

Dispersion and settling characteristics of evaporating droplets in ventilated room

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Abstract

Movement and evaporation of small droplets in the room air are investigated in this paper through CFD simulations. A modified drift-flux model is presented with the droplet evaporation rate and the drift velocity expressed as simple algebra functions of droplet diameter, which is integrated in the transport equations of droplet number density and droplet bulk density. Evaporating droplets are treated as a continuum phase with one way coupling with the carrier phase, i.e. air. Our numerical simulations reveal that the distribution of the large evaporating droplets in the ventilated room air is characterized by a combination of the settling feature when droplets are first generated and released and the dispersion feature after the droplets are evaporated to be either very fine or become droplet nuclei. For droplets less than 50 μm in diameter, the dispersion feature is dominant in the test room that we simulated, while for droplets larger than 100 μm in diameter, the settling feature dominates. For evaporating droplets between these two sizes, the spatial distribution of droplets tends to be located at the lower part of the test room than that of small neutral aerosol particles. Within this size range, a lower initial position of the droplets in the room results in a higher deposition rate of the droplets on the floor.

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1. Introduction

The widespread of pollutant in nature and industrial process causes great concern of indoor air quality due to possible long exposure to aerosol particles which can cause significant health problems. Many previous works [1–3] have focused on investigating motion of particles in indoor environment. Contaminated droplets generated from processes such as coughing of a patient with chest infection, indoor spays, etc. are generally treated as aerosol particle due to their eventually shrinkage to a very small size [4] and their initial diameter is generally less than 100 μm . Droplets greater than 100 μm in diameter are generally considered being quickly settled and finally deposited on the floor. However droplets evaporate during their travel and movement in the room air which can be relatively dry. Droplets less than 100 μm in diameter can still have considerable

gravitational settling velocity at the beginning, which can make their transport behavior different from those very small and neutral aerosol particles. Previous studies show that small aerosol particles tend to distribute uniformly in a fully mixed room, while large particles with a greater settling velocity tend to settle in the lower part of the room. Particles greater than 10 μm in diameter shows obvious different distribution pattern from those smaller aerosol particles (without gravitational settling velocity) in a ventilated room [1,3]. Since the diameters of evaporating droplets reduce during the course of droplets transmission, the simulation of a constant-sized solid particle–gas flow cannot describe the dispersion behavior of the evaporating droplets. This paper focuses on the modeling of spatial distribution of droplets in a ventilated room considering both the gravitational settling and evaporation of droplets. A modified drift-flux model is presented to study the dispersion characteristics of evaporating droplets.

Murakami et al. [1] and Holmberg et al. [2] have studied the effectiveness of drift-flux model in predicting the

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Nomenclature			
\dot{m}_C	droplets mass density loss rate	Sc	Schmidt number of carrier phase
\dot{m}_d	single droplet evaporation rate	Sh	Sherwood number
A_d	droplet surface area	T	temperature
C	droplets bulk density	t	time
C_p	specific heat	\mathbf{V}	room air velocity vector
d_d	droplet diameter	\mathbf{V}_d	drift velocity vector
g	gravitational acceleration	Γ	binary diffusion coefficient
h	heat transfer coefficient	λ	thermal conductivity
h_m	mass transfer coefficient	μ	molecular viscosity of air
L	latent heat of droplet evaporation	ν_{eff}	effective kinematic viscosity
m_d	single droplet mass	ρ_d	droplet material liquid density
n	droplets number density	ρ_v	droplet material vapor density
Nu	Nusselt number	<i>Subscripts</i>	
Pr	Prandtl number	d	droplet
Re	Reynolds number	∞	surrounding air
		g	carrier gas phase

particle dispersion and deposition in ventilated rooms [1,2]. In a drift-flux model, the solid particles are considered as a continuum phase with the convection velocity as the sum of the gravitational settling velocity of the particles and the velocity of the carrier phase (air) at the local position. The gravitational settling velocity of different particle sizes leads to various particle distribution pattern in a ventilated room. In contrast to solid particles, the settling velocity of which remains at a constant value, the gravitational settling velocity of evaporating droplet reduces as its diameter reduces as a function of both space and time. This paper proposes a modified drift-flux model considering the variation of droplet diameters. The correlation between the settling velocity of the evaporating droplet and its varying diameter is included based on the consideration of the droplet evaporation process in the room air. The distribution of evaporating droplets in a ventilated room is predicted with a computational fluid dynamics method by using this modified drift-flux model.

