surface, developed in the liquid towards the hotter region (which is called here an “*outward flow*”). This was contrary to what is expected since

the liquid surface tension is a monotonically decreasing function of temperature.

To address this issue, Kawamura *et al.* carried out a combined study with a ground-based laboratory experiment and a two-dimensional numerical simulation¹³⁾. In this ground-based experiment, an *outward flow* was observed in the film. Their 2-D numerical simulation, however, predicted an *inward flow*; the computed flow was in the opposite direction of the experiment. Then, Ueno *et al.* conducted an experiment of water film sustained in a rectangular frame to investigate this phenomenon^{14,15)}. One side of the frame was heated and the other side was cooled. A thermocapillary flow developed in the film, and *inward* and *outward flow* patterns were observed depending on the volume ratio.

As seen from the above discussion, questions still remain for the reasons why an *outward flow* developed and why could not be predicted numerically. Studies conducted thus far did not examine the mechanisms determining the flow direction, and did not provide a clear explanation for the development of an *outward flow* in the experiments.

In this direction, with the purpose of shading light on the mechanism determining the direction of the thermocapillary flow develops in a thin circular liquid film, we have conducted a three-dimensional numerical simulation. In the simulation we have particularly focused on the effect of meniscus shape since we have previously found that the surface geometry (shape) affected the flow patterns in the half-zone method³⁾ (which is a simplified model for the floating-zone crystal growth method) and also in a thin liquid film^{5,15,16)}. Thus, the inclusion of the effect of meniscus in the present simulation led to a successful prediction for the flow direction in the film.

2. Numerical Analysis

Schematics of the computational domains are shown in Fig. 1. The following assumptions were made in the model: (1) The effect of gravity is negligible since the space experiment was conducted under microgravity and the buoyancy driven convection in the water film was not seen, (2) The heat loss from water or solid wire into the ambient gas is negligible, (3) The physical properties, except that of surface tension, are constant, and the values at 293 K corresponding to the previous experiments of Kawamura *et al.*¹³⁾ are used, (4) Free surfaces do not deform, and (5) The ambient gas is passive.

Heat transfer in the solid wire is analytically approximated by one-dimensional unsteady heat conduction, and the following unsteady function is obtained for temperature:

$$T = T_0 + q \cdot \frac{(\sqrt{6\alpha t} - r|\theta|)^2}{2k\sqrt{6\alpha t}} \quad (1)$$

where heat flux q was 1.0×10^4 W/m². The derivation of Eq. (1) is given in Yamamoto *et al.*¹⁶⁾.

2.1. Computational domain

The basic computational domain is a very thin non-skewed cylinder. In this domain, the solid-liquid and liquid-gas interfaces were assumed to be flat. A schematic diagram of the domain is shown in Fig. 1 (a). We then focused on the meniscus shape. Estimating the actual meniscus shape is very

difficult because many factors affect the film shape, such as contamination, wire surface roughness, and temperature, and the accurate free surface shapes were not measured in the space experiment¹²⁾. Thus, we selected some geometric patterns of the computational domain and investigated what geometry affects the flow direction. The computational domain was similar to a thin cylinder and the free surface edge was skewed. In this case, the solid boundary wall was assumed to be flat and the meniscus shape was represented by a smooth Bezier curve. The schematic of this computational domain is shown in Fig. 1 (b). In the same way, the swollen water film is shown in Fig. 1 (c). Figure 1 (d) shows the two-dimensional domain, which is a simplified model in a cross section of a three-dimensional liquid film. Therefore, the two-dimensional domain has two free surfaces, and temperature on the sidewall increases with time. This is used to analyse generation of vortex shown later.

