Nano-scale Aerosol Deposition Model for CFD in Indoor Environmental Analysis

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ABSTRACT

The overarching objective of this study was to develop a numerical model based on computational fluid dynamics to predict aerosol concentration distributions in indoor environments. Towards this end, this paper proposes a wall surface deposition model of nano-scale aerosol that can predict unsteady deposition flux of aerosol indoors; it also reports the results of sensitivity analyses for targeting a plug-flow-type chamber.

KEYWORDS

Nano-scale aerosol, Deposition model, CFD, Indoor environment

INTRODUCTION

The air quality in the overall indoor environment is called the indoor air quality (IAQ) and has attracted increasing attention with the increasing health consciousness of residents. We spend most of our time indoors and hence IAQ has a great impact on health because of the large amount of inhalation by steady breathing. In the wide spectrum of IAQ problems, this research focuses on indoor aerosol pollution issues that have a large influence on the health of indoor residents. Many studies have reported associations between aerosol in indoor environments and adverse health effects. With regard to the aerosol problems in indoor environments, a prediction method of aerosol distribution and exposure concentration level for residents is required for designs that ensure healthy indoor air quality. The aerosol concentration distribution is usually formed by various factors, for example, convection, diffusion, chemical reaction, gravitational sedimentation, thermophoresis, and electrophoresis. Concerning the particularity of indoor environments compared with outdoor environments, the ratio of wall surface area to the volume of the room or space is usually much larger. From this point of view, aerosol deposition phenomenon is one of the critical components to determine aerosol concentration level in an occupied zone or breathed air; hence, the development of an aerosol deposition model for numerical simulation is an important research issue in the field of IAQ.

The overarching objective of this study is to develop a numerical model based on computational fluid dynamics (CFD) to predict aerosol concentration distributions in indoor environments. Towards this end, this paper describes a novel wall surface deposition model of nano-scale aerosol that can predict unsteady deposition flux of aerosol indoors; it also reports the results of sensitivity analysis targeting a simple 2-dimensional rectangular duct model.

PREVIOUS STUDIES OF DEPOSITION MODELS

There have been many studies of adsorption/desorption of gaseous chemical compounds and various numerical models incorporating adsorption isotherm have been proposed. Concerning the aerosol deposition phenomenon, there have been research reports published since the

1980s [Okuyama et al., 1986, Shimada et al., 1988, Otani et al., 1989] and, in recent years, A.C.K. Lai published an elaborate and comprehensive review article that focuses on a deposition model for indoor environments. The aerosol deposition mode in an indoor environment is described by the concepts of particle loss coefficient or deposition velocity and these parameters are classified as functions of aerosol size and turbulent properties.

Deposition velocity of aerosol particles is defined by the aerosol deposition flux and reference concentration, and the wall boundary condition of aerosol deposition is described as follows:

$$J = -v_d \cdot n \, . \tag{1}$$

Here, J indicates deposition flux of indoor aerosol, v_d denotes deposition velocity, and n is number concentration of aerosol.

In general, the concept of deposition velocity is analogous to the mass transfer coefficient by which surface zero concentration is considered and hence incorporates not only Brownian diffusion but also the effects of turbulent diffusion and gravitational sedimentation.

Base on the previous reports, for indoor aerosol from 10 nm to 10 μm in diameter, the deposition velocity as a function of particle diameter has a concave downward profile and is minimized within the range of 0.1 to 1.0 μm. This is because the effect of gravitational sedimentation becomes predominant for larger aerosol (aerosol diameter >> 1 μm) and the effect of Brownian diffusion becomes critical for smaller aerosol (aerosol diameter << 0.1 μm).

