Parameter analysis of droplet impact of aqueous fluids onto textile fiber surfaces for advanced modeling of droplet-substrate interaction of textiles

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Abstract

A number of structure parameters of textile surfaces and a number of jetting fluid parameters define the impact and spreading of aqueous droplets on textile fiber surfaces. Parameter and dimension analysis as well as advanced CFD and DPD modeling results provide data that form a basis for parameter analysis. Structure parameters and fluid properties have been varied in several computation runs. Experimental verification data on fluid distribution is shown for combinations of textile and model fluids.

Introduction

Impact and spreading of droplets on surfaces occur within a process window, defined by 2 dimensionless numbers (Fig. 1)[1]:

Re - Reynolds number = inertial forces/viscous drag

We - Weber number = inertial forces/surface tension

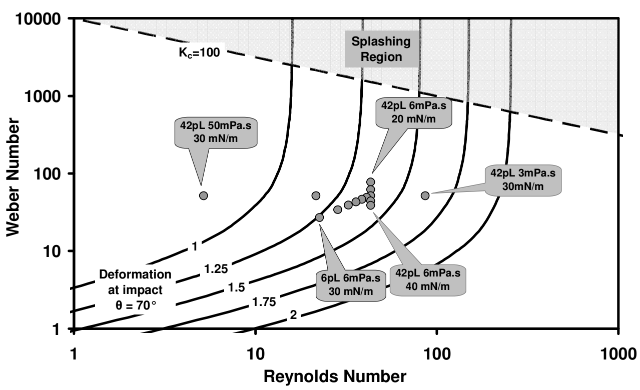

Figure 1. *Process window in Re-We plane for droplet impact on a flat plane [1].*

It should be said that the physical dimensions in the above numbers are based on either the droplet size (for flat planes) or on the size of characteristic elements on rough planes. In fact, fiber sizes and spaces between fibers actually define the fluid flow during impact and spreading. Inertia dominates the vertical flow and deformation after impact, whilst capillary (surface tension) forces dominate the flow during recoil or spreading. Capillary flow in the fiber structure is governed by Darcy's Law with a wetting front separating saturated and unsaturated regions on the fibers: there is a disjoining pressure that arises from microscopic and physiochemical interactions on the rough or porous fiber surface. This results in a sorption model based on the Washburn equation for single capillaries. The macroscopic (apparent) contact angle of the droplet on the rough (porous) substrate or fiber differs considerably from the corresponding smooth and solid surface, made of the same species.

It is difficult to describe the droplet penetration into the highly anisotropic structure of the yarns. Wicking phenomena in capillaries along fibers strongly perturb the species distribution against the application of geometrically uniform print patterns. The capillary flow is applied to the outer space of a series of parallel solid cylinders, which are twisted. An example of a FEM construction of a yarn, with a number of polyester fibers, is shown in fig. 2.

Figure 2. *Geometry of a FEM construction of a yarn in textile.*

A simplified geometrical model is needed for estimating the wicking effect after impact. The fluid is penetrating the yarn in all directions and one of them is more distinguished, which is observed as the wicking effect. Figure 3 shows the scale of the droplet on the yarn surface, and that the fibers can be considered as straight. These fibers can be modeled as porous cylinders, which is a model of the absorptivity of the fluid in e.g. cotton. Also, the large-scale wicking effect on the straight fibers is seen to be similar to the wicking on the more or less realistic bent fibers shown in figure 2.

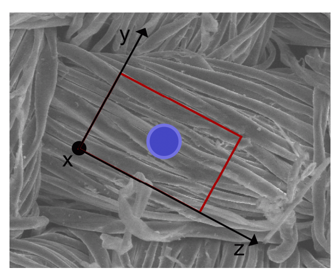

Figure 3. *Simplified computational domain for straight fibers geometrical model, marked by red rectangle.*

The deposition process has several different characteristic time scales (Fig. 4). Dividing the process into sub processes enables firstly to solve them separately and secondly to couple the results by setting initial conditions for the processes with the results of the previous one. The penetration and wicking (A-B) is analyzed by simulation of the droplet behavior into a group of straight non-porous cylinders (Fig. 5). Results from this simplified model gives information about the relation between the wicking effect and the fluid and structure parameters.