The diameter and film thickness (10 mm and 1 mm, respectively) of the film used in the numerical simulation is much smaller than those (50 mm and about 0.5 mm (because wire diameter was about 0.6 mm)) of the space experiment because of reduction of the computational cost. In the terrestrial experiment conducted by Kawamura *et al.*¹³⁾, the direction of thermocapillary flow in a 10 mm circular water film was *outward flow*, and the film thickness did not affect the direction of thermocapillary flow as shown in Section 3. 3. In addition, the numerical simulation showed that the developed flow direction in 10 mm water film corresponded to that in 50 mm water film. Therefore, it is considered that the downward scaling does not affect the direction of thermocapillary flow in a circular water film. Since we are interested in finding out the mechanism determining the flow direction, such a downward scaling in the size of the film is acceptable.

Fig. 1. Schematics of the film geometry: (a) flat film, (b) with meniscus, (c) with film swelling, and (d) in a two-dimensional cross-section.

In the analysis, the solid wire was assumed to be a heat-conducting rigid solid, and the liquid domain being pure water was assumed to be a heat conducting, incompressible, Newtonian fluid. The physical properties are presented in Table 1 and Table 2.

Table 1. Physical properties of water (293 K)¹⁷⁾

Property (Symbol)	Value	Unit
Thermal diffusivity (α)	1.43×10^{-7}	m^2/s
Dynamic viscosity (ν)	9.95×10^{-7}	m^2/s
Density (ρ)	9.98×10^2	kg/m^3
Surface tension coefficient of temperature (σ_T)	9.93×10^{-5}	kg/s^2
Prandtl number (Pr)	6.96	-

Table 2. Physical properties of stainless steel wire (293 K)¹⁷⁾

Property (Symbol)	Value	Unit
Thermal diffusivity (α)	4.40×10^{-6}	m^2/s
Thermal conductivity (k)	2.00×10^1	$\text{kg}\cdot\text{m}/(\text{s}^3\cdot\text{K})$

2.2. Model equations

The governing equations of the liquid phase are the following momentum, continuity, and energy balance equations:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v} \quad (2)$$

$$\nabla \cdot \mathbf{v} = 0 \quad (3)$$

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \alpha \nabla^2 T \quad (4)$$

Along the top and bottom free surfaces, thermocapillary forces are in effect, that is, the velocity gradient in the normal direction to the free surface is proportional to temperature gradient:

$$\mu \frac{\partial \mathbf{v}_\tau}{\partial \mathbf{n}} = -\sigma_T \frac{\partial T}{\partial \tau} \quad (5)$$

The free surfaces were assumed to be adiabatic:

$$\nabla_n \cdot T = 0 \quad (6)$$

On the wire wall, no-slip condition is imposed for the flow velocity, and the temperature boundary condition is expressed by Eq. (1).

Initial temperature is uniform with a value of 293 K, and the water film is stationary initially in all regions.

2.3. Numerical procedure

The governing equations given in Eqs. (2) - (4) were discretized by the finite volume method, and the velocity and pressure fields were coupled by the PISO algorithm. The values on cell interfaces were calculated by a second-order central difference scheme. For the discretization of time derivative, a first-order implicit Euler method was applied. All the numerical simulations were conducted by a free source software, OpenFOAM[®]. Computational grids were non-orthogonal structured grids in multi blocks and clustered near the wall because local fine grids were required to capture small vertical flows near the wall. Examples of the computational grids used in the present simulation are shown in Fig. 2 and the total number of grid points is about 200000 ~ 350000. Especially in the case of water film with meniscus, the resolutions of computational grids were fine in meniscus because the free surfaces were complicated shapes. Depending on meniscus shape, total grid number varies. The grid

dependency was checked, and the verification is shown in Section 3.1.

3. Results and Discussion

3.1. Verification of the numerical code

Verification of the numerical code was shown in Yamamoto *et al.*¹⁶⁾ and grid convergence was assessed with

Fig. 2. Computational grids: (a) flat film, (b) with meniscus, and (c) with film swelling.

