MIXING AND DEPOSITION OF BROWNIAN PARTICLES IN MODEL ALVEOLUS

YOSHIO OTANI, HITOSHI EMI AND TAKAYA TANAKA
Department of Chemistry and Chemical Engineering, Kanazawa University, Kanazawa 920

Key Words: Aerosol, Deposition, Mixing, Alveolar Model

Inhaled submicron particles readily penetrate into alveolar regions of the human lung, where the behavior of these particles is largely influenced by mixing between inhaled air and residual air. In the present work, an experimental technique to study mixing and deposition of Brownian particles in an expanding/contracting balloon as a model alveolus was developed by employing a "wash-out" experimental technique. Further, applying a simple number balance equation of particles, the mixing volume and deposition coefficient during a breath were obtained. It was found that (i) there exists a critical value in the duration of balloon expansion/contraction over which Brownian diffusion of aerosol enhances mixing between aerosol and clean air, and the critical duration of balloon expansion/contraction is longer for a larger expansion/contraction volume of the balloon; and (ii) at the same expansion/contraction volume of the balloon, the deposition coefficient per breath is larger for a larger expansion/contraction volume.

Introduction

Submicron particles tend to deposit selectively in the alveolar region of the human lung. The motion of particles with a diameter smaller than 0.5 μm is governed mostly by diffusion. However, the behavior of these particles in the alveolar regions is not simple because of the movement of the alveolar walls as well as air-mixing between tidal and residual airs.

Cincotai[1] experimentally studied fluid flow in a latex sphere of a model alveolar sac, and suggested that inhomogeneous expansion and contraction of the latex sphere lead to mechanical mixing even at a very low Reynolds number (10^{-4}–10^{-3}). Yu *et al.*[3,4] numerically solved flow field and concentration distribution in a spherical vessel of a model alveolus. They showed that there exists significant mechanical mixing and that all particles with a diameter smaller than 0.05 μm which enter the alveolus are deposited.

However, no experimental works for determining air mixing and deposition efficiencies of aerosol in a model alveolus have been reported, because even for a model alveolus with a simple geometry, movement of the alveolar wall and the unsteady nature of the flow field lead to considerable difficulty in measuring aerosol concentration. In the present work, the alveolus is modelled by a distensible latex balloon, and air mixing and deposition of Brownian particles in the model alveolus were experimentally investigated by employing a "wash-out" experimental technique. Based on the experimental results, a model for the mixing and deposition of Brownian particles in the expanding/contracting balloon was proposed.

Received August 18, 1989. Correspondence concerning this article should be address to Y. Otani. T. Tanaka is now with NOK Corp., Fujisawa 251.

1. Model Alveolus and Experimental Procedures

Since an alveolus is considered as a vessel which expands and contracts periodically, it is modelled by. a spherical latex balloon as shown in **Fig. 1**. The whole experimental set-up is shown in **Fig. 2**. The model alveolus is made of a moulded natural latex rubber balloon with diameter of 20 mm. The ratio of throat diameter to balloon diameter is 0.75 and that of throat length to balloon diameter is 0.5, referring to the paper by Cinkotai.[1] The balloon is attached to a side tube of a circular glass tube with Teflon tape and placed in a cylinder filled with water. The cylinder is connected to a syringe, and the balloon is expanded and contracted by moving the piston of the syringe with a linear head operated by a reversible motor.

Clean air in the main tube flows in a single direction and the outlet flow is maintained at a constant rate of 5 cm^3/s. All of the exiting air flows into a condensation nucleus counter (TSI Model 3020). Since the inlet flow rate of the test tube varies with expansion

