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Submicron particle dynamics for different surfaces under quiescent and turbulent conditions

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HIGHLIGHTS

- Modeling both coagulation and deposition to predict aerosol behavior accurately.
- Both coagulation and deposition are significant for submicron particles.
- Surface roughness and turbulence have a cumulative effect in increasing deposition.
- Increasing turbulence helps reduce aerosol peak concentration faster.

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ABSTRACT

Experiments were conducted using CsI aerosols in a small scale test chamber to simulate behaviour of aerosols in the containment of a nuclear reactor. The primary focus of the study was on submicron particles (14.3 nm–697.8 nm) due to their hazardous effect on human health. Different wall surfaces, viz., plexiglass, concrete and sandpaper were chosen to study the effect of surface roughness on dry deposition velocity under both quiescent and turbulent conditions. An analytical approach to calculate dry deposition velocity of submicron particles for rough surfaces has been proposed with an improvement in the existing parameterization for shift in the velocity boundary layer. The predicted deposition velocity with the improved parameterization was found to have better agreement with published measured data of Lai and Nazaroff (2005) compared to the existing parameterizations (Wood, 1981; Zhao and Wu, 2006b). There was a significant reduction in root mean square error (RMSE) between predicted, using the improved parameterization and measured deposition velocity (upto 100%) compared to earlier ones. The new analytical deposition approach was coupled with volume conserving semi-implicit coagulation model. This aerosol dynamic model was evaluated against explicit particle size distribution for the first time for rough surfaces. Normalized RMSE between simulated and measured particle size distribution varied in the range of 2%–20% at different instances. The model seems to closely predict submicron particle behaviour in indoor environment.

1. Introduction

In a nuclear reactor, under postulated accident conditions, the cooling to the reactor fuel can be lost and the fuel gets overheated. This overheating can lead to fuel damage causing release of radioactive fission products in the form of aerosols (Sapra et al., 2008). These aerosols get transported through the broken coolant system and reach the containment which is the final barrier in their release to the public domain. The study of the behaviour of aerosols in the containment is a subject of research worldwide (Fischer and Kanzleiter, 1999). These studies are important to characterize the source term into the environment so that the effect of radioactivity in the public domain can be quantified and possibly mitigated by confinement within the containment. The aerosol particles released during such scenarios are reported to have a diameter in the size range of 0.1 μm–20 μm, covering both the continuum and

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Nomenclature

A	Surface area (m^2)
β	Coagulation kernel (m^3 s^{-1})
b	Effective roughness height (μm)
C	Particle number concentration (cm^{-3})
D	Brownian diffusivity of particle (cm^2 s^{-1})
d	Particle diameter (nm)
e	Shift in velocity boundary layer (μm)
e^+	Dimensionless parameter for shift in velocity boundary layer
ε	Turbulent (eddy) diffusivity of particle (cm^2 s^{-1})
$f_{i,j,k}$	Volume fraction of colliding particles of bin i & j partitioned into bin k
J	Particle flux given by Fick's law (cm^{-2} s^{-1})
k^+	Dimensionless surface roughness height
k_s	Mean surface roughness height (μm)
Q	Sampling rate of instruments (m^3 s^{-1})
r^+	Dimensionless radius of particle
Sc	Schmidt number
t	Time (s)
u^*	Friction velocity (cm s^{-1})
V	Chamber volume (m^3)
v	Volume of a particular size bin (m^3)
v	Velocity of particle (cm s^{-1})
λ	Ventilation rate (h^{-1})
τ	Particle relaxation time (s)
Δt	Time step (s)
ν	Fluid kinematic viscosity (m^2 s^{-1})
y	Distance from the wall or surface (μm)

Subscripts

ceil	Ceiling (top surface of the chamber)
floor	Floor (base of the chamber)
wall	Vertical walls of the chamber
d	Deposition
p	Particle
s	Settling
t	Turbulent

slip flow regimes (Brockmann and Tarbell, 1984). From a health perspective, the submicron particles are of great concern due to their high number density, and ability to penetrate deep into the lungs and induce oxidative stress with cellular damage (Song et al., 2011). Natural attenuation of radioactive material occurs due to deposition of aerosols on the internal surface of a reactor (Slama et al., 2014). The aerosol inventory in the containment atmosphere depends on the aerosol released into the containment and aerosol removal processes like deposition, gravitational sedimentation, and leaks.

