Analysis of Wetting and Coalescing Behavior of Minute Ink Droplets by MPS Simulation

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(Received Feb. 9, 2016)

To obtain the desired images from inkjet printers, it is important to control the coalescing and wetting behaviors of the ink droplets. However, predicting these behaviors quantitatively through an experimental approach is difficult because of the speed and the minuteness of such phenomenon. Therefore, the establishment of a simulation technology to predict these behaviors is in demand. In this study, an MPS simulation method was developed based on a particle method that considered the effect of surface tension acting on the liquid–liquid and liquid–solid interfaces. Quantitative prediction of the coalescing and wetting behaviors was made possible using this technology.

Keywords: Simulation, Wetting characteristics, Inkjet printing, Fluid dynamics,

1. Introduction

Because of its advantage of being able to avoid damage to media due to contact and heat, inkjet printing technology is used for a wide variety of applications, such as printed electronic circuits, digital fabrication, etc. In inkjet printing systems, the minimum unit of an image structure is an ink droplet that is spread on a surface of the media, forming images by continuously coalescing ink droplets in a linear fashion. To avoid the occurrence of image defects such as unevenness and discontinuity, it is important to control the wetting and coalescing behaviors of the ink droplets. Surface tension is considered to be one of the key factors affecting these behaviors. However, quantifying the effect of the surface tension accurately using an experimental approach is difficult because of the minuteness and the speed of the phenomenon. Variations of wetting and coalescing characteristics, in combinations with the ink and media, are also considered to be a contributing factor to the difficulty. Virtual experiments by computer simulation that take into consideration various parameters of ink and media are effective for evaluating the phenomenon. However, a simulation method with practical accuracy for calculating highly non-linear phenomenon such as wetting and coalescence has not yet been developed. Therefore, the establishment of a simulation model that is able to predict the wetting and coalescing behaviors of minute droplets quantitatively is in demand.

To develop a simulation model that is sufficient for practical use, it is necessary to calculate the deformation of free surface ink droplets accurately. In this study, the authors focused on a particle–based MPS (Moving Particle Semi–implicit) method that has the advantage of simulating the fluid dynamics involving the free surface deformation. To consider the effects of interacting force caused by surface tension acting along the surface, a new improved potential model was developed. Additionally, a simulation model based on lubrication theory was also developed to calculate the semi-static deformation of droplets with low computational load.

2. Simulation model

2.1 MPS method

Recently, particle–based simulation is focused on one method for calculating fluid dynamics. Particle–based simulations enable avoidance of the necessity to solve advective terms in Navier–Stokes equation since calculation points are handled by the Lagrangian approach. Therefore, the blurring of fluid surfaces caused by numerical diffusion that are generally considered to be a problem of the Eulerian method, such as FEM (Finite Elemental Method), do not occur. Additionally, special algorithms are not required for calculating the non-linear deformation of the shape of the free surface when coalescing or separation of droplets occurs. For these reasons, the authors considered that particle–based simulation is suited for analysis in this study.
The MPS method proposed by Koshizuka is a particle-based simulation method. In the MPS calculation, stability and accuracy of calculations are guaranteed using implicit algorithm to solve the pressure gradient term in the Navier-Stokes equation. Calculating flow in the MPS method is shown in Fig. 1. Differential operators such as gradient and Laplacian are discretized by an interaction model using a weight function \( w \) and a number density \( n \). \( w \) and \( n \) are calculated by equations (1) and (2) respectively.

\[
w(r) = \begin{cases} \frac{r}{r_{i}} - 1 & (0 \leq r < r_{i}) \\ 0 & (r_{i} \leq r) \end{cases}
\]

\[n_{i} = \sum_{j=1}^{N}(w(|\mathbf{x}_{i} - \mathbf{x}_{j}|))
\]

In these equations, \( r \) is the distance between two particles, \( r_{i} \) is the effective range, and \( \mathbf{x} \) is the positional vector of particles. The gradient and Laplacian of arbitrary physical quantity \( q \) are formulated as below.

\[
\langle \nabla q \rangle = \frac{D}{n_{i}} \sum_{j=1}^{N} \left( \frac{q_{j} - q_{i}}{|\mathbf{x}_{j} - \mathbf{x}_{i}|} \right) w(|\mathbf{x}_{j} - \mathbf{x}_{i}|)
\]

\[
\langle \nabla^{2} q \rangle = \frac{2D}{n_{i}} \sum_{j=1}^{N} (q_{j} - q_{i}) w(|\mathbf{x}_{j} - \mathbf{x}_{i}|)
\]

