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Three-dimensional Simulation of Heat and Moisture Transfer in the Human Bronchial Tree

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Abstract. A mathematical model of heat and mass transfer in human airways has been developed. Three–dimensional calculations of the distribution of heat and humidity of inhaled air in the human bronchial tree have been performed. The modeling has been performed on the basis of the analytical model of the complete bronchial tree developed earlier by the authors by the numerical method of stage–by–stage calculation. A comparison with experimental data on heat transfer in lungs shows that the model describes the change in the air temperature along the bronchial branch quite well. The process of breathing with a heated helium–oxygen mixture has been considered. This mixture is used to treat patients with bronchial asthma and COVID–19. It has been shown that the temperature of the heated helium–oxygen mixture in human lungs decreases faster than that of heated air. The results show that the thermal effect is observed not in the entire human bronchial tree, but only in the upper airways.

Keywords: bronchial tree, mathematical modeling, human lungs, heat and moisture transfer, thermoheliox, thermal helium–oxygen mixture.

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Introduction

Air is warmed up (or cooled down) and humidified (or excess moisture is condensed on the bronchial walls) in the human respiratory tract. Violation of this function of human lungs (along with other factors) can cause respiratory system diseases. Experimental studies of heat transfer in human lungs are limited in their capabilities [1,2] owing to the complex structure of the human respiratory tract and methodological difficulties of experimental research.

Modeling the human bronchial tree

The human bronchial tree consisting of bronchi connected by bifurcations (branching, diverging into two outgoing bronchi) has a complex tree–like structure. To describe the human bronchial tree, [3] proposed a model of symmetrical dichotomy, where the bronchi in one generation (the number of bronchial bifurcations) have identical parameters. There are 24 such bifurcations, i.e.,

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the bifurcation parameter of the bronchial tree varies from 0 to 23. The bronchial parameters of the symmetrical dichotomy model are described by the following expressions [?, ?, ?].

The model of [3] ignores the spatial distribution of bronchial tree branches. [7] extended the one–dimensional Weibel model to a realistic three–dimensional model of the lung. This model described the rules for constructing a three–dimensional analog of the Weibel model, where the main rule says that the subsequent bronchial bifurcation rotates by an angle of 90° relative to the previous one. However, [7] described only the rules for constructing the bronchial tree, but did not provide a formula for constructing an individual bifurcation.

Previously, the authors developed an analytical technique for analytical construction of the bronchial tree with symmetrical dichotomy [?, ?, ?]. Analytical formulas for constructing the complete bronchial tree were derived. All surfaces of the bronchial tree were coupled with the second order of smoothness (had no acute angles and sharp edges). Final analytical formulas allow constructing the human bronchial tree of any complexity (up to alveoli). The numerical method for step–by–step calculation of air motion in the human bronchial tree was proposed [?, ?, ?]. This methodology allows a sequential calculation of the air flow in a separate complete branch of the bronchial tree.

Mathematical model of heat and mass transfer in human lungs

In what follows, we consider the flow of a gas (air and thermal helium–oxygen mixture) in the human bronchial tree. The air in the bronchial tree is assumed to be incompressible: this is true due to the small pressure drop in the human lungs (the pressure change in the bronchi during breathing is about 10^{-5} atm).The flow in the human bronchi is considered as laminar [?]. The temperature of the bronchial wall is constant and equal to the body temperature of 37° C. The bronchial wall is considered as a "wet wall", and the relative concentration of water vapor on the wall is equal to unity (saturated vapor concentration). The thermodynamic characteristics (heat capacity, thermal conductivity, density, etc.) of the gas are assumed to be constant and independent of the temperature and concentration of water vapor in the gas.

For steady problems, the incoming air flow rate is assumed to be constant during the entire breathing process (about 1 second). Unsteady problems were solved using the quasi–stationary method [?]: the inspiratory/exhalatory flow spirometry was divided into N sections, and the gas flow rate was assumed to be constant in each section.