PROPOSING A DEPOSITION MODEL THAT CONSIDERS SURFACE ASPECT

In this study, we propose a novel deposition model of indoor aerosol with a size range from gas scale to nanometer scale (< 100 nm) for wall surface boundary conditions of CFD simulation. Here we focus on Brownian diffusion and gravitational sedimentation, and other parameters, for example, thermophoresis, turbophoresis, electrophoresis, coagulation, and inertial collision, are disregarded. Although generally Brownian diffusion becomes the dominant process in deposition to a solid surface in the case of nanometer-sized aerosol, in this study, a deposition model incorporating gravitational sedimentation is developed in consideration of extendibility. For simplification, the uniform flow inside the channel cavity and isothermal conditions are assumed in the following development of a formula.

Improvement of Deposition Velocity $\mathbf{v_d}$

The surface geometry of building materials must be reproduced by a numerical grid design in a range of possible resolutions, and the integration of surface roughness effect into the deposition model is needed for the microscopic phenomenon below the resolution with a numerical grid.

If the first grid point on the wall surface adopted in the indoor air flow analysis is set inside the viscous sub-layer (wall unit y+<<1), the surface geometry of the building material can be reproduced by a numerical mesh and hence the flow profile becomes linear. In this boundary condition, the flow profile at the vicinity of the wall surface can be analyzed by CFD simulation and the microscopic difference of surface characteristics of building materials must be modeled independently of flow profile information.

As shown in Figure 1, the order of deposition velocity changed in accordance with the change of building materials. Although the experimental conditions were not united for the results shown in Figure 1, there are certain amounts of rationality in separate modeling of flow information and microscopic surface characteristics of building materials when the flow field conditions are almost the same in these experiments.

In this hypothesis, deposition flux is expressed as follows:

$$J = -S' \bar{v}_d \cdot n \, . \tag{2}$$

Here, $\overline{v_d}$ denotes deposition velocity for a smooth surface, *S'* indicates the ratio of effective surface area of a rough surface to that of a smooth surface of building materials.

Novel Nano-scale Aerosol Deposition Model for CFD in Indoor Environment

In this section, constant flow along a flat plate is considered. The hypothetical deposition layer at the surface boundary between solid phase (building material) and air phase is introduced as shown in Figure 1 and it is assumed that the control volume (C.V.) of CFD consists of an imperceptible area element *dS*, thickness *dh*, and volume *dV*. The first grid point as the hypothetical deposition layer is assumed to be set inside of the viscous sub-layer (wall unit y+<<1).

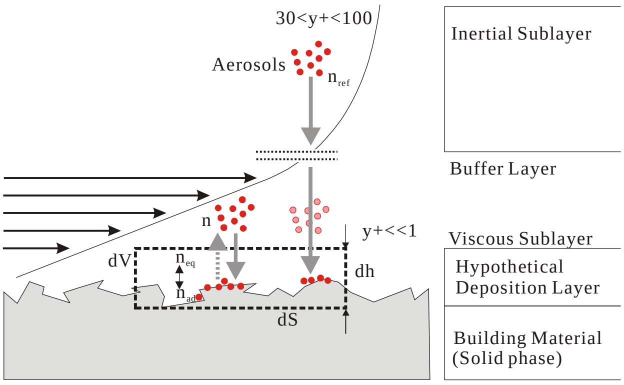


Figure 1 Transport phenomenon of aerosol at the vicinity of wall surface and hypothetical deposition layer

In this condition, the convective flow inside the C.V. is negligible and deposition phenomenon is described by Brownian diffusion. In addition, local equilibrium and one-dimensional deposition in the normal direction against the wall surface are assumed in C.V. (y+<<1 at *dh*).

The aerosol transportation in C.V. is described by the following transport equation of aerosol.

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x}\left(D_a \frac{\partial n}{\partial x}\right) + \frac{\partial}{\partial x}\left(V_g n\right) - adv \qquad (3)$$

Here, n is the number concentration of aerosol [m^{-3}], D_a is Brownian diffusion coefficient of aerosol [m^2/s], and ρ_a indicates air density [kg/m^3]. In this formula, gravitational sedimentation (settling velocity) *Vg* [m/s] is also considered for enhancing to larger particles in the future. In this modeling, impacts of diffusion flux and gravitational settling flux act in parallel.

adv denotes mass transfer at the interfacial surface of air and solid surface and is expressed on the basis of the potential model approach as follows:

$$adv = -\alpha S\left(n_{eq} - n\right), \qquad (4)$$

where α is mass transfer coefficient at the interfacial surface between solid phase and air phase [m/s], S is the contact area pre-unit volume of building material [$m^2/m^3{}_{(CV)}$], and n_{eq} is the equilibrium concentration [m^{-3}]. The aerosol concentration in C.V. is assumed to be identical to n_{eq} by local equilibrium.