Deposition of particles onto the indoor surfaces of the reactor can effectively reduce the exposure to harmful aerosols unless resuspended. The essential mechanisms for deposition in the nuclear containment have been listed as Brownian and turbulent diffusion, turbophoresis, gravitational sedimentation, thermophoresis, convective transfer due to condensation of the vapours on the inner surface of the reactor, and centrifugal force in case of flow around a curved surface (Simons and Simpson, 1988; Alipchenkov et al., 2009).

Crump and Seinfeld (1981) derived a general formula for rate of aerosol deposition due to Brownian and turbulent diffusion as well as gravitational sedimentation in a turbulently mixed vessel. However, this model is valid when the inertial effects are insignificant. Indoor particle deposition onto smooth surfaces was modelled in Lai and Nazaroff (2000) and Mayya et al. (2004) taking into account deposition only due to Brownian diffusion, turbulent diffusion, and gravitational settling. A modified version of this model (popularly known as the three-layer model), taking turbophoresis also into consideration, has been proposed (Zhao and Wu, 2006a). It is an improved model, which correctly models the three different zones classified according to the particle relaxation times (turbulent diffusion regime, turbulent diffusion-eddy impaction regime, and particle inertia moderated regime).

Deposition onto rough surfaces has been studied both experimentally and theoretically, and similar trends of increase in deposition velocity with increase in particle sizes, turbulence and size of roughness were observed (Shimada et al., 1988; Shimada et al., 1989; Zhao and Wu, 2007; Hussein et al., 2009a,b). However, the numerical model proposed by Shimada et al. (1988) focused only on diffusion ignoring the gravitational sedimentation. Experimental studies were done in a 8 m^3 test chamber facility and they also showed similar results (Lai et al., 2002). Particle deposition on rough surfaces was found to be less than that on the smooth surfaces for small particles and low airflow condition. For large size particles and high airflow conditions, particle deposition on rough surfaces increased upto three times to that on smooth surfaces. Experimental studies for particle deposition in ventilation ducts have been carried out and the results modelled by applying a roughness of 180 μm as opposed to the hydraulic roughness of about 1600 μm measured by the axial pressure drop in the ventilation ducts (Sippola and Nazaroff, 2004). Wood (1981) assumed that for a rough surface, the virtual origin of the velocity profile is shifted by a distance $e(=0.55k_s)$ away from the wall, where k_s is the roughness height. This was incorporated in the boundary condition in the three-layer model of Lai and Nazaroff (2000) in order to study coarse particle deposition onto rough surfaces (Lai, 2005). Experiments were carried out using four sandpapers with different roughness scales (Lai and Nazaroff, 2005), but the model predicted satisfactory results only for the finer sandpapers. Zhao and Wu (2006b) have modelled particle deposition onto rough surfaces in ventilation ducts as an improvement of the three-layer model proposed in Zhao & Wu, (2006a) by incorporating surface roughness in the boundary condition. A new equation stated in Eq. (1) was fitted on the experimental data of Grass (1971) and Wan (1981) in order to calculate the shifted distance in the boundary layer (Zhao and Wu, 2006b). Both e^+ and k^+ are dimensionless parameters, which are described later in detail (Section 2.2.2).

$$\frac{e^+}{k^+}=\begin{cases}0 & k^+<3 \quad \text{Hydraulically smooth}\\ 0.3219\ln\left(k^+\right)-0.3456 & 3<k^+<30 \quad \text{Transition}\\ 0.0835\ln\left(k^+\right)+0.4652 & 30<k^+<70 \quad \text{Transition}\\ 0.82 & k^+>70 \quad \text{Completely rough}\end{cases} \tag{1}$$

The results predicted by the improved model agreed better with the measured data of Sippola and Nazaroff (2004) than the traditional model suggested by Wood (1981), but were not satisfactory. It was suggested that this may be due to the fact that Eq. (1) was obtained under the condition that the roughness was made up by