



Thermophoretic capture of submicron particles by a droplet



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HIGHLIGHTS

- The available formula overestimates the thermophoretic capture efficiency.
- The relative deviation varies remarkably with temperature difference and Re .
- Assumption of uniform particle concentration distribution leads to the deviation.
- A corrected formula for thermophoretic capture efficiency is established.

ARTICLE INFO

Article history:

Received 29 June 2016
 Received in revised form
 1 September 2016
 Accepted 4 October 2016
 Available online 5 October 2016

Keywords:

Particulate matter
 Droplet
 Thermophoresis
 Deposition efficiency

ABSTRACT

Thermophoresis is an important mechanism for submicron particle capture by droplets. The thermophoretic deposition efficiencies under varying Reynolds (Re) numbers and temperature differences are obtained from the direct numerical simulation of the submicron particle flowing around the droplet. Comparison of the results calculated under the same conditions through the classical thermophoretic deposition efficiency formula and by numerical simulation shows that the Davenport formula always returns greater values than the numerical simulation, by a relative deviation of 19.8%–63.8%. The relative deviation decreased first and then increased with increasing difference in temperature, and increased gradually with increasing Re . The deviation resulted from the assumption that the particle concentration on the droplet surface is equal to that of the incoming flow in the formula deduction process. The convection of the gas and the thermophoresis of the particles together determined the migration of the particles in the boundary layer, and so determined the particle concentration distribution on the surface of droplets. Thus, the particle concentrations on the surface of droplets are actually lower than those of the incoming flow and are distributed bimodally on the surface. The dimensionless particle concentration on the surface of droplets decreased with increasing Re , and increased first then decreased later with increasing difference in temperature. The dimensionless thermophoretic driving velocity and Re were adopted to correct the formula. The results calculated by the corrected formula were consistent with the numerical simulation employed in this paper, such that the maximum relative deviation was reduced from the original 66.8% to less than 8%.

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1. Introduction

Particulate matter is a critical pollutant in the atmospheric environment of many countries (Agudelo-Castaneda et al., 2013; Li et al., 2014). Fine particle pollution is becoming more stringent. Wet scrubbing and wet deposition are efficient methods of removing particles from industrial flue gas and from the atmosphere (Park et al., 2005; Queen and Zhang, 2008; Bae et al., 2010; Guo et al.,

2014). Particle capture by a single droplet is the foundation of both processes (Jaworek et al., 2006); studies on single droplet capture are significant for developing industrial wet scrubbing technologies and understanding the capacity and mechanisms of wet deposition in the atmospheric environment.

In wet deposition and wet scrubbing processes, particle-carrying gas flows around the droplet. Particles can collide with the droplet surface during flow, under inertia, interception, Brownian mechanism, electrostatic mechanism, diffusio-phoresis and thermophoresis (Kraemer and Johnstone, 1955; Pranisha and Kamra, 1996; Chate and Murugavel, 2011; Carotenuto et al., 2010). The single droplet efficiency is a basic input parameter in predicting

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the efficiency of wet deposition and wet scrubbing (Lee et al., 2006). For the convenience of calculation, the deposition efficiencies of single droplets under the effect of different capture mechanisms were organized to the empirical concise formula (Park et al., 2005). Deposition efficiencies are the function of dimensionless numbers in the capture process. The classical deposition efficiency calculation includes the following: the formula proposed by Slinn (1977), which is used for calculating the inertial deposition efficiency, interception deposition efficiency, and Brown diffusion deposition efficiency; and the thermophoretic deposition efficiency formula proposed by Davenport and Peters (1978). The total particle deposition efficiency of single droplets is the sum of the calculated deposition efficiencies under different mechanisms. Both the formulaic and numerical calculations of efficiency show that thermophoresis is the most important mechanism for sub-micron particle capture by droplets. Bae et al. (2009) estimated the relative contribution of thermophoresis in the wet deposition process through the thermophoretic deposition efficiency formula and found that the removal coefficient of 1- μm particles increased from 10^{-7} to 10^{-6} at 5 °C of temperature difference. In the industrial wet spraying process, a few degrees of temperature difference between the droplets and the gas results in a higher submicron particle deposition efficiency. Pilat and Prem (1976) performed a numerical simulation on the deposition efficiencies of single droplets on particles of different sizes as the temperature difference increases from 5 °C to 60 °C; the deposition efficiency of 1- μm size particles increased by two orders of magnitude, from 0.001 to 0.25, under the effect of thermophoresis.