The heat transfer in the bronchi is described by the Navier–Stokes equations

$$\begin{aligned} &\nabla \cdot \vec{v} = 0, \\ &\rho_i \left[\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} \right] = -\nabla p + \mu_i \nabla^2 \vec{v}, \end{aligned} \tag{1}$$

where $\vec{v}$ is the gas velocity and p is the gas pressure. The subscript "i" here and below is "a" for air and "t" for the helium–oxygen mixture, μ_i is the dynamic viscosity coefficient, and ρ_i is the density. The bronchial walls are subjected to the no–slip condition

$$\vec{v} = 0. \tag{2}$$

The heat transfer in the bronchi is described by the equation

$$\rho_i c_{pi} \left(\frac{\partial T_i}{\partial t} + \vec{v} \cdot \nabla T_i \right) + \nabla \cdot \vec{q}_i = \tau_i : \nabla \vec{v} \tag{3}$$

where T_i is the temperature, $\vec{q} = -\lambda_i \nabla T_i$ is the heat flux due to thermal conductivity, λ_i is the thermal conductivity coefficient, c_{pi} is the specific heat capacity, and $\tau_i = \mu_i \left(\nabla \vec{v} + (\nabla \vec{v})^T \right) - \frac{2}{3} \mu_i (\nabla \cdot \vec{v}) I$ is the viscous stress tensor.

The moisture transfer in the bronchi is carried out only by diffusion and is described by the equation

$$\frac{\partial c_i}{\partial t} + \vec{v} \cdot \nabla c_i + \nabla \cdot \vec{g}_i = 0, \tag{4}$$

where c_i is the relative humidity, $\vec{g}_i = -D \nabla c_i$ is the water vapor diffusion flux vector, and $D = 2.86 \cdot 10^{-5}$ m$^2/s$ is the water vapor diffusion coefficient in the gas.

The temperature of the bronchial wall is assumed to be constant. The boundary conditions on the bronchial wall are

$$-\vec{n} \cdot \vec{q}_i = H_i (T_w - T_i), \tag{5}$$

where T_w =37°C is the temperature of the bronchial wall, $\vec{n}$ is the vector of the normal at the boundary, and $\vec{q}_i = -\lambda_i \nabla T_i$ is the vector of the conductive heat flux to the isothermal bronchial wall. The heat transfer coefficients H_a and H_t are taken from [11] and are calculated by empirical formulas for circular tubes with water-wetted walls in the laminar flow regime:

$$H_i^{(n)} = 0.7 \frac{\lambda_i}{R_n} \left(2\mathrm{Re}_i^{(n)} \frac{R_n}{L_n} \right)^{0.4} Pr_i^{0.33} \varepsilon_1^{(n)} \varepsilon_2^{(n)}. \tag{6}$$

The coefficients depend on the number n of the bronchial tree bifurcation. The parameters in Eq. (6) are defined as follows: $\mathrm{Pr}_i = \dfrac{\mu_i c_{pi}}{\lambda_i}$ is the Prandtl number; the radius R_n and length L_n of the n–th bronchus are given by [?,?,?], $\mathrm{Re}_i^{(n)} = \dfrac{2\rho_i U_n R_n}{\mu_i} = \dfrac{\rho_i Q}{2^{n-1} \pi \mu_i R_n}$ is the Reynolds number, $\varepsilon_1^{(n)} = 0.1 \left(\dfrac{L_n}{2\mathrm{Re}_i^{(n)} R_n} \right)^{-1/7} \Bigg/ \left(1 + 1.25 \dfrac{L_n}{\mathrm{Re}_i^{(n)} R_n} \right)$ is the correction for the hydrodynamic stabilization section, $\varepsilon_2^{(n)} = 1 + 3.54 R_n \big/ r_c^{(n)}$ is the correction for the tube curvature, and $r_c^{(n)}$ is the radius of curvature of the tube axis calculated based on the branching angle and bronchial length. For the bronchial geometry considered here [?], the radius of curvature is equal to

$$r_c^{(n)} = \frac{R_{n+1} (1 + 1.5 \cos \chi_n) - R_n}{1 - \cos \chi_n} + \frac{L_{n+1}}{\tan \chi_n}, \tag{7}$$

where $\chi_n = 35^0$ for the bronchial model in question.

