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A model-based prediction of droplet shape evolution during additive manufacturing of aligned fiber-reinforced soft composites

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ABSTRACT

The objective of this paper is to develop a mathematical model capable of predicting the temporal shape evolution of a droplet during the additive manufacturing of aligned fiber-reinforced soft composites. Given the ellipsoidal shape of the droplets encountered during the additive manufacturing process, the three time-dependent output parameters of interest include the height of the droplet (H), and its two relevant diameters $D_{//}$ and $D_{\perp}$ that are measured in the directions parallel and perpendicular to the fiber axis, respectively. The model calculations start with a substrate parametrization step involving a characterization of the diameter of the fibers, fiber bundles and fiber spacing encountered in the printing zone. This coupled with the knowledge of the inkjet printing parameters and the fluid properties of the ink allow for the subsequent calculations. The droplet shape is parametrized as an ellipsoidal cap. For every discrete time-step calculation, the model uses the equations of energy and volume conservation as well as an experimentally calibrated relation for the ratio $\frac{D_{//}}{H}$. The model also involves a free energy barrier calculation at every time increment that checks for the pinning of the $D_{\perp}$ diameter. The validation experiments involved single droplet impingement studies using three inks under distinctly different inkjet printing conditions and substrates profiles. In general, the model prediction errors are observed to be under 7%. The free energy barrier calculation is a critical component of the model. In some cases, it contributes to a >50% reduction in the model prediction errors.

1. Introduction

Fiber-reinforced soft composites (FrSCs) are a new class of composite materials made up of hierarchical, polymer fiber networks embedded within another soft polymer matrix [1,2]. These composites are relevant to applications such as artificial muscles, sensors/actuators, 4D printing, bio-printing and bio-mimetic materials [3–5]. Recently, the additive manufacturing of FrSCs has been demonstrated using a novel hybrid process that combines the conventional inkjet-based deposition of UV curable polymers with the direct-writing of micro/sub-micron fibers [6]. While this manufacturing process has been proven to 3D print FrSCs, the interactions between the droplets (ejected by the inkjet nozzle) and the fibrous substrates are not well understood.

Recently, Picha et al. [7] performed an experimental study focused on the spreading of droplets under conditions encountered during the additive manufacturing of aligned FrSCs. Their droplet-substrate interaction study revealed that for FrSCs containing aligned fibers, the droplets preferentially spread in the direction parallel to the fibers. Furthermore, key substrate characteristics such as fiber spacing and fiber bundling influenced the temporal evolution of the droplet shape. While such experimental insights are valuable, they have limited application to the development of process control strategies that primarily rely on mathematical models to predict the process outcomes [8]. For the case of FrSCs, such models should predict the temporal evolution of the droplet diameter (parallel and perpendicular to the fibers) and height, under conditions relevant to additive manufacturing.

The modeling of droplet spreading has been investigated since the early 1900s [9,10]. The largest category of such models explores droplet deposition on plain substrates with prediction of the final droplet radius and contact angle [11]. Other models have explored droplet spreading on substrates with concentrically distributed surface components [12] and even thermodynamic approaches to droplet spreading on micro-patterned surfaces [13,14]. In addition, there are models that look at droplet spreading in the presence of fibrous structures suspended in air [15,16]. However, the aforementioned models deal predominantly with either sessile droplets and as such are not suitable for process planning related to additive manufacturing of FrSCs.