Fig. 3. The velocity profiles with different number of grids in y direction at the film surface on the upper line at 0.1 s with: (a) meniscus shape ($h_m = 0.1$ mm, $w_m = 0.5$ mm, and $\delta = 0.1$ mm), and (b) film swelling ($\delta = 0.1$ mm, $w_s = 1.0$ mm, and $h_s = 0.1$ mm).

different grids cases. The grid convergence assessment was conducted in the both cases of water film with meniscus and swelling. The geometry with meniscus was selected as $\delta = 0.1$ mm, $w_m = 0.5$ mm, and $h_m = 0.1$ mm, and the geometry with swelling was selected as $\delta = 0.1$ mm, $w_s = 1.0$ mm, and $h_s = 0.1$ mm. These geometries were selected because very strong and complicated flow developed with coarse grid.

In the case of meniscus, four grid levels were examined, and the total grid numbers were about 34000, 170000, 180000, and 250000 points (coarse, normal, fine, and very fine). The grid number gradually increased in each direction as becoming finer numerical grid. The total numerical grid number of normal and fine grid are similar, however, normal grid resolution is finer in the parallel direction to the free surface and fine grid resolution is finer in the normal direction to the free surface. The flow directions are the same in all grid levels, however, the quantitative values were different for each grid levels. Figure 3 (a) shows the velocity profile in the y -direction along the line shown in the left figure with different grid levels. The velocity with fine grid nearly corresponds to that with very fine grid. Therefore, the lines of fine and very fine grid are expressed in one line. The result shows grid resolution of fine grid is sufficient to capture the flow. The other grid convergences with meniscus were checked. Finally, about 200000~350000 total grid points were needed for fine grid resolution. In the same way, grid convergence was checked for the case of swelling. The total grid number was about 50000, 110000, 200000 (coarse, normal fine). Figure 3 (b) shows the grid resolution of normal grid is enough. We finally concluded about 120000~200000 total grid points were needed in the case of swelling.

Using this verified simulation code, we first examined to see if the unsteady heat transfer at the wall and the three-dimensional fluid flow structure in the domain played any role in determining the thermocapillary flow direction.

3.2. Thin liquid film with flat free surfaces

In this section we discuss the case where the water film was assumed sustained in the circular wire with flat free surfaces, and the solid boundary is a flat wall. The circular film thickness was 0.1 mm and the diameter was 10 mm. The computed streaklines and temperature contours at 2.5 and 5 s after heating were plotted in Fig. 4. The started points of streaklines are allocated randomly in the liquid film. The increment of temperature contours was selected as 0.5 K. The computed streaklines seems to be straight lines in a radial direction. This shows that flow did not develop in the circumferential direction. The computed streaklines also exhibit a three-dimensional structure. However, this is not obvious since the figure was seen only in the normal direction to the free surface. The streaklines were therefore examined from another direction to see the behavior of the flow near the wall. The velocity vectors in the cross-section of $\theta = 0^\circ$ of the circular region are shown at 5 s in Fig. 5. As seen from the figure, a symmetric vortex pair developed near the wall. These computational results may be explained as follows. Since the temperature gradient along the free surface near the heated edge was steeper, the thermocapillary effect caused flow towards the center of the film along the free surface and a

return flow developed in the inner region where the temperature gradient was shallower. As a result, a symmetric vortex pair developed in the film. Except vortex pair, the fluid in the film was almost stationary. Then, the computed flow pattern was *roll flow* near wall.

As seen from the above results, the simulation under the above conditions did not predict the flow pattern of the space experiment of Dr. D. Pettit. In order to shed further light on the issue, we have also considered the contribution of film thickness. We carried out simulations with different film thicknesses (0.1 mm – 0.4 mm). However, the numerical results showed that the film thickness did not affect the flow direction (all numerical result showed *roll flow*). These results indicate that the consideration of the unsteady heat transfer at the ring and three-dimensional flow structures in the film were not sufficient to predict the *outward flow* of the experiments. It seems there are other factors affecting the flow direction.

3.3. Effect of meniscus

In this section, the effect of the following three parameters of meniscus was investigated: film thickness δ , meniscus width w_m , and meniscus height h_m . In this case, the simulation

Fig. 4. *Roll flow* development in complete thin cylindrical shape at 2.5s: of (a) streaklines and (b) temperature contours, and at 5s for (c) streaklines and (d) temperature contours (with 0.5 K increments).

