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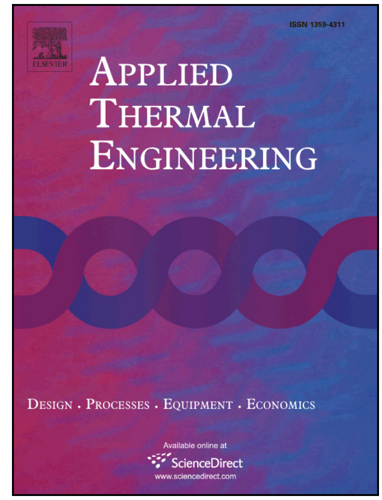

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Numerical Simulation on Circulation Flow and Mass Transfer inside Atmospheric Water Drops

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Abstract: When a water droplet moves in atmosphere with pollutant, internal circulation is formed due to surface shear stress. This enhances internal mass transfer greatly, and improves the spray droplet SO_2 absorption. In this paper, the internal circulation and diffusion of SO_2 in a water droplet were numerically studied. The distribution of tangential velocity at the interface and the effect of interior circulation on sulfur dioxide transfer are analyzed under different Reynolds numbers. The numerical results indicate that there are two symmetrical vortexes inside the droplet when there is a relative motion between gas and liquid phase. The distance between the vortex core and the droplet center is around $2/3R_d$, and the vortex velocity increases with the Reynolds numbers. The study shows sulfur dioxide absorption by the droplet is controlled by two mechanisms, w are (1) the radial diffusion due to concentration gradient; and (2) mass transport induced by internal circulation. The characteristic times of radial diffusion and vortex formation are compared. The comparison indicates that the internal circulation dominates sulfur dioxide mass transfer inside the water droplet. The internal circulation influences the sulfur dioxide mass transfer greatly with the increase of Reynolds number. On the other hand, the effect of deformation rate on mass transfer is insignificant because of the characteristic time are of the same order with the same Reynolds number.

Key words: droplet, internal circulation, VOF, sulfur dioxide, mass transfer, numerical simulation

Introduction

Due to extensive burning of fossil fuels, the atmosphere is filled with aerosol particles and air pollutants. These aerosol particles and air pollutants have caused severe environmental problems such as acid rain and haze, which have aroused extensive attention in China [1-5]. In all air pollutants, sulfur dioxide and nitrogen oxides are the major harmful elements. It is well known that acid rain is formed when sulfur dioxide and nitrogen oxides are absorbed by rain droplets. It is a great challenge to control air pollutants. Accordingly, the precise prediction on sulfur dioxide or nitrogen oxides absorption plays a vital role in understanding and controlling acid rain pollutions.

Sulfur dioxide or nitrogen oxides absorption by droplets is a series of processes related to mass transfer between gas and liquid phases. In the past several decades, a variety of theoretical models such as the film theory, penetration theory and eddy diffusion theory have been developed to describe the process of mass transfer [7-9]. The aforementioned mass transfer theories focused on the droplet interface at macro scale. The unsteady aqueous-phase oxidation of sulfur dioxide around a stagnant droplet contains five stages, which are gas-phase diffusion; mass transfer at the interface; aqueous dissociation reaction; aqueous-phase diffusion; and aqueous chemical reactions, as shown in Figure 1 [10]. Although this problem has been extensively studied adopting theoretical, experimental and numerical method and many important results have been accomplished, there are relative few studies connected to mass transfer of drops with internal circulation.

According to the published literature, internal circulation or vortex inside a drop was introduced by velocity boundary layer when the air flows around a droplet. Four approaches were used to study the internal circulation of a falling droplet. Of such, the boundary layer theory, numerical method, and experimental measurement obtained agreeable results for droplets with radii < 500μm [11]. The internal circulation in an evaporating drop was also reported in details [12-16]. There exists only a few papers concerned mass transfer of droplet with internal circulation. A convective-diffusion equation was developed to describe the gas absorption accounting the internal flow given by

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