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Simulation of fine polydisperse particle condensational growth under an octadecane–nitrogen atmosphere

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ABSTRACT

The evolution of particle size distribution (PSD) of fine polydisperse particles at high number concentrations ($>10^5 \text{ cm}^{-3}$) was simulated through a combined model employing direct quadrature method of moments (DQMOM) with heat and mass transfer equations. The PSD was assumed to retain log-normal distribution during the heterogeneous condensation process. The model was first verified by exact solution and experimental data prior to investigating the influence of initial conditions on final PSD under an octadecane–nitrogen atmosphere. Low particle number concentrations and high vapor concentrations were beneficial to shift the PSD to larger particles having a narrower distribution. Additionally, vapor depletion has more influence on the final PSD than the heat release parameter for a number concentration of 10^6 cm^{-3} . This study may assist the design process of a gas–solid separating cyclone, to eliminate dust from high-temperature volatiles by pyrolysis of solid fuels.

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Introduction

Oil shale, a sedimentary rock embedded with organics named kerogen, is widespread in the world as unconventional energy (Dyni, 2003; Han, Jiang, & Cui, 2009; Niu, Wang, Han, & Jiang, 2013). Solid heat carrier pyrolysis technologies are superior in utilizing small-size oil shale particles, and in obtaining high shale oil yields comprising high heat-value gas products when compared with gas heat carrier processes (Lai et al., 2015; Niu et al., 2013). However, the high dust content in shale oil severely restricts the application of this process (Li, Deng, & Yu, 2012). Therefore, the separation of dust from pyrolysis vapor is of great importance.

Many conventional methods are efficient in eliminating large particles from gases, however, the removal of fine particles remains a challenge (Chen, Shu, & Yang, 1993; Wu, Pan et al., 2016). Heterogeneous condensation—which can induce water vapor condensation on the particle surface—is an effective method to improve the separation efficiency of fine dust from flue gas (De Joannon, Cozzolino, Cavaliere, & Ragucci, 2013; Liu, Chen, & Lu,

2017; Wu, Pan, et al., 2016; Wu, Yang, Yan, Hong, & Yang, 2016). Fine particles serve as a condensation nucleus upon ingress into the condenser and form droplets that encapsulate solids (Jendoubi et al., 2011; Lédé, Broust, Ndiaye, & Ferrer, 2007). In this process, particles enlarge with respect to both mass and size as a function of continuous vapor condensation, and additionally, particles having liquid films increase their probability to inter-agglomerate.

According to this principle, the idea of staged condensation is proposed for the pyrolytic volatile removal of dust, with components having high dew points being first to condense on the particle surface. Thus, such components are captured in high-temperature collectors in more numbers, while fewer particles having the minimum amount of heavy components and maximum dust-free light components are concentrated in low temperature collectors. In fact, the influence of staged condensation temperature on the fractionation of bio-oil has been previously studied (Chang, Wu, Lin, Wan, & Lee, 2012; Johansson et al., 2017; Pollard, Rover, & Brown, 2012; Sui et al., 2014; Westerhof et al., 2011).

Conversely, the particle size distribution (PSD) of pretreated particles by staged condensation may influence the separation efficiency of gas phase dust separation. Application testing (Chen et al., 1993) has shown improved elimination of fine particles across a wide range of diameters in the presence of a cyclone with pre-condensation of water vapor on the particles. Additionally, except for enlargement of the particles after condensation, particles will

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grow to a narrower size distribution than the initial size distribution of the particles before condensation (Heidenreich & Ebert, 1995), which also benefits cyclone performance. The key of the innovative route is the control of condensation in determining the PSD evolution under stage-decreased temperatures.

The evolution of PSD can be described by the population balance equation (PBE), which can be solved by several methods including the moment method (Marchisio & Fox, 2005; McGraw, 1997), multi-class method (Kumar, Peglow, Warnecke, Heinrich, & Mörl, 2006; Qamar & Warnecke, 2007), weighted residuals method (Pourmehran, Rahimi-Gorji, Gorji-Bandpy, & Ganji, 2015; Pourmehran, Rahimi-Gorji, Hatami, Sahebi, & Domairry, 2015; Rahimi-Gorji, Pourmehran, Gorji-Bandpy, & Ganji, 2015; Rahimi-Gorji, Pourmehran, Hatami, & Ganji, 2015; Rahimi-Gorji, Pourmehran, Gorji-Bandpy, & Ganji, 2016), and the Monte Carlo simulation method (Meimaroglou & Kiparissides, 2007). Presently, the study on PSD evolution of fine polydisperse particles at high number concentrations during heterogeneous condensation is rather scarce. An analytical model to simulate the condensational growth of polydisperse aerosols was proposed in the continuum and transition regime (Jung, Park, & Kim, 2006; Park, Lee, Shimada, & Okuyama, 2001; Park, Lee, Shimada, & Okuyama, 2002), and a log-normal distribution was applied to describe particle distribution. The model was appropriate to a low number concentration, while neglecting vapor depletion and latent heat release. However, for higher particle number concentrations this assumption is not appropriate. A discrete method was adopted, which did not cap number concentration, and classified the entire PSD in linear intervals (Tammaro, Di Natale, Salluzzo, & Lancia, 2012). However, significant computation time is necessary for a wide PSD system (Geng, Nie, & Marlow, 2012).