Fig. 5. Symmetric vortex pair in the cross-section at the upper encircled region in complete thin cylindrical shape of velocity vector at 5 s.

Fig. 6. *Outward flow* development for the case with a sharp-edged meniscus: of (a) streaklines at 2.5 s, (b) temperature contour at 2.5 s, (c) streaklines at 5 s, and (d) temperature contour at 5 s.

Fig. 7. *Inward flow* development for the case with a gently sloping meniscus: of (a) streamlines at 2.5 s, (b) temperature contour at 2.5 s, (c) streamlines at 5 s, and (d) temperature contour at 5 s.

results showed that both *outward* and *inward* flows could be obtained depending on the values of these parameters.

For the following values of the parameters: $\delta = 0.1$ mm, $w_m = 0.05$ mm, and $h_m = 0.2$ mm, the numerical result showed an *outward* flow, for which the snapshots of the computed streaklines and temperature contours at 2.5 s and 5 s are shown in Fig. 6. Isotherms were plotted with the increment of 0.5 K. As seen in these figures, a symmetric vortex pair was emerged near the wall similar to that without meniscus. The size of the symmetric vortex pair with meniscus was smaller compared with that without meniscus. In addition, the interval

of the temperature contours was smaller near the heat source. It means that the temperature gradient near the heat source towards the center became larger. On the other hand, for the following parameters: $\delta = 0.1$ mm, $w_m = 0.5$ mm, and $h_m = 0.1$ mm *inward* flow developed. The flow is shown in Fig. 7 in the same way as Fig. 6. Figure 7 shows that the heated water near heated wire flows toward the center of the liquid film.

The results for the flow direction obtained numerically are summarized in Fig. 8. In Fig. 8, cross sign means *inward* flow, triangle sign means unstable flow, and circle sign means *outward* flow. Figure 8 (a) shows that an *outward* flow developed with small w_m and Fig. 8 (b) and (c) show an *outward* flow developed with large h_m . Figure 8 (d) shows an *inward* flow in all condition. We can summarize the results as follows. The film thickness δ did not play any role in determining the flow direction. When h_m is large and w_m is small, an *outward* flow develops. Our numerical simulation results can be roughly expressed in three categories based on the ratio of h_m/w_m . An *inward* flow develops for $h_m/w_m \ll 1$, and an *outward* flow develops for $h_m/w_m \gg 1$, and both *inward* and *outward* flows develop for $h_m/w_m \approx 1$. When a small perturbation such as numerical errors was added in the case of $h_m/w_m \approx 1$, the flow direction was easily changed and became unstable, and the strength of unstable flow is very weak except for a symmetric vortex pair. Therefore, one can state that the condition of $h_m/w_m \approx 1$ represents a transitional state (saddle point). Although the criteria of flow direction switching is an important issue in thermocapillary flow physics, a precise threshold was not investigated in the present study since it was beyond our main objective, and the threshold was dependent on geometrical and physical conditions.

As mentioned earlier, the film diameter and the film thickness were reduced (compared with the experiment) because of the limitation of the numerical simulation

Fig. 8. Effect of meniscus shape on the flow direction: (a) for $h_m = 0.1$ mm, (b) for $w_m = 0.05$ mm, (c) for $w_m = 0.1$ mm, (d) for $w_m = 0.5$ mm. The symbols are $\times$: *Inward* flow, $\blacktriangle$: *Unstable* flow, and $\bullet$: *Outward* flow.

