

ABSTRACT

Title of Dissertation: SIMULATION OF POLYMERIC DROP DYNAMICS: EFFECT OF PHOTOPOLYMERIZATION, IMPACT VELOCITY, AND MULTI-MATERIAL COALESCENCE

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Over the past couple of decades, additive manufacturing has emerged as one of the most promising manufacturing tools and has rightfully garnered the attention of researchers across various fields ranging from biochemistry and medicine to energy and infrastructure. Especially, direct-ink-writing methods (*e.g.*, inkjet printing, aerosol jet printing, or AJ printing, etc.) have been widely studied because of their ability to print highly complex geometries with finer resolution. In order to design a more efficient droplet-based direct ink writing system, it is essential to understand the deposition process and the post-deposition dynamics of the drop. The post-deposition drop dynamics dictate the spreading radius of the drop and hence the print resolution. Such an understanding is even more critical when there are multiple drops interacting with each other, given the fact that such interactions determine the presence/absence of surface defects in addition to determining the print resolution. Moreover, to have a holistic understanding of the post-

deposition process, it is essential to further account for the droplet solidification mechanisms (for example, through effects such as *in-situ* curing) that might interplay with multiple drop dynamics events (such as drop spreading, drop coalescence, drop impact, etc.).

In this dissertation, computation fluid dynamics (CFD) frameworks have been developed to investigate the facets dictating the post-deposition dynamics of one (or several) solidifying polymer drops, with these dynamics show-casing the different post-deposition events that are intrinsic to the droplet-based additive manufacturing processes. First, we considered a situation where the polymeric drop undergoes simultaneous spreading and photopolymerization, with the timescales of the spreading and photopolymerization events being τ_s and τ_p respectively. The findings from this work confirmed the significant impact of the ratio of timescales (τ_s and τ_p) on the thermo-fluidic-solutal dynamics of the polymeric drops. Moreover, the evolution of the curing front showed distinct behaviors as a function of the timescale ratio.

Subsequently, the effect of the interaction of multiple polymeric drops during the post-deposition event, as seen in the typical printing process, was investigated. Specifically, we studied the effect of drop impact on the coalescence dynamics of two polymeric drops of identical and different sizes. The study revealed the presence of two distinct stages of coalescence. The early-stage coalescence was found to be enhanced with an increase in the impact velocity; however, the late-stage coalescence behavior remained unaffected by the impact velocity. Further, the coalescence dynamics of polymeric drops of different materials, as witnessed in multi-jet printing, was probed. This study shed light on the mechanisms that drive the mixing process at different stages of drop coalescence.

Finally, we evaluated the effects of the *in-situ* photopolymerization on the coalescence dynamics of multiple polymeric drops deposited on a substrate. Here too the comparative values of the drop dynamics timescale and the photopolymerization became important. Our results show three-distinct regimes characterizing the bridge growth which was further validated through physics-based theoretical scaling. This study would provide key insights into the direct-ink writing process and would aid in designing parameters for polymer-based additive manufacturing and product repair.