The absorption and spreading of aqueous finishing fluids onto textile fiber surfaces

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Abstract

The mechanism of ink absorption at the fiber surface, and also the penetration of ink into the fiber structure are key phenomena of textile finishing technology. To obtain high quality finishes, it is important to understand the relative importance of the parameters that define the absorption rate and spreading ratio of droplet shaped fluid elements that impact the textile surface.

A simple model that combines Darcy's Law and harmonic droplet oscillator frequency forms a precursor to further advanced Dissipative Particle Dynamic (DPD) modeling. Experimental data for several combinations of textile and model fluids are presented. The key technical challenges to be addressed and overcome in the near future are discussed.

Introduction

A droplet impacting onto a substrate at speeds of a few meters per second is a dynamic process, with spreading initially greater than that belonging to the equilibrium rest state. This comes from conversion of droplet kinetic energy into interfacial surface energy through deformation.

Impact and spreading processes on surfaces occur within a process window which can be defined by 2 dimensionless numbers:

Re - Reynolds number: Describes the inertial forces in a fluid flow with respect to the viscous drag occurring in the fluid during impact and spreading and is given by:

$$Re = \rho \cdot v \cdot D / \eta \qquad (1)$$

Where ρ is drop density, v drop velocity, D drop diameter and η drop viscosity.

We - Weber number: Describes the inertial forces in the fluid with respect to surface (tension) forces on the fluid interface during impact and spreading.

$$We = \rho \cdot v^2 \cdot D / \sigma \qquad (2)$$

Where σ is droplet surface tension.

In there early work Pasandideh-Fard et al. [1], considered the spreading of 2-mm droplets on solid surfaces for industrial processes such as spray cooling, sprinkler systems, spray forming and pesticide spraying. The impact speed of 1 m/s was low enough that no splattering occurred, with simulation and experiment in good agreement. Inertia was found to dominate spreading after impact, whilst capillary (surface) forces dominate droplet recoil. A comparison between theory and experiment was done by measuring the wetted surface diameter D(t) at successive stages during droplet deformation. The spreading factor or ratio $\xi(t)=D(t)/D_0$ was plotted against time, Figure 1. And giving rise to a simple expression for the maximum spread factor ξ:

$$\xi = D_{max}/D = \{ (We+12) / (3\cdot(1-\cos\theta) + 4\cdot We/Re^{1/2}) \}^{1/2} \qquad (3)$$

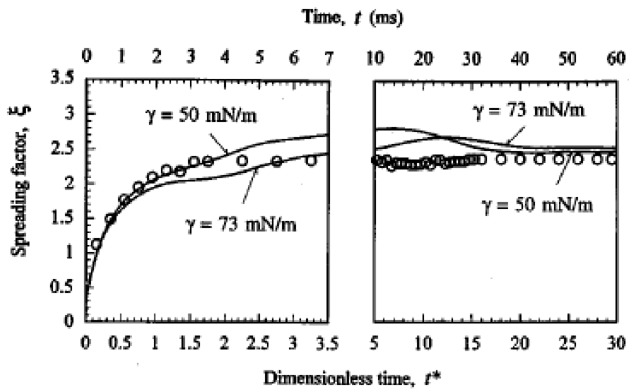


***Figure 1**. Measured spreading factor during impact of a droplet with 1000 ppm of surfactant, compared with model using surface tension of 50 and 73 mN/m (Figure from [1]).*

The onset of splashing can be described by the parameter K_c [1], shown in Figure 2:

$$K_c = We^{1/2} \cdot Re^{1/4} \qquad (4)$$

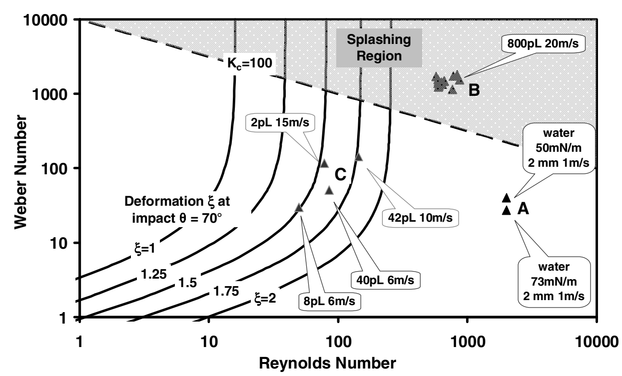


***Figure 2**. Process window in Re-We plane for impact processes of droplets, with varying fluid properties and impact conditions (deformation and splashing criterion according to [1]), A: Ref. Experiment [1], B: CIJ-qualified processes, C: Qualified processes of DOD generations.*

