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Numerical investigation of the interaction, transport and deposition of multicomponent droplets in a simple mouth-throat model

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ABSTRACT

A basic analysis of inhaled multicomponent droplet-vapor interaction and subsequent aerosol deposition is very important for the understanding of natural phenomena as well as for health-care related applications. Employing a highly idealized mouth-throat (MT) model as a test bed, the transport and deposition mechanisms of a water-droplet are simulated, considering ethanol, sodium chloride and fluorescein as components. The flow-field equations are solved with a validated transition SST model which can predict the effects of flow rate, relative humidity (RH), and wet *vs.* dry airway walls on aerosol deposition efficiency (DE). The simulation results indicate that the hygroscopic growth of sodium chloride particles is sensitive to the saturation pressure of water vapor. A high flow rate decreases the RH in the airways as well as the average growth ratios of deposited and escaped droplets; but, still increases the DE. When compared to a dry boundary condition, the wet airway-wall increases the DE up to 4.6% when RH = 30% and the flow rate is 60 L/min. It also increases the average growth ratio of deposited droplets notably, i.e., larger than 0.5 for most conditions, while its effect on the average growth ratio of deposited droplets is not apparent. A high inlet RH can significantly enhance the hygroscopic growth of the droplets and DE, especially when it is larger than the RH threshold for the hygroscopic component. Besides, it can elevate the growth ratios of deposited and escaped droplets at the same time, which could be utilized to reduce the deposition of submicron hygroscopic aerosol in the upper airway.

1. Introduction

From air pollutants to cigarette smoke particles and pharmaceutical aerosols, many inhalable aerosols contain soluble and/or volatile components. As the humidity conditions in the human airways are normally higher than in the ambient atmosphere, these components can interact with water vapor, causing a change in aerosol size. Thus, aerosol - vapor interactions can significantly influence the trajectories of the aerosols and hence lung deposition.

Numerous experiments and simulations have been carried out to investigate the mechanisms of such aerosol - vapor interactions and to improve the efficiency of inhalers. For example, Cheng, Kleinstreuer, Kim and Zhang (2004a) numerically analyzed the effect of evaporation on JP-8 fuel droplet deposition in a human upper airway model. Later on, Kleinstreuer, Kim and Zhang (2006a) studied evaporative and hygroscopic effects on saline droplet deposition in upper airways, and concluded an increase in solute

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Nomenclature

A	surface area of the droplet
a_1, a_2, a_3	constants determined by particle Reynolds number
α_m	mass thermal accommodation coefficient
C_1,C_2	constants in Eq. (31).
C_c	Cunningham correction factor
C_D	drag coefficient
C_{Dd}	drag force coefficient for droplet
Cd_ω	cross-diffusion term
C_m	Fuchs-Knudsen number correction
C_μ	coefficient in the turbulent model
$c_{d,i}$	specific heat of the component i in the droplet
D	inlet diameter
D_e	mass diffusivity of component e
D_w	mass diffusion coefficient for water vapor
$\widetilde{D}_k$	modified term of destruction of turbulence kinetic energy
D_ω	dissipation of ω
d_d	droplet diameter
$E_{\gamma1}$, $E_{\gamma2}$	transition source and destruction source terms
f_i	damping functions for fluctuating velocity in near-wall region, $i = u, v, w$
f_u	streamwise damping function
f_v	damping function normal to the nearest wall
f_w	damping function normal to f_u and f_v
G_i	zero-mean, unit variance independent Gaussian random numbers
$\vec{g}$	gravitational acceleration
i	van't Hoff factor
K_e	Kelvin effect correction for component e
K_w	Kelvin effect correction for water vapor
Kn	Knudsen number
k	turbulence kinetic energy
l_e	eddy length scale
L_e	latent heat of evaporable component e
M_e	molar mass of the component of interest e
m_d	mass of the droplet
$m_{d,i}$	mass of the component i in the droplet
$\overline{n}_e$	the average mass flux of evaporable component e on the droplet surface
n_e	mass flux of evaporable component e
Nu	Nusselt number of the droplet
Pr	Prandtl number
P_k	production of turbulence kinetic energy
$\widetilde{P}_k$	modified term of P_k with intermittency
$P_{ve,sat}(T_d)$	saturation pressure of component e under temperature T_d
$P_{\gamma1}$, $P_{\gamma2}$	transition source and destruction source terms
$P_{\theta t}$	source term in Eq. (5).
p	fluid pressure
R	universal gas constant
R_e	gas constant of component e
R_w	gas constant of water vapor
r_∞	radius of the air around the droplet
Re_d	droplet Reynolds number
$\mathrm{Re}_{\theta t}$	critical Reynolds number
$\widetilde{Re}_{\theta t}$	transport scalar for momentum thickness Reynolds number
RH	relative humidity
Sc	Schmidt number
Sc_t	turbulent Schmidt number
Sh	Sherwood number of the droplet
T_a	temperature of the surrounding air
T_d	droplet temperature
T_L	fluid Lagrangian integral time
t	time
t_{cross}	eddy crossing time
t_1, t_2, t_3	constants in Eq. (30).
u	fluid velocity
$\vec{u}_d$	velocity vector of the droplet
u_i	instantaneous velocity of the fluid, $i = x, y, z$
$\bar{u}_i$	time average velocity
u_i'	fluctuating component
x_e	mole fraction of e in the droplet
x_s	mole fraction of soluble component, i.e., NaCl in the validation case
x_w	mole fraction of water
$Y_{e,surf}$	mass fraction of the evaporable component e on the interface of the droplet
$Y_{e,\infty}$	mass fraction of the evaporable component e in the surrounding gas
Y_w	mass fraction of the water vapor
$Y_{w,surf}$	mass fraction of the water vapor on the interface of the droplet
$Y_{w,\infty}$	mass fraction of the water vapor in the surrounding air
y	distance to the nearest wall
y^+	dimensionless wall distance

Greek

α_m	mass thermal accommodation coefficient
ΔT	temperature change in one time step
γ	intermittency
γ_e	activity coefficient of component e
γ_w	water activity coefficient
ξ_i	random numbers from standard normal distribution
λ	gas mean free path
λ_g	thermal conductivity of the surrounding gas
μ	dynamic viscosity of the fluid
μ_t	turbulent viscosity
υ	kinematic viscosity of the fluid
υ_t	turbulent eddy viscosity
ρ	fluid density
ρ_d	droplet density
ρ_g	density of surrounding gas
$\rho_{vw,sat}$	saturation water vapor density
σ	surface tension of the droplet
σ_k	turbulent Prandtl number for k
σ_ω	turbulent Prandtl number for ω
τ	particle relaxation time
τ_e	eddy lifetime
τ_w	wall shear stress
ϕ	heat flux
ω	specific dissipation rate