Here, \( D \) is the dimension number, and \( \lambda \) is the corrective coefficient calculated by function (5).

\[
\lambda = \frac{\sum_{j=1}^{N} (w(|\mathbf{x}_{j} - \mathbf{x}_{i}|))}{\sum_{j=1}^{N} w(|\mathbf{x}_{j} - \mathbf{x}_{i}|)}
\]

Wetting and coalescing deformations occur as results of surface tension acting along the liquid and solid interfaces. In this study, to solve these behaviors accurately, the surface tension \( \sigma(r) \) is calculated for the product of potential coefficient \( K \) and a potential function \( \phi(r) \) as shown in equation (6).

\[
\sigma(r) = K\phi(r)
\]

\( K \) is determined from the characteristics of the ink and media. To express the principle of surface tension to minimize the surface area, the interaction force acting between neighboring particles must be an attracting force. However, as particles become excessively close and overlapped, numerical instability is induced. Therefore, the potential function is defined on the basis that the direction of the interaction force continuously changes depending on the distance between two particles so that the force becomes repulsive when they are excessively close as shown in Fig. 2.

To calculate wetting behavior, the interface tension between droplets and the media must be considered. The balance of surface tension at the three-phase interface shown in Fig. 3 is formulated by equation (7). Here, variables with subscripts \( f \) and \( s \) represent those related to the liquid surface, non-wetted solid surface and wetted solid surface respectively, and \( \theta \) is the contact angle.

\[
\sigma_{r-f} \cos \theta = \sigma_{r-s} - \sigma_{r-s}
\]

In present potential model, equation (7) is converted into equation (8).

\[
K_{r-f} \cos \theta = K_{r-s} \phi - K_{r-s} \phi
\]

The potential coefficient \( K_{r-f} \) is determined from surface tension of a fluid. Even though it is necessary to measure surface tensions of wetted and non-wetted medium surfaces to quantify \( K_{r-s} \) and \( K_{r-s} \), it is difficult to measure them for all combination of ink and media. In this study, the differences in potential coefficients between the wetted and non-wetted solid
surface $\Delta K_i$ was defined as shown in equation (9).

$$K_{f_{i-1}} - K_{f_{i-2}} = \Delta K_i$$  \hspace{1cm} (9)

Given that the static contact angle $\theta$, $\Delta K_i$ is easily determined using the equation (10).

$$K_{f_{i-1}} \cos \theta = \Delta K_i \phi$$  \hspace{1cm} (10)

The interaction force between fluid particles and non-wetted solid particles is calculated using $\Delta K_i$ and there is no need to calculate that between fluid and wetted solid particles. The condition of solid particles either wetted or non-wetted is judged by setting a threshold of the number density $n$ formulated as equation (2).\(^1\)\(^2\)

**2.2 Semi-static coalescing model**

In a general ink jet printing system, ink droplets are continuously jetted from the printing head, which scans in a linearly manner, so the image is formed by a number of line images. Therefore, to predict the occurrence of image defects in a line image, such as discontinuity and unevenness, is very important. However, to calculate the printing process of a line image is time consuming and it is necessary to consider a number of droplets, and vast amounts of hours. To solve this problem, the authors developed a semi-static coalescing model based on the lubrication theory for calculating prolonged deformation of coalesced droplets with low computational load.

In this model, a line image is discretized in the scan direction, and the volume transfer between neighboring slice elements with an arbitrary thickness $\Delta t$ is considered by one-dimensional analysis. This model is not able to handle the inertial effect produced by the jetting speed of a droplet. Therefore, the wetting behavior immediately after landing on the media is calculated by the MPS method and the results are used to determine the initial shape of line image in the semi-static model.

A schematic view of the model is shown in Fig. 4.

Premising that the arc-like shape of the element is circular, curvature radius $R$, curvature $\kappa$, sectional area $A$, volume $V$, height $h$ and width $W$ shown in Fig. 5 have relationships shown in equations (11)–(15).

$$R = \frac{W^2 + 4h^2}{8h}$$  \hspace{1cm} (11)

$$\kappa = \frac{1}{R}$$  \hspace{1cm} (12)

$$\theta = \sigma \sin \frac{W}{2R}$$  \hspace{1cm} (13)

$$A = R^2 \theta - \frac{W(R-h)}{2}$$  \hspace{1cm} (14)

$$V = A \Delta z$$  \hspace{1cm} (15)

The internal pressure at each element is calculated as the product of curvature $\kappa$ and surface tension $\sigma$ as shown in equation (16).

