TRAJECTORIES AND DEPOSITION SITES OF SPHERICAL PARTICLES MOVING INSIDE RHYTHMICALLY EXPANDING ALVEOLI UNDER GRAVITY-FREE CONDITIONS

S. HABER*, D. YITZHAK* AND A. TSUDA**

* Department of Mechanical Engineering, Technion, Haifa 32000, Israel, mersh01@tx.technion.ac.il
** Department of Environmental Health, Harvard School of Public Health, Boston, MA 02115, USA, atsuda@hsph.harvard.edu

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ABSTRACT...Trajectories and deposition sites of 0.5-2 m in diameter particles moving inside the lung alveoli under gravity-free conditions are investigated. In particular, we show the interplay between alveoli rhythmical expansion (a flow model suggested by Haber et al. J. Fluid Mech. 45:245-268, 2000) and particle deposition vis-à-vis predictions based on non-stretching alveoli models. It is shown that small, inertia-less, non-Brownian particles can never enter rigid alveoli in micro-gravity circumstances since the flow field consists of isolated closed streamlines that separate the cavities from the airways. However, for expanding alveoli, the streamline map is significantly altered, allowing diversion of particles from the airways toward the alveoli walls. A new collision mechanism of geometrical entrapment is revealed manifesting that particle deposition tends to occur inside alveoli located up the acinar tree and at the distal area of the alveolus rim.

INTRODUCTION

Breathing in a polluted environment under micro-gravity circumstance has gained significance with the onset of space programs in which astronauts were haphazardly exposed to aerosolized particles floating in the space cabin. Beeckmans [1] studied the effect of reduced gravity that exists on the Moon on particle deposition inside the lung. He concluded that more particles 7 m in diameter and smaller tend to settle inside the alveoli on Earth than on the Moon and vice versa for particles larger than 7 m. Darquenne et al.[2], [3] and [4] examined the effect of high gravity and microgravity upon particles 0.5-3 m in diameter. In Darquenne et al. [2], Fig. 1 demonstrates that the number of deposited particles increases with concomitant increase in gravity and particles size.
However, in a micro-gravity case deposition is only slightly affected by particle diameter. In Darquenne et al.[3], Figures 2 and 3 indicate that deep penetration of a bolus of particles results in higher deposition and dispersion. Similarly, in Darquenne et al. [4], Fig.3 illustrates that deposition is higher with increased penetration and is only slightly dependent upon particle diameter. Obviously, in all these articles the singular effect of particle deposition in the acinar region was not attempted and the results pertain to the combined effect of particle deposition in the lung upper airways and the acinus. At best, the increased dispersion and deposition with penetration depths hints that the acinar region may have a profound effect on particle deposition. Alas, there are no conclusive or rigorous results demonstrating how deposition depends upon acinar airway generation or particle size. Generally, particle inertia is considered as the main mechanism that may cause particles of diameter larger than 3 μm to cross streamlines and impact the alveolar walls in microgravity circumstance while finer particles of diameter lower than 0.5 μm are mainly affected by Brownian motion. Thus, particles about 1 μm in diameter would follow fluid streamlines closely in the absence of gravity. Previous flow models, that assumed rigid configuration of the acinus, predicted that isolated closed streamlines exist inside the lung alveoli, separating the cavities from the adjacent airways (e.g. Fig. 2 from Pozrikidis [5], data re-plotted by Haber et al. [6]).
More recently the effect of alveolar rhythmical expansion was incorporated into the alveoli flow model (Tsuda et al., [7] and Haber et al., [6]; Henry et al., [8], Lee and Lee [9]) that exhibit streamlines entering the alveolus (e.g. Fig. 3 from Haber et al., [6]). In Haber et al., [10] we have demonstrated (e.g. Fig. 3) the important effect of alveolar expansion on trajectories of particles moving under gravity. Indeed, in many cases, a flow model of rigid alveoli predicts that particles would skip the alveolus and move along the airway during inhalation (Figure 4 from Haber et al. [10]) whereas in an expanding/contracting alveoli model the particle would enter the alveolus, obviously, due to flow generated by the expanding alveolus.

Figure 2: Streamline map of shear flow over a hemispherical cavity (from Pozrikidis [5]).