2. Formulation

As in the drift-flux model, the droplets are treated as a continuum phase. As only dilute droplets loading are considered here, droplets have a negligible effect on the room airflow field. Thus, the droplets–air interaction is considered to be one-way coupling. Because of evaporation, the mass transport equation of droplets has a source term related to the evaporation rate of droplets. Droplets are assumed not to break up or coagulate during their evaporation and movement process. When the droplets completely evaporated, we assume that droplet nuclei form as a result of drying up. Under these assumptions, we deduce that the number of the droplets does not increase nor decrease during droplets evaporation. Therefore the droplets transport equations of the droplets number

density n and bulk density C can be written as

$$\frac{\partial n}{\partial t} + \nabla \cdot (n(\mathbf{V} + \mathbf{V}_d)) = \nabla \cdot \left(\frac{\nu_{\text{eff}}}{\sigma_n} \nabla n \right) + S_n, \quad (1)$$

$$\frac{\partial C}{\partial t} + \nabla \cdot (C(\mathbf{V} + \mathbf{V}_d)) = \nabla \cdot \left(\frac{\nu_{\text{eff}}}{\sigma_C} \nabla C \right) + S_C + \dot{m}_C, \quad (2)$$

where n is the number of droplets per unite volume, C is the droplets mass per unite volume, S_n and S_C are the source terms of droplets generation, \dot{m}_C in Eq. (2) is the droplet mass density loss rate due to evaporation. The droplets transport and dispersion are governed by the flow field of the carrier gas phase. Because the droplets phase to the room air is one-way coupling, the room air velocity \mathbf{V} and the effective kinematic viscosity ν_{eff} in Eqs. (1) and (2) are calculated independently with the standard two-equation k – ϵ turbulence model [5]. The two dimensionless numbers σ_n and σ_C are the turbulence diffusivity of the droplets number and mass density, which are both set as 1.0 in the present study. \mathbf{V}_d is the drift velocity for the droplets phase relative to the air phase, $\mathbf{V}_d = \mathbf{V}_{\text{droplet}} - \mathbf{V}$. The droplets mass density loss rate \dot{m}_C in a computational cell equals to the droplets number density n in that cell times the corresponding single droplet evaporation rate \dot{m}_d .

The single droplet evaporation rate \dot{m}_d and drift velocity \mathbf{V}_d in a computational cell is related to the local droplet diameter, while droplets number density and mass density of that cell provide the required information. With the assumption of droplet being spherical, a single droplet mass and diameter in a computational cell is $m_d = (\pi/6)d_d^3\rho_d = C/n$. For a droplet of a given initial diameter, its evaporation rate \dot{m}_d and drift velocity \mathbf{V}_d vary as its diameter decreases. The algebra relationship between the two can be obtained by solving the momentum and mass conservation equations of a single droplet through its evaporation process.

Previous study shows if the ratio of the droplet density to the density of the carrier fluid is large, the Stokes drag and the gravity forces are dominant, and the other forces can be assumed negligible [6]. For indoor contaminant droplets, their density is much larger than the air density. Therefore the momentum equation for a single droplet can be written as [7]

$$\frac{dV_{\text{droplet}}}{dt} = \frac{V - V_{\text{droplet}}}{\tau_d} + g. \quad (3)$$

The droplet relaxation time $\tau_d = (\rho_d d_d^2 / 18\mu)$. Substitute the droplet drift velocity into the Eq. (3), for a steady-state room airflow, we have

$$\frac{dV_d}{dt} = -\frac{18\mu}{\rho_d d_d^2} V_d + g - (V \cdot \nabla)V. \quad (4)$$