When K_c exceeds some critical value (100), then splashing occurs. The impact processes with droplets belonging to CIJ-qualified processes (blue in Figure. 2) show splashing behavior, while other droplet categories lay in the stable deformation regions (gold and pink in Fig. 2).

Capillary spreading and flow in the porous substrate is considered as governed by Darcy's Law with a wetting front separating saturated and unsaturated regions. The pressure field (P) depends on hydrostatics, surface tension and the disjoining pressure (π) that arises from microscopic interactions in the submicron scale inside the rough or porous structure (e.g. Van der Waals).

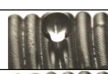
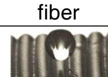
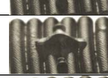
Modeling sorption into the porous substrate is based on the Washburn equation for a single capillary, from equations (5) and (6), appropriately coupled with the contact area of the droplet above the porous substrate.

$$\mathbf{v} = - K/\eta \cdot \text{grad } P \quad (5)$$
$$P = \rho g h - \sigma \cdot \Delta h - \Pi \quad (6)$$

Holman et al. [2] found that the macroscopic (apparent) contact angle of a liquid on a rough or porous substrate differs considerably from the corresponding smooth and solid surface.

The challenges for ink jet applications to textiles are two fold: (1) drop impact and motions of fluid with retained functionality, (2) morphology and chemistry encountered on fiber interfaces. Carr et al. have studied the impact of relatively big drops on silicon wafers and on monofilament surfaces, with varying impact position, Table 1 [3]. The location of impact on a rough surface affects spreading ratio and final resting diameter.

Table 1: Impact of a 2.3mm water droplet on a wafer and on a 1.25mm polyester fiber (speed=0.87m/s, Re=2000, We=24, [3]).

Time (ms)	HDMS coated silicon wafer	between fibers	on center of fiber
0			
5			
9			
800			

In order to accurately predict drop-fiber interaction fabric geometry must be precisely defined. The points of the fiber paths in the yarn are calculated using minimum strain energy principle. Fibre geometry is represented by periodic splines. Figure 3 shows a section of a cotton fabric and illustrates the use of splines. Software tools for such geometric models of fabrics form an interface between mechanical, flow dynamical, thermal and other applications [4].

Verleye et al [5] calculated the permeability of textile reinforcements by solving Navier-Stokes/Brinkmann equations in a unit cell of defined geometry and given local tow permeability (Figure 4).

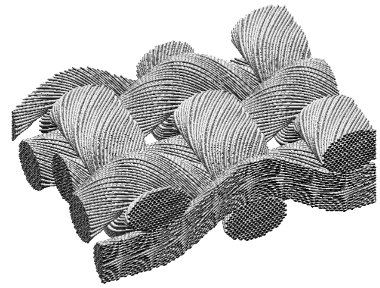


***Figure 3**. Section of a cotton fabric.*

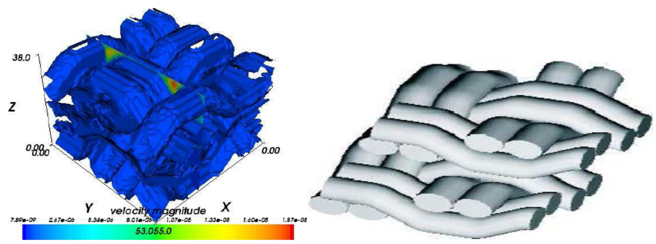


***Figure 4**. Unit cell as base for permeability model [5].*

Spreading Model

The process of impact and sorption of a droplet is summarized as follows (Figure 5):

(1) Kinetic energy of the droplet is converted into thrust pressure energy above the substrate, while fluid is either penetrating under influence of thrust into the substrate or spreading outwards.