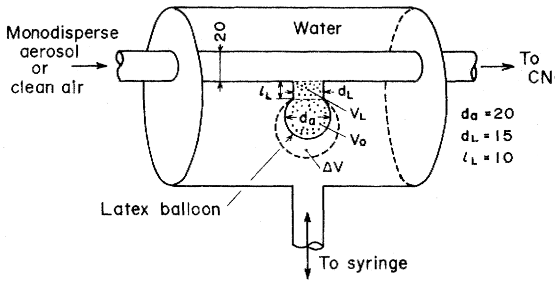

Fig. 1. Model alveolus

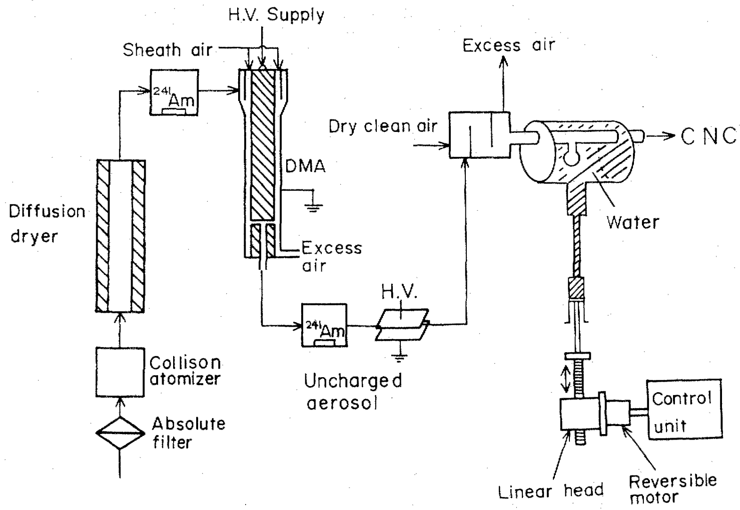

Fig. 2. Flowchart of experimental setup

and contraction of the balloon, air sufficient to cover the flow rate in the test tube during the balloon expansion is introduced into the mixing chamber, and excess air with variable flow rate is discarded from the chamber.

The rate of expansion and contraction of the balloon is controlled by the speed of rotation of the reversible motor, and the expansion/contraction volume is adjusted by changing the piston stroke. Since the piston moves at a constant rate, the change in volume of the balloon is also linear.

There are two ways to study mixing in a model alveolus, namely the "wash-in" and "wash-out" approaches, as in a breathing test for the human lung. The "wash-out" is performed in such a way that a balloon is first filled with aerosol and then clean air is passed through the main tube. While the balloon is expanded and contracted the aerosol concentration is monitored at the outlet of the test tube. The "wash-in" experiment is such that clean air is filled into the balloon and aerosol is passed through the main tube. In the present work, both "wash-in" and "wash-out" experiments were attempted. However "wash-in" experiments yielded data that were insensitive to the mixing in the balloon, i.e., the aerosol concentration at the test tube outlet varied slightly because only a small amount of aerosol was exchanged by residual clean air in the balloon. Further, because of the difficulty in generating constant-concentration aerosol, small fluctuations of inlet aerosol concentration affected the experimental data greatly. In "wash-out" experiments, however, small amounts of effluent aerosol particles from the balloon can be detected because the aerosol concentration at the test tube outlet is measured while passing clean air.

The procedure in a "wash-out" experiment is as follows.

1) Fill aerosol into the balloon. Passing DMA (differential mobility analyzer) classified monodisperse aerosol through the test tube while monitoring the concentration at the test tube outlet, the balloon is expanded. After the balloon is inflated, the aerosol flow is switched to clean air. Waiting for 3 min until no particles are detected at the outlet of the test tube, the filling process is completed.

2) The balloon is expanded and contracted at a given frequency and expansion/contraction volume, and effluent aerosol concentration from the balloon is continuously monitored by a CNC at the test tube outlet.

3) After a given number of "breaths", the residual aerosol in the balloon is expelled by contracting the balloon and the effluent aerosol concentration is measured.

The number of particles initially trapped in the balloon is obtained by multiplying the aerosol concentration by the initial volume of the balloon. However, because particle deposition occurs during the filling process, it is necessary to correct the deposition loss of particles. Therefore, after completing the filling process the balloon was contracted and the aerosol was expelled to obtain fractional particle loss during the filling process. The predetermined fractional particle loss was used to calculate the initial number of particles in the balloon.

The CNC was operated only in a pulse count mode (i.e., aerosol concentration was less than 10^3 particles/cm^3) and the aerosol concentration was recorded every two seconds on a recorder.