The bronchial wall is considered a "wet wall." The water vapor concentration at the air–liquid surface interface is assumed to be 100 %, i.e., on the bronchial wall

$$c_i = c_w = 1. \tag{8}$$

For the moisture transfer Eq. (4), the boundary conditions on the bronchial wall are

$$-\vec{n} \cdot \vec{g}_i = K_i (1 - c_i), \tag{9}$$

where $\vec{g}_i = -D \nabla c_i$ is the vector of the water vapor diffusion flux on the wall.

The mass transfer coefficients K_a and K_t are taken from [11] and are calculated by empirical formulas for circular tubes with water–wetted walls in the laminar flow regime

$$K_i^{(n)} = 0.7 \frac{D}{R_n} \left(2\mathrm{Re}_i^{(n)} \frac{R_n}{L_n} \right)^{0.4} \mathrm{Sc}_i^{0.33} \varepsilon_1^{(n)} \varepsilon_2^{(n)}, \tag{10}$$

where $\mathrm{Sc}_i = \dfrac{\mu_i}{\rho_i D}$ is the Schmidt number.

The thermodynamic and transport properties of air and the helium–oxygen mixture (20 vol.% oxygen and 80 vol.% helium) used in the calculations are listed in Table 1. The parameters for the helium–oxygen mixture are taken from [12].

Table 1. Thermodynamic and transport properties of air and the helium–oxygen mixture (20 vol.% oxygen and 80 vol.% helium)

	Density ρ_i, kg/m^3	Dynamic viscosity coefficient μ_i, Pa·s	Specific heat capacity c_{pi}, J/(kg·K)	Heat transfer coefficient λ_i, W/(m·K)
air ($i = a$)	1.225	$1.7894 \cdot 10^{-5}$	1010	0.026
t–He/O$_2$ ($i = t$)	0.377	$2.25 \cdot 10^{-5}$	2345	0.114

In the work [13, 14] obtained an approximate one-dimensional solution for the distributions of temperature and relative humidity in human lungs (symmetrical dichotomy was taken as a model of bronchi [3].

A one-dimensional solution [13, 14] for the gas temperature is

$$T_i^{(n)} = T_w + (T_0 - T_w)\, e^{-\varphi_i^{(n)}}, \ \ \varphi_i^{(n)} = \frac{2\pi R_n H_i^{(n)} \left(L_{tree}^{(n)} - L_{tree}^{(0)}\right)}{2^{-n} Q \rho_i c_{pi}} \tag{11}$$

and a solution for the relative humidity is

$$c_i^{(n)} = 1 + (c_0 - 1)\, e^{-\psi_i^{(n)}}, \ \ \psi_i^{(n)} = \frac{2\pi R_n K_i^{(n)} \left(L_{tree}^{(n)} - L_{tree}^{(0)}\right)}{2^{-n} Q}, \tag{12}$$

where T_0 and c_0 are the initial temperature and relative humidity at the entrance to the bronchial tree, $L_{tree}^{(n)}$ is the length of the bronchial tree from the beginning of the inlet bronchus to the end to the n–th bifurcation calculated by analytical formulas [?, ?].

Calculation methodology for the air flow, heat transfer, and moisture transfer in human lungs

The numerical methodology for stage–by–stage calculation of the human bronchial tree presented in [?, ?] is based on the following procedure. One of the branches of the human bronchial tree constructed according to the method [?, ?] is chosen. The air flow, heat transfer, and mass transfer are calculated sequentially in one bifurcation (starting from the 0th to the 23-rd bifurcation). The inlet of the next bifurcation is subjected to the conditions of velocity, temperature, and humidity fields, as well as the pressure at one point at the inlet from the calculation of the previous bifurcation. The known flow rate $Q/2^{n+1}$ is set at the bifurcation outlet. Thus, 24 steps (the bifurcation number varies from 0 to 23) are needed to calculate one branch of the bronchial tree. According to the bronchial tree construction technique [?, ?], a similar solution would be obtained for any other bifurcation of the same generation n. In this case, only the velocity vector is rotated in accordance with the branch geometry.