$$p = 2\kappa$$  \hspace{1cm} (16)

The volume transfer resulting from the internal flow caused by the pressure gradient from element $i$ to element $i-1$ is calculated by equation (17).

$$\Delta V_{i-1,i} = C(p_{i-1} - p_i) \frac{A_{i-1} + A_i}{2} \Delta t$$  \hspace{1cm} (17)

Here, $C$ is defined as a coefficient of flow, which depends on the characteristics of the ink such as viscosity, $p$ is internal pressure, and $\Delta t$ is a discretized time. The volume of element $i$ after the volume transfer is calculated by equation (18).

$$V' = V + \Delta V_{i-1,i} + \Delta V_{i+1,i}$$  \hspace{1cm} (18)

From $V'$, the geometric factors of the element are calculated by equation (11) to (15) to estimate the new pressure. Subsequently, whether the element width is changed or not after the volume transfer is judged considering wetting characteristics such as forward and backward contact angle using relationships shown in equation (19). In equation (19), $\theta_f$ and $\theta_t$ are forward and backward contact angles respectively.

$$\begin{array}{ll}
\theta_f < \theta_t & \text{changed} \\
\theta_f < \theta < \theta_t & \text{not changed} \\
\theta < \theta_t & \text{changed}
\end{array}$$  \hspace{1cm} (19)

By continuing this calculation flow while maintaining the contact angle until a static state is obtained, the shape of the line image is calculated.\(^3\)

3. Validation

3.1 Experiment for validation

To validate the accuracy of the present simulation model, wetting and coalescing behaviors were measured experimentally and compared with calculated results. Time variation in the shapes of wetting droplets that landed on a medium surface was observed using the apparatus shown in Fig. 6. Using a high speed camera, the apparatus is capable of capturing images of deforming minute droplets at an interval of $1 \mu s$.

The velocity of the internal flow of coalescing droplets was measured in the experimental apparatus shown in Fig. 7 using...
the PIV (Particle Image Velocimetry) method. In the PIV method, fluid velocity is quantified by tracing displacement of particle assemblages which are dispersed in the fluid.

3.2 Validation results of wetting behavior

To validate the calculation accuracy of the wetting behavior, time variations of shape of spreading single droplet with various parameters were compared. The experimental result was quantified using the device shown in Fig. 6. The comparison was conducted for 200 μsec after the landing of a droplet on the medium surface. Validation conditions are shown in Table 1. In this validation, the contact angles were varied to compare wetting behavior under hydrophilic and hydrophobic conditions by changing combination of media and ink.

Validation results of the hydrophilic and hydrophobic conditions are shown in Fig. 8(a) and Fig. 8(b) respectively. From these results, it is clarified that droplets spread gradually in a hydrophilic condition, and the shapes of droplets are substantially constant in a hydrophobic condition. Furthermore, it is confirmed that measurements and simulation results quantitatively agree. An average of relative errors between the measurements and simulations was 7.2%. It is considered that the calculation of wetting behavior of a single droplet was possible with sufficiently high accuracy by the present simulation model.

3.3 Validation results of coalescing behavior

To validate the coalescing behavior, internal flow velocity distributions in two coalesced droplets were compared. The internal flow velocity was quantified by the PIV method using the device shown in Fig. 7. It is well known that the smaller droplet is absorbed into the larger droplet by pressure differences when coalescing occurs. To confirm that the
Table 2  Verification conditions of coalescing behavior.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter (µm)</td>
<td>400.0, 240.0</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>1.0×10³</td>
</tr>
<tr>
<td>Viscosity (Pa · s)</td>
<td>8.93×10⁻³</td>
</tr>
<tr>
<td>Surface tension (mN/mm)</td>
<td>72.2</td>
</tr>
</tbody>
</table>

![Graph showing velocity distribution](image)

**Fig. 9** Comparison result of coalescing behavior.

The measured and calculated contours of internal flow velocity distribution of coalescing direction observed in a plane parallel to the stage are shown in **Fig. 9**. In these results, the dark color indicates the flow heading forward in the left direction, and the dotted lines represent the surface of each droplet. It is confirmed that the typical flow heading from the smaller droplet to the larger droplet are generated in both the measurement and the simulation.

**Fig. 10** is a comparison result of the coalescing directional velocity on a line passing through the center of two droplets. In **Fig. 10**, x denotes the scan direction and the position of x=0 denotes the contact interface of two droplets, and the smaller droplet landed on the right side of the graph. The maximum velocity of the internal flow in the smaller droplet toward the larger one is approximately 6 mm/s in both results. The relative error in the distributions of the internal flow was less than 10% of the measured velocity. It was clarified that the present simulation method is capable of calculating the coalescing process with high accuracy.

