Simulation of the deposition of aerosol droplets in a person's bronchial tree

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Abstract. The work is devoted to the mathematical construction of the human bronchial tree, calculating the flow of gas in the lungs and modelling the deposition of drops of medicinal aerosols in the human bronchial tree. Analytically built a symmetrical human bronchial tree. To calculate the flow of gas in the lungs and the deposition of aerosols, the method of phasing out the flow in one branch of the bronchial tree is used. Three-dimensional numerical calculations of air flow and aerosol droplets in human lungs were carried out. It is shown that the number of past drops depends (except for the flow, size of drops) on the duration of inhalation.

1. Introduction

For the treatment of a wide range of human diseases, the inhalation (aerosol) method of drug administration is now increasingly used. This method of treatment has a number of serious advantages over other ways of administering drugs, as it acts directly at the very place of pathology (for the treatment of pulmonary diseases) or delivers the medicine directly to the blood, through the pulmonary alveoli. Knowing how and where drops or particles of medication are deposited in the respiratory system is fundamental to the correct dosage of medicines.

The human respiratory system consists of the upper (nose, nasopharynx, larynx) and lower (trachea, bronchial tree and alveoli) airways. The human bronchial tree has a complex tree-like structure. From the trachea to the alveoli, the bronchial tree has 24 branches (bifurcations). Individual bronchi in the section are not, generally speaking, circles. In pathology (e.g. asthma) there is a narrowing of the bronchi and a change in the shape of the passage section of the bronchi.

The complexity of numerical modeling of the current in the bronchial tree is determined by the geometric growth of the calculation area with a decrease in the size of the bronchus (the number of bronchus increases twice after each branching). Existing numerical models are limited to 7 generations for asymmetrical bronchial tree and 16 for symmetrical wood, while the full human bronchial tree consists of 23 generations. One-dimensional flow models are used to model the current in subsequent generations (in smaller bronchus). Existing methods of building a bronchial tree are empirical in nature and are tied to the possibilities of constructing complex geometry with a specific commercial CFD simulation package. Existing models of the bronchial tree do not describe the "star" internal structure of the bronchiol and thus do not describe the lungs normally and especially in pathology. To calculate the deposition of particles or drops of aerosol in a person's bronchial tree, it is necessary to
use three-dimensional calculations, because only such calculations give a real picture of the movement of particles or droplets in the bronchi of a person.

2. Building a human bronchial tree

For computer simulation of the flow of air and deposition of aerosol droplets in the bronchial tree of a person it is necessary to build a three-dimensional model of bronchus with bifurcations. The quality of the built bronchial tree affects the accuracy and speed of calculation. The situation is aggravated by the different scale of the upper and lower bronchus, which together leads to a loss of accuracy of numerical calculations. Taking into account the non-cylindricalness of the bronchi further complicates the construction of a three-dimensional model of the bronchial tree. The analytical representation allows you to build a bronchial tree up to the alveoli. For numerical calculations, analytical formulas allow to build a grid of any complexity up to the smallest bifurcations and bronchus. The construction of the analytical model of the human bronchial tree is detailed in the works [1, 2]. Examples of analytical construction of the human star-shaped bronchial tree are shown in Figure 1.

![Figure 1. An example of the construction of a human star-shaped bronchial tree. Shown here is the bronchial tree of a person from 0 to 5-th bifurcation (bifurcations of one order are highlighted in one color).](image)

![Figure 2. An example of building a separate full branch of the human star-shaped bronchial tree. Shown here is a full branch of the human bronchial tree from the 0 to the 23-rd bifurcation.](image)

3. Calculating the flow of gas in a person's bronchial tree

Previously, a numerical method of sequential calculation of human bronchial tree was proposed [1, 2]. Due to low speeds and pressures, air compressibility is usually neglected. By construction, the bronchial tree has a symmetrical structure, so the air flow through all bronchi $n$-generation is the same. The calculation is carried out from $n$ to $n+1$-st generation. At the entrance to the $n$ generation is set a field of speeds and average pressure in the entrance section, at the exit – expense. After the calculation at the exit we will get a field of speeds and average pressure in the section. These values are transferred to $n$ 1st generation. Thus, you can (if desired and patient) calculate the current in the entire bronchial tree of a person or at least in one branch from the 0 to the 23-rd generation. The size of the bronchi and bifurcation decreases with the increase in the number of bifurcation (the diameter of the bronchi 0 bifurcation is 18 mm, and the 23-rd is only 0.419 mm). The calculation is carried out for a separate bifurcation, so that the grid and the accuracy of the method on bifurcation do not degrade much, which allows almost no loss of accuracy of calculation up to the 23-rd bifurcation.
The results of the calculation of pressure in the bronchial tree are shown in Figure 3. On Figure 3 the value of the given pressure in the bronchial tree is shown. The given pressure is equal to 