2. Experimental Results

Typical output of the CNC is shown in **Fig. 3**. In the figure, the first ten peaks correspond to the effluent aerosol concentration from the balloon during balloon expansion/contraction and the last peak is for the residual aerosol particles in the balloon. Although the

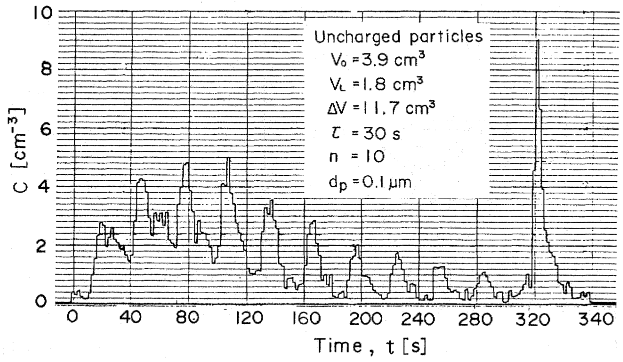

Fig. 3. Typical output of CNC during balloon expansion and contraction

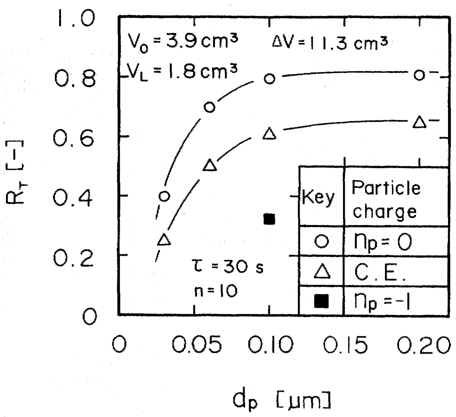

Fig. 4. Effect of particle charge on recovery of aerosol from a balloon. C. E. designates Boltzmann charge equilibrium particles.

peaks are not separated from one another because of the internal mixing of aerosol in the CNC, we can see that there are ten peaks—equal to the number of "breaths"—and that the time period between any two peaks is equal to the duration of balloon expansion and contraction.

Expansion and contraction of the latex balloon may cause electrostatics on the surface, resulting in enhanced deposition of aerosol particles. Prior to measurements of mixing and deposition of aerosol in the balloon, the influence of electrostatic force on the deposition of particles was studied by measuring recoveries of particles with different charge states. The recovery R_T is the ratio of number of particles flowing out from the balloon including particles expelled after ten breaths to initial number of particles in the balloon. **Figure 4** compares the recoveries of uncharged, singly charged, and Boltzmann charge equilibrium particles during ten breaths. For any charge state of particles, the recovery decreases with decrease in particle size, and at $d_p = 0.1\,\mu$m the recovery of singly charged particles is considerably lower than that of uncharged ones, suggesting that electrostatic force (Coulomb force) is exerted on the charged particles. To examine whether electrostatic force (mainly induced force) is exerted on the uncharged particles, the recoveries of uncharged particles were measured at various residence times of aerosol in a balloon with constant volume and were compared with the analytical solution for diffusional particle deposition in a spherical vessel.[2] This is shown in **Fig. 5**. The abscissa in the figure is the dimensionless residence time of aerosol particles in the balloon. As seen from the figure, the experimental data are in good agreement with the theoretical curve, indicating that the deposition of uncharged particles takes place by pure diffusion. Therefore, Figs. 4 and 5 suggest that, although the balloon has an electrostatic charge, the electrostatic effect on particle deposition can be eliminated if uncharged particles are used as a test aerosol. Accordingly, the experiments to measure mixing and deposition of aerosol were conducted by using only uncharged particles.