(2) The outward flow, with viscous dissipation, causes an oblate droplet shape with extra free surface energy. The flow into the substrate is not available for the droplet deformation.

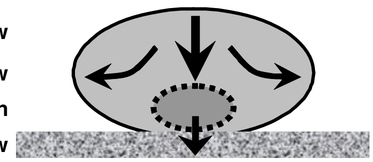


***Figure 5**. Relevant flows during the process of impact and sorption of a droplet onto a porous substrate.*

(3) The deceleration of the downward flow results in a thrust region above the substrate. The round "window" of the entrance of the flow into the substrate depends on the wetting angle between fluid and substrate.

(4) The substrate flow occurs during the first half cycle of the vibration of the droplet during impact. The flow time and the "window" size define the amount of fluid into the substrate.

(5) The remaining fluid initially forms a globe segment, and spreads out according to the rest energy after substrate flow. The resulting area of the oblate droplet represents an amount of surface

energy that can be decreased by breaking up into single small droplets. This reveals a splashing process.

Impact on a hydrophobic substrate gives a narrow window for substrate flow, while a more or less neutral substrate, θ=90° leads to a wider substrate flow window. It is then expected that after impact not enough free fluid is left for formation of an oblate droplet onto the substrate. In that case no splashing is expected.

Viscous dissipation is very low due to the high Re number of the impact process. Only large-sized droplets from [1] are expected to splash in all cases, the 42-, 40- and 8-pL droplets are expected to splash only on hydrophobic substrates.

DPD Modeling

The approach of Dissipative Particle Dynamics (DPD) modeling was introduced by Groot and Warren [6], who were looking for an approach to adequately model such phenomena on the mesoscopic time and length scale, i.e. longer than atomistic and shorter than the "big" world of hydrodynamics and mechanics:

DPD works by (1) 'lumping' similar atoms together into particles ("united atoms"), and (2) allowing the particles to interact with each other via rather soft forces, because the positions and influences of nearby atoms are smeared out. The correct thermodynamic and hydrodynamic parameters on the mesoscopic scale are obtained by inhibiting the correct compressibility of the liquid, and the correct solubility's of the components into each other (in case of mixtures). The removal of the hard core interaction allows a considerable large time-step, four orders of magnitude more than that of simulation of Molecular Dynamics. The following assumptions are made:

1. Newton's equation of motion governs the time evolution of interacting particles in DPD, so at every time-step the set of positions and velocities, $\{\mathbf{r}_i, \mathbf{v}_i\}$ follows from the positions and velocities at earlier time.
2. The force acting on a particle is given by the sum of conservative, drag and pair-wise additive random force, i.e. $f_i = \sum_j(F^C_{ij} + F^D_{ij} + F^R_{ij})$ where the sum runs over all neighboring particles within a certain distance R_c. All forces depend on coordinate differences. It is also possible to define an extra spring force F^S_{ij} between neighboring particles.
3. The drag force F^D_{ij} and the random force F^R_{ij} are coupled in such a way that their combined effect results in a constant-temperature system (thermostat) [6] [7].
4. The particle mass, temperature and interaction range, as units of mass, energy and length, are set to 1, i.e. m = 1, $k_BT = 1$, and $R_c = 1$ and the time is expressed in units of $\tau = R_c\sqrt{(m/k_BT)}$.

Advanced DPD modeling is used to investigate the absorption and spreading phenomena of impacting micro droplets of fluid onto textile fiber surfaces, Figure 6. A simulation of such a droplet onto 4 fibers is shown in Figure 7. The interaction of 3 phases has to be described in the underlying droplet impact model: (1) droplet fluid, (2) surrounding air, and (3) solid fiber surface material. Free energy and interaction energy of the phases govern the absorption and spreading of the fluid during the impact process.