The room air velocity and velocity gradient are generally small. In our test room to be studied, $(V \cdot \nabla)V$ is in the order of 10^{-2} m/s^2 in the vertical direction, much smaller than the gravitational acceleration. In the horizontal direction, we assume the droplets can quickly catch up with the surrounding air velocity. Therefore the momentum equation only need to be solved in the vertical direction with where the last term on the right hand of Eq. (4) is negligible. Consequently the droplet drift velocity equation is simplified to vertical settling velocity equation as

$$\frac{dV_d}{dt} = -\frac{18\mu}{\rho_d d_d^2} V_d + g. \quad (5)$$

The droplet diameter in the above equation depends on the mass transfer and heat transfer from a droplet as

$$\dot{m}_d = \rho_d \frac{d}{dt} \left(\frac{\pi}{6} d_d^3 \right) = -A_d h_m (\rho_{v,s} - \rho_{v,\infty}), \quad (6)$$

$$m_d C_{p,d} \frac{dT_d}{dt} = A_d h (T_\infty - T_d) + L \dot{m}_d. \quad (7)$$

The droplet evaporation rate (mass loss per unite time due to evaporation) is driven by the difference between the droplet material vapor density in the surrounding air $\rho_{v,\infty}$ and the vapor density at the droplet surface $\rho_{v,s}$. The vapor density at the droplet surface is assumed as saturated vapor density of the droplet temperature T_d . Hence the droplet heat Eq. (7) is also needed to be solved to provide the corresponding temperature. For the calculation of the mass transfer coefficient h_m and the heat transfer coefficient h in Eqs. (6) and (7), the widely-used Ranz–Marshall correlations [8] for the Sherwood and Nusselt numbers are applied.

$$Sh = \frac{h_m d_d}{\Gamma} = 2 + 0.6 Re_d^{1/2} Sc^{1/3},$$

$$Nu = \frac{h d_d}{\lambda_g} = 2 + 0.6 Re_d^{1/2} Pr_g^{1/3}. \quad (8)$$

The gas phase Schmidt and Prandtl numbers in terms of the viscosity (μ), specific heat (C_{pg}), thermal conductivity

(λ_g) and binary diffusion coefficient Γ , i.e. are defined as $Sc = \mu / \rho_g \Gamma$ and $Pr_g = \mu C_{pg} / \lambda_g$. The droplet Reynolds number is defined as $Re_d = \rho_g d_d |V_d| / \mu$.

By integrating Eqs. (5)–(7) in time with the fourth-order Runge–Kutta numerical scheme, the single droplet evaporation rate \dot{m}_d and the drift velocity V_d are obtained as a functions of the droplet diameter d_d . Substitute the algebra relation $\dot{m}_d(d_d)$ and $V_d(d_d)$ into Eqs. (1) and (2) for the corresponding droplet diameter d_d in a computational cell, the droplets number density and bulk mass density equation are solved, and the spatial and temporal distribution of the evaporating droplets in the ventilated room can thus be presented.

3. Numerical experiments

We performed a numerical simulation of the dispersion of evaporating droplets in an isothermal ventilated room. The airflow is considered to be steady state. The test room as shown in Fig. 1 has a dimension of $X \times Y \times Z = 4 \text{ m}$ (width) $\times 10 \text{ m}$ (length) $\times 3 \text{ m}$ (height). There is an inlet of $0.5 \text{ m} \times 1.5 \text{ m}$ at the upper level of one side wall and an outlet of $1 \text{ m} \times 1.5 \text{ m}$ on the bottom level of the opposite wall. The inlet air velocity is 1 m/s with a turbulence intensity of 10%. The air temperature in the room is assumed to be 296 K . The room airflow field is calculated with the standard two-equation $k-\epsilon$ turbulent model [5]. The droplets generation rate is assumed to be constant with zero initial velocity. The generation rate (number of droplets) is normalized as unity per second.