(computational cost). Here we discuss the effect of this reduction. The following conditions were investigated: $w_m = 0.1$ mm, $h_m = 0.2$ mm, and δ varying between 0.1 to 0.6 mm. When δ was less than or equal to 0.3 mm, the flow pattern did not change significantly. On the other hand, when δ was larger than 0.3 mm, the flow pattern was affected. It was noted that a rolling flow pattern was observed when δ was larger than 0.3 mm. In the flow pattern, the vortex pair expanded to the whole film area (*roll flow*). As a conclusion, the size of the symmetric vortex pair became smaller with decreasing δ . In the space experiment, the wire diameter was about 0.6 mm. When h_m is larger than 0.15 mm, the film thickness δ is smaller than 0.3 mm. Therefore, sharp meniscus ($h_m/w_m \ll 1$) could develop *outward flow* in the space experiment.

Next, the film diameter was changed from 10 mm to 50 mm to compare the result of the space experiment with the numerical results. The particle tracers' movement obtained numerically is shown in Fig. 9. In Fig. 9, captions i, ii, iii, and

Fig. 9. Time development of particle tracers movement: space experiment (dark shapes)¹²⁾ and numerical (light colored shapes).

Fig. 10. Computed temperature gradient and velocity on the drawn lines (shown above) along free surfaces: (a), (c) $y = 0$, (b), (d) $x = 0$.

iv mean time development, and i means initial and iv means final tracers' pattern. The meniscus shape in the calculation is the same as that in Fig. 6. Figure 9 shows that the tracer pattern obtained from the numerical simulation is almost the same as that observed in the experiment and the order of the computed flow velocity is the same that of the experiment. From these results, we can conclude that our numerical analysis predicts well the observation of the space experiment.

The temperature gradient distribution and the flow velocity variation along the free surface with meniscus are shown in Fig. 10. The liquid film geometry used was selected as $\delta = 0.1$ mm, $w_m = 0.05$ mm, and $h_m = 0.2$ mm, which corresponds to the cases in Fig. 6. As seen in Fig. 10, temperature gradient takes maximum or minimum values near the wall while a small value in the central region. Similar to the temperature gradient distribution, the flow velocity is larger near the wall and weaker in the center. The highlighted sections with solid

Fig. 11. Outward flow development for the case with film swelling ($h_s = 0.1$ mm, $w_s = 1.0$ mm, and $\delta = 0.3$ mm): for (a) streaklines at 2.5 s, (b) temperature contour at 2.5 s, (c) streaklines at 5 s, and (d) temperature contour at 5 s.

lines in Fig. 10 indicate the vortex region. Comparing these results, it may be concluded that the size of the vortex pair was closely related to temperature gradient, and the magnitude of temperature gradient was proportional to the magnitude of velocity. The figure also indicated that near the wall region (meniscus region) temperature gradient and velocity in the radial direction were very small. Sharp meniscus caused this temperature and velocity profiles. Sharp meniscus shape caused small temperature gradient in meniscus in the radial direction. Then, velocity in the radial direction became small.

3.4. Effect of swelling

In this section, we consider the effect of swelling on thermocapillary flow direction. When the amount of water used in a liquid film is large, the water film geometry becomes swelling. The film shape is assumed to be swelling geometry, although the actual film shape in the space experiment¹²⁾ was not measured. The numerical domain is shown in Fig. 1 (c).

The swelling shapes are defined by three parameters: h_s , w_s , and δ . In this simulation, the film shapes are determined arbitrarily, and the three parameters are following parameters: $\delta = 0.3$ mm, $h_s = 0.1$ mm, and $w_s = 0.1 \sim 2.5$ mm. The numerical result ($\delta = 0.3$ mm, $h_s = 0.1$ mm, and $w_s = 1.0$ mm) is shown in Fig. 11. The figure shows streaklines and temperature distribution at 2.5 s and 5 s. The increment of temperature contours was 0.5 K, and the seed of streaklines were given randomly. The figure indicates that the flow toward heated area, *outward flow* developed. *Outward flow* developed with a symmetric vortex pair near heated area in the same way as *outward flow* with sharp meniscus. When the numerical simulations with various swelling shapes were investigated in the range of these parameters, all numerical results showed *outward flow*.

