CHARACTERISTICS OF TURBULENT PARTICLE TRANSPORT IN HUMAN AIRWAYS UNDER STEADY AND CYCLIC FLOWS

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ABSTRACT
Motion of monodispersed micron-sized particles suspended in air flow was studied on transparent model of human airways using Phase-Doppler Particle Analyser (P/DPA). Time-resolved velocity data for particles in size range 1 to 8 µm were processed using Fuzzy Slotting Technique embedded in Kern software (Nobach, 2002) to estimate power spectral density (PSD) of velocity fluctuations. Optimum setup of the software for these data was found and recommendations for improvements of future experiments were given. Typical PSD plots are documented and mainly differences among (1) steady-flow regimes and analogous cyclic breathing regimes, (2) inspiration and expiration breathing phase and (3) behaviour of particles with different size are described for several different positions in the airway model.

Systematically higher content of velocity fluctuations in the upper part of frequency range (30 – 500 Hz) was found for cyclic flows in comparison with corresponding steady flows. Expiratory flows in both the (steady and cyclic) cases produce more high-frequency fluctuations compared to inspiratory flows. Negligible differences were found for flow of particles in the inspected size range 1 to 8 µm at frequencies up to 500 Hz. This finding was explained by Stokes number analysis. Implied match of the air and particle flows thereby confirms a possibility to use the P/DPA data as air flow velocity estimate.

INTRODUCTION
Transport and deposition of aerosol in human airways has been of research interest for several decades. Main present motivation for elucidation of related phenomena is increasing tendency of therapeutic drug application in form of inhaled aerosol.

Published works show that air flow in the multiple-bifurcating airway system is very complex problem showing turbulent, transient and laminar behaviour depending on breathing conditions, morphology and position in the airways. Complex flow structures containing different types of vortices, flow detachment, wakes, bidirectional flow, recirculation zones and even velocity oscillations were observed (brief review in Jedelsky et al., 2010a). Continuous movement from simple airway models and steady flows to realistic models and lifelike cyclic flow regimes is seen on present CFD simulations and experimental studies. Realistic, CT based, lung models were proved to be a must for true results of flow and particle transport. Significant quantitative and qualitative differences in aerosol transport/deposition data under steady flows frequently studied in the past and lifelike oscillatory flows were reported. Fate of the inhaled particles depends on character of the flow; for instance diffusion mechanism of small particle deposition is influenced by flow turbulence. Turbulence affects airflow flow patterns as well as wall shear stress (Lin et al., 2007) and is responsible for increased local particle deposition (Gemci et al., 2002, Chan et al., 1980).

Several methods have been applied for flow studies in airway models. Intrusive Hot Wire Anemometry (HWA) was used for in vitro air flow measurements in the past while optical measurement methods prevail today. The most common is Particle Image Velocimetry (PIV), Laser Doppler Velocimetry (LDV) (Corieri and Riethmüller, 1989, Lieber and Zhao, 1998, Tanaka et al., 1999, Corcoran and Chigier, 2000) and P/DPA (Gemci et al., 2002) are less frequent. Complexity of the realistic models perplexes application of optical methods for aerosol transport studies. PIV requires an application of liquid with refraction index equal to the one of the model walls instead of air as really breathed fluid. LDV or P/DPA, as point-wise techniques are more suitable for research in composite optical system of transparent model with air as a carrier medium. These methods also offer direct particle flow measurement with high temporal resolution and high data rate. Aside basic flow characteristics as mean and rms velocities also moments and spectral properties could be estimated therefore. PIV as planar technique offers global look on flow structures while Laser-Doppler based techniques give information on velocities of individual particles in chosen point.

We have processed exemplary P/DPA data acquired during our earlier study¹ with aim to elucidate character of the turbulent particle transport in human airways. PSD of particle velocity fluctuations was estimated for several data sets. Arbitrary PSD plots are shown to describe nature of the particle-air flow. Differences between steady and cyclic flows

¹ This measurement of transport of monodispersed micron-sized liquid particles dispersed in air was made in realistic transparent human airway model for a range of steady and cyclic flows and particles of various sizes. P/DPA was used to acquire time resolved data of particle velocity (Jedelsky et al., 2010a).
in several positions of the airway model and influence of flow regime and particle size on the PSD are discussed. Several recommendations for future to improve the PSD estimations are given.