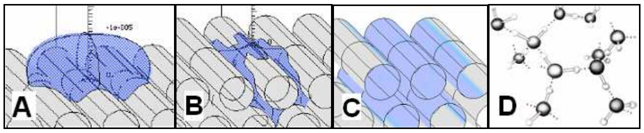

Figure 4. *Typical times of phases of droplet deposition. (A) Impact 0.1 µs, (B) Penetration and wicking 100 ms, (C) Drying 1-10 s, (D) Chemical bonding.*

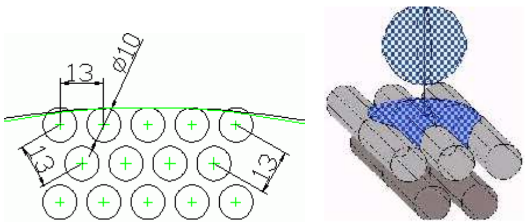

Figure 5. *Dimensions used in straight fiber model. The difference between real geometry and simplified geometry is small.*

Geometry of the textile is thus simplified (Fig. 5) and the influence of curved fiber surface can be neglected.

CFD analysis

The CFD model of droplet impact and wicking includes the next features: (1) Newtonian flow, (2) Water/air surface tension, (3) water/air/fiber contact angle, (4) Gravity. Calculations where carried out with a CFD-ACE+ solver. The numerical simulations where performed in order to find the most important fluid and printing parameters from droplet geometry after impact and penetration into the yarn surface. The 3 parameters, which are found to be most important in the analysis, are (Fig. 6 thru 8):

-- Wetting angle: 15°, 45° and 70°
-- Viscosity: 1, 3 and 6 mPa·s
-- Droplet volume: 6, 24 and 40 pL
-- Fiber distance 2 and 3 µm

Other parameters are: droplet velocity 6 m/s and surface tension 30 mN/m. The results are compared for t = 10-40 ms, which is a time when steady state is obtained.

4 Parameters are used to describe the resulting dot shape: (1) Height above the textile, (2) Depth of penetration, (3) Diameter across the fibers, (4) Diameter along the fibers.

Only the 40 pL droplet reaches then 2nd fiber row, and that for low wetting angle of 15°. There is almost no penetration between the fibers (high droplet above textile) for high wetting angle of 70° and for all droplet volumes. For other wetting angles there is deeper penetration between the fibers, and more or less longitudinal wicking.

Similar dependencies can be observed for viscosities of 1, 3 and 6 mPa·s. The viscosity influences the longitudinal wicking and penetration – for higher viscosities this distance is smaller within a certain time span. However, it can be observed that for sufficiently long time the *same* wicking may be observed for different viscosities. So there is, in principal, only a dependency on droplet volume in fig. 7. But wetting angle remains the most important parameter, see fig. 6.

Smaller capillaries lead to deeper fluid penetration and longer wicking distance as can be seen from figure 8. Moreover, smaller capillaries cause less inter-fiber space that should be compensated with more fluid flow into the other directions.

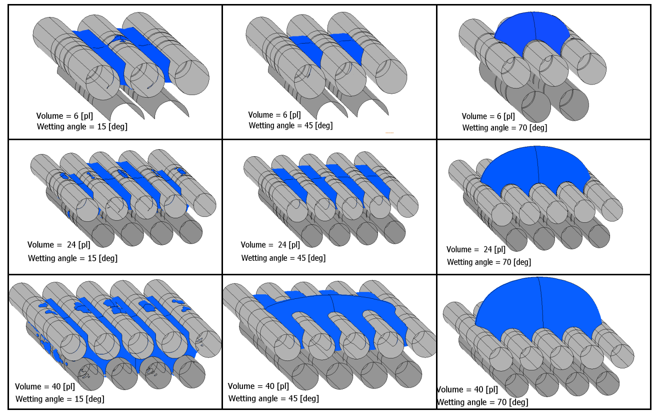

Figure 6. *Wetting angle influence for wetting angle 15°, 45° and 70° and 6, 24 and 40 pL droplet volume with 3 µm fiber distance and viscosity 1 mPa·s.*

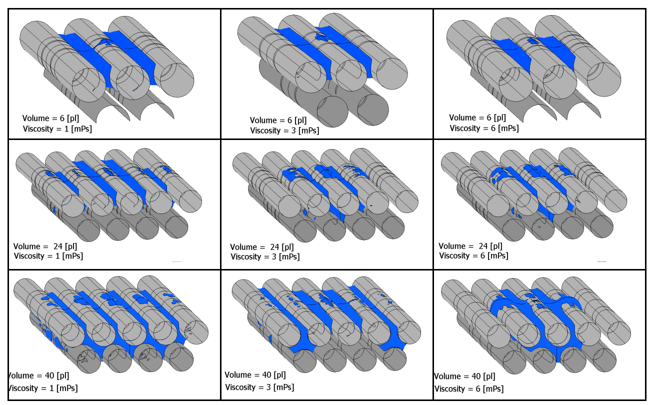

Figure 7. *Viscosity influence for droplet volumes 6, 24 and 40 pL with 3 µm fiber distance and 15° wetting angle.*

