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AI-assisted determination of refractive index and mass concentration of individual spray droplets using TSTOF light-scattering signals☆

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ABSTRACT

In this work, we investigate whether light-scattering signals recorded by a Time-Shift–Time-of-Flight (TSTOF) instrument contain sufficient information to recover refractive index and mass concentration and demonstrate how artificial intelligence (AI) can exploit this information. Accurate determination of the refractive index and mass concentration of individual dynamic droplets is essential for the characterization of transparent and suspension droplets in industrial spray processes. Conventional optical diagnostics cannot provide these quantities for individual droplets in motion, and current TSTOF-based instruments are generally limited to size, velocity, and opacity, especially under dense spray conditions. Controlled measurements were performed on suspension droplets with concentrations from 0% to 100% and on transparent droplets from water–glycerin mixtures with refractive indices between 1.30 and 1.40. For each droplet, light-scattering signals were recorded as it traversed an elliptical Gaussian beam. AI models were trained on different combinations of these signals. The results demonstrate that AI-enhanced TSTOF diagnostics enable real-time, composition-sensitive characterization of dynamic droplets and significantly extend the capabilities of current optical spray measurement systems.

1. Introduction

In spray characterization, accurate determination of the refractive index (m) and mass concentration of individual dynamic droplets is as essential as measuring droplet size (d) and velocity (v). These parameters enable discrimination between transparent droplets according to their liquid composition and between suspension droplets according to their solid loading or mass concentration of solid particles. While static droplets can be isolated for detailed optical analysis, dynamic droplets move with a finite velocity within a spray or flow and cannot be extracted from the flow for compositional measurements. For individual static droplets levitated acoustically (Zaitone et al., 2006; Zaitone, 2009; Yu, 2013) or electromagnetically (Heinisch, 2008; Bakić et al., 2008; Bakić, 2010), the refractive index can be derived from rainbow scattering, and the mass concentration from the Lambert–Beer relation. To determine the refractive index from an ensemble of droplets in a flow, rainbow-based methods (Roth et al., 1991; Wu et al., 2016) can be applied, provided that the droplets exhibit nearly identical properties and the flow remains sufficiently stable. However, no commercial instrument currently allows refractive-index or concentration measurements for individual droplets in motion, despite the high relevance of these quantities in applications such as bioprinting, coating, agricultural spraying, and powder production. In bioprinting, for example, monitoring the refractive index of transparent print droplets could provide insights into the state of organic material during medical manufacturing, while in suspension-based processes the mass concentration is crucial for powder production and quality control. For dynamic but localized droplets, such as droplets generated in a stable droplet chain, light-scattering flow cytometry can be applied (Fulwyler, 1968; Herzenberg et al., 1981). In such configurations, the droplets follow well-defined trajectories and can be analyzed under controlled conditions similar to microfluidic systems.

Moreover, the measurement of refractive-index and/or concentration measurements are directly relevant to heat and mass transfer in turbulent multiphase flows. Local droplet composition and refractive index are closely linked to solvent/solute concentration, temperature-dependent properties, evaporation and condensation behavior, and,

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