Drop coalescence on non-absorbent coated substrates

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Abstract

Drop coalescence and ink reflow significantly affect the image quality in inkjet printing, especially on coated and non-absorbent substrates. In this study, the coalescence of inkjet-printed drops on a non-absorbent substrate was numerically simulated and compared with machine tests. Using a commercial software Flow-3D, the coalescing drop pairs are simulated by solving the mass and momentum conservation equations with Volume-of-Fluid method tracking the liquid-air interface. The effects of drop spacing and time interval on the geometry of coalescing drops are numerically investigated. Results show that when the second drop lands next to a pre-deposited drop, liquid in the second drop migrates towards the first drop driven by its internal capillary pressure and inertia. As a result, a geometrical shift towards the first drop and reduced drop spreading length are observed in the merged drop. The geometric shifts of coalesced droplets were qualitatively proved in a machine test using statistical image analysis. Both the reduced drop spreading length and the geometric shift contribute to the trailing edge displacement, defined as the wetting edge shift of the second drop away from its ideal location. It is also indicated in the simulation that drop spacing and time interval influence the geometric shift, drop spreading length, and thus trailing edge displacement. This trailing edge displacement plays an important role in determining the continuity of the printed lines, e.g. non-coalescence of printed drops due to large trailing edge displacement will lead to broken patterns or functional failures of printed electronics. This study provides valuable information in designing jetting sequence in the printhead, and optimizing printing processes for uniform line and solid formation.

Introduction

One of the challenges in inkjet printing on coated media [1] is aqueous ink droplets do not penetrate into the coated paper and ink reflow occurs when two drops coalesce resulting in broken lines and streakiness in the final prints. The high boiling point co-solvents in aqueous inks are difficult to dry which limit the printing speed and exacerbate the coalescence and reflow. Inkjet printing on packaging film materials and 3D printing could potentially face the similar challenge, i.e., the substrates are non-absorbent and ink reflow occurs due to coalescence which can affect the uniformity of the printed lines and solids; in 3D printing, the coalescence and intermixing of support and build materials can lead to rough surface on the final printed objects and intermixing of different build materials can potentially lose the printing precision.

Experimental studies on drop coalescence mainly focused on millimeter-sized water drops [2-3] and coalescence of two equilibrium drops driven by viscous forces [4]. Very few machine tests on coalescence of inkjet-printed picoliter drops have been examined [5]. Numerically, Lee and Son [6] investigated the effect of substrate wettability on drop coalescence with level-set method. However, the effect of jetting parameters, such as drop spacing and jetting time interval, on drop coalescence still remains unknown.

In this paper, our model describing the impact and coalescence of inkjet-printed drops on a non-absorbent substrate was validated by published experimental results. The effects of drop spacing and time interval on geometric shift and trailing edge displacement were studied. Finally the simulation results were compared with machine tests.

Numerical Modeling

Model Description

The liquid-air interface is treated as a free surface in Flow-3D, and Volume-of-Fluid (VOF) Method is used as the numerical approach. The fractional volume, *F*, equals to 1.0 within the liquid phase, and 0.0 in air phase, as shown in Fig. 1. *F* changes from 0.0 to 1.0 at the liquid-air interface [7]. This interface is obtained by calculating the transport equation of the local volume fraction of the liquid phase.

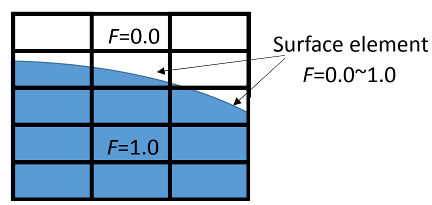

Fig. 1 Schematic of Volume-of-Fluid method

The continuum and Navier-Stokes equations (mass and momentum conservation) along with the transport equation of *F* [7] are solved in Flow-3D.

$$\nabla \cdot \boldsymbol{U} = 0 \quad (1)$$

$$\rho\left(\frac{\partial \boldsymbol{U}}{\partial t} + (\boldsymbol{U} \cdot \nabla)\boldsymbol{U}\right) = -\nabla P + \mu \nabla^2 \boldsymbol{U} + \rho g - \sigma(\nabla \cdot \boldsymbol{n})\boldsymbol{n}\delta_s \quad (2)$$

$$\frac{\partial F}{\partial t} + \boldsymbol{U} \cdot \nabla F = 0 \quad (3)$$

Where $\boldsymbol{U}$ is velocity vector, ρ is fluid density, P is pressure, μ is dynamic viscosity, σ is liquid surface tension, $\boldsymbol{n}$ is unit vector normal to the interface, and δ_s is surface Dirac Delta function. The last term in Eq. 2 represents the interfacial capillary force.