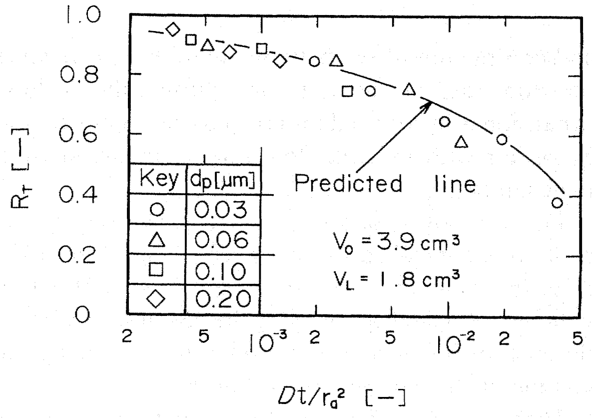

Fig. 5. Recovery of aerosol from a balloon with constant volume as a function of dimensionless residence time of aerosol in the balloon. The solid line is the theoretical line for diffusional deposition in a spherical vessel.[2]

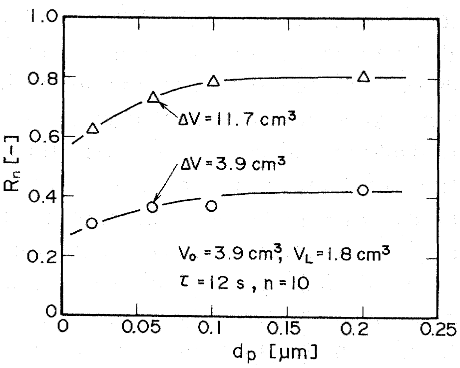

Fig. 6. Fractional recovery of aerosol particles from an expanding/contracting balloon during ten breaths

Figure 6 shows the recoveries of aerosol particles from the balloon during ten breaths R_n as a function of particle size. R_n is the ratio of the number of particles expelled in ten breaths to the initial number of particles. The figure shows that (i) at a constant d_p, R_n is larger for a larger ΔV, and (ii) at a constant ΔV, R_n of 0.1 μm particles is equal to that of 0.2 μm particles, and for $d_p<0.1$, R_n decreases as d_p decreases. The result (i) is explained by a difference in mixing intensity in the balloon. For a larger expansion/contraction volume at the same duration of balloon expansion/contraction, clean air flows into the balloon at a faster rate, resulting in a significant convective mixing of residual aerosol and clean air. Therefore, at $\Delta V=11.7\,\mathrm{cm}^3$, most of the aerosol in the balloon is expelled in the first ten breaths, while at $\Delta V=3.9\,\mathrm{cm}^3$ a large portion of aerosol particles remains in the balloon. The result (ii) implies that for particles with a diameter larger than 0.1 μm, mixing between aerosol and clean air is determined by convective air-mixing, because particle size, i.e. particle diffusion, does not affect R_n. However, since diffusion is significant for particles with a diameter smaller than 0.1 μm, diffusional loss of particles onto the balloon wall influences R_n. The same experimental implications can be obtained from **Fig. 7**, where the ratio of number of residual aerosol particles in the balloon after ten breaths to the initial number of particles is plotted against particle size. The residual fraction f_r is smaller for a larger ΔV because of stronger convective air-mixing at $\Delta V=11.7\,\mathrm{cm}^3$, and there is a sharp decrease in f_r at $d_p=0.1\,\mu$m because of diffusional particle loss in the balloon.

3. Discussion

To characterize the behavior of aerosol particles in the balloon from the experimental results shown in the preceding section, it is necessary to account for both the mixing and the diffusional deposition of aerosol particles. The mixing and deposition model constructed to represent the aerosol behavior is schematically illustrated in **Fig. 8**. Assumptions underlying the model are that (1) "breaths" are the repeated cycles of an identical mixing and deposition process of aerosol, (2) at both the initial and final stages of each breath, aerosol concentration is uniform in the balloon, (3) during a breath, clean air with volume of ΔV enters the balloon, volume V_{mix} of which is completely mixed with the aerosol, and (4) at the end of each breath, aerosol of volume V_{mix} with concentration C_i leaves the balloon. From these assumptions and referring to Fig. 8, the number balance of particles at i-th breath is expressed by the following equation.

$$C_{i-1}(V_0+V_L)=C_i(V_0+V_L)+C_iV_{\mathrm{mix}} \\ +\eta C_{i-1}(V_0+V_L) \quad i=1,2,3\cdots \tag{1}$$

where η is the fractional particle deposition based on the number of particles at the initial stage of each breath. Rearranging Eq. (1), the concentration ratio, $\gamma=C_i/C_{i-1}$, is given by

$$\gamma=\frac{C_i}{C_{i-1}}=\frac{(1-\eta)(V_0+V_L)}{V_0+V_{\mathrm{mix}}+V_L} \tag{2}$$

if we define fractional recovery at i-th breath, f_i, as the ratio of number of particles expelled during i-th breath to the initial number of particles, it is expressed as

$$f_i=\frac{C_iV_{\mathrm{mix}}}{C_0(V_0+V_L)}=\gamma^i\frac{V_{\mathrm{mix}}}{V_0+V_L} \tag{3}$$