\[ p_{\text{given}} = p_0 - p_n \]

where \( p_0 \) is the pressure of inhaled air, \( p_n \) is the pressure on the way out of \( n \) bifurcation. For comparison on Figure 3 the calculation of the current in a separate branch of the bronchial tree is given. In the work [3], the calculation was carried out by iterative method for the entire branch of the bronchial tree. In the [3] calculation was carried out for the turbulent flow of gas for incomplete branch up to 14 bifurcation. It is evident that the laminar current mode gives half the value of the drop-in pressure, compared to the turbulent calculations. Perhaps this is true, because the human body over the years of evolution has developed breathing with the least energy. For the star-shaped (in pathology) section of the human bronchi (Figure 3) the given pressure above the "normal" pressure drop.

![Figure 3](image)

**Figure 3.** The results of the numerical calculation of the flow of air in the bronchial tree of a person at the consumption of 50 l/min. Calculating the given pressure depending on the bifurcation number.

4. Precipitation of aerosol drops in human bronchi

To calculate the deposition of aerosol droplets in a person's bronchial tree, a typical NE-C24 compressor (“Omron” production) is taken for example. The characteristics of the nebulizer are as follows: the size of drops 3 microns, the volume consumption of aerosols 0.3 ml/min. The typical air flow when inhaling aerosols through a nebulizer is taken equal to 50 l/min. The duration of the breath ranged from 1 to 3 seconds.

Aerosol drop equations

\[
m_p \frac{d\vec{v}_p}{dt} = \vec{F}_o,\\
\]

where \( m_p \) is the particle mass, \( \vec{v}_p \) is the velocity of the particle, \( \vec{F}_o = m_p(\vec{v} - \vec{v}_p)/\tau_p \) is the drag force, \( \tau_p = \rho_p d_p^2/18\mu \) is the particle velocity response time, \( \mu \) is the fluid viscosity, \( \rho_p \) is the particle...
density. These ratios are true for the slow flow of gas drops. The drops don't break apart, they don't stick together. When falling on the wall drops of aerosol stick to it.

The time of the drop's flyby through the bronchi can be estimated by the average speed of the gas flow in the bronchi. The average speed of gas flow in the bronchi is equal to

$$\bar{w}_n = \frac{Q}{2^n R_n^2}.$$  \hspace{1cm} (2)

Then the time of flying the drops through the $n$ bronchi will be equal

$$t_n = \frac{L_n}{\bar{w}_n}.$$  \hspace{1cm} (3)

For the flow of gas $Q = 50 \text{ l/min}$, the flow of drops to the bronchi is no less then $t_n \approx 1.98 \text{ s}$.  

The calculations were carried out for one branch of the bronchial tree. The duration of the breath ranged from 1 to 3 seconds.

The results of the calculation are shown in the Figure 4. It can be seen that with the increase in the number of bifurcation (down the bronchial tree) the number of past drops of aerosol almost linearly falls. Inhale time 1 and 2 seconds is not enough for drops of aerosol to reach the alveoli. When inhaled for 1 second, aerosol drops reach only the 21-st bifurcation. When inhaled for 2 seconds, drops of aerosol reach the 22-nd bifurcation. And only with a breath duration of 3 seconds about 45% of drops reach alveoli. When you use 50 liters of air, a person needs 0.83 liters of air every second. The maximum deep breath of a person is about 2 liters.

![Figure 4](image-url)
It is evident that for the initial bifurcations the nature of subsidence drops is not monotonous. Beginning with the 7-th bifurcation, the nature of subsidence is almost linear. After the 21-st bifurcation, the drops do not have time to fly to the alveoli during the breath. Therefore, the proportion of settled and under-achieving alveoli drops tend to be a unit. In the 23-rd bifurcation and in the alveoli drops during inhalation time (2 seconds) do not have time to fly. To improve the performance of the nebulizer, it is necessary to increase the breath time and/or reduce the size of aerosol droplets.

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