Calculation results of heat and moisture transfer in the human bronchial tree

Numerical calculations of the flow in the human bronchial tree were performed. Fig. 1 show the calculated profiles of steady inhalation of hot air ($T_0 = 96°$C) with the relative humidity $c_0 = 0.2$ and the flow rate $Q = 24$ l/min. The symmetry of the flow, pressure, temperature, and humidity in the left and right outlet bronchi is clearly visible from the figure. Such symmetry is obtained for all calculated bronchi, which confirms the validity of the stage–by–stage calculation of the bronchial tree and the concept of constructing the bronchial tree [?, ?]. As a result, it is possible to avoid calculations in the entire bronchial tree (the total number of branches of the bronchial tree is 2^{23}): the results calculated for one branch can be transferred to any other branch. This concept allowed pioneering calculation of the entire tree, up to the 23-rd bifurcation [?, ?].

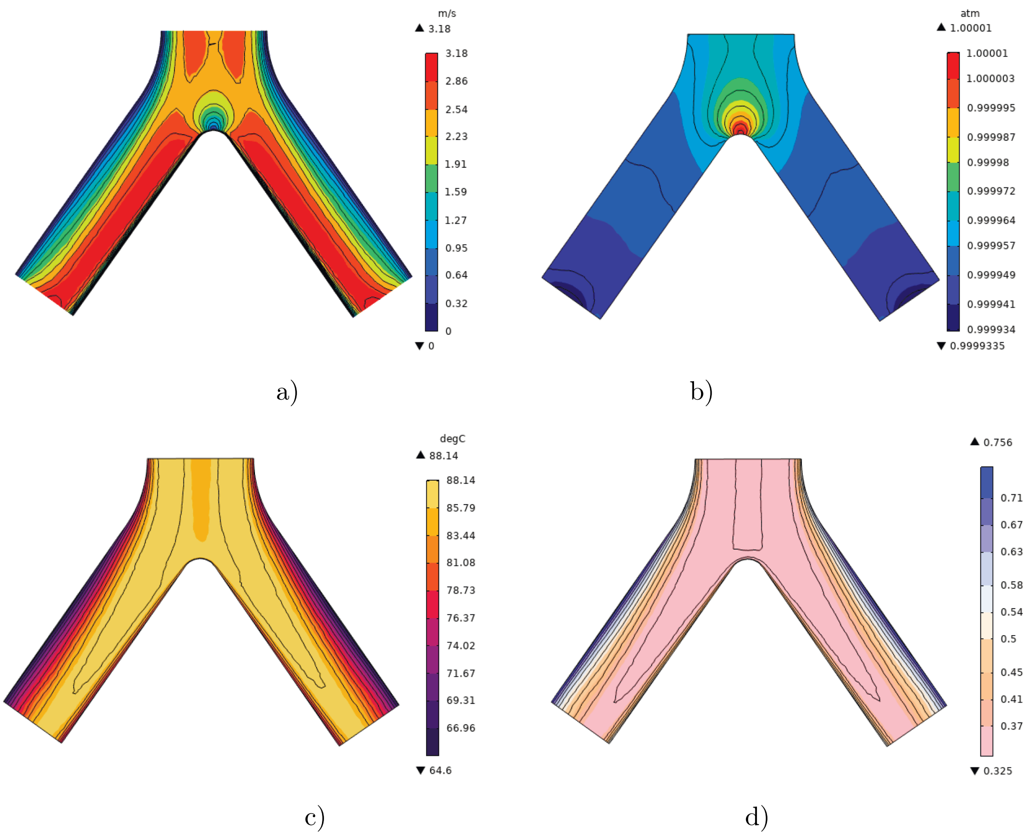
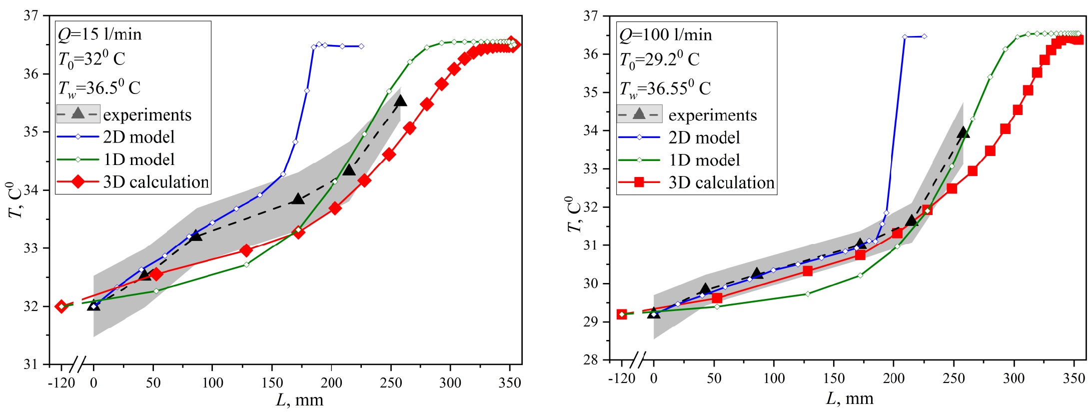