The deposition amount on the surface of a building material is expressed as follows by using deposition phase concentration n_{ad} [m^{-2}].

$$S\frac{\partial n_{ad}}{\partial t} = adv \qquad (5)$$

Here, instantaneous equilibrium in C.V. is adopted and the time change of aerosol concentration in the air phase is assumed to be negligible. When equation (3) is subjected to volume integration in C.V., equation (6) is derived and equation (7) is also derived from equation (5) in a similar way.

$$0 = D_a \frac{\partial n}{\partial x} dS + V_g n dS - adv \cdot dV \qquad (6)$$

$$S\frac{\partial n_{ad}}{\partial t} dV = adv \cdot dV \qquad (7)$$

From equations (6) and (7), the following equation is introduced.

$$-\left(Da\frac{\partial n}{\partial x}+V_g n \right)\Bigg|_B = -\left(S\frac{\partial n_{ad}}{\partial t} \right)\frac{dV}{dS} = -S'\frac{\partial n_{ad}}{\partial t} \qquad (8)$$

Here, *S'* indicates the ratio of effective surface area of rough surface and smooth surface of building materials and the same parameter as in equation (2).

Relationship between Concentrations of Deposition Phase and Air Phase

In order to close the equations, it is necessary to introduce the relationship between deposition phase concentration n_{ad} and air phase concentration of aerosol n (= n_{eq}). In this study, a simple relationship as shown in equation (9) is introduced.

$$n_{ad} = f\left(n_{eq}\right) \qquad (9)$$

The function of f in Equation (9) indicates an adsorption isotherm in the case of gas phase adsorption/desorption phenomenon.

Here, when a simple linear relationship between n_{eq} and n_{ed} is introduced, equation (10) is derived from equation (9) and deposition flux is also defined in equation (11).

$$n_{ad} = k_h \cdot n_{eq} = k_h \cdot n\big|_{B-} \qquad (10)$$

$$-\left(Da\frac{\partial n}{\partial x}+V_g n \right)\Bigg|_B = -S'\frac{\partial n_{ad}}{\partial t} = -S' k_h \frac{\partial n_{eq}}{\partial t} \qquad (11)$$

Here, k_h denotes a model coefficient of the linear relationship between n_{eq} and n_{ed} and corresponds to Henry's coefficient of gas phase adsorption isotherm.

Although equation (9) is a hypothetical assumption and not validated by experimental data, a higher-precision model can be developed by introducing higher-order function f in equation (9).

For example, when the sigmoid function like Langmuir-type adsorption isotherm is adopted, equation (12) is derived from equation (9) and deposition flux is also defined in equation (13).

$$n_{ad} = \frac{n_{ad0} k_l n_{eq}}{1 + k_l n_{eq}} \qquad (12)$$

$$-\left(Da\frac{\partial n}{\partial x}+V_g n \right)\Bigg|_B = -S' \frac{n_{ad0} k_l}{\left(1 + k_l n_{eq}\right)^2} \frac{\partial n_{eq}}{\partial t} \qquad (13)$$

Here, k_l and n_{ad0} are the model coefficients.

In numerical analysis integrating the proposed deposition model, equation (11) or (13) is adopted as the boundary condition of a wall surface in an indoor environment.

SENSITIVITY ANALYSIS

In order to analyze the impact of model parameters of the proposed deposition model, sensitivity analysis was carried out for targeting a simple flow field.