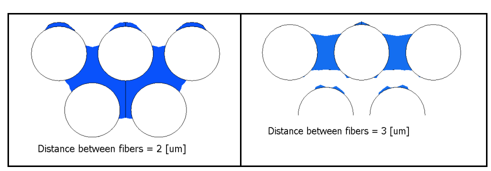

Figure 8. *Different fluid distribution for two different distances between fibers, 2 and 3 µm, other parameters where kept constant (6 pL, 6 mPa·s, WA=15°).*

The final dot shape strongly depends on the analyzed parameters.

CFD analysis shows that the droplet behavior into the group of straight fibers is highly nonlinear with respect to varied input parameters. This comes from the fact that droplet spreading across the fibers is limited by the stepwise choice of the fluid for passing the fiber barrier in order to fill the next fiber spacing and the underlying 2nd fiber row.

DPD Analysis

The Dissipative Particle Dynamics (DPD) analysis method uses a mesoscopic model of hydrodynamics with molecular dynamics methods (Monte-Carlo Simulations). It uses a set of equations for updating positions of clusters of molecules or “lumps” of fluid [2]. Parameterization of the underlying droplet impact model has been carried out by adjusting the interaction at the water/air/fiber interface.

The DPD model of droplet impact and wicking includes the next items: (1) Newtonian flow, (2) Water/air surface tension, (3) water/air/fiber contact angle.

The varied parameter of the DPD analysis is:

-- Wetting angle: 30° thru 170°

Other parameters are: (1) Viscosity 6 mPa·s, (2) Surface tension 30 mN/m, (3) Droplet volume 6 pL, (4) Fiber distance 3 µm, (5) Fiber diameter 10 µm, (6) Droplet velocity 5 m/s. The results are compared for t = 11.2 ms.

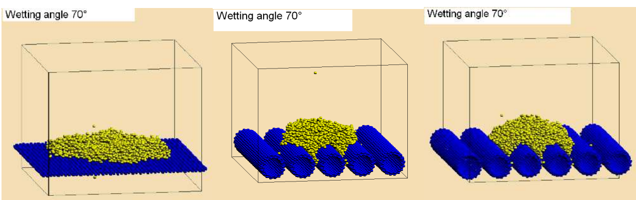

Figure 9. *Simulation result after 11.2 ms of an impact of a 10 pL droplet on a flat surface and on a series of fibers (fiber centered and space centered).*

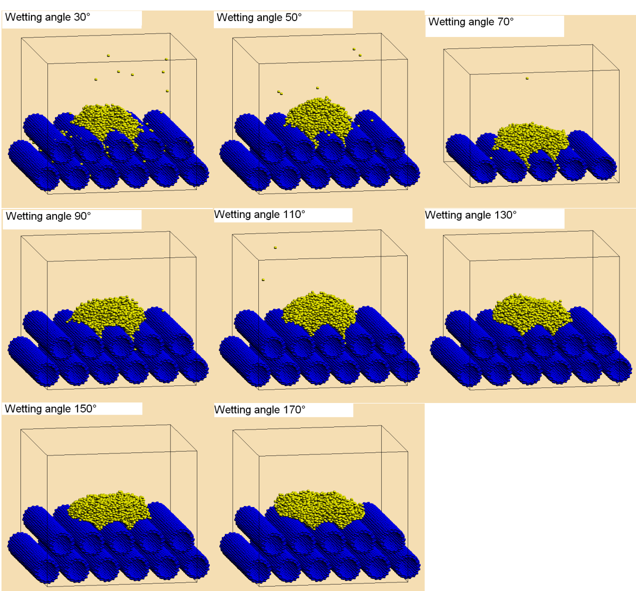

Figure 10. *Simulation result after 11.2 ms of an impact of a 10 pL droplet on a series of fibers with variation of wetting angle.*

Figure 9 shows the droplet spreading on a flat surface and on a series of fibers. The spreading across the fibers is much more limited compared to the flat surface case. Simulations for the fiber centered case lead to wicking into 2 fiber space channels, while in the space centered case there is wicking also into the central space channel, so in total 3 wetted space channels.