3.5. Two-dimensional simulation in a cross-section plane

For a further examination of the generation of the symmetric vortex pair near the wall, a two-dimensional simulation was conducted for the cross-section of the film in the y - z plane. The use of a two-dimensional model was for simplicity and also for reducing the computational cost. The computational domain is the rectangular film that was taken as the cross-section of three-dimensional domain, as shown in Fig. 1 (d). The numerical grid was uniform, and the grid numbers were 400 and 20 in the y - and z - directions, respectively. It was assumed that the top and bottom surfaces are free surfaces and the sides are solid boundaries wall. Initial temperature was uniform at the value of 293 K. The temperature at the hot wall increased linearly with time. Figure 12 shows the computed streaklines, velocity vectors, and temperature contours at 1 s. Isotherms were plotted with an increment of 0.5 K. As seen, a symmetric vortex pair develops near the wall, and it was due to the temperature gradient along the free surfaces. As seen in Fig. 12 (c), the temperature gradient is steeper near the wall while it gets shallower away from the boundary. Similarly, the flow velocity is stronger near the wall and becomes weaker towards the center (Fig. 12 (b)). A return flow develops due to the difference in the flow strengths near the free surface in the region where the flow slows down. Then, a symmetric vortex pair emerges, as seen in Fig. 12 (a), due to the decreasing temperature gradient.

Figure 13 shows temperature gradient and velocity profile along the free surface with various film thicknesses (0.1, 0.2, 0.4 mm). When the film thickness was changed, temperature gradient slightly changed, while the velocity profile changed dramatically. The velocity increased and the vortex pair became large with the expansion of the film thickness. This means that thin film thickness prevents the fluid from near wall from flowing toward the cold area and symmetric vortex pair occurs. Therefore, the reason why symmetric vortex pair emerged near the heated wire is related to thin film thickness. Since symmetric vortex pair advects heat, the spreading of temperature is the same as that of vortex. These results of the two-dimensional simulation can be adopted for the three dimensional numerical results.

3.6. Discussion

3.6.1. Vortex pair generation

In the previous section, we discussed a vortex pair by two-dimensional numerical simulation. Then, the conclusion is that very thin water film caused a symmetric vortex pair near the heated wire. Next, a symmetric vortex pair of three-dimensional numerical simulation with flat free surfaces is discussed as mentioned in Section 3.2. Figure 14 shows the thicknesses of the temperature boundary layers along a free surface. In this figure, three thicknesses of the boundary layers are expressed. One is calculated with the assumption of flat free surfaces. This thickness is defined as the distance between wall and the point where temperature is $T_0 + 0.01\Delta T$, where ΔT is the temperature difference between maximum and

Fig. 12. Two-dimensional simulation at 1 s: for (a) streaklines, (b) velocity vector, and (c) temperature contour.

Fig. 13. (a) Temperature gradient and (b) velocity along film surface with various film thicknesses.

Fig. 14. Thickness of temperature boundary layer along a free surface on the upper line: calculated by numerical simulation, calculated analytically, and of 1.3 times analytically calculated thickness.

minimum value. Other is calculated analytically with approximation in the assumption that convection is neglected, and the other is 1.3 times the analytically calculated value. The analytical thickness is expressed by the following equation¹⁷⁾:

$$\delta = \sqrt{6\alpha t} \quad (7)$$

From the figure, the computed thickness is about 1.3 times the analytically calculated thickness. This result shows that the heat expansion is due to heat conduction without convection because the thickness of the temperature boundary layer is proportional to the square root of time. It is considered that the difference between 1.3 times value and the original value is due to the development of a symmetric vortex pair. These results indicate that at first the heat is transported by heat conduction, then a symmetric vortex pair develops in the area where the heat is transported. Finally, the symmetric vortex pair causes the difference of thickness of temperature boundary layer between 1.3 times the analytically calculated value and original analytically calculated value.