Target Flow Field

In this numerical analysis, the flow field and aerosol concentration distribution are analyzed for a two-dimensional rectangular duct model. This target model is reproduced by the inside space of an experimental setup of a rectangular duct made of stainless steel. The outline of the experimental duct model is shown in Figure 2. This chamber has one supply inlet and one exhaust outlet. The cross section of this chamber is 0.02 m (*x*) × 0.1 m (*y*) and with a total length of 6.0 m including a running section (z=1.0 m) and a test section (z=5.0 m) with a building material.

Outline of Numerical Analysis

The modeling methodology is based on the Eulerian moment form of the dynamic equation for aerosol transport and dynamics in conjunction with solving the Reynolds averaged Navier-Stokes equations (RANS) for bulk fluid modeling. The Navier-Stokes governing equations were discretized by a finite volume method and flow fields were estimated using the low Reynolds number-type k-ε model (Abe Kondo Nagano model). The QUICK scheme was used for the convection term, and a SIMPLE algorithm was used. To analyze the flow field in the boundary layer and to enable the application of the aerosol deposition model at the wall surface in equation (11), the center of the computational cells closest to the wall surface should be at a non-dimensional distance (wall unit) of $y^+<1$, where $y+ = u^* y_1/\nu$ and y_1 is the distance normal to the wall surface, ν is the kinematic viscosity, and $u^* = \sqrt{\tau_w/\rho}$ is the friction velocity. Here, ρ is the air density and τ_w is the wall shear stress. In general, the order of Brownian diffusion coefficient is about 10^{-5} to 10^{-6} [m^2/s] while the order of molecular diffusion coefficient of gas phase contaminant is about 10^{-8} [m^2/s]. Meeting the requirement of y+<<1 with this Brownian diffusion scale deviates greatly from the usual grid size used with CFD simulation. Hence, kinematic viscosity defined by air density and molecular viscosity was used to evaluate y+.

In order to analyze the aerosol dynamic equation numerically in conjunction with CFD based on RANS model, these equations are ensemble-averaged. For the cross-correlation function of time fluctuation of scalar concentration and wind velocity caused as a result of the ensemble-averaging operation, eddy-viscosity representation is adopted using turbulent eddy viscosity ν_t and turbulent Schmidt number σ_t. In general, a value of about 0.2-1.3 is adopted for turbulent Schmidt number and the value 0.7 or 0.9 has been used for most of the CFD studies for turbulent mass diffusion. Here, σ_t =1.0 was used. Concerning the aerosol dynamic equation, convection term, diffusion term, and surface deposition model were considered and other influential factors, for example, reaction-generation term, coagulation loss and gain term, thermophoresis, and electrophoresis, were disregarded in this study because the experimental condition of supply inlet aerosol concentration was reasonably low and nominal time constant (τ_n) was also short enough (= 5 sec).

The number of meshes was set to 52 (x) and 152 (z) and structured mesh was used for the analysis. The analysis was carried out in two dimensions. The air inlet velocity and turbulent intensity were set to U_{in} = 1.0 m/s and 10%, respectively, which are the same as those used in the experiments.

The concentration of aerosol at the inlet position was set to 1.0 [-] as the normalized concentration and kept constant.

Analytical conditions are shown in Table 1.