Figure 10 shows the droplet spreading on a series of fibers (fiber centered) when the wetting angle is varied between 30° and 170°. The blocking effect of the fibers, in the cross direction of the fibers, for the spreading effect in that direction, is obvious for all low wetting angles. It is also seen that there is limited wicking in the space channels in that cases. Probably is this due to the used DPD method for fluid modeling.

Validation of wicking distance

Main difficulty in the comparison between numerical and experimental results is an accurate measurement of the wetting angle of the fluid on the fiber surface. In addition, model analysis showed that the wetting angle is one of most important parameters in the deposition process. Fig. 11 shows the deposition of 10 pL droplets onto a 100% cotton fabric for a droplet spacing equal to 80 µm. The droplets have no overlap; therefore these results are good for comparison with single droplet numerical simulations. The black ink has a surface tension of 28 mN/m and a viscosity of 6.3 mPa·s. Available results give a rough estimation of the wetting angle. The wicking distance along the fibers is indicated in the images. The experimental values are of the same order as the numerical CFD results for wetting angle equal to 70°.

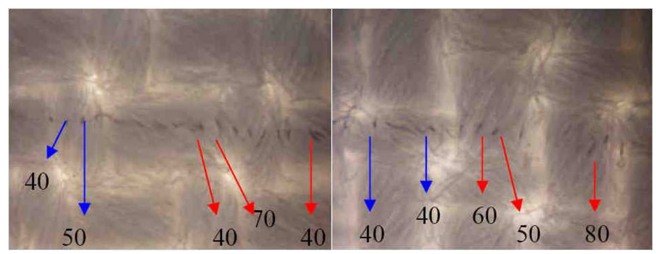

Figure 11. *Deposition of a 10 pL droplet onto a cotton fabric. Droplet spacing is 80 µm.*

Species distribution by Raman spectroscopy

The Raman spectroscopy method was selected as a way to specifically observe and measure the functional species distribution on the fabric surface as well as inside the fabric volume. This method uses a single frequency radiation to irradiate the sample. Radiation scattered from the molecule is detected. It is known where the bands should be present in the Raman spectrum, but in practice one may observe many peaks with uncertain origin in the Raman spectrum. These form a unique pattern for every chemical compound. The substance identification is then provided by comparison of the recorded spectrum with spectra from a data base [3]. Raman spectroscopy can not only be used for substance identification but also for phase or ionic species identification.

Additional information can be obtained from Raman maps that are collected from a volume of a sample. The mapping time depends on the amount of sampling points and the time of collecting the spectrum at one point, which is related to the chemical character, concentration and purity of the species, and also to the quality of the equipment. The map consists of Raman spectra recorded in each of the points and chosen peaks are compared. The distribution of species is shown by colors, which are connected to the amount of the species.

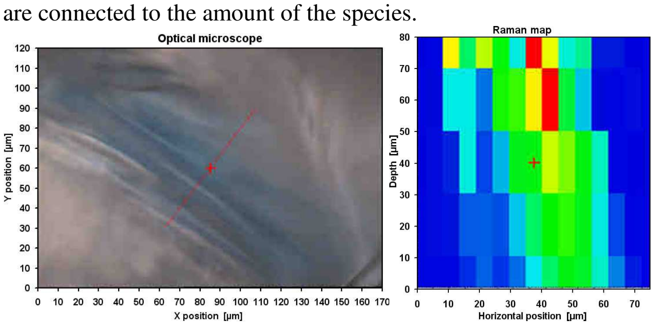

Figure 12. *40 pL droplet on a polyester fabric: picture of dot from optical microscope and Raman map of dot over cross-section along red line.*

Investigated samples of polyester and cotton fabric where printed with UV curable cyan ink, containing phthalocyanine blue pigment (12 cP, wetting angle 15-25°). The pigment is visible as well as detectable by Raman spectroscopy (Fig. 12). Very intensive peaks where observed in the spectrum, resulting in short mapping times. Moreover, phthalocyanine blue, cotton and polyester have separated peaks, which is a favorable condition for measuring the species concentration. Geometry was collected for 3 dots (Table 1), using Dispersive Raman Spectrometer Nicolet Almega.

Table 1. 40 pL droplet on a polyester fabric: geometry of 3 dots.

	Dot #1	Dot #2	Dot #3
Along fibers	150 µm	180 µm	160 µm
Across fibers	25-30 µm	25-35 µm	45 µm
Depth	>60 µm	>60 µm	90 µm

Comparison with numerical results

Dot geometry after penetration and wicking appeared to be more or less random because of textile geometry. Mean values and standard deviations of the dot sizes were calculated for the UV curable cyan ink over a number of dots on the textile surface.