The model is constructed in 3D configuration assuming half symmetry of the droplets. The ink properties are chosen based on a typical aqueous ink for inkjet printing: drop volume (V) 7 pL, dynamic viscosity (μ) 8 cP, surface tension (σ) 27 mN/m, density (ρ) 1050 kg/m^3, and drop impact speed (v) 5 m/s. The ink drops impact and coalesce on a smooth non-porous surface with a static contact angle of 10°. Drop evaporation is neglected since its characteristic time is 4-5 orders of magnitude longer than that of drop impact and 2-3 orders of magnitude longer than wetting [8].

Model Validation

Impact inertia and capillary flow are the driving forces for the coalescence of inkjet-printed drops. Here, to validate the drop impact model, the single drop dynamics including drop impact, spreading and wetting on a non-porous solid substrate are simulated and compared with experimental results by Son *et al.* [9], as in Fig. 2. An adjusted substrate contact angle has been used to accommodate the dynamic contact angle. Upon impact, the water drop of 46 µm diameter and 1 m/s impact velocity, quickly spreads driven by inertia followed by slow capillary wetting. The computed droplet spreading and height in the center of the droplet agree reasonably well with the experimental results [9].

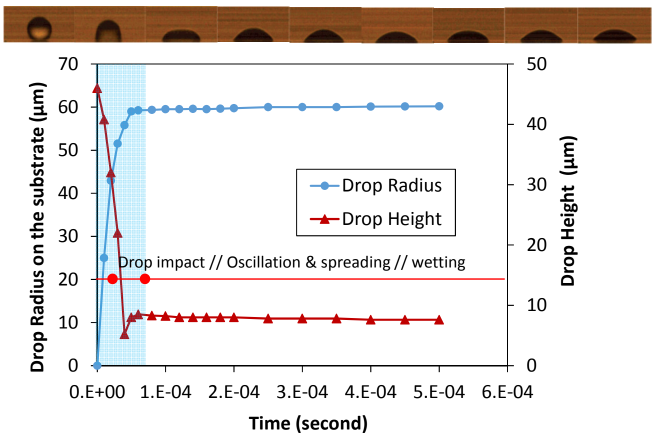

Fig. 2 Single drop dynamics validation. The inserted inkjet drop images [9] are from drop impact till ~66 µs with 8.25 µs interval (i.e. shaded area).

Drop coalescence model is validated with the experimental data [4] of two 240 µm droplets of diethylene glycol (DEG) with an equilibrium static contact angle of 56° and a distance of 225 µm. As these two drops start to coalesce near their equilibrium wetting states, the entire coalescence process corresponds to the viscosity-dominated creeping flow regime without drop dynamics effect. The coalescing drop bridge r_m and drop height R_y from our simulation and referencing experimental results [4] are plotted against time in Fig. 3. Similar scaling laws from simulation and experiments demonstrate this model captured the critical physics in the two drop coalescence process.

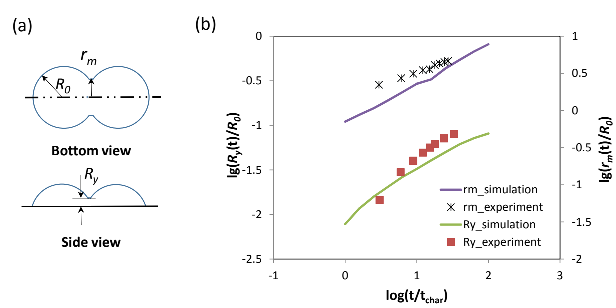

Fig. 3 (a) Schematic of two drop coalescence under viscosity-dominated creeping flow; (b) comparison of drop bridge r_m and drop height R_y by modeling (this work) and experiment [4].

Results and Discussion

Two Drop Coalesce

The first ink drop impacts on the substrate with the conditions specified in the Model Description. Similar to the process in Fig. 2, the initial fast spreading resulted from inertia followed by slow capillary wetting. The Weber number $\frac{\rho v^2 D_0}{\sigma}$ is 23.08; Reynolds number $\frac{\rho v D_0}{\mu}$ is 1.56; and the Ohnesorge number $\frac{\mu}{\sqrt{\rho \sigma D_0}}$ is 3.08, which compare the kinetic energy to the surface energy at impact, inertial to viscous forces, and viscous forces to inertial and surface tension forces, respectively. According to the parameter space in We-Oh plane [10], the drop impact and coalesce in this study are driven by both impact and capillary wetting, with more contribution from drop impact. The equilibrium diameter of this single drop on the substrate is about 74 µm.