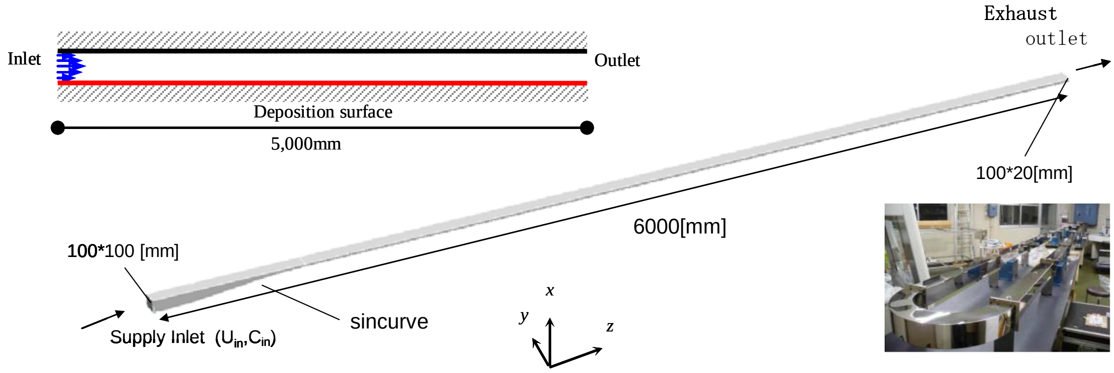


Figure 2 Model analyzed (2-dimensional flow field inside rectangular duct)

Table 1 Numerical and Boundary Conditions

Turbulence Model	Low Re k-ε model (Abe-Kondh-Nagano model, 2-dimensional Cal.)
Mesh	52(x)×152(z)
Scheme	Convection Term: QUICK
Inflow Boundary	U_{in} =1.0 [m/s], k_{in} =3/2× (U_{in}×0.1)^2,ε_{in} =$C_\mu^{3/4}$×$k_{in}^{3/2}$/l_{in}, C_μ=0.09, l_{in} =0.02[m]
Outflow Boundary	U_{out} = free slip, k_{out}= free slip, ε_{out} = free slip
Wall Treatment	Velocity, no slip; Aerosol, proposed deposition model (linear type, see eq.(11))
Aerosol	Dp=1 - 2,000 (see Table 2)

Table 2 Setting of Model Parameters and Cases Analyzed

D_p [nm]	Gas	1	2	3	7	20	70	300	2000
V_g [m/s]	0	6.4×10^{-9}	1.2×10^{-8}	1.9×10^{-8}	4.5×10^{-8}	1.3×10^{-7}	5.3×10^{-7}	4.3×10^{-6}	1.2×10^{-4}
D_a[m^2/s]	1.0×10^{-5}	5.0×10^{-6}	1.0×10^{-6}	5.0×10^{-7}	1.0×10^{-7}	1.0×10^{-8}	1.0×10^{-9}	1.0×10^{-10}	1.0×10^{-11}
$S'k_h$ [-]	1.0×10^{-5} - 1.0×10^{4}								

D_p: particle diameter, V_g: gravitational sedimentation, D_a: Brownian diffusion coefficient

Cases Analyzed

In this study, a deposition model that assumed a linear relationship between n_{ad} and n_{eq} in equation (11) was used for sensitivity analysis. In the linear model shown in equation (11), there are two model parameters: S' and k_h. $S'k_h$ was assumed to be one parameter and the sensitivity analysis was carried out. In this analysis, Brownian diffusion coefficient D_a corresponding to aerosol diameter was changed within the range from 10^{-11} to 10^{-5} [m^2/s]. The parameters of cases analyzed are shown in Table 2.

Concerning the wall surface treatment of deposition model, three cases were set: one-sided deposition (floor) of diffusion flux in rectangular model (Case 1), one-sided deposition (floor) of diffusion and gravitational settling flux in rectangular model (Case 2), and two-sided deposition (floor and ceiling) of diffusion flux and one-sided deposition (floor) of gravitational settling flux in rectangular model (Case 3).