Systematic differences of about 20 µm in the dot size were observed between the top and the valley of the yarn, while the standard deviation is large (Fig. 13, 14).

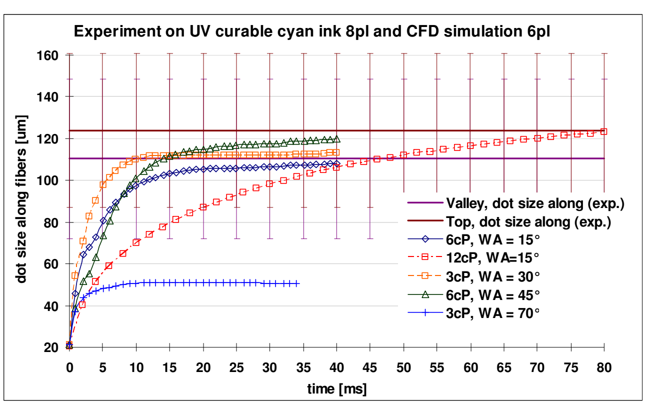

Figure 13. *Calculated dot geometry versus measurements: dot size along fibers.*

Calculated dot geometry has been plotted until t = 40, 50 and 80 ms, what is seen to be enough for the stationary situation. Wetting angle is the only relevant parameter. Dot size along fiber (wicking length) is the best indicator. Calculated dot geometry, using wetting angle = 15°, 30° and 45° falls in the range of the dot size measurements.

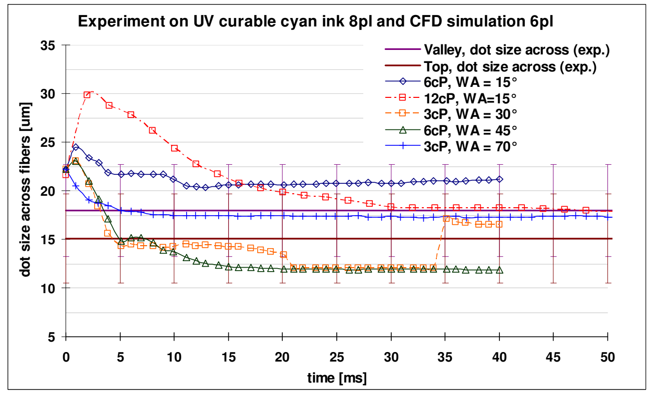

Figure 14. *Calculated dot geometry versus measurements: dot size across fibers.*

Dot size across fiber (dot width) is not a good indicator because of the fiber barriers that fluid encounter during spreading in that direction. Its is obvious that calculated dot geometry for all wetting angles falls in the range of the dot size measurements.

Conclusions

CFD analysis is an effective tool for identifying critical textile structure and jetting fluid parameters in droplet deposition processes. Penetration and wicking phenomena into a group of straight non-porous cylinders form the base for extensive calculations on more or less random fiber layers in complex textile geometries. DPD analysis has limited applicability as a tool for identifying wicking phenomena in the space channels between the fibers.

Optical microscopy and Raman spectroscopy are essential in the determination of species distribution on the fabric surface and inside the fabric volume as a way of verification of drop deposition concepts to be developed.

Dot geometry validation has become a challenge because of the limited accuracy of dot size measurements. Also the nonlinear behavior of the fluid viscosity and surface temperature, and its temperature dependency, make it difficult to use adequate input for numerical results.

The rough estimations of wetting angles have been used in the underlying paper. Because of its importance to droplet deposition processes and being a parameter in numerical simulations, fluid-fiber wetting angles should be confirmed by e.g. porometry measurements with several kinds of fluids and use of Zisman plots.

Acknowledgement

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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, Dr. Heil now has a position as research scientist digital finishing at Xennia Holland BV in Nijverdal, the Netherlands. Backgrounds are fluid dynamics, energy systems, process engineering and nonwovens. Current topics are "characterization of and fluid flow in textile materials" and "advanced printing systems"

Armen Jaworski received his M.Eng from the Warsaw University of Technology in 2006 and now is finishing his Ph.D in adjoint methods for aerodynamics. Since 2007 he is working in CIM-mes Projekt on development of numerical models for ink-jet printing on textiles. His aeronautical background mainly on numerical methods and optimization and experience with development of CFD software is giving new insight into engineering problems existing in textile industry.