The calculation of the room airflow field and solution of the transport equations of droplets is performed by using the commercial software Fluent 6.0.12 with user defined functions. The transport equations of the droplets number density and bulk density are solved using the user-defined scalar transport modeling in Fluent. The droplets number density and bulk density are set as zero at the inlet. Zero normal gradients are used as the boundary conditions at side walls, the ceiling, the outlet and the floor for droplets. If droplets have a gravitational settling velocity (the

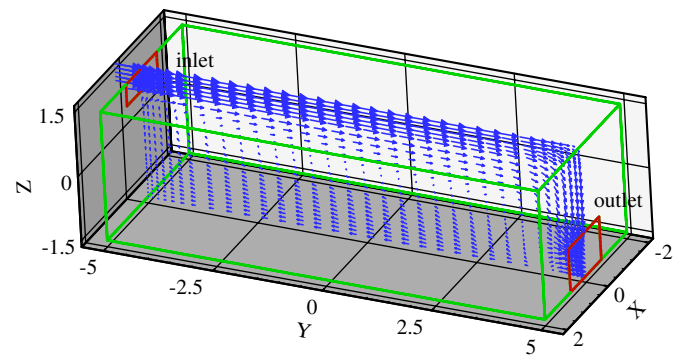


Fig. 1. Geometry of the test room and the flow field in the mid- X -plane of the room that cut through the supply inlet and the exhaust outlet. The flow exhibits a recirculation in the room in the mid- X plane.

diameter is not zero) while they reach the floor, the droplets are removed from air due to a downward flux. The droplets number density flux through the floor is calculated as $-(V_z + V_d)n + v_{eff}/\sigma_n \partial n/\partial z$. Due to the zero air flux and zero droplets density normal gradient at the floor surface, the droplets deposition onto the floor is considered as only a result of gravity as $-nV_d$. The total droplets number deposit rate is the integration of droplets gravity flux $-nV_d$ through over the floor surface area. This boundary condition suggests that the droplets cannot be resuspended from the floor.

In the calculation of single droplet evaporation rate and drift dropping velocity, the fourth-order accurate Runge–Kutta numerical scheme is used to solve Eqs. (5)–(7). The initial temperature of all droplets is set as 303 K, which is about the temperature of droplets released from human breath or coughing. The droplet material properties are taken as constant. We assume that the droplets contain mainly water and the water properties are used for the droplets material in the present work. The droplets vapor density in the surrounding air is determined by the relative humidity of the moist air, which is assumed constant everywhere uninfluenced by the droplets evaporation as only dilute droplets are considered. Most of the air-conditioned rooms require the relative humidity to be between 50% and 60%, therefore a 55% relative humidity is chosen in our study. In order to show the influence of relative humidity upon the droplets dispersion, a 75% relative humidity is also considered for comparison.

The dispersion characteristics of evaporating droplets with the original diameter of 100, 80 and 50 μm are studied in the ventilated room. For comparison, the simulation of the dispersion of small neutral aerosol particles without settling velocity and the simulation of the dispersion and deposition of large particles with a diameter of 80 or 50 μm are also performed in the same model room using the drift-flux model.

4. Results and discussion

4.1. Droplet evaporation rate and drift velocity

The correlation between the single droplet evaporation rate and drift settling velocity is obtained by the solution of Eqs. (5)–(8). As shown in Fig. 2, the droplet evaporation rate approaches a linear decrease as a function of its diameter, apart from the very beginning when the droplets are first released when the evaporation process is rapid. In the droplet evaporation linear decreasing, we have the relationship $(d(d^3)/dt)/d = \text{const.}$, which means the droplet diameter change follows the d^2 law after that time. This d^2 law phenomenon is achieved by the droplet remaining at a balance temperature with the ambient temperature after a time of temperature dropping from its initial higher temperature. By observing Eqs. (6) and (7), we note that the balance temperature is related to the balance between the droplet surface vapor density and the vapor density in

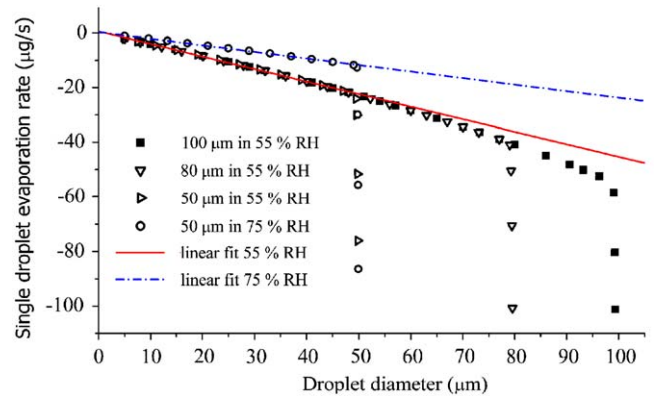


Fig. 2. Droplet evaporation rate as a function of the diameter change for different droplet initial sizes in the 55% and 75% relative humidity (RH) air.