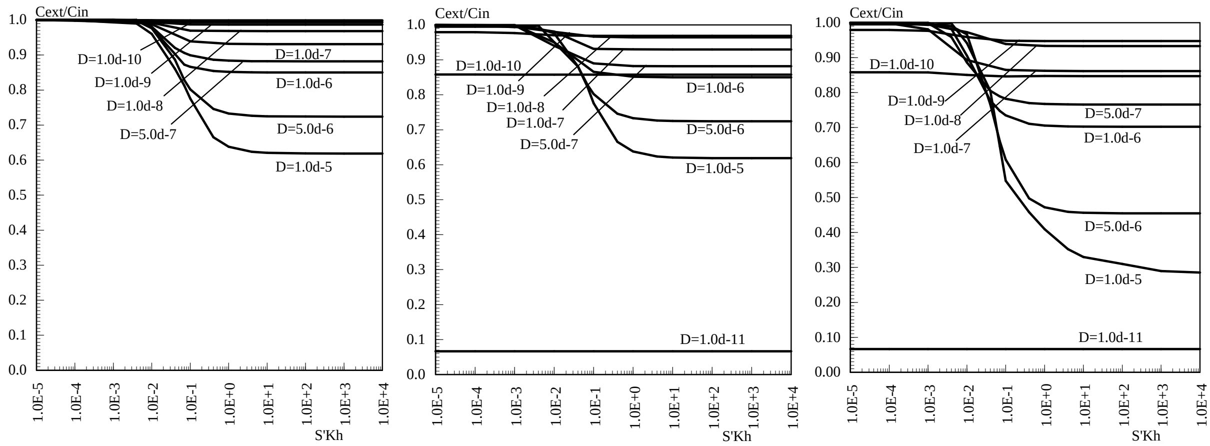
RESULTS

The results of sensitivity analysis are shown in Figure 3. In each case, Brownian diffusion coefficient Da was changed from 10^{-11} to 10^{-5} [m^2/s] and $S'k_h$ was changed from 10^{-5} to 10^4. The vertical axis in Figure 4 indicates aerosol concentration decay passing through the deposition surface from the inlet to the outlet position (C_{ext}/C_{in}, C_{in} indicates supply inlet concentration, C_{ext} denotes exhaust outlet concentration of aerosol). The representative concentration distributions of aerosol in the duct model are shown in Figure 4. The aerosol concentrations in Figure 4 are normalized by supply inlet concentration.

In Case 1 for one-sided deposition of diffusion flux onto a floor, the aerosol concentration at the exhaust outlet (C_{ext}/C_{in}) decreased gradually when the aerosol diameter became small (Brownian diffusion coefficient became larger). The model parameter of linear model $S'k_h$ had high sensitivity between the range from 10^{-2} to 10^0, and concentration gradient on the wall surface became almost zero (adiabatic boundary condition) within the range of $S'k_h < 10^{-3}$, and wall surface concentration became almost zero (perfect sink boundary condition) at the range of $S'k_h > 10^1$ as shown in Figure 4 (1).

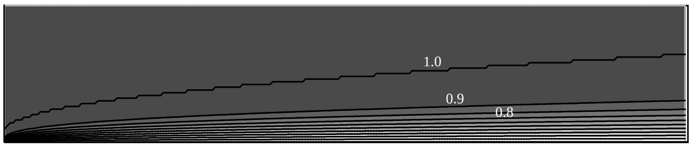
In Case 2 with one-sided deposition of diffusion and gravitational settling flux onto a floor, the change of the aerosol concentration at the exhaust outlet (C_{ext}/C_{in}) as a function of $S'k_h$ showed a similar trend to that in Case 1 for a relatively fine aerosol, that is, within the range of 10^{-8} to 10^{-5} [m^2/s] of Da, because the gravitational sedimentation was disregarded in this region. On the other hand, gravitational settling flux became larger than Brownian diffusion flux in the range of μm diameter of aerosol. In this numerical analysis, concerning the aerosol of μm size, the diffusion and gravitational sedimentation flux were assumed to act separately and in parallel and the zero gradient concentration at the wall surface was adopted for the boundary condition of gravitational sedimentation. Hence, the decrease of the aerosol concentration at the exhaust outlet (C_{ext}/C_{in}) was determined by the effect of gravitational sedimentation in the range of μm size aerosol.

In Case 3 that considered two-sided deposition of diffusion and gravitational settling flux onto a floor and one-sided deposition of diffusion onto a ceiling, the decrease of the aerosol concentration at the exhaust outlet (C_{ext}/C_{in}) became larger than that of Case 2 for the upper side deposition by Brownian diffusion.