The second drop is deposited to the right of the first drop with a specified spacing and time interval. Fig. 4 shows the velocity and pressure contours of coalescing drops with 42 µm spacing and 200 µs time interval from front and top views. The strong inertia and higher pressure in the second drop due to its larger liquid-air interface curvature drive the ink flowing into the first drop. As a result, the coalesced drop spreads non-symmetrically at the left and right edge in Fig. 5, contributing to the geometric shift, i.e., the shift of the center of merged drop from the center of the two individual drops.

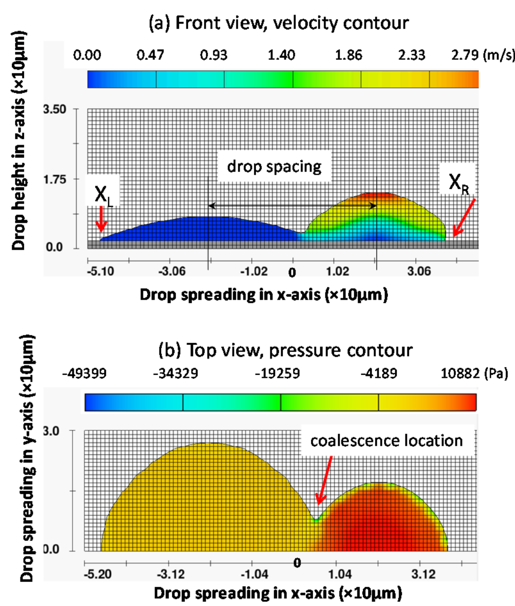

Fig. 4 Drop coalescence (a) front view with velocity contour, (b) top view with pressure contour.

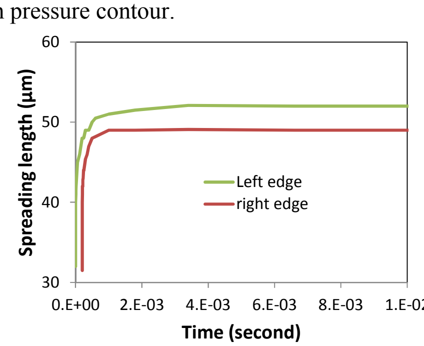

Fig. 5 Displacement of left and right edges of the coalesced drop

Due to coalescence, the spreading length of the merged drop (L) can be smaller than the ideal spread length, the sum of the spreading length of a single drop and drop spacing (D+Ls). This reduced spreading length, (D+Ls)-L, is known as "drawback" [5]. In printing, continuity of a printed line is determined by the shift of the merged drop edge. Line breaks up if the following drop cannot reach the edge of the merged previous drops. In this work, a new parameter, trailing edge displacement is defined as the wetting edge shift of the second drop from its ideal wetting location, which is half of the drawback plus the geometric shift. In the coalesced drop in Fig. 4, a drawback of 14.4 µm and geometric shift of 1.3 µm as shown in Fig. 5 contribute to the right edge shift of the second drop 8.5 µm towards the first drop, which can significantly affect the coalescence with the third and following drops.

Effect of Drop Spacing and Time Interval on Trailing edge displacement

The effect of drop spacing and time interval on the geometric shift and trailing edge displacement were systematically studied, by varying drop spacing of 21, 32, 42 and 52 µm and time interval of 33, 200, 1000, and 10000 µs. The merged drop dynamics are simulated until 0.005 seconds after coalescence, where the spreading reach equilibrium as indicated in Fig. 5.