4. Application

As shown in the preceding chapter, the authors concluded that the present simulation method has sufficiently high accuracy to calculate wetting and coalescing behavior, and considered that it has a capability of predicting image defect. In this chapter, the prediction results of typical defects of a line image in inkjet printing system are presented.

4.1 Prediction results of discontinuity of a line image

Calculated results of the shape of coalesced droplets by MPS method were compared with experimental results. In this comparison, five droplets were periodically jetted at a time interval and jet pitch shown in **Table 3**.

**Fig. 11** shows calculated and measured results of time variations of coalesced shapes of droplets looking from straight above them. In **Fig. 11**, the coalesced shapes of droplets are shown at time intervals of 1ms, and the results shown on the left side are simulation results and those of right side are experimental results. In the simulation results each droplet is
### Table 3  Simulation conditions for predicting line image.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of droplets (µm)</td>
<td>25.0</td>
</tr>
<tr>
<td>Number of droplets</td>
<td>5</td>
</tr>
<tr>
<td>Viscosity (Pa · s)</td>
<td>10.1 × 10⁻³</td>
</tr>
<tr>
<td>Surface tension (mN/mm)</td>
<td>34.4</td>
</tr>
<tr>
<td>Jet pitch (µm)</td>
<td>30.0</td>
</tr>
<tr>
<td>Jet frequency (kHz)</td>
<td>1.0</td>
</tr>
</tbody>
</table>

### Table 4  Calculation condition of predicting line image.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of droplets (µm)</td>
<td>25.0</td>
</tr>
<tr>
<td>Number of droplets</td>
<td>5</td>
</tr>
<tr>
<td>Viscosity (Pa · s)</td>
<td>10.1 × 10⁻³</td>
</tr>
<tr>
<td>Surface tension (mN/mm)</td>
<td>34.4</td>
</tr>
<tr>
<td>Contact angle (degree)</td>
<td>20.0</td>
</tr>
<tr>
<td>Jet pitch (µm)</td>
<td>(a) 20.0, (b) 30.0, (c) 50.0</td>
</tr>
<tr>
<td>Jet frequency (kHz)</td>
<td>10.0</td>
</tr>
</tbody>
</table>

Fig. 12  Predicting results of width unevenness of line image.

The simulation was conducted using the result of the MPS simulation as an initial shape of the line image until it had reached a steady-state. The comparison conditions and results are shown in Table 4 and Fig. 12 respectively.

In Fig. 12, the shape of line images formed by coalesced droplets was observed from above. The results of left side are simulation results, and those of right side are experimental results. Fig. 12(a), (b) and (c) are the results using a jet pitch of 20, 30, 50 µm respectively. From Fig. 12(a), it can be seen that the width of the line image is almost uniform, and in this case it is clear that the jet pitch is adjusted appropriately. However, as shown in Fig. 12(b), the jet pitch is narrower than the appropriate pitch, and it turns out that a specific position of the line swells. This deformation is caused by internal flow toward the swollen part due to the pressure gradient. Expansion occurs continuously as long as movable fluid exists. In Fig. 12(c), when the jet pitch is larger than the appropriate value, a cyclic wavy line is formed. It is considered that the lines become wavy when sufficient flow of ink is not generated toward the narrow area at the interface of two neighboring droplets because of the effect of the wetting characteristics such as a forward or a backward contact angle. From these results, the relationship between jet pitch and shape of line image obtained by simulation has good correspondence with that of experiment. Therefore, it has been concluded that the shape of a line image can be predicted using the present model.
5. Conclusion

To predict behaviors of minute ink droplets such as wetting and coalescing, the MPS simulation method with a novel potential model of the surface interaction force was developed. By the novel potential model, it becomes possible to consider a difference of interface tension between wetted and non-wetted solid surface. From the validation of the calculation accuracy of present simulation method with measurement result and the calculation to predict image defects of a line image, the following results were obtained.

1) The wetting behavior of a single droplet was calculated with high accuracy under both hydrophilic and hydrophobic conditions.

2) The calculated internal flow velocity in two coalescing droplets was in accord with the measurement results.

3) The prediction of the occurrence of image defects of a line image depending on the jet pitch became possible by using the MPS method and the semi-static deformation model.

From these results, it is concluded that the developed MPS simulation technology is useful in designing parameters of inkjet processes and ink characteristics to avoid image defects.

References


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