Fig. 1. Velocity (a), pressure (b), temperature (c), and relative humidity (d) profiles in the 2–nd bifurcation of the bronchial tree

The 3D temperature calculations (numerical solution of Eqs. (1), (3), and (4) with the boundary conditions (2), (5), and (9)) were compared with experimental data [1], with 1D solutions (11), (12), and with 2D solutions [?]. [1] reported results on the measurement of the inhaled air temperature in human lungs. A flexible probe containing six temperature sensors was developed. The probe could be safely inserted into the tracheobronchial tree of normal people. This device was used to record the temperature from the vocal slit (glottis) to the distal bronchi under various inhalation conditions. Tawhai in [?] developed a 2D model of heat and mass transfer in the bronchi using these experimental data as an example. A 2D equation of heat and mass transfer in a cylinder was solved. It was assumed that the temperature and humidity distributions over the cylinder cross section, as well as the air velocity, were of the Poiseuille flow type, each with its own exponent. These exponents were found in the course of the solution. The bronchial structure was based either on the symmetrical geometry [3] or the anatomical geometry [?]. The temperature distributions in the lungs were compared with the experiments [1] and calculations [?]. The temperature measurements in [1] and [2] were performed along the bronchial tree, with the first temperature sensor placed at the beginning of the 0 th bifurcation. To calculate the temperature and humidity using Eqs. (3) and (4), it is necessary to specify the temperature and humidity distributions at the inlet of the 0-th bronchus. The distributions of these parameters over the bronchus cross section before the inlet of the 0-th bronchus are not known. The power–law distribution over the bronchial cross section, as suggested in [1], is rather controversial (this issue was also discussed in [1]). Therefore, to solve Eqs. (3) and (4), the temperature T_0 and relative humidity c_0 at the tracheal inlet (the initial calculation point was referred to −120 mm) were set constant over the cross section. This allowed us to minimize the influence of the initial temperature and humidity distributions on the subsequent bronchi.