EXPERIMENTAL APPARATUS

Our experimental device (Fig. 1) uses a computer controlled motor (6) which drives piston through pneumatic cylinder (5) as a source of oscillating air flow\(^2\). Monodispersed aerosol particles of di-2-ethyl hexyl sebacate (DEHS) ranging from 1 to 8 µm are generated by condensation generator (4). One-half of the particles is mixed with the air in a chamber (3) using static mixer and flows into the airway model (Fig. 1 left). The second half flows into bladder (2), that collects the particle-air mixture for the second breathing cycle phase. The particle-air flow is incompressible, subsonic, isothermal, viscous, with particle/air density ratio of 760 and the DEHS aerosol is non-evaporating/non-condensing. ID Dantec P/DPA (7) was used for measurement of particle size and mainly for time resolved measurement of axial velocity component of the particle motion during breathing cycle in several cross-sections of the model\(^3\).

RESULTS AND DISCUSSION

Exemplary results of the two-phase air-particle flow under cyclic breathing are seen in Fig. 2. The measurement was made in point A (placed in trachea centreline, 20 mm above carina, see Fig. 1) in regime 1 litre & 4 s, and 3 µm particles were used. Time-resolved axial velocity as well as axial turbulence intensity of individual aerosol particles passing through the measurement volume of P/DPA are displayed in the plot; an assumption that particles follow the air flow with no significant slip is made here and discussed later on. Particle velocity data are so used for air velocity and turbulence intensity estimation. It is seen that particle velocity during the cyclic flow approximately corresponds to the sinusoidal shape of the cyclic breathing. Positive velocity values stand for inspiration, negative stand for expiration.

Extensive documentation of further results of the particle transport supported with explanation of effect of various factors (particle size, steady/cyclic flows, spatial and temporal nature of the flow) was already made in (Jedelsky et al. (2010b)). Average axial turbulence intensities in point A at steady and cyclic inspiration flows are compared in Table 1 to illustrate typical results of these basic flow characteristics. Small differences between both the cases and also among different flow rates and particles of different sizes were found. Turbulence intensity covers range 0.07 – 0.11 for all the cases and no significant correlation between flow regime and the turbulence intensity is seen. It is interesting as Reynolds number varies significantly: from 1200 (15 l/min) to 4800 (60 l/min). The relatively high and regime independent turbulence intensity can be attributed to the complexity of the upstream geometrical structures of larynx.

Probability density function (PDF) of particle velocity was evaluated for steady flow conditions 30 l/min in point A (Fig. 3). The velocity distribution corresponds to log-normal distribution with moderate inclination of the maximum to higher velocities. This bias is caused by specific P/DPA sampling rate; where for spatially uniform particle

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\(^2\) Three steady breathing regimes (15, 30 and 60 litre/min) and three corresponding cyclic sinusoidal breathing regimes were used (tidal volume 0.5 litre and breathing period 4 s, 1 litre & 4 s and 1.5 litre & 3 s).

\(^3\) P/DPA was chosen instead of simpler LDV to verify particle size and also to reduce unwanted sources of noise in PSD estimation such as reflections and multiple-particle scattering. For more information on the P/DPA setup, data processing and the airway model see Jedelsky et al. (2010a) and Jedelsky et al. (2008) resp.

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<table>
<thead>
<tr>
<th>Size (µm)</th>
<th>Steady Inspiration (litre/min)</th>
<th>Cyclic Inspiration (^4)</th>
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<tbody>
<tr>
<td></td>
<td>15</td>
<td>30</td>
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<tr>
<td>2</td>
<td>0.104</td>
<td>0.085</td>
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<tr>
<td>4</td>
<td>0.107</td>
<td>0.110</td>
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<tr>
<td>7</td>
<td>0.109</td>
<td>0.092</td>
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\(^4\) The turbulence intensity in cyclic inspiration flow is calculated as an average value during a phase window (0.3π - 0.7π) averaged for ten consequent cycles.

\(^5\) Tidal volume (litre) & period of cycle (sec)
concentration the data rate is proportional to actual flow velocity. Different particle sizes give similar PDF shapes with no significant systematic differences.