3.6.2. Mechanism of outward flow development

In the previous section, heat conduction is dominant in the area where a symmetric vortex pair develops. If only heat conduction is considered, the temperature gradient along a free surface is calculated by differentiating Eq. (1) with respect to position x , and substitute the following equation into Eq. (1).

$$r|\theta| = x \quad (8)$$

The calculated temperature gradient is expressed by the following equations:

$$\frac{dT}{dx} = -\frac{q}{k} \left(1 - \frac{x}{\sqrt{6\alpha t}} \right) \quad (0 \leq x \leq \sqrt{6\alpha t}) \quad (9)$$

$$\frac{dT}{dx} = 0 \quad (\sqrt{6\alpha t} < x) \quad (10)$$

From these equations, the temperature gradient has the maximum value at $x = 0$, and this means that temperature gradient reaches the maximum value at wall. Figure 15 shows the temperature gradient profiles in cross sections in each case. Figure 15 (a) and (b) express the temperature gradient in the case of *outward flow* with sharp meniscus, (c) and (d) express

Fig. 15. Temperature gradient of cross section near heated wall at 2 s, and 4 s; the flow patterns were (a), (b) *Outward flow*, (c), (d) *Unstable flow*, and (e), (f) *Inward flow*.

the case of unstable flow, and (e) and (f) express the case of *inward flow*. From the figure, in the case of *inward flow*, the maximum temperature gradient exists in the meniscus; on the other hand, the maximum temperature gradient exists out of meniscus in the case of *outward flow*. The position of the maximum temperature gradient determined the flow direction. From above discussion, the maximum temperature gradient should exist at the vicinity of the heated wall. However, the areas of the maximum temperature gradient vary in each shape. The area where the maximum temperature gradient gradually moves to the outside of meniscus as meniscus shape becomes sharper. In the case of a similar flat free surface, the maximum temperature gradient exists near the heated wall in Fig. 15 (e) and (f). These results indicate that a narrow meniscus caused the temperature in the meniscus to be uniformed, then the temperature gradient in the meniscus becomes smaller. Thermocapillary flow becomes stronger along the free surface where the value of temperature gradient is large. The conclusion is that if the position of the maximum temperature gradient exists in the meniscus, thermocapillary force along the upper and lower free surfaces acts in the same direction, then this causes an *inward flow*. On the other hand, the mechanism of an *outward flow* development is explained as follows: (1) Temperature gradient in the radial direction was very small in the meniscus because the meniscus width was very small, (2) The thermocapillary flow in the radial direction became very weak in the meniscus, (3) A symmetric vortex pair emerged near meniscus because film thickness is very small, (4) The thermocapillary flow in the circumferential direction developed according to the circumferential temperature gradient, (5) Vortex pair flows in the circumferential direction with circulating, (6) An *outward flow* developed. Once the *outward flow* developed, the flow pattern remained unchanged under the condition of $h_m/w_m \gg 1$. The reason for this is that the *outward flow* causes a steep temperature gradient towards the film center near the wall. As the size of the vortex depends on temperature gradient as discussed before, the growth of vortex is suppressed and the circumferential temperature gradient caused an *outward flow*. In the case of swelling film, temperature gradient near the heated area becomes steep and thermocapillary force along the free surface acts in the oppose direction. This is contrary to the water film with meniscus. Therefore, the flow toward the center of the water film does not develop. The other mechanisms developing *outward flow* in the swelling water film is the same as the mechanisms in the water film with meniscus (mechanisms (2) – (6)).

4. Conclusion

A numerical simulation study has been carried out to explain the flow direction of thermocapillary flow in a thin circular water film with meniscus and swelling. The consideration of unsteady heat transfer alone in the solid wire and three-dimensional flow structures did not explain the development of an *outward flow*. However, in this simulation study the consideration of the effects of meniscus and swelling well predicted the development of an *outward flow*, and the

experimental flow directions. Sharp meniscus and film swelling cause *outward flow*, corresponding to the direction of space experiment. In the case of *outward flow*, the symmetric vortex pair occurs near the heated wire due to thin film thickness, and the symmetric vortex pair flows in the circumferential direction with circulating. In this way, *outward flow* emerges. The changing of flow direction is determined by the position of temperature gradient.

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