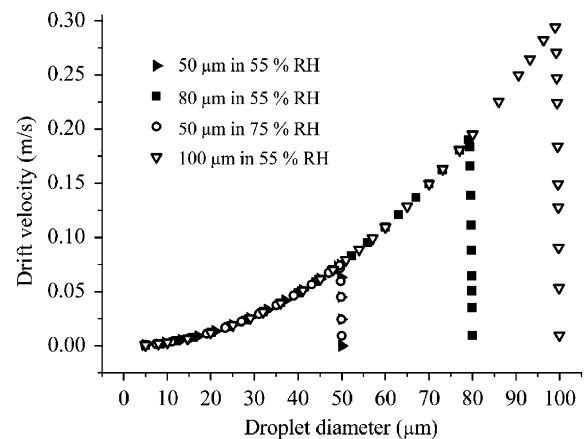


Fig. 3. Droplets drift velocity changes as the droplet diameter reduces from their different initial diameters in the 55% and 75% relative humidity (RH) air.

the ambient air depending on the relative humidity in the air. This balance temperature is actually the wet-bulb temperature, lower than the ambient temperature.

For the droplets of 100 μm in diameter, it takes more time to achieve the balance temperature, as the larger droplet Reynolds number Re_d results in a higher heat transfer coefficient h between the droplet and the surrounding air. Therefore the evaporation rate of droplets of 100 μm in diameter deviates from the linear relation with diameter changes as shown in Fig. 2.

The droplet evaporation of droplets with an initial 50 μm diameter is also calculated in the 75% relative humidity air. It is noted that the relative humidity of the ambient air greatly affects the droplet mass loss rate. Fig. 2 shows the evaporation rate of the droplet declines flatter in the 75% relative humidity air. Hence the life time of the 50 μm diameter droplet is about 8 s in the 75% relative humidity air, twice the time of that in 55% humidity air, which is only about 4 s.

The change of the droplet drift velocity with the droplet diameter is shown in Fig. 3. After the sharp increase near to

the settling velocity of the initial diameter droplet, the droplet drift velocity starts to decrease as the droplet diameter decreases. The droplet size and relative humidity of the surrounding air do not affect the algebra relation between the droplet drift velocity and the droplet diameter, except at the very beginning. This phenomenon is also a result of droplets evaporating at the balance temperature, where droplet diameter follows d square law as $d_d^2 = d_0^2 - kt$. Substitute this equation into Eq. (4), the differential Eq. (4) can be solved as $V_d = g/(k(A - 1))d_d^2$, where $A = 18\mu/\rho k$. Because A is in the order of 10^5 , much greater than unity, therefore the drift velocity V_d can be simplified as $V_d \approx g/(Ak)d_d^2 = g\tau_d$, which is the exact form of particle settling velocity except that the relaxation time τ_d for evaporating droplet changes as its diameter reduces.

4.2. Dispersion and deposition characteristics of droplets

As a comparison, we first consider particles without evaporation. The dispersion of very small particles without drift velocity and large particles of 50 and 80 μm with the settling velocity are simulated. The source of particles locates in the geometrical center of the room. As shown in Fig. 4, the larger the particles size, the more the derivation of the particle path from the airflow. Our simulation shows that most particles of 50 μm and all the particles of 80 μm deposit to the floor in the end, while small particles can get out the room through the outlet, only.

Fig. 5 shows the distribution of the evaporating droplets in the test room with their source also located in the room center. Our simulation reveals that for droplets of 50 μm in the 55% relative humidity air, the distribution is nearly identical to that of small aerosol particles without drift velocity. The 50 μm droplets in the 55% relative humidity

air evaporate so fast that the drift dropping velocity decreases quickly out of its effective values. After 5 s in the air, the initial 50 μm droplets behave exactly like neutral aerosol particles. But in the 75% relative humidity room air, the droplets clearly tends to the lower part of the room as shown in Figs. 5a and b, although the distribution still shows similarity to that of neutral small aerosol particles. The evaporation process of 50 μm droplets finishes in a small region in the 75% relative humidity room air near the source as their diameter reduces to less than 6 μm out of that region as shown in Fig. 6a.

