Mechanisms of Aerosol Particle Deposition in the Oro-Pharynx Under Non-Steady Airflow

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Comparison of experimental and computational results of aerosol deposition in the oro-pharyngeal cast of human published recently (Sosnowski TR, Moskal A, Gradon’ L. (2006) Inhal Toxicol; 18: 773–780) demonstrated the applicability and relevance of considering realistic breathing patterns in analysis of aerosol flow and deposition within the human head airways. This issue is extended in the current paper, focused on a detailed analysis of spatial and temporal distribution of particle deposition in the oro-pharynx during inspiration. CFD modeling was used to determine both the 3D airflow structure and the local particle deposition fluxes at two different inspiratory patterns. Behavior of aerosol (particle size: 0.3–10 μm, material density: 2200 kg m⁻³) was analyzed applying Lagrangian approach and considering Brownian effects for submicron particles. Results indicate that particles of different sizes are deposited in different parts of the oro-pharynx, depending on the point in the inspiration cycle. Larger particles (3–10 μm) are separated efficiently in the naso-pharyngeal bend due to inertia, which predominate in the middle phase of inspiration. Submicron particles are deposited more uniformly in the oro-pharyngeal space, and their separation from the air is enhanced in a short transition period between inspiration and expiration. It suggests the importance of mixing of inspired and expired air streams for particle deposition pattern. Comparison of our computational results of deposition to the approximation derived from the in vivo data (Stahlhofen W, Rudolf G, James AC. (1989) J Aerosol Med; 2: 285–308) shows a good agreement for particles, for which the inertia is a predominant mechanism of deposition. The results of this work lead to a more detailed description of the dynamics of oro-pharyngeal aerosol deposition during inspiratory part of the breathing cycle. The recognition of that problem is essential for prediction of toxic or pharmacological local effects of inhaled aerosols.

Keywords: inhalation; oro-pharynx; aerosol dynamics; deposition distribution

INTRODUCTION

Breathing with air contaminated by aerosol particles leads to health effects that eventually result in the development of lung diseases (McClellan, 2000). Deposition of inhaled particles on the surface of the respiratory system is the first step in the chain of events creating the health hazard. The detailed recognition of deposition mechanisms in different parts of the respiratory tract is therefore essential for understanding the toxic potential of inhaled aerosol. It also allows for evaluating the strategies of therapy since the majority of drugs for treatment of lung diseases are also introduced by inhalation (Smith and Bernstein, 1996).

Most experimental studies of aerosol deposition in the respiratory system, beside the costly in vivo measurements, rely on the use of airway cast replicas (Gradon and Yu, 1989; Swift, 1996; Cheng et al., 1999; Gracic et al., 2004, Sosnowski et al., 2006). Theoretical methods using computational fluid dynamics (CFD) are also extensively developed thanks to the increase of computer power. CFD calculation results give a possibility of detailed analysis of the local gas flow and particle deposition in different parts of the respiratory tract. Two issues need to be stressed as the important features of the discussed problem:

(i) Particle deposition is governed by the local dynamics of aerosol particles that are carried through the complex geometry of the airways by inspiratory/expiratory airflow;
(ii) The dose (mass) of deposited particles is not necessarily the most appropriate measure of potential health effects caused by deposition of inhaled particles.

Considering the first problem, it should be noted that the probability of deposition of a particle with the given size and density depends both on the airflow geometry and the actual local airflow conditions. However, in the widely accepted approach (e.g. Cheng et al., 1999; Grgic et al., 2004; Zhang et al., 2005, Zhang and Finlay, 2005) only the average airflow rates (usually equal to the minute ventilation) are used to quantify the regional and total particle deposition. Although it may be in part justified by an overall agreement between predicted deposition efficiencies and rather sparse in vivo results (additionally characterized by a large scatter due to inter-subject variability), one must admits that the physical picture of the process is substantially different. In reality, the airflow during breathing is characterized by the variable rate and alternating direction. These aerodynamic features are especially important for the local deposition fluxes. Zhang and Finlay (2005) suggested recently that a striking discrepancy between their in vitro results and the previously published in vivo data should be attributed to the unsatisfactory representation of airflow conditions in the cast studies. It is obviously true, if the results of volunteer studies (natural breathing) are compared with the results obtained with casts at the constant airflow rates. It is therefore essential to include all airflow features in both the experimental and computational studies.

The second mentioned issue concerns the submicron particles, which are often present in the occupational environment, e.g. during welding, grinding, combustion processes and in diesel emissions (Mauderly et al., 2000; Zimmer and Maynard, 2002; Maynard and Kuempel, 2005). Their toxic potential is attributed to the high surface area per unit mass (Kreyling et al., 2004). Such particles are capable of inducing apparent health effects, although their weight fraction in the total mass of deposited material is almost negligible. In such cases, the number rather than mass of deposited particles should be taken into account. This leads, however, to several technical problems in the methods of aerosol generation and measurements, which are typically used in deposition studies. It can be also a reason why the significance of such particles has been neglected for a long time.