**Estimation of PSD of Velocity Fluctuations**

Laser-Doppler based techniques provide flow velocity data with comparatively high temporal resolution so they can serve for estimation of the moments and spectra of the turbulent velocity fluctuations. Our particle mixing system delivers homogeneous air-particle mixture with concentration $c$ in range $10^3 - 10^7$ particles/cm$^3$ into the airway model. This dilute aerosol (mean free path in order of hundreds particle diameters) give typical data rate of P/DPA measurement in kHz range. Mean data rate is $\bar{n} = \bar{v} \cdot \bar{c} \cdot S$, where $S$ is area of the measurement volume projected in the flow direction and $\bar{v}$ is mean particle velocity.

P/DPA is a tracer-based method with irregular particle arrival times. Presuming an equal particle distribution in space with constant concentration and mean data rate of the measurement $\bar{n}$, the intervals $\Delta t$ between the particles are distributed exponentially: $p(\Delta t) = \frac{\bar{n}}{\Delta t} \cdot e^{-\frac{\bar{n}}{\Delta t}}$. The most probable interparticle arrival time is zero so information about very high frequency fluctuations is contained in the data. Nevertheless maximum reliable frequency is $\bar{n}/2\pi$ according to Adrian and Yao (1987). The irregularity of the sampling time caused by naturally seeded particles in flow brings difficulties with estimation of the PSD of the velocity fluctuations. We employed a slot correlation technique for estimation of the PSD as described by Benedict et al. (2000) and calculated the PSD using Kern software (Nobach, 2002).

**PSD Evaluation using Kern Software**

The software has a number of options and variables to set with no guideline for optimum setup. However resulting PSD is very sensitive to the input parameter values. Large data set was tested to find out the best setup. Published HWA and LDA data of identical flow (Nobach, 2006) were compared first. After successful agreement between these HWA and LDA results we have focused on our P/DPA data. A set of three consequent data records was chosen to describe the PSD estimation process. The data were acquired in point A for steady flow regime 30 l/min and 1 µm particles. Each file has 16384 samples and measurement period 5.8 s (average sampling frequency 2825 Hz).

Fig. 4 shows PSD of the velocity fluctuations versus frequency, $f$, using log-log plot. Average PSD curve based on the three records together with standard deviation is calculated. We have realised that any unique setup does not produce the PSD in whole frequency range provided by the measured data. So each spectra is composed of two curves; the lower frequency part (3.3 – 35 Hz) was calculated using: SC, $F=5000$, $K=2048$, $N_f=1000$, standard options +vw +ln +fst +fbat +lte +cft, the upper frequency part was calculated as: SC, $F=5000$, $K=2048$, $N_f=1000$, standard options. Individual PSD plots (not shown here) are very consistent in the frequency range 15 – 750 Hz as indicated by the standard deviation curves. Fluctuations in amplitude that were observed in each PSD plot change record to record and therefore are not inherent property of the flow. Low frequency fluctuations in the PSD amplitude (up to about 15 Hz) are a product of natural variations of flow that cannot be fully reflected by this relatively short data record. The results differ significantly also for frequencies higher than about 1 kHz due to lack of useful data from P/DPA measurement. The differences can be partially caused also by the processing algorithm. This part of plot is not realistic and cannot be used for analysis.

Variable windowing (vw) used in this calculation leads to smoothening and averaging of fluctuations in individual spectral lines. Larger fluctuations are preserved. Amplitude of velocity fluctuation in the inspected point shows only very mild decreasing tendency with frequency up to about 30 Hz, then slightly higher and relatively constant-slope decrease according $f^{-2}$ in range 30 – 300 Hz and more distinct decrease with constant slope $f^{-7/3}$ for frequencies higher than 300 Hz. No distinct peak in the PSD is obvious. Very similar shape of

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5 SC = Slot Correlation, $F$ is the frequency used to define the time lag between samples in the autocorrelation function (ACF), $K$ is the number of samples in the ACF, $N_f$ is the number of samples in the spectrum, for better description see Nobach (2002).
the PSD was found also at other measurement points, for other particle sizes and other flow regimes in trachea.

Cumulative turbulence kinetic energy (TKE) was calculated for given data. Amplitude of oscillations at frequencies higher than 800 Hz was approximated using the $f^{0.5}$ rule. Low frequency oscillations up to 140 Hz participate on 50% of the total TKE and 90% is covered in range up to 620 Hz.