The distributions of large particles of 80 μm are totally different from the small neutral aerosol particles because of their large settling velocity. For 80 μm evaporating droplets, the downward trend is strong at the beginning of the droplet dispersion as shown in Fig. 5c. However as the droplets become smaller and smaller during evaporation, the small particles dispersion characteristics begin to replace the large particles settling behavior. Fig. 6b shows the droplets diameters distribution of initial 80 μm droplets at 40 s. It indicates that although the 80 μm droplets fall to the floor at the beginning, most of them do not deposit to the floor as their diameter reduces to less than 6 μm when they close to the floor. The remaining droplets nuclei follow the airflow and disperse like small neutral particles.

The distribution of 100 μm droplets is more like large particles as shown in Figs. 5 and 4, because of the large settling velocity. Most of these droplets can reach the floor before they shrink to less than 6 μm in diameter in our simulations as shown in Fig. 6c at a time of 40 s.

Since for evaporating droplets between 50 and 100 μm , the settling feature can act only in certain region of the droplets distribution, a lower droplets initial position in the room increases the droplets deposition rate. Dispersion and

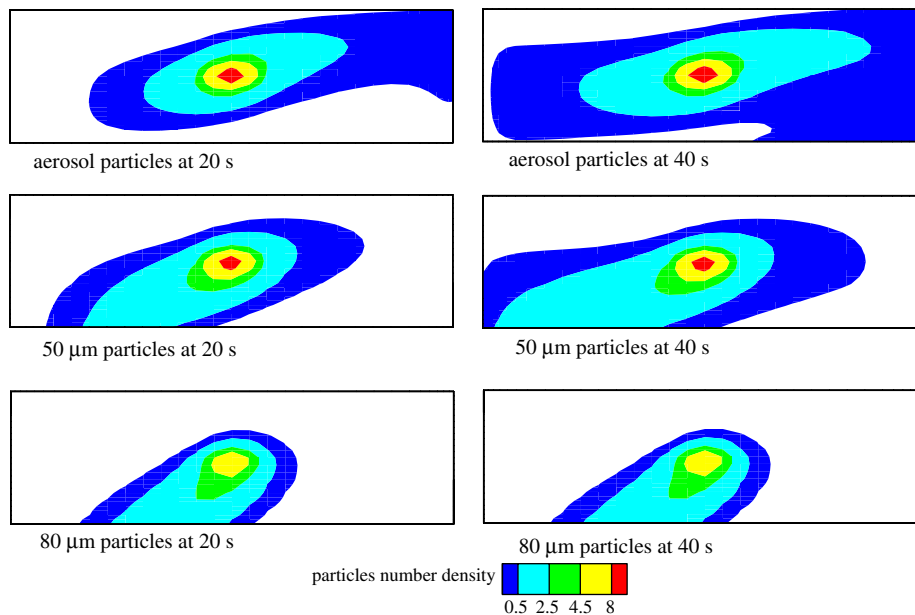


Fig. 4. Distribution of solid particles in the central X plane of the test room at 20 and 40 s after the particles are released at the room center. For top figures, “aerosol particles” refer to those neutral particles without gravitational settling.