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Nomenclature

$<>_{t^*}$	Variables in the $<>$ brackets represent model calculated values at time t^*
a	Ellipsoid semi-axis length along x-axis
Arc_j	Length of the embedded arc of fiber *j*
b	Ellipsoid semi-axis length along y-axis
c	Ellipsoid semi-axis length along z-axis
c_1, c_2, c_3	Coefficients in the differential equation
$\widehat{c}_1, \widehat{c}_2, \widehat{c}_3$	Estimates of the coefficient variables c_1, c_2 and c_3 obtained by least squares error minimization
$Chord_j$	Embedded chord length of fiber *j*
CSA_j	Cross-sectional area of the non-embedded portion of fiber *j*
d_0	Undeformed droplet diameter
$d_{f,avg}$	Average diameter of fibers in the droplet landing zone
d_j	Diameter of fiber *j*
$D_{//}$	Diameter of the droplet in the direction parallel to fiber alignment
$D_{\perp}$	Diameter of the droplet in the direction perpendicular to fiber alignment
E_v	Viscous dissipation energy
g	Gravitational acceleration
H	Height of the droplet
h_j	Embedded portion of the diameter of fiber *j*
KE_0	Initial kinetic energy
$Length_j$	Length of fiber *j* that is under the liquid droplet
$l^{\%}_{fiber}$	Percentage of the transition length seen by the fiber
$l^{\%}_{substrate}$	Percentage of the transition length seen by the substrate
L_A^{lv}	Arc length of the liquid-vapor interface at droplet edge location A
m	Mass of droplet
n_f	Number of distinct fiber groupings
$n_{f\text{-}covered}$	Total number of fibers covered by the liquid droplet
SA_{lf}	Surface area of the liquid-fiber interface
SA_{ls}	Surface area of the liquid-substrate interface
SA_{lv}	Surface area of the liquid-vapor interface
SE_0	Initial surface energy
SE_1	Final surface energy
$S_{f,avg}$	Average fiber-to-fiber spacing
t	Time
t^*	Non-dimensional time
u	Droplet velocity
V_0	Initial droplet volume
V_1	Final droplet volume
$V_{f\ total}$	Total volume of fibers underneath liquid droplet
w_j	Width of fiber grouping *j*, [$j = 1,2...,n_f$]
x_j	X-coordinate of fiber grouping *j*, [$j = 1,2...,n_f$]
y_1	$D_{//}/H$ value at $t^* = 1$
y_{1000}	$D_{//}/H$ value at $t^* = 1000$
γ_{lf}	Surface tension at the liquid-fiber interface
γ_{fv}	Surface tension at the fiber-vapor interface
γ_{lv}	Surface tension at the liquid-vapor interface
γ_{ls}	Surface tension at the liquid-substrate interface
γ_{sv}	Surface tension of substrate-vapor interface
$\Delta F_{A\rightarrow B}$	Difference in the free energy between points A and B
Δt^*	Time increment for calculations
θ_a	Droplet contact angle along X-axis
θ_b	Droplet contact angle along Y-axis
$\theta_{e,fiber}$	Steady state contact angle for liquid and fiber
$\theta_{e,substrate}$	Steady state contact angle for liquid and substrate
μ	Liquid viscosity
μ_{water}	Viscosity of water at 25 °C
ρ	Droplet density
φ	Capillarity adjustment coefficient

Recently, there have been two droplet-spreading models used for manufacturing process planning purposes. In 2010, Ghai et al. [17] developed a model for predicting the steady-state diameter and height of droplets under conditions encountered during atomization-based delivery of cutting fluids. Carter et al. [18] adapted the work of Ghai et al. [17] for droplet deposition applications involving the near-field electrohydrodynamic jet-based (E-jet) printing process. While the Ghai et al. [17] and Carter et al. [18] models hold promise, these models only deal with: i) droplet depositions on flat substrates; and ii) the prediction of the steady-state shape parameters of the droplet. For the FrSC additive manufacturing application, not only should the model be adapted for fibrous substrates but it should also be capable of predicting the temporal evolution of the droplet shape, since the time delay for curing of the UV polymer is a critical process parameter that influences the additive manufacturing outcomes.

In light of the current state of knowledge, the objective of this paper is to develop a mathematical model capable of predicting the temporal shape evolution of a droplet deposited on fibrous substrates encountered during the additive manufacturing of aligned FrSCs. The model combines the ellipsoidal droplet shape parametrization developed by Ghai et al. [17] with equations of energy conservation, volume conservation, and experimentally-calibrated relations between the droplet shape parameters. The predictions of the temporal droplet shape evolution parameters are corrected at every discrete time-step using the free energy barrier (FEB) calculations. These FEB calculations check for the possibility of the fibers arresting the spread of the droplet. The validation experiments show that the model prediction errors are under 7%. Furthermore, the FEB calculations are seen to critically influence the model accuracy, in some cases reducing the prediction error by >50%.

The remainder of this paper is organized as follows. Section 2 presents the critical timescales of interest to the additive manufacturing of FrSCs. Section 3 provides an overview of the droplet modeling approach followed by Section 4 that presents the substrate and droplet shape parametrization scheme. Section 5 presents the details of the model development and calculation, followed by Section 6 that deals with model validation results. Finally, Section 7 presents the specific conclusions that can be drawn from this study.

2. Droplet shape evolution timescale

The experimental work of Picha et al. [7] identified that there are three droplet shape parameters that are of interest for single droplet spreading cases involving aligned FrSCs, (Fig. 1a), viz., : 1) $\mathbf{D}_{\perp}$: Diameter of the droplet measured perpendicular to the direction of the aligned fibers; 2) $\mathbf{D}_{//}$: Diameter of the droplet measured parallel to the direction of the aligned fibers; and 3) **H**: Height of the droplet. Fig. 1b depicts the typical experimental plot of the two diameters, when plotted against dimensionless time, t^*, defined as $\left(\frac{tu}{d_0}\right)$ [19], where t is the time of spread, u is droplet velocity, and d_0 is the undeformed droplet diameter. It should be noted that in Fig. 1b, the horizontal axis is a logarithmic scale. While the height