Calculation made with the same setup as previous results but without vw produced PSD plots containing strong scatter in the amplitude. No significant coherence of this “noise” in spectra among different records was found. Averaging of PSD from the three records (Fig. 5) reduces this scatter so processing of multiple data files or long measurements is important for statistically correct results. Variable windowing is even stronger instrument for the data smoothening mainly at high frequencies as indicated in the plot.

**Steady Flows**

Several P/DPA data sets were used to find out influence of flow regime and particle size on PSD of velocity fluctuations and to describe differences between inspiration and expiration flows and spatial variations of the PSD. Data in main-stream positions with relatively simple flows without wakes and recirculation zones were used throughout the paper.

**Flow Regimes.** PSD plots for three inspiratory flow rates (15, 30 and 60 l/min, particles with diameter 4 µm) in point B (placed in trachea 4 mm from the centreline, 20 mm above carina, see Fig. 1) are compared on Fig. 6. All three cases give similar PSD values for low frequencies (up to ~30 Hz) but higher flow rates produce significantly higher energy in upper part of the spectra. PSD is almost constant up to 200 Hz for 60 l/min but drops down suddenly for 15 l/min and 30 l/min after reaching 20–30 Hz. The difference among different regimes is especially distinct for frequencies higher than 200 Hz. Velocity fluctuations in range 30–300+ Hz are therefore responsible for rising TKE with increase in flow rates. The same behaviour was also found in other measurement positions for both inspiratory and expiratory flows.

**Particle Size.** Steady inspiration flow of particles with 1, 4 and 8 µm in diameters was measured in point B at 30 l/min. No distinct differences in PSDs up to about 500 Hz (the maximum available correct frequency) are seen (Fig. 7). Differences at lower part of the spectra are due to short record as already mentioned. This result (found also in other measurement positions and for expiration flow) is important and confirms that particle up to 8 µm in diameter respond the same way to the most energetic frequencies.

**Stokes Number.** Behaviour of particles in solid-gas two-phase flow for different particle sizes at various breathing conditions can be explained and discussed by means of Stokes number ($Stk$). Mean $Stk$ (spatially and temporally averaged) in the case of flow in air through a tube of diameter $D$ for a particle having aerodynamic diameter $d_p$ and density $\rho_p$ is

$$Stk = \frac{\rho_p C_c d_p^2 \bar{V}}{18 \mu D} = \frac{4 \rho_p C_c d_p^2 \bar{V}}{18 \pi \mu mD^2}$$

(1)

where $\mu$ is air dynamic viscosity, $m$ is number of the branches in given branching level of the model, $\bar{V}$ is the mean flow rate, $\bar{V}$ is mean (spatially and temporally) particle velocity and $C_c$ is Cunningham correction factor (Theodore, 2005). Particles in our model have 0.0005 < $Stk$ < 0.12, particular $Stk$ value depends on the branching level, particle size and flow rate (Jedelsky et al., 2010b).
Turbulent particle-air flow containing vortices of certain characteristic dimension, $D$, will produce fluctuations of the particle velocity measured by P/DA probe at frequency $f = \gamma / D$, with corresponding $St_k = \rho C d v / \gamma$. Such defined $St_k$, contrary to the one given by Eq. 1, does not directly depend on flow regime and position in the lung model. Size of vortices is 2.1, 4.2 and 8.4 mm for flow-rates of 15, 30 and 60 l/min respectively at $f = 500$ Hz and corresponding $St_k$ is 0.002 for $D_k = 1$ µm, 0.016 for 3 µm, and 0.08 for 7 µm respectively. Such reasonably small $St_k$ suggests that the particles should follow the air flow closely at frequencies up to hundreds Hz as confirmed by our observations (Fig. 7).

**Other Factors.** There is not enough space to describe spatially resolved results in this paper so only illustrative plot with PSD acquired in two points of the same cross-section (A and B) for inspiration flow at 30 l/min is shown on Fig. 8. Point B give higher intensities of velocity fluctuations in whole range and mainly at frequencies higher than 200 Hz, but shape of the PSD plot is consistent with the other point.