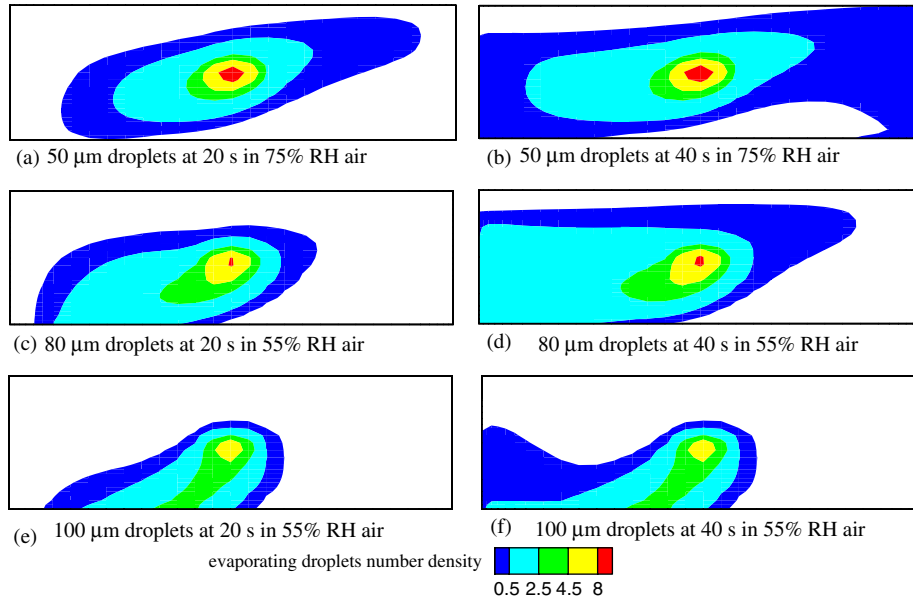


Fig. 5. Distribution of number density of evaporating droplets of different initial diameters in the center *X* plane of the test room.

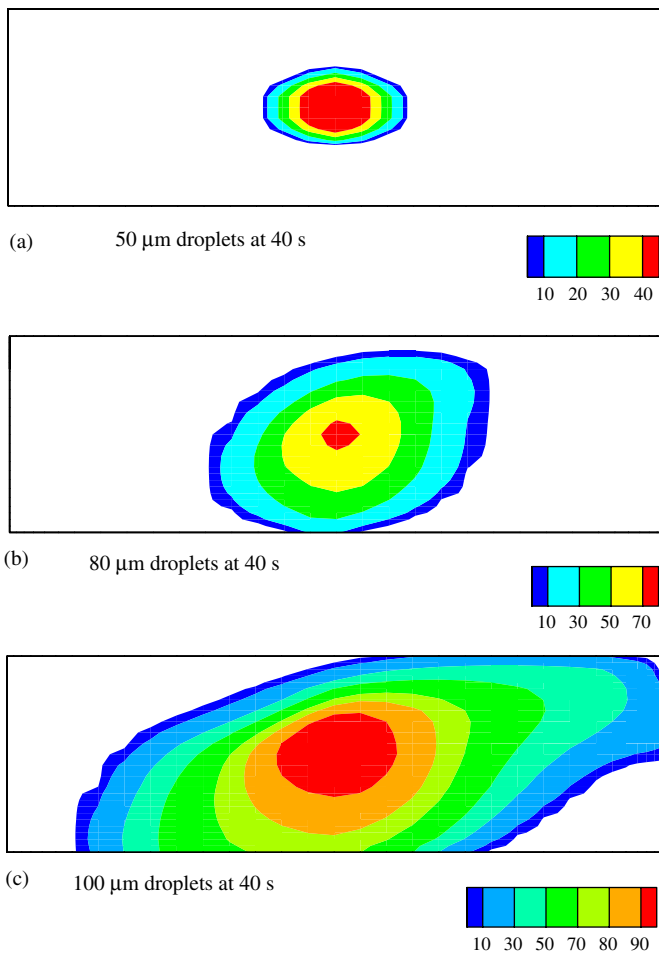


Fig. 6. Spatial distribution of droplets diameter corresponding to Fig. 5b, d and f in the central *X* plane of the test room at 40 s.

deposition of 80 μm droplets are simulated for the generation source above the floor 1.0, 0.8 and 0.5 m in the central *X* plane, as shown in Fig. 7. The droplets

settling feature is affected by both droplet characteristics and room airflow. From our numerical results, we learn that 80 μm droplet has a about 0.95 m/s average drift dropping velocity during the 11 s evaporation time to less than 5 μm, which means the droplets settling feature can last about 1 m down from their initial position in quiescent air. But because of the carrier air in the lower part of the test room has a positive vertical velocity as shown in Fig. 7a, most of the droplets nuclei remain in the room air for the initial position 1.0 m above the floor. The ratio of deposition rate to the generation rate for 80 μm droplets numbers at 40 s in the model room is 15.4%, 62.4% and 86.1% for initial position 1.0, 0.7 and 0.5 m above the floor, respectively.