Both problems indicated here have already been addressed recently (Sosnowski et al., 2006), where we have reported selected issues of CFD modeling and experiments related to oro-pharyngeal flow and deposition. We have proposed there an experimental procedure based on the application of the silicone-rubber cast and the programmable pump (‘artificial lung’) to mimic real-like flow conditions. We have also discussed some problems of computational method and its limitation.

The current paper is focused on the detailed discussion of mechanisms responsible for the influence of inspiratory airflow variability on local and temporal deposition of aerosol particles in the model of human oro-pharynx. The selection of the oro-pharyngeal region for such analysis was motivated by the fact that particle deposition in that part of the respiratory system determines the aerosol ability of penetration to the tracheobronchial tree (Dolovich and Rhem, 1998), which is the primary region of lung disease development and, at the same time, the major target of aerosol therapy (Zanen and Laube, 2002). At the same time, the oro-pharynx is built as a strongly inhomogeneous air duct, in which the discussed dynamic effects are intensified.

METHODS

Owing to advances in measuring techniques, refined airway models became available in recent years. Magnetic resonance imaging (MRI) has been used for 3D visualization of the human oro-pharyngeal airspaces (e.g. Ehtezazi et al., 2004; Pritchard and McRobbie, 2004). The results indicate a complicated shape of that region of the airways, which has a strong influence on the deposition pattern. In addition to inter-subject variability, the geometry of the oro-pharynx was shown to be dependent also on the inhalation conditions even for the same subject. It is therefore difficult to indicate any specific geometry that could be used as a general model of the human oro-pharynx.

In this study we used the geometry developed at the Human Anatomy Department at Medical Academy of Warsaw, as described previously (Sosnowski et al., 2006). The 3D computational mesh has been constructed using Gambit software from Fluent Inc. (Lebanon, NH) and contained ~200 thousands tetrahedral elements (Fig.1).

Computations of the airflow field and aerosol particles dynamics, during realistic inhalations, have been performed with the commercial CFD package Fluent (Fluent Inc.). The simulated breathing curves have been characterized by the volume of inhaled air \( V_{inh} \, [dm^3] \) given by Sosnowski et al., (2006):

Curve ‘a’:

\[
V_{inh}(t) = 1.383 \cdot \left[ 1 - \cos \left( \frac{\pi}{3.41} \cdot t \right) \right] \tag{1}
\]

Curve ‘b’:

\[
V_{inh}(t) = 1.368 \cdot \left[ 1 - \cos \left( \frac{\pi}{2.75} \cdot t \right) \right] \tag{2}
\]

where: \( t \) is inhalation time in seconds. The instantaneous value of the airflow rate can be calculated by
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RESULTS AND DISCUSSION

Total deposition efficiencies of particles with different size, \( \eta_{\text{tot}}(d_p) \), for both inspiratory patterns and two material densities (1100 and 2200 kg m\(^{-3}\)) have been presented and discussed previously (Sosnowski et al., 2006). The relationships between the efficiency of particle deposition and particle diameter have a typical shape, with a minimum (efficiency <25%) for the particles in the size range 0.5–1 \( \mu \)m. The efficiency of deposition is higher for smaller particles due to strong effects of turbulent diffusion. Deposition efficiency of coarse particles (>5 \( \mu \)m) also gradually increases, to >95% for 10 \( \mu \)m particles. This is caused by the predominance of impaction as a separation mechanism. Calculated deposition efficiency and the change in particle size distribution (PSD) of a polydisperse aerosol have been successfully verified against the experimental data obtained with the oro-pharyngeal cast of the exactly matching geometry (Sosnowski et al., 2006).

In the current work we want to focus our considerations on the temporal and spatial distributions of particle deposition in the studied geometry. Figure 2 shows the temporal distribution of the relative deposition efficiency in the whole oro-pharynx during the inspiratory part of the breathing cycle. Calculations consider also the effect of transition between inspiration and expiration with incorporation of the mixing effect at this transition moment. Each bar in Fig. 2 represents the efficiency, which is normalized in respect to the absolute collection efficiency, \( \eta_{\text{tot}} \), for particles with the given size \( d_p \), and averaged over the indicated time-interval.

This drawing illustrates the intensity of deposition of particles with diameters 0.3, 1, 3 and 10 \( \mu \)m during...
Fig. 2. Calculated temporal distribution of deposition of particles with different diameter in the model oro-pharynx during non-steady flow. Upper line in each figure shows the spatially-averaged velocity at the entrance to the object.
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The spatial distribution of the relative deposition efficiency during the whole inhalation in each characteristic segment of the studied geometry (Fig. 1A–C) is shown in Fig. 3. It illustrates the deposition intensity along the oro-pharynx.

The distribution of temporal deposition (Fig. 2) clearly indicates that the most effective deposition size depends on the phase of inhalation. Deposition of 10-μm particles is almost independent of the actual airflow rate, which can be explained by the particle mass being high enough for the effective impaction at the walls of the airway, even at relatively low airflow rates. As indicated in Fig. 3, the region of the most efficient deposition of 10-μm particles is located in segment B (naso-pharyngeal bend characterized by the narrowing and a strong curvature of the duct), and virtually no particles are deposited beyond it, as they are not able to penetrate to segment C.