Therefore, cumulative fractional recovery up to n-th breath, $R_n=\sum_{i=1}^{n}f_i$, becomes

$$R_n=\sum_{i=1}^{n}f_i=\frac{V_{\mathrm{mix}}\gamma(1-\gamma^n)}{(V_0+V_L)(1-\gamma)} \tag{4}$$

The fraction of residual aerosol particles remaining in the balloon after n-th breath f_r is given by

$$f_r=\frac{C_n}{C_0}=\gamma^n \tag{5}$$

In the above equations, the quantities obtainable from

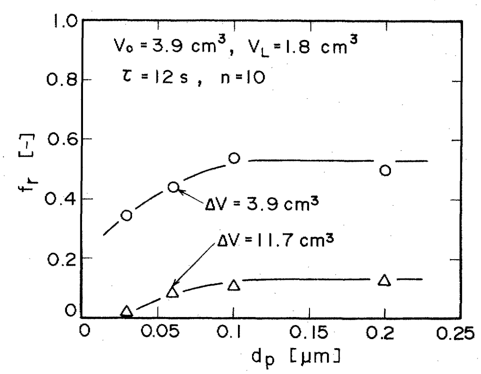

Fig. 7. Residual fraction of particles in a balloon after ten breaths

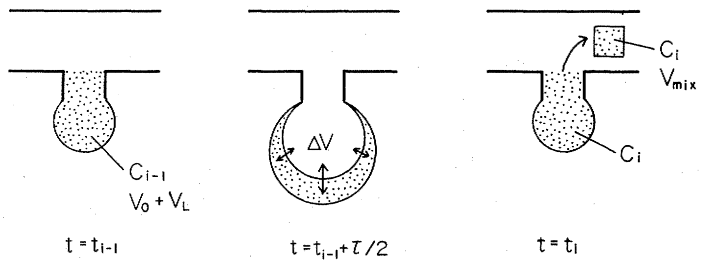

Fig. 8. Schematic illustration of mixing between aerosol and clean air in a balloon

the experiments are R_n and f_r as shown in Figs. 6 and 7. Therefore, by using Eq. (4), the value of V_{mix} was calculated from R_n and γ, which was obtained from f_r by Eq. (5). Then the values of V_{mix} and γ were substituted into Eq. (2) to obtain η.

Figures 9 and 10 respectively show the dependences of V_{mix} and η on τ. V_{mix} does not change with particle size up to $\tau=12$ s for $\Delta V=3.9\,cm^3$ and up to $\tau=30$ s for $\Delta V=11.7\,cm^3$, and for a longer τ, V_{mix} increases with decreasing particle size. If convective air-mixing determines the mixing between aerosol and clean air, there is expected to be no dependence of V_{mix} on d_p. Therefore, Fig. 9 indicates that convective mixing is dominant when τ is shorter than 12 s for $\Delta V=3.9\,cm^3$ and 30 s for $\Delta V=11.7\,cm^3$. For a longer τ, particle diffusion enhances mixing between aerosol and clean air. In Fig. 10, η is higher for smaller particles and increases with τ. Further, an increase in ΔV brings an increase in η. The increase in η with ΔV is attributed to an increase in the deposition surface area.

