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Numerical investigation of droplet pre-dispersion in a monodisperse droplet spray dryer

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ABSTRACT

Monodisperse droplet spray dryers have great advantages in particle formation through spray drying because of their ability to produce uniform sized particles. Experimental analyses of this system have shown that droplets atomized through the piezoceramic nozzle need to be sufficiently well dispersed before entering the drying chamber to achieve sufficiently dried particles. However, the dispersion dynamics cannot be readily observed because of experimental limitations, and key factors influencing the dispersion state currently remain unclear. This study carried out numerical simulations for droplet dispersions in the dispersion chamber, which allow this important process to be visualized. The systematic and quantitative analyses on the dispersion states provide valuable data for improving the design of the dispersion chamber, and optimizing the spray drying operation.

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Introduction

Spray drying allows a large quantity of liquid to be dried in a single unit, and is used to produce a wide range of powder products. Spray drying has applications in food, pharmaceutical, and chemical industries (Chen & Patel, 2008; Liu, Wu, Selomulya, & Chen, 2011; Paudel, Worku, Meeus, Guns, & Van den Mooter, 2013; Rogers, Wu, Lin, & Chen, 2010; Wu, Amelia et al., 2011). In a typical spray drying process, the solution to be dried passes through a spray nozzle, which facilitates its atomization into a spray of tiny drops. Introducing a stream of hot gas into the main drying chamber provides the necessary activation energy via heat and mass transfer to evaporate the solvent. This produces low-moisture particles at the dryer outlet. A primary objective of spray drying is to achieve sufficiently dried powders to meet specified standards, and to obtain particles of desirable and consistent morphology. There is typically a desirable particle size, for instance to maximize the efficacy of drug delivery (Lei, Gao, Wu, Wu, & Chen, 2016). However, the particle morphology is highly influenced by the dryer configuration (in

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terms of nozzle type and flow pattern) and operating settings (in terms of input conditions).

The validation of laboratory-wide spray drying by traditional models has been hampered by the wide variation in the morphology and size of the atomized droplets (Huang, Kumar, & Mujumdar, 2004; Jin & Chen, 2009a, 2009b). A large number of droplets are continuously ejected from the nozzle orifice, and they experience distinctive trajectories and heating histories (Jin & Chen, 2009b). The collected particles then exhibit different sizes and morphologies. Generating uniform sized droplets requires a simple robust set-up that provides precise control of the spray drying operation. This requirement has led to the development of a laboratory scale monodisperse spray dryer (MDSD) (Patel & Chen, 2008a; Rogers, Fang, Lin, Selomulya, & Chen, 2012; Rogers, Wu, Lin, & Chen, 2012; Shakiba, Mansouri, Selomulya, & Woo, 2016; Woo, Rogers, Lin, Selomulya, & Chen, 2011; Woo, Rogers, Selomulya, & Chen, 2012).

A schematic representation of the monodisperse nozzle, dispersion chamber, and main drying chamber is shown in Fig. 1. A detailed description of the MDSD can be found elsewhere (Woo et al., 2011; Woo, Rogers et al., 2012b). Typical monodisperse dryers have been designed such that droplets pass through a dispersion chamber, before entering the main chamber. This design exploits the full benefits of spray drying, as droplets pre-dispersed in the dispersion chamber reportedly yield sufficiently dried powders. An

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Nomenclature

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Ap	Droplet/particle surface area (m ²)
$C_{\rm p}$	Specific heat under constant pressure (J/(kgK))
$d_{\rm p}$	Droplet/particle diameter (m)
Ê	Energy
$\Delta H_{\rm L}$	Latent heat of water vaporization (J/kg)
h	Heat transfer coefficient $(W/(m^2 K))$
$h_{\rm m}$	Mass transfer coefficient (m/s)
$\overrightarrow{J_i}$	Diffusion flux of species <i>j</i>
\vec{k}_{eff}	Effective conductivity
Ν	Number of the droplets/particles
т	Mass (kg)
Ņ	Mass flow rate (kg/s)
$Q_{\rm p}$	Droplet position
R	Universal gas constant
Т	Temperature (K)
t _r	Residence time (s)
Χ	Moisture content (kg/kg, db)
Greek symbols	
α	Coefficient for linear shrinkage models
ρ	Density (kg/m ³)
Subscrints	
h	Bulk
d	Dispersion chamber
n	Particle/droplet
P r	Pasidonco
I C	Surface
3	Vapor
V	Vapor Water
vv	VValei

inefficient water removal process can be necessary in the absence of droplet pre-dispersion. In a similar manner, tuning the operating settings that control droplet distribution has been found to significantly affect the conditions of the resulting powder (You et al., 2014). However, key factors that could influence droplet dispersion remain unclear and unexplored, due to experimental limitations in visualizing the dispersion dynamics. Numerical modeling has therefore been developed to better understand the intricacies of this process.

Modeling and simulations can provide insights into spray drying systems, and are useful for prediction, control, and optimization (George, Chen, Xiao, Woo, & Che, 2015). Computational fluid dynamics (CFD) tools such as ANSYS Fluent or a version of CFX, FLOW3D, COMSOL Multiphysics, etc. (for 1-3 dimensions (1-3D)), and even EXCEL and MATLAB (usually for 1-2D), have frequently been used to model spray drying (Huang, Kumar, & Mujumdar, 2003; Huang et al., 2004; Mezhericher, Levy, & Borde, 2010a; Mezhericher, Levy, & Borde, 2010b; Patel & Chen, 2008a, 2008b; Putranto & Chen, 2013; Woo, Che, Daud, Mujumdar, & Chen, 2012). Wall deposition, agglomeration, powder quality degradation, and so on have been studied to a large extent, and the focus of these studies has been restricted to the main drying zone (Jin & Chen, 2010; Sadripour, Rahimi, & Hatamipour, 2012; Ullum, Sloth, Brask, & Wahlberg, 2010; Woo et al., 2011; Woo, Che et al., 2012; Woo, Rogers et al., 2012b). The current study focusses on the dispersion segment of the MDSD, as there has been little or no previous study in this aspect. Little or no simulation work has been reported for the dispersion domain. In the few studies where the MDSD has been considered, unrealistic dispersion states were adopted in which the authors assumed four (i.e. the 2D model of Woo et al. (2011) and five (i.e. the 3D model of Yang, Xiao, Woo, and Chen (2015) injection points at the inlet of the main drying chamber. These were intended to approximate the state of dispersion, but are clearly not accurate models. The significant size difference between the dispersion chamber and main dryer also makes numerical coupling of the entire system in a single set very cumbersome. Such modeling has thus far yielded little or no success. A systematic approach of the situation requires starting one thing at a time, to gain a broader understanding of this aspect.



Fig 1. Schematic diagram of the monodisperse spray dryer and expanded view of the dispersion zone (left), and its mesh (right).

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