Figure 3: Streamline map of the combined flow generated by expanding alveoli and ductal shear flow over a hemispherical cavity (from Haber et al. [6]).
A broader discussion on aerodynamic models used in the past to describe the flow field inside lung alveoli and a comprehensive discussion on the forces exerted on a particle is presented in Haber, Yitzhak and Tsuda [10]-henceforth referred to as HYT- and would not be repeated. The main goal of this paper is to explore the effect of alveoli expansion on particle’s fate and to elucidate a new mechanism of geometrical entrapment that is the sole mechanism responsible to deposition of inertia-less non-Brownian particles inside alveoli. In chapter 2 we provide a brief depiction of the aerodynamic model used in this paper to describe the flow field inside a rhythmical expanding alveolus and the equations that govern the motion of a particle in a gravity-free environment. In chapter 3 particle fate is addressed and the results are discussed, underlying the difference between the current flow model and rigid wall alveoli models. In Chapter 4 we present the main conclusions.

**METHOD**

The aerodynamic model employed in this paper to describe the flow field inside rhythmical expanding alveoli was suggested by Haber *et al.* [6] and its main characteristics are recapitulated in HYT. The geometrical model of an alveolus and its neighboring duct is shown in Fig. 4. It consists of a hemisphere attached at its rim to a plane wherein both undergo cyclic expansion and contraction motions. The radius of the alveolus depends on time and is approximately given by the following expression,

\[ R = R_0(1 + \beta \cos(\omega t)) \]  

characterized by a single dimensionless parameter \( \beta \), that is determined by the breathing flow rate.
We shall, henceforth, assume common values for the mean alveolus radius, \( R_0 = 100 \mu m \), the dimensionless amplitude, \( \beta = 0.1 \) and the breathing frequency, \( \omega = 2\pi/5 \) to reduce the number of parameters examined. We also assume that the far upstream or downstream flow inside the duct adjacent to the alveolus is given by a cyclic shear flow (Figure 4)

\[
v_y = -G_0 R_0 \frac{z}{R} \sin(\omega t + \delta)
\]

that is slightly out of phase (observed in alive rabbit lungs, Miki et al., [11]) with that of the radial velocity of the alveolus wall \( \dot{R} = -R_0 \beta \omega \sin(\omega t) \).

As in HYT we assume that \( \delta = 100^\circ \) for the phase angle. The alveolus expansion velocity (1) and the shear flow (2) induce a very complex flow field \( v \) inside the alveolus (e.g. figure 3) that is wholly dependent on a single dimensionless shear parameter \( \gamma \),

\[
\gamma = \frac{G_0}{\beta \omega}.
\]

In essence, the \( \gamma \) parameter reflects alveolus placement along the acinar tree (See figure 2 in HYT for a distinctive correlation that exists between \( \gamma \) and the generation number of lung airways). For rigid alveoli \( \beta = 0 \) and \( \gamma \to \infty \) while for stretching alveoli \( \beta \) is non-zero and the value of \( \gamma \) varies according to changes in the shear rate \( G_0 \) along the acinar tree. Generally, the value of \( \gamma \) decreases with increasing generation number since the flow rate inside the airways diminishes with each successive bifurcation.

Haber et al. (2000) obtained a generic solution \( v^H \) describing the flow field inside an alveolus of radius unity that its wall expands with a unit radial velocity. Pozrikidis [5] derived a generic solution \( v^P \) depicting the flow field induced inside a hemispherical cavity of radius unity that is affected by a unit downstream shear rate flow. Thus, the combined Stokes flow field is given by,

\[
v = \beta \omega R_0 \left[ v^H \sin(\omega t) + \gamma v^P \sin(\omega t + \delta) \right].
\]

The dimensionless equation that governs the motion of a particle of diameter \( D_p \) in a gravity-free environment possesses the simplified form,

\[
\frac{d\hat{r}_p}{dt} = \beta \left[ \sin(\dot{\hat{r}}_p / \hat{R}) + \gamma \sin(\dot{\hat{r}} + \delta) \right] \frac{v^H}{R_0} \cdot \hat{R} = \frac{R}{R_0} = 1 + \beta \cos \dot{\hat{r}},
\]

since particles 0.5-2\( \mu m \) in diameter are strongly affected by aerodynamic forces while inertia forces and Brownian displacements are negligibly small (see HYT).

The caret symbol in (5) is used to define the dimensionless variables,

\[
\hat{r}_p = r_p / R_0, \quad \hat{t} = \omega t, \quad \hat{R} = R / R_0 = 1 + \beta \cos \dot{\hat{r}}.
\]

where \( r_p \) is the instantaneous location of the particle center.
The solution of (5) depends upon seven dimensionless parameters: Three parameters stand for the particle initial position \((\hat{x}_{p0}, \hat{y}_{p0}, \hat{z}_{p0})\); Additional three characterize the flow field, namely, the dimensionless expansion amplitude \(\beta\), the shear parameter \(\gamma\), and the phase angle \(\delta\). The seventh parameter stands for dimensionless particle diameter \(\alpha = \frac{D_p}{R_0}\). This last parameter is introduced via the condition that finite size particles may not penetrate the alveoli walls.