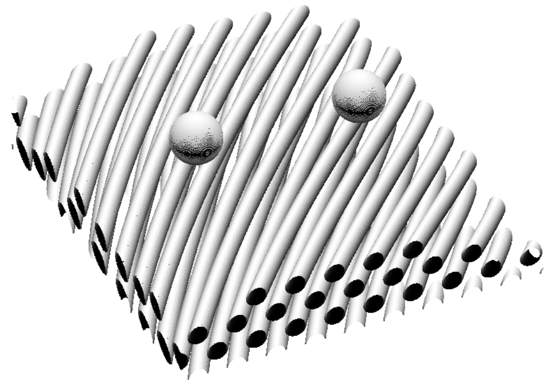


Figure 6. *10-pL droplets onto a fiber surface of a cotton yarn.*

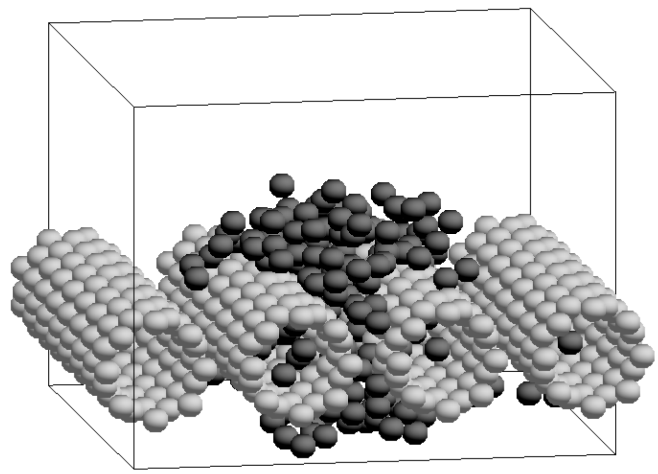


Figure 7. *Simulation result after time evolution of an impact of a downward moving 10-pL droplet onto 4 cotton fibers.*

Figure 7 shows the spreading and penetration of the DPD particles around and between the fibers in this configuration. Also, part of the particles has crossed the fiber surface, representing absorption effects, connected with this type of modeling of mesoscopic fluid transport.

Experimental

It is interesting to investigate the spreading of droplets of black ink onto the yarns of a fabric. Saturation of the fiber surface and the successive penetration of the fluid into the fiber layers can be deduced from droplet deposition experiments with varying dot spacing. Results for 10-pL droplets with centre to centre dot spacing of 90, 30, 20 and 10 µm are shown in Figure 8.

The substrate is a 100% cotton fabric. The black pigment/water-based ink has a surface tension of 28 mN/m and viscosity of 6.3 mPa·s.

At 90 µm dot spacing no droplet overlap is observed, for all other conditions there is overlap. Ink penetration between the fiber layers is derived from the percentage of black pixels as a function of dot density, and for 2 kinds of fabrics (Figure 9).

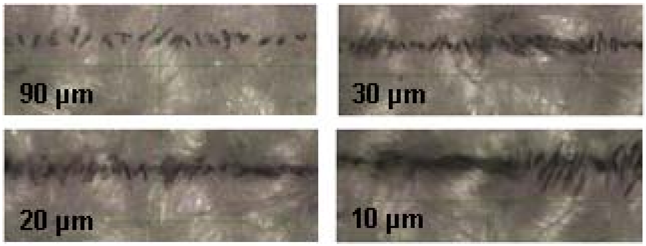


***Figure 8**. 10-pL droplets onto a cotton yarn with varying dot space.*

The relationship between ink spreading and dot density is essentially *linear* in case of spreading onto the 1st fiber layer, thus *no* droplet penetration, with a negative deviation for yarn 2 (cotton-warp) showing droplet penetrations.

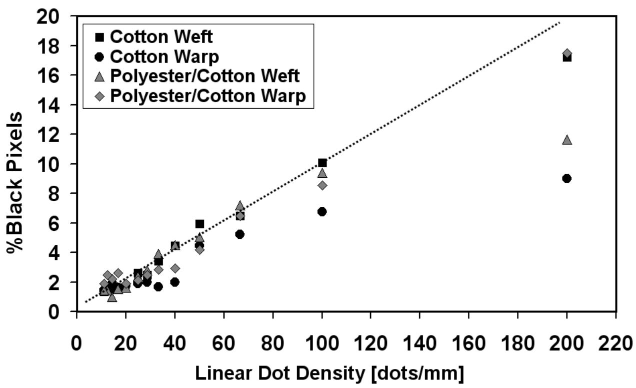


***Figure 9**. Amount of black pixels as a function of linear density of 10-pL droplets onto 2 kinds of fabrics and at weft and warp directions.*

The cotton-weft and polyester/cotton-warp directions show almost no penetrations, while the cotton-warp and polyester/cotton weft directions show penetrations until the 2nd fiber layer (9% versus 20% black means equal distribution between 1st and 2nd layer and 7% versus 10% black means 70% of ink on 1st and 30% on 2nd layer).