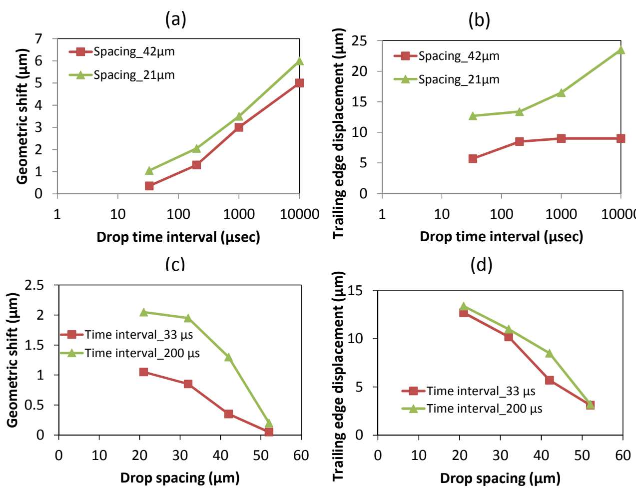

Fig. 6 Geometric shift and trailing edge displacement with various spacing and time intervals.

Fig. 6 compare the geometric shift and trailing edge displacement of the two drop coalescence with various spacing and time intervals. All the trailing edge displacements use spacing of 42 µm as the ideal edge location of the second drop. As shown in Fig. 6a and 6b, longer time intervals enhance the geometric shift as well as the trailing edge displacement. As the time interval increases, the first drop spreads more before the second drop impact. After two drops contact, inertia and larger capillary pressure gradient between the two drops, resulted from smaller contact angle on the first drop side, pushes more liquid flowing from the second drop to the first drop. Thus, the spreading of the second drop is limited. Both more spreading of the first drop and less spreading of the second drop drive the merged drop center shifting more towards the first drop. At the same time, this increasing geometric shift promotes the increasing of the trailing edge displacement. If the two drops are printed on the substrate simultaneously, the symmetric spreading and coalescence will eliminate the geometric shift, but the drawback will remain.

With the same time interval, increasing drop spacing (Fig. 6c and 6d) prolongs the time for the second drop to spread before coalescence. Therefore, carrying less inertia and smaller capillary pressure gradient, the second drop flows into the first drop less, leading to a smaller geometric shift for the merged drop. On the other hand, the increasing drop spacing enlarges the spreading length of the merged drop. Hence, these decreasing geometric shift and increasing spreading length enable significant decrease in trailing edge displacement. This could prevent breakup of the printed lines, however, too large spacing will separate individual drops from coalescence.

The trailing edge displacement could be overestimated in the simulation, because it neglects ink solvent evaporation and penetration into substrates, which reduces drop spreading.

Comparison with Machine Tests

A test pattern in Fig. 7 was designed to study the geometric shift with an Image On Web Array (IOWA) sensor [11]. A set of single dashes in the process direction (Fid-1) were printed to determine the cross-process jet position of individual nozzles; a set of paired dashes (Fid-2) consisting of two adjacent jets are employed to examine the coalescence of two dashes. A solid strip is inserted between these two dash patterns for image quality measurement (e.g. streakiness) as well as exercising the nozzles to avoid clogging and mis-directionality.

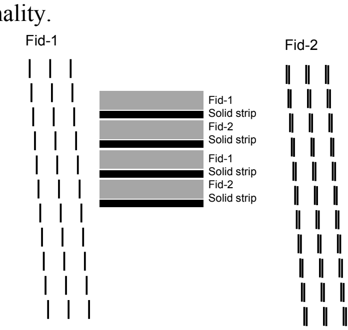

Fig. 7 Test pattern for coalescence study

Black and Cyan aqueous inks were printed by a Kyocera printhead KJ4B with 2656 nozzles arranged in four trapezoids. Printing resolution is 600 dpi by 600 dpi in x and y directions, with a processing speed of 1.26 m/s. A coated offset printing paper with a surface porosity of less than 3% from a scanning electron microscope (SEM) measurement was selected as non-absorbent substrate (or less absorbent substrate). The printed test pattern was captured by an integrated IOWA sensor and processed to determine the center of both the single and double pixel dashes with an accuracy of a few microns [12, 13]. The locations of each jet are captured from Fid-1, i.e., x_1 and x_2 in Fig. 8; and the centers of the dash pairs are captured from Fid-2, as denoted as x_{12}. The dash spacing, x_{nn} is defined as x_1-x_2. Due to random variations in the drop ejection angle, a large range of x_{nn} is sampled across the printhead. In the absence of coalescence the double dash will have an apparent center that is the average of the individual jets. With coalescence, the later deposited drops can move toward the earlier deposited drops and the apparent center of the merged dashes will produce a shift, i.e., geometric shift, $\Delta x = \frac{x_1+x_2}{2} - x_{12}$.

Dash pairs are laid down sequentially because they are jetted from different rows on the head. The jetting time intervals between these two dashes are obtained from the printhead nozzle layout and jetting sequence. Positive time interval represents the left dash laid down before the right one, and vice versa.