It is interesting to note that the respiratory frequency \(\omega\) has no direct impact on the solution under gravity-free conditions. It merely serves to scale the time. Also note that particle and alveoli sizes affect the solution through the value of \(\alpha\) only.

Notwithstanding, we shall use the physical particle diameters instead of \(\alpha\) with \(R_0=100 \mu m\). However, the solution would be similar for various values of \(R_0\) and \(D_p\) as long as the value of \(\alpha\) is preserved. Equation (5) is solved using Matlab’s ODE45 procedure, a self-starting Runge-Kutta method, and the desired accuracy is obtained with 1000X1000 grid-points for the velocity fields \(v^H\) and \(v^P\) and relative and absolute tolerances of \(10^{-8}\) and \(10^{-16}\), respectively (see HYT for in-depth investigation).

RESULTS AND DISCUSSION

Particle motion within the lung in a micro-gravity environment is distinctly different from that obtained in HYT that addressed gravity effects on particle trajectories and deposition. In a gravity-free environment 0.5-2 \(\mu m\) particles simply move along path lines, namely, their center of volume follow closely the trajectories of fluid particles. Consequently, it seems that no deposition can occur in this case. Notwithstanding, since particles are of finite size, their external surface may contact the alveoli walls and be captured. This geometrical entrapment mechanism must obviously depend upon the particle diameter - for a given alveolus radius - and on the alveoli expansion mechanism (or, more precisely, upon the dimensionless parameters \(\alpha\) and \(\gamma\)).

The dependence of particle trajectories upon alveoli expansion

Figure 5 illustrates the trajectory of a 2 \(\mu m\) particle during five breathing cycles for three different values of the alveolus shear parameter \(\gamma\). The particle is initially located at (0.3, 0.3, -0.7) and performs a complex non-periodic motion. For the smallest value tested \(\gamma = 20\), the particle performs a small number of orbits mainly contained in the \(yz\)-plane as it slowly drifts in the \(x\)-direction. For larger values of \(\gamma\), the number of orbits increases. This observation is hardly surprising since large \(\gamma\) values is a result of stronger shear flows and consequently higher vorticity values. The slow drift in the \(x\) direction (or \(-x\) direction, for particles initially located at the -\(x\) side of the alveolus) stems from the combined effect of expansion and shear flows and the asynchrony between the flows. Had the phase angle \(\delta\) been zero the particle would have performed a periodic motion, never depositing or leaving the alveolar cavity (Haber et al. [6]). Similarly, in the absence of an expansion mode, a closed streamline region is formed inside the cavity that is completely separated from the flow in the adjacent duct (Fig. 2, Pozrikidis [5]). Thus, a particle placed outside the alveolus, can never enter the alveoli and its deposition inside the alveolus would have been impossible. However, according to our flow model which accounts for expansion and contraction of the alveoli, slow motion of the particle toward the rim may eventually cause its entrapment or its escape from the alveolus.
Note, that the residence time of particles inside the alveoli may be quite large, a fact that may play an important role in deposition enhancement due to Brownian motion of sub-micron particles. A follow-up paper will address this very important deposition mechanism.

In the next chapter particle fate is discussed vis-à-vis its initial location, size and various values of the shear parameter $\gamma$ indicating alveoli location along the acinar tree.

**The dependence of particle fate upon initial position, alveoli expansion and particle size**

Figures 6a-c address the effect of various initial positions and $\gamma$ values on the fate of 2 $\mu$m particles. Particle locations are evenly distributed at the $x=0.2$ plane and the calculation is terminated after at most 10 breathing cycles. The symbol attached to a point signifies whether a particle, initially located at that point, is still moving inside the alveolus (*), has left the alveolus and moves down- or up-stream inside the adjacent alveolar duct (.) or has deposited (+). Very complex and rich maps are obtained. In some regions, particles behave uniformly. For instance, particles located initially near the cavity opening are more likely to leave and many located near its bottom are likely to stay on or deposit. However, in a region near the saddle point (shown in Fig. 3), particles placed at close proximity to each other may behave in a completely non-uniform manner. This sensitivity to initial conditions is the hallmark of chaotic flows. Indeed, figure 6c shows a blow up of a small region near the saddle point. It manifests the entanglement and the totally unpredictable behavior of very close points.