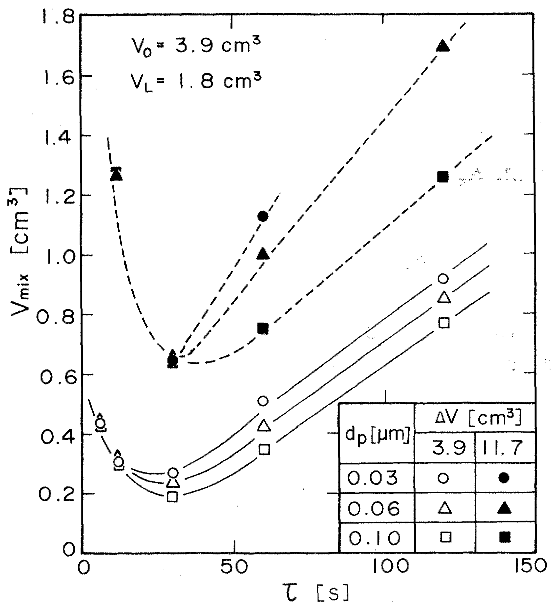

Fig. 9. Mixing volume V_{mix} as a function of duration of balloon expansion/contraction

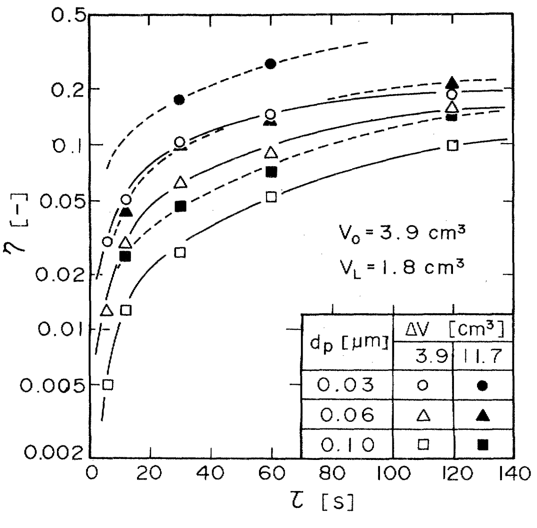

Fig. 10. Deposition coefficient η as a function of duration of balloon expansion/contraction

Conclusions

An experimental technique to study mixing and deposition of Brownian particles in an expanding/contracting balloon as a model alveolus was developed by employing a "wash-out" experimental technique. By applying a simple number balance equation of particles to the experimental results, the mixing volume between aerosol and clean air and the deposition coefficient were obtained. Following are the main conclusions on the mixing and deposition of Brownian particles in the expanding/contracting balloon.

(1) There exists a critical value of the duration of balloon expansion and contraction over which Brownian diffusion of aerosol enhances mixing between aerosol and clean air.

(2) The critical value of the duration of balloon expansion/contraction is larger for a larger expansion/contraction volume.

(3) An increase in expansion/contraction volume of balloon enhances particle deposition because of a larger deposition surface area.

Acknowledgement

This work is financially supported by a Grant-in-Aid for Scientific Research on Priority Areas, Ministry of Education, Science and Culture. The authors wish to express great appreciation for the fabrication of latex balloons by Okamoto Co. Ltd.

Nomenclature

C	=	Particle number concentration	[m^{-3}]
C_i	=	Average particle number concentration in balloon at the end of i-th breath	[m^{-3}]
D	=	Brownian diffusivity	[m^2/s]
d_a	=	Diameter of balloon	[mm]
d_L	=	Diameter of balloon throat	[mm]
d_p	=	Particle diameter	[m]
f_r	=	Fraction of residual aerosol particles in balloon after n breaths	[—]
f_i	=	Fractional recovery of aerosol from balloon at i-th breath	[—]
i	=	Breath number	[—]
l_L	=	Length of balloon throat	[mm]
n	=	Number of breaths	[—]
n_p	=	Number of electrons on a particle	[—]
R_T	=	Overall recovery of aerosol from balloon ($=R_n+f_r$)	[—]
R_n	=	Fractional recovery of aerosol during n breaths	[—]
r_a	=	Radius of balloon	[m]
t	=	Time	[s]
V_0	=	Initial balloon volume	[cm^3]
V_L	=	Volume of balloon throat	[cm^3]
V_{mix}	=	Mixing volume between aerosol and clean air in balloon	[cm^3]
ΔV	=	Expansion/contraction volume of balloon	[cm^3]

γ	=	Ratio of aerosol concentration in balloon at i-th breath to that of $(i\text{-}1)$th breath	[—]
η	=	Deposition coefficient	[—]
τ	=	Duration of balloon expansion and contraction	[s]

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