5. Conclusions

In this work we have extended the drift-flux computational model for motion of solid particles to evaporating droplets. In order to deal with the changing diameters of evaporating droplets, the transport equations of droplets number density and bulk density with the drift-flux model are solved together to obtain the spatial distribution of droplets diameter. We believe that the novelty of our model is the use of the two transport equations. The droplets drift velocity and evaporation rate in the transport equations are treated as the algebra functions of the droplet diameter, which is obtained by a numerical solution of single droplet evaporation in the room air. This modified drift-flux model is proposed to simulate dispersion and deposition of the evaporating droplets in a ventilated room. The cases for droplets of different initial diameters are computational simulated with a comparison to the small neutral aerosol particles and large settling particles.

The CFD simulation results reveal that the droplet evaporation time and drift dropping velocity are the key

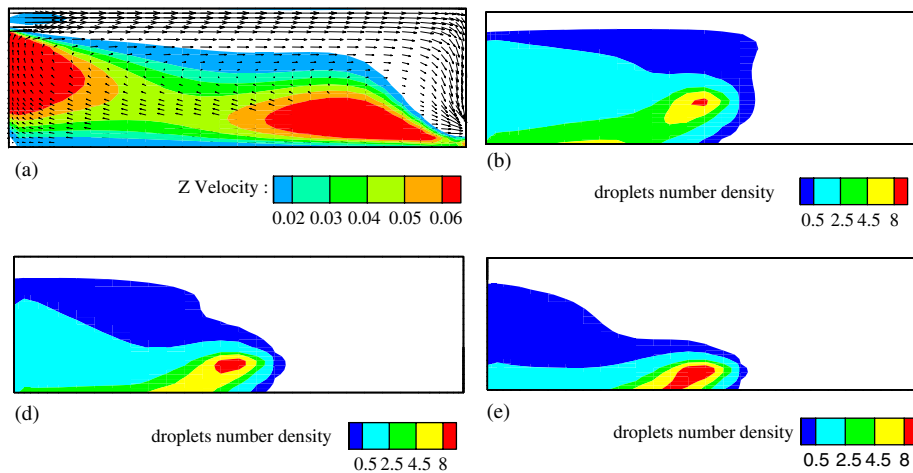


Fig. 7. Distribution of 80 μm droplets at 40 s in the central X plane for different droplets source positions in the test room. (a) Velocity vector and contour of the positive vertical velocity (m/s) of room air in the central X plane, (b) droplets source at 1.0 m above floor, (c) droplets source at 0.7 m above the floor and (d) droplets source at 0.5 m above the floor.

parameters for the distribution of evaporating droplets in the ventilated room. Because of the diameter variation during the droplet movement, the distribution characteristics of large evaporating droplets is the combination of the settling feature at the beginning and the dispersion feature at a later time. The final distribution pattern of evaporating droplets in ventilated room depends on the combination of the two features. For droplets less than 50 μm , the dispersion feature is dominant due to their very short evaporation time and small settling velocity, therefore evaporating droplets of these sizes distribute in a similar manner as the neutral aerosol particles. For droplets as large as 100 μm , the settling feature is dominant due to the longer evaporation time and considerable large dropping velocity, their distribution consequently behave like large depositing particles in a room scale. For droplets between these two sizes, the distribution tends to be at the lower part of the room than that of small neutral aerosol particles. Within this size range, a lower initial position of the droplets in the room results in a higher deposition rate to the floor. It is also noted that the relative humidity of the room air has a strong influence upon droplet evaporation time that it considerably affects the distribution of evaporating droplets.

Therefore it is of reasonable accuracy to consider evaporating droplets as neutral aerosol particles, which are initially smaller than 50 μm in relative dry room air. This modified drift-flux model is promising for larger droplets or droplets in humid air. It can be used to investigate the droplets concentration in the occupied zone of a room and in the breath zone of human. Future study with human and more practical room air will be prepared

to see the effect of evaporating on the possible risk of human inhalation of contaminated droplets.

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