In this paper, a model was built to simulate PSD condensational growth at high number concentrations based on previous studies (Jung et al., 2006; Park et al., 2001, 2002). To solve the condensation equation, the direct quadrature method of moments (DQMOM) (Marchisio & Fox, 2005) coupled with the heat and mass transfer equations was applied, in addition to utilizing the log-normal distribution. The model was first verified by exact solution and experimental data from literature, and thereafter, was adopted to estimate the effects of initial particle and vapor conditions on the evolution of PSD under an octadecane–nitrogen atmosphere.

Model development

A schematic diagram of heterogeneous condensation in a tube is illustrated in Fig. 1. Carrier gas in the presence of vapor and particles is fed into the cylindrical tube at a constant wall temperature, which is lower than the gas mixture (Kim, Hong, Kwon, & Park, 2011). With axial downward particle flow along the tube, supersaturation of the vapor phase is achieved and the particles enlarge by condensation. The process involves both heat and mass transfer and the condensational growth of particles.

Heat and mass transfer modeling

Temperature and vapor pressure profiles in the cylindrical tube can be obtained by solving the Navier–Stokes equation (Ghadirian & Arastoopour, 2016, 2017; Milioli, Milioli, Holloway, Agrawal, & Sundaresan, 2013). The physical properties of the gas and vapor at the mean temperature are assumed to be constant in a fully developed laminar flow (Lewis & Hering, 2013; Tammaro et al., 2012). Additionally, the boundary conditions are on the basis of the assumption that the vapor is saturated at a constant film temperature along the tube wall. With the aforementioned assumptions in

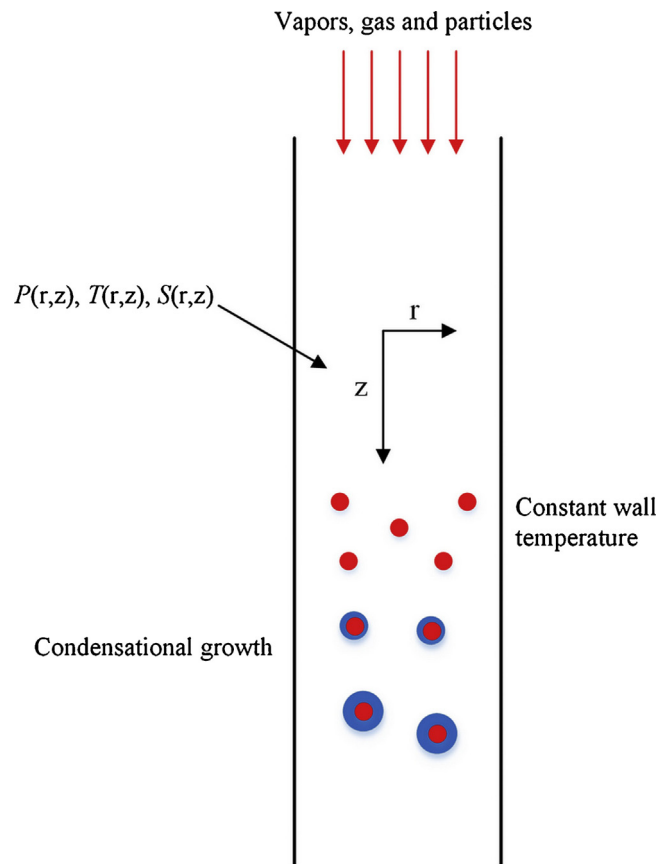


Fig. 1. Schematic diagram of heterogeneous condensation in a tube.

mind, the heat and mass transfer equations can be written as (Bird, Stewart, & Lightfoot, 2002):

$$2U [1 - (r/R)^2] \frac{\partial T}{\partial z} = \alpha \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right), \quad (1)$$

$$2U [1 - (r/R)^2] \frac{\partial P_v}{\partial z} = D \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial P_v}{\partial r} \right), \quad (2)$$

where z and r are the axial and radial coordinates, R is the tube radius, α and D are the thermal diffusivity of gas and mass diffusivity of vapor, respectively, and U is the average velocity of the gas flow.

Boundary conditions for Eqs. (1) and (2) are listed as:

$$T(r, 0) = T_0, \quad (3)$$

$$P(r, 0) = P_0, \quad (4)$$

$$T(R, z) = T_w, \quad (5)$$

$$P(R, z) = \min \{ P_0, P(T_w) \}, \quad (6)$$

$$\frac{\partial T}{\partial r} \Big|_{r=0} = 0, \quad (7)$$

$$\frac{\partial P}{\partial r} \Big|_{r=0} = 0, \quad (8)$$

where T_0 and P_0 are the gas temperature and the vapor pressure at the tube inlet, T_w is the wall temperature and $P(T_w)$ is the saturation pressure of vapor at wall temperature T_w .

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