Comparison of inspiratory and expiratory flows in point A for 30 l/min (Fig. 8) shows much higher amount of TKE contained at high frequencies for the expiration flow. This difference can be explained by different way of the turbulence generation which is due to laryngeal jet flowing to trachea during inspiration and due to mixing of streams from daughter branches for expiration flow.

**Cyclic Flows**

Flow during breathing cycle changes from positive (inspiratory phase) to negative (expiratory phase) and in major part of upper airways transition from laminar to turbulent occurs with increasing Reynolds number. High-velocity parts of the cycle near inspiration/expiration peaks are the most important for particle deposition. PSD of cyclic velocity fluctuations was evaluated using Kern similar way as above on fragments of cycle considering the flow here as quasi-steady. PSD estimates acquired such way give only overall information on average content of TKE in the spectra in the inspected fragment of time. Length of time window is a compromise to fulfil the quasi-steady flow character and acquire enough data for reasonable PSD estimate7.

Fig. 9 shows such PSD averaged from four records. Data measured in point C (Bronchus Intermedius, centreline, see Fig. 1) for particle velocity in time window 0.3 - 0.7 π (peak inspiration) were processed. These data with mean data rate about 6.7 kHz enabled reliable spectra evaluation up to 1 kHz. Short time window - 0.6 sec leads to only 4096 samples in each record and problematic evaluation for frequencies lower than 40 Hz. Large scatter in the PSD spectra and large record-to-record differences were found. The spectrum shows relatively constant values up to 300 Hz. Slow decrease with frequency above 300 Hz compared to the steady data is seen. Relatively high amplitudes of low frequency fluctuations (below 30 Hz) with local minimum at about 40 Hz were observed here and at other measurement points/ regimes. These fluctuations are supposed to be related with large-scale vortices propagated through the tubes and their influence is recognisable also on time plots of the droplet velocity, where these vortices lead to deformations of the mean velocity from the original sinusoidal course.

7 A sort of short-time Fourier transform or Hilbert transform working with non-equidistant sampling would be useful to estimate PSD of velocity fluctuations for individual breathing phases but these are not at disposal yet.
Exhalation phase of the cyclic flow produces more high-frequency fluctuations than the inspiration flow (Fig. 10) from the same reason as in the steady flow case (Fig. 8).

Corresponding steady and cyclic flows 15 l/min and 0.5 l/4 sec respectively with 3 µm particles were compared in point A (Fig. 10). Cyclic flows contain more high-frequency velocity fluctuations then the steady flows for both the flow directions. PSDs differ from frequencies about 50 Hz and about half-order difference appears at 100 Hz already.

CONCLUSIONS

Extensive data on particle flow in time domain are contained in P/DPA results acquired in steady and cyclic flows in realistic airway model. Possibilities of estimation of velocity fluctuation PSD from these data was presented. The PSD spectra were found a useful representation of the fluctuating flow and a tool to describe character of the turbulent particle transport in human airways. Kern software was chosen to calculate PSD and optimised for our results.

Similar fundamental character of TKE spectra was found for all processed data with systematic quantitative differences for (1) inspiration and expiration flows, (2) different positions in the airway tubes and (3) different flow regimes.

Amplitude of velocity fluctuations in PSD representation is relatively constant up to certain frequency (~ 30 – 50 Hz depending on flow regime), followed by moderately decreasing trend (up to ~ 300 Hz for steady and ~ 500 Hz for cyclic flows) and more rapid drop afterwards. The PSD curves are generally smooth with no distinct peaks identified in any analysed main-stream data file.

The PSD in the inspected frequency range (~ 2 – 700 Hz) is practically independent of the particle size for 1 - 8 µm particles. This effect is explained by low Stk values for observed cases. This finding is particularly important as it implies that the aerosol particles up to 8 µm closely follow the air motion and they behave according to the air flow. Particle flow data for whole range of flow rate regimes in our case can be therefore used for determination of the local air velocity. This is useful for description of air flow structures as well as for comparison with numerical simulations of flow.

Successfulness of PSD estimation relies with available data. Present P/DPA results with mean data rate 0.5 – 10 kHz (depending on position, particle size and flow conditions) allow for max. usable frequency 0.1 – 1.6 kHz. The most energetic fluctuations are covered by this range but no data on high-freq. fluctuations can be resolved. High concentration aerosol, larger measurement volume and/or multiple data sets are needed to increase the limiting frequency for PSD.

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