Conclusions

Existing knowledge on droplet impact behavior is extending the traditional boundaries of flat, solid and homogeneous surfaces. DPD modeling offers great opportunities for studying the mesoscopic effects that are connected to the impact of droplets onto complex fiber layer structures. Measuring the distribution of ink droplets with varying composition on varying textile substrates is an essential tool for verification of proposed advanced drop deposition concepts.

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Symbols

Re	Reynolds number	[-]
We	Weber number	[-]
v	Velocity	[m/s]
D	Diameter	[m]
ρ	Density	[kg/m^3]
η	Viscosity	[Pa·s]
σ	Surface tension	[N/m]
ξ	Spread factor	[-]
θ	Contact angle	[degr]
K_c	Splashing criterion from [1]	
$\mathbf{v}$	fluid velocity (vector)	[m/s]
K	Permeability	[m^2/s]
P	Pressure	[Pa]
g	acceleration of gravity	[m/s^2]
h	Fluid height of droplet	[m]
Δh	Capillary length	[m]
Π	Disjoining pressure	[Pa]
$\mathbf{r}_i$	Position of DPD particle i	[m]
$\mathbf{v}_i$	Velocity of DPD particle i	[m/s]
f_i	Force acting on DPD particle i	[N]
F^C_{ij}	Conservative force between i and j	[N]
F^D_{ij}	Drag force between i and j	[N]
F^R_{ij}	Pair-wise random force between i and j	[N]
R_c	Interaction distance (size) of DPD particle	[m]
m	Mass of DPD particle	[kg]
k_B	Boltzmann constant	[J/K]
T	Temperature	[K]
τ	Unit of time in DPD simulation	[s]

References

[1] M. Pasandideh-Fard, Y.M. Qiao, S. Chandra and J. Mostaghimi, "Capillary Effects during Droplet Impact on a Solid Surface", Phys. Fluids, 8, 650 (1996).

[2] R.K. Holman, M.J. Cima, S.A. Uhland and E. Sachs, "Spreading and Infiltration of Inkjet-Printed Polymer Solution Droplets on a Porous Substrate", J. Colloid Interface Sci., 249,432 (2002).

[3] W.W. Carr, J.F. Morris F.J. Schork and W.C. Tincher, "Textile Ink Jet Performance and Print Quality Fundamentals, NTC Project C99-GT08, June 2002.

[4] X. Chen, "Geometrical and Mechanical Modeling of Woven Fabrics", EPSRC Final Report: Engineering the Performance and Functional Properties of Technical Textiles, February 2006.

[5] B. Verleye, D. Roose and S. Lomov, "Numerical Modeling of Permeability of textile Reinforcements", Engineering Science Models for Textile Structures, Nottingham, April 2005.

[6] R.D. Groot and P.B. Warren, "Dissipative Particle Dynamics: Bridging the Gap between Atomistic and Mesoscopic Simulation", J. Chem. Phys., 107, 4423 (1997).

[7] R.D. Groot, "Applications of Dissipative Particle Dynamics", Lect. Notes Phys., 640, 5 (2004).

Author Biography

Kees Heil graduated from Eindhoven University of Technology with M.Sc. in 1979 and Ph.D. in 1984. After working in several areas of process technology and fluid engineering in the last two decades, he now has a position as a research scientist at Ten Cate's Digital Finishing Laboratory in Nijverdal, the Netherlands. Backgrounds are fluid dynamics, global energy systems, process engineering and nonwoven technology. Current topics are "fluid flow in textile materials" and "advanced printing systems".