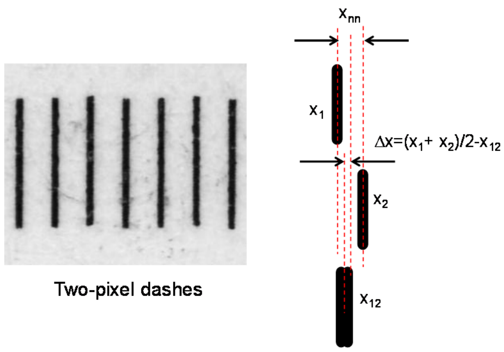

Fig. 8 (a) Two-pixel wide dashes captured with IOWA; (b) schematic of analyzing coalescence algorithm.

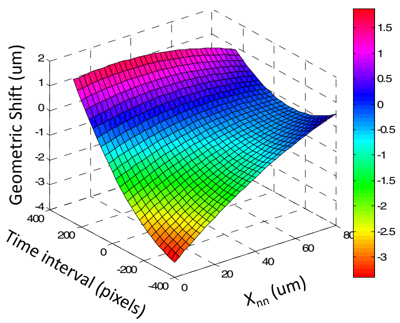

Fig. 9 Surface plot of drop geometric shift as a function of x_{nn} and time intervals.

A surface plot of the geometric shift is shown as a function of the dash spacing and time intervals (in pixels) in Fig. 9. Each time interval pixel corresponds to 33 µs when printing at 600 dpi, and the machine test covers the range from -13200 to 13200 µs. One observes that when two dashes are laid down closely with a small x_{nn}, coalescence occurs. Statistically, the center of the coalesced dash pair always shift towards the first deposited dash, as evidenced by positive geometric shift along with positive time intervals and vice versa. Smaller drop spacing and longer time intervals lead to larger geometric shifts, which agrees well with the simulation results in Fig. 6. The geometric shifts from the machine test and simulation are both in the range of a few microns, which shows first-order agreement to the simulation results. It is worth noting that this numerical model is simplified based on many assumptions, and a complete agreement of the experimental with numerical data is not expected. When two dashes are roughly simultaneously deposited (i.e., time interval closes to zero), there is no favoring of the direction of coalescence which results in minimum geometric shift for all the x_{nn}.

At a large x_{nn}, no coalescence occurs as confirmed by the relative flat surface plateau (i.e., minimum geometric shift) when $x_{nn} > 60$ µm in Fig. 9. It is worth pointing out that x_{nn} has a normal distribution centered about 42 um. The fraction of dash pairs with x_{nn} less than 20 um and larger than 60 um represent only ~ 8% among the total dash pairs. That probably explains some deviation when the drop spacing are extremely small or large, due to sparse data and measurement noise. However, it still provides a solid proof of our numerical findings on the geometric shift during drop coalescence.

Conclusion

Drop coalescence on a non-absorbent substrate has been studied numerically and compared with machine tests. Results show that when the second drop lands next to a pre-deposited drop, liquid in the second drop migrates towards the first drop due to its internal capillary pressure and inertia. This geometric shift of the merged drop was validated in the machine tests. The trailing edge displacement, which represents the wetting edge shift of the second drop away from its ideal location, occurs as a result of geometric shift and reduced spreading length. Longer time intervals and shorter drop spacing result in larger geometric shift and trailing edge displacement. The modeling work can potentially provide guidance in printhead design and developing printing process for printed electronics and 3D printing where uniform, continuous lines and solid films are highly desirable.

Acknowledgement

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Jun Ma is a research scientist at Xerox. Jun is focused on simulation-based design of electromechanical systems. She joined Xerox in 1996 and is more involved in Inkjet Print Head development in the past 5 years. Jun received her master's degree from Rensselaer Polytechnic Institute in 1995.

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Hong Zhao received her Ph.D. in the Mechanical and Aerospace Engineering from Rutgers University in 2007. She joined Virginia Commonwealth University as an assistant professor in 2014. Before that, she was a research scientist and project lead at Xerox Corporation. Zhao has authored and co-authored 28 peer-reviewed journal publications and conference papers, 31 issued patents and patent applications. Her research interests include superhydrophobic and superoleophobic surface design, inkjet drop dynamics, self-assembly of colloidal particles, inkjet printing and electrohydrodynamic printing for functional devices and additive manufacturing.