The number of particles that deposit due to geometrical entrapment increases with $\gamma$. In other words, less deposition occurs in an alveolus located in a higher generation airway by this mechanism (This result by no means states that the *total* number of particles trapped in the distal region of the acinus is smaller, since this region comprises of an increasing number of alveoli). A significant change occurs when $\gamma$ increases from a small value as 20 to 100 i.e. as the particle moves to a lower generation of the alveolar tree. A possible explanation for the significant effect of $\gamma$ is as follows: As $\gamma$ increases, particle pathline contain an increased number of orbits (Fig. 5), this, in turn, enhances its probability to stay close to the wall and eventually deposit. As $\gamma$ increases from 20 to 100 the flow vorticity increases 5 times and the number of orbits increases accordingly. A smaller effect would be observed with a change from $\gamma=100$ to 200 that increases the vorticity by a factor of two. In case $\gamma$ is about 10, the flow is controlled by the flow induced by alveolar expansion/contraction, no closed pathlines are observed (Haber et al. [6]), and deposition due to geometrical entrapment is minimal.
Figure 5: Trajectories for gravity-free conditions

(a) $\gamma = 20$, (b) $\gamma = 100$, (c) $\gamma = 200$
Figure 6: The effect of various particle initial positions and $\gamma$ on particle fate for particle size $D_h = 0.5\mu m$ under gravity-free conditions. A blow up of a small area of figure 6c illustrates the sensitivity of the results to particle initial positioning.

Deposition sites for several $\gamma$ values and initial locations are depicted in figure 7. It elucidates that particles tend to deposit unevenly over the alveolus wall with the largest concentration occurring near the alveolus rim.
Figure 7: Deposition sites of $0.5\mu m$ particles, initially positioned according to figure 6, under gravity-free conditions for various $\gamma$ values.
The effect of particle size on its fate and the deposition sites is addressed in figures 8 and 9 where two particles, $1\mu m$ and $2\mu m$ in diameter, are examined for $\gamma=100$.

![Figure 8: The effect of particle initial position and size on its fate ($\gamma=100$).](image)

They manifest that smaller size particles are less inclined to deposit due to the geometrical entrapment mechanism and that deposition sites occur mainly near the distal side of the alveolus. Darquenne et al. [2], [3], [4], observed that particle size has only a slight effect on particle deposition in a micro-gravity environment. However, one should notice that [2], [3], [4] have monitored the total number of particles deposited inside the lung as a whole, namely, entrapment at the upper airways, bifurcation regions and the acinus whereas our prediction pertain to the alveolar region only. Thus, alas, no rigorous or meaningful comparison can be made with their experiments.
In summary, the foregoing results manifest the importance of alveolar expansion that combined with the geometrical entrapment mechanism yield non-zero deposition of particles inside lung alveoli. Had the flow model disregarded acinar expansion, zero deposition due to geometrical entrapment would have been predicted.

Figure 9: Deposition sites for $\gamma = 100$, and $D_h = 1[\mu m]$. $D_h = 2[\mu m]$ under gravity-free conditions.
CONCLUSIONS

Under gravity-free conditions, particles in the 0.5-2 $\mu$m size range are strongly affected by aerodynamic drag forces and to a much lesser extent by their inertia (the Stokes number is of the order of $10^{-4}$, see Haber et al. [10]) and Brownian motion. Consequently, particle trajectories follow fluid pathlines closely and geometrical impaction is the only mechanism that may affect their deposition. If no expansion of the alveolus is considered, particles initially located inside the airways would travel back and forth along the alveolar ducts, performing a cyclic reversible motion during the breathing cycle, never penetrating the alveoli during the breathing process since the flow streamlines inside the alveolus, are known to be completely separated from that inside the duct. Thus, no deposition can be predicted by rigid wall alveoli models.

However, if alveoli expansion is accounted for, particles may be diverted toward the cavity region. Since chaotic particle motion may ensue, the fate of the particles is very sensitive to their initial location. Particle deposition due to geometrical impaction may occur with their majority entrapped at the distal area of the alveolus rim.

REFERENCES


2. Darquenne, C., Paiva, M., West, J. B., & Prisk, G. K., Effect of microgravity and hypergravity on deposition of 0.5 to 3 $\mu$m -diameter in the human lung, J. Appl. Physiol., 83 (1997) 2029-2036.


5. Pozdrikidis, C., Shear flow over a plane wall with an axisymmetric cavity or a circular orifice of finite thickness, phys. Fluids, 6 (1994) 68-79.