The thermophoretic deposition efficiency formula proposed by Davenport and Peters (1978) is presently the only empirical formula for predicting the thermophoretic deposition efficiency of single droplets. Through experiments and numerical simulation, Wang et al. (1978) studied the deposition efficiency of droplets of 0.1 mm–1 mm size on 0.5- μm particles, under a 3 °C temperature difference between the environment and the droplet surface. Comparison between the experimental data and the predicted values by the Davenport thermophoretic deposition efficiency formula showed that the latter overestimated the former by a relative deviation of 24.1%–47.8%. Viswanathan (1999) performed a numerical simulation of the deposition efficiency of droplets on particles of 0.1 μm –1 μm size under a temperature difference of 10 °C–80 °C and with a droplet Reynolds number (Re) of 1.54–400 (characteristic size is the droplet diameter). The predicted values by the thermophoretic deposition efficiency formula (Davenport and Peters, 1978) were found to overestimate the numerical calculation results by 10%–50%. The classical deposition efficiency calculation is based on specific assumptions, theoretical analysis, and experimental data. Numerical simulation (Wang et al., 2015) of particle capture by single droplets show that the discrepancy between the research hypothesis and the actual process will likely result in deviations in the calculated values by the classical deposition efficiency formula and the actual values. Correction is needed based on the thermophoretic deposition behavior. The thermophoretic deposition efficiency of single droplets is the basis for analyzing industrial spraying and wet deposition process of fine particles. Further discussion should thus be made on the reason for the large deviation in the calculated value by the traditional thermophoretic deposition efficiency formula. A more accurate prediction method of the thermophoretic deposition efficiency of droplets is also urgently needed.

Previous literature (Wang et al., 2015) has studied the thermophoretically driven migration of submicron particles when flowing around droplets under different conditions by direct numerical simulation. Based on the simulated migration of submicron particles, the present paper reports the thermophoretic deposition

efficiency of particles flowing around a droplet under different temperature differences and Re numbers. The differences between the results of direct numerical simulation and that calculated by the thermophoretic deposition efficiency formula are presented. The causes for the calculation error in the thermophoretic deposition efficiency formula are analyzed. A quantitative correction method applied to the thermophoretic deposition efficiency formula is put forward.

2. Governing equations and numerical method

2.1. Equations of particle motion and gas flow

In wet deposition and wet scrubbing processes, the gas that carries particles flows around the droplet as shown in Fig. 1. When the temperatures of the droplet and the atmospheric gas differ, the particles deviate from the streamline due to inertia, Brownian force, and thermophoretic force, causing the particles to collide with the droplet surface. The particles are assumed to be captured once they touch the droplet surface, which aligns with common wet deposition and wet scrubbing processes. The droplet is assumed to be a sphere with a constant diameter because the reduction in diameter from evaporation is negligible, actual deformation is slight in droplets with diameters less than 2 mm, and circulation inside the droplet is weak compared with outside flow (Pruppacher and Klett, 2010). The coordinate system is established with the center of the droplet as the origin. The equations of hydrodynamics can be expressed as follows:

$$\vec{\nabla} \cdot \vec{u} = 0 \quad (1)$$

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \vec{\nabla}) \vec{u} = -\frac{1}{\rho_f} \vec{\nabla} p + \nu \Delta \vec{u} \quad (2)$$

$$\frac{\partial T}{\partial t} + (\vec{u} \cdot \vec{\nabla}) T = \frac{\lambda}{\rho_f c_p} \Delta T \quad (3)$$

where t is the time, \vec{u} is the gas velocity relative to droplet, ρ_f is the density of gas, p is the pressure, ν is the kinematic viscosity of gas, T is the local gas temperature, c_p is the specific heat capacity, and λ is the thermal conductivity.

The particles in the gas flowing around the droplet are tracked by Lagrangian equation. As per the results of Pilat and Prem (1976), the thermophoretic force is two to three orders of magnitude greater than the Brownian diffusion force acting on submicron particles when the temperature difference is above 10 °C. Therefore, Brownian diffusion force is ignored in this study. The particle motion equation is given as:

$$m_p \frac{d\vec{v}}{dt} = \vec{F}_D + \vec{F}_T \quad (5)$$

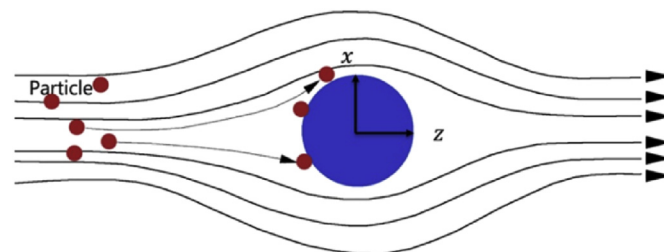


Fig. 1. Schematic diagram of the capture of particles by a droplet.

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