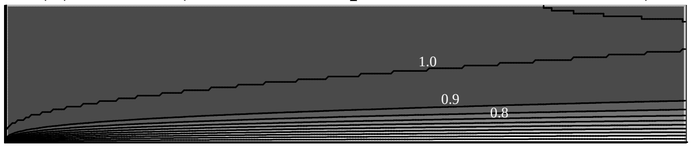


(1) Case 1 (2) Case 2 (3) Case 3

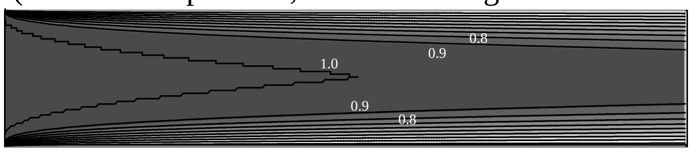
Figure 3 Results of sensitivity analysis



(1) Case 1 (one-sided deposition, diffusion flux)



(2) Case 2 (one-sided deposition, diffusion and gravitational settling flux)



(3) Case 3 (two-sided deposition of diffusion and gravitational settling flux (on floor), and one-sided deposition of diffusion (on ceiling))

Figure 4 Results of aerosol concentration distribution in duct model

(Vertical axis in Figure 5 enlarged 50 times to facilitate visualization)

DISCUSSION

For the adsorption/desorption model for gas phase contaminant, in general, the adsorption phase concentration on a wall surface is analyzed by using the concept of adsorption isotherm. In other words, wall surface concentration of gas phase contaminant will be analyzed explicitly. On the other hand, wall surface concentration will generally be set to zero when analyzing diffusion flux. The behavior of μm size particles is known to be ruled by physical factors and hence the deposition model of previous reported study was discussed in terms of physics properties of wall surface-aerosol interaction, especially in aerosol engineering. However, the diameter of aerosol contaminants has a wide spectrum from a few nanometers to micrometers and above, and the distinction between gas phase contaminant and nano-scale aerosol will not be clear.

Although there seems to be a boundary between gas phase molecules and aerosol particles at about 2 nm for contaminants of comparatively simple structure, the macromolecules that reach a size of 100 nm and above have the characteristics of gas phase molecules. From this point of view, the development of a wall surface deposition model for numerical simulation that could apply continuously from gas phase to nano-scale aerosol (<100 nm) is necessary.

We have a research plan to report the results of two types of fundamental experiment: (i) dynamic chamber experiment with rectangular duct model, and (ii) static chamber experiment with Tedlar bag (polyvinyl fluoride).

In the Tedlar bag experiment, deposition velocity and effective surface area *S'* will be identified for various building materials, that is, materials of smooth surface and rough surface, by measuring time series of aerosol concentration in the bag enclosing the target size aerosol and building material.

In the rectangular duct experiment, the model parameter $S'k_h$ will be identified by measuring the concentration decrease from the supply inlet to the exhaust outlet opening and using the identification chart of $S'k_h$ and C_{ext}/C_{in} as shown in Figure 4. Then, conclusively, *S'* and k_h will be separately identified by the above two types of experiment.

The experimental validation of this sensitivity analysis and identification of model parameters will be reported in the future.

CONCLUSION

In this paper, a novel deposition model for nano-scale aerosol to analyze the surface concentration explicitly was proposed and the results of sensitivity analyses were also reported. The findings obtained in this work can be summarized as follows:

(1) The deposition model that incorporated a linear relationship between n_{ad} and n_{eq} was confirmed to have high sensitivity in the range from 10^{-2} to 10^{0} of the model parameter $S'k_h$.

(2) Deposition flux of relatively large aerosol (>100 nm) was determined by gravitational sedimentation and the effect of model parameter of $S'k_h$ was almost negligible for this relatively large aerosol size.

(3) In future, we will report the experimental validation of this sensitivity analysis by using two types of experiment (dynamic chamber experiment with rectangular duct model, and static chamber experiment with Tedlar bag) and identification of model parameters

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