The situation is different for smaller particles (with a lower mass). In the case of 3-μm particles, the efficiency is increased during the central part of the inspiratory curve, i.e. for the highest flows. This suggests that impaction still remains an important deposition mechanism for such particles; however higher velocities are required to make this mechanism predominate. It can be noticed that for a faster inhalation (Fig. 2, curve ‘b’), the deposition remains effective also during a decline of the airflow, which resembles the results obtained for larger particles. Again, the bend area (Segment B) is the main region of the deposition, however some particles are able to penetrate and deposit in the posterior part of the oro-pharynx (Segment C).

Particles with diameter of 1 μm are collected with a lower overall efficiency (Sosnowski et al., 2006), and, as seen from Fig. 2, their deposition takes place mainly during flow decrease and the transition to expiration. The preferred region of deposition is located in segment C, but particles are appreciably deposited also in two other parts of the oro-pharynx. Similar results have been found for submicron particles (0.3 μm), although their deposition is more uniform along the airway. Deposition of the smallest particles is governed by the diffusive effects; however the observed enhancement during flow reversal suggest also the strong influence of air mixing effect, and, as a result of this, the reduction of the thickness of diffusional boundary layer. This can be attributed to aerodynamic effects caused by the interaction between inspired and expired air, which are stronger for the faster transition (curve ‘b’). Such effects seem unimportant for particles of high inertia (e.g. d_p = 10 μm), which are deposited with almost equal efficiency in all stages of inspiration.

The most important outcome from the presented set of data is that the common assumption of constant (averaged) flow leads to a significantly simplified physical picture of aerosol behavior in the oro-pharynx. One should be aware that, even if the residence time of a particle in the given geometry may be in the sub-second range, its dynamics is determined by the local aerodynamic conditions, which are continuously changing during breathing. This effect is less significant for large particles, which are efficiently deposited even at low flow rates, therefore flow variations do not change their deposition noticeably. This explains why the common approach to prediction of particle deposition by considering only the mean airflow rate can be useful for coarse aerosol particles. However, analysis of submicron particles and their importance for health effects requires a more realistic description, such as the one presented here. It can be found from it that change of the averaged value of flow rate (curve ‘a’: 48.7 dm³ min⁻¹, curve ‘b’: 59.7 dm³ min⁻¹) only slightly influences regional distribution of deposition of fine particles in the oro-pharynx. On the other hand, temporal variations in airflow during inhalation have a profound influence on the temporal deposition rate (e.g. it increases when flow declines and reverses, but is reduced for the periods of fast flow). Figure 4 compares the computational results of particle deposition to the relationship, which was fitted to the experimental data obtained in vivo (Stahlhofen et al., 1989). This fitted curve is expressed by:

\[ \eta = 1 - \frac{1}{3.5 \times 10^8 (d_{ae}^2 Q)^{1/7} + 1} \]  (3)

where \( d_{ae} \) denotes aerodynamic diameter of particle [μm], and \( Q \) stands for the mean volumetric airflow rate [cm³ s⁻¹].

The presented comparison shows a satisfactory agreement for the inertial parameter \( \xi \geq 1000 \), where:

\[ \xi = \rho_p d_p^2 Q \]  (4)

(\( \rho_p \) and \( d_p \) denote particle density [g cm⁻³] and diameter [μm], respectively). The agreement does not hold for \( \xi < 1000 \), because for small particles the inertia is no longer the predominant mechanisms of deposition.

CONCLUSIONS

This study was focused on the explanation of the mechanisms responsible for dynamic effects during particle flow and deposition in a model of human oro-pharynx under realistic, non-steady-flow patterns. Based on CFD results, it was demonstrated that the local particle deposition depends both on particle size and the actual aerodynamic conditions related to the given time-interval of inspiration. Different mechanisms of particle separation from the
aerosol stream become effective in various phases of breathing. Large particles are less sensitive to airflow variations due to their high inertia resulting in good separation efficiency in the naso-pharyngeal bend. On the other hand, the behavior of submicron particles is more sensitive to airflow variations.

The modeling approach proposed in this work gives the opportunity of further discussions regarding the

Fig. 3. Calculated distributions of relative regional deposition of aerosol particles with different diameter in the model oropharynx during non-steady flow.
influence of breathing patterns and aerosol properties on the local distribution of deposition in other model geometries of the human oro-pharynx. This allows for the tracing of evolution of the primary PSD from the respiratory tract inlet down to the trachea. The computational results agree well with the in vivo data by Stahlhofen et al. (1989). Our data for submicron particles extend this picture by indicating a higher deposition than expected from the models developed for large particles and restricted to inertial effects. Deposition of submicron particles, caused primarily by Brownian diffusion, is strongly influenced by local aerodynamic effects, which were usually overlooked by assuming conditions of the stationary flow. The methods and results presented in this work allow for a more detailed and realistic description of aerosol flow and deposition in the complex geometry of the human oro-pharynx during dynamical conditions of breathing. Such information is necessary for the understanding of toxic or pharmacological effects of inhaled aerosols.

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