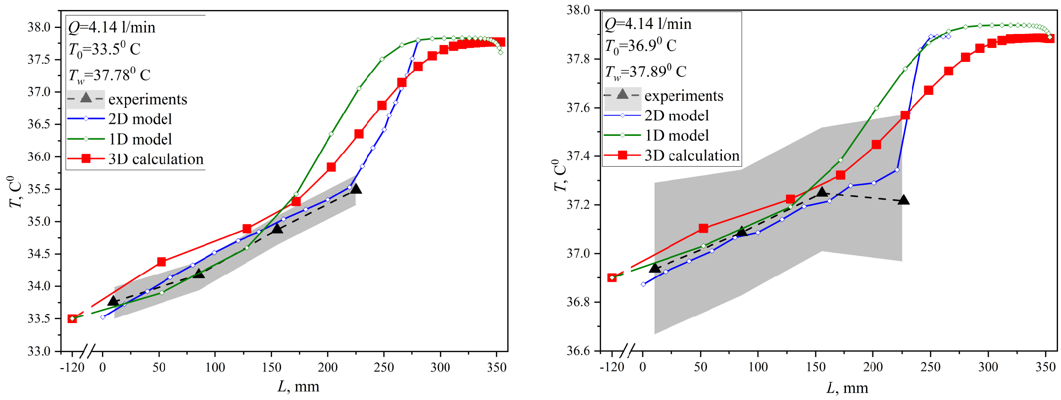
The results of the comparison are presented in Fig. 2, which shows the bronchial temperature T_a and relative humidity c_a of air averaged over the cross section at the outlet of the n-th bronchus. The parameters at the bronchial inlet are the same as those for Fig. 1. The 1D model and 3D calculation used the same heat transfer coefficients $H_a^{(n)}$ (6) and mass transfer coefficients $K_a^{(n)}$ (10).



a) b)

Fig. 2. Changes in the inhaled air temperature versus the length of the bronchial tree branch. The air flow rate is $Q = 15$ l/min (a) and $Q = 100$ l/min (b). The relative humidity of inhaled air is $c_0 = 0.8$

Fig. 3 shows the results of the experiments [2] on the temperature distribution in the human bronchi. Here we also present the calculations obtained by the 2D [?], 1D model (11), and the proposed methodology. As in Fig. 2, the 1D and 2D solutions predict a sharp rise of temperature as compared to the present model. For the experiments (Fig. 3b), the calculated temperature lies within the error margin; for the experiments (Fig. 3a), the calculated temperature lies slightly higher than the experimental values.



a) b)

Fig. 3. Changes in the inhaled air temperature versus the bronchial tree branch length at the air flow rate $Q = 4.14$ l/min. The inhaled air temperature is $T_0 = 33.5^0$ C (a) and $T_0 = 36.9^0$ C (b). The relative humidity of inhaled air is $c_0 = 0.9$

Thermal helium–oxygen breathing

A new way to treat COVID–19 patients was developed in a Russian clinic [16]. The method consists in using a thermal helium–oxygen mixture (thermoheliox — t–He/O_2). Thermogeliox has been used for more than 20 years to treat some lung diseases [16, 17]. This method involves patient breathing of a gas mixture of helium and oxygen (21% of oxygen and 79% of helium) at temperatures between 75°C and 96°C. The lower density of helium compared to that of air reduces the breathing resistance. The thermal conductivity of helium is five times that of air, which speeds up heat transfer in the lungs [11].

Breathing with air and the thermal helium–oxygen mixture at the temperature $T_0 = 96°$C and relative humidity $c_0 = 0.2$ at the flow rate $Q = 24$ l/min was compared. The results of calculation of the reduced pressure (atmospheric pressure minus the pressure at the bronchus outlet) in situations of breathing with air and the thermal helium–oxygen mixture are shown in Fig. 4.

The thermoheliox viscosity is 1.26 times higher than that of air, while the density is three times lower (Tab. 1). Therefore, the pressure drop for helium increases to a smaller extent as compared to air. As the length of the bronchus branch increases, the pressure difference between air and thermoheliox genesis is leveled off. This is due to expansion of the flow in the bronchi. According to [?, ?, ?], for example, the ratio of the bifurcation inlet area to the bifurcation outlet area is $R_0^2/\left(2R_1^2\right) = 1.09$ for the first bronchi and $R_0^2/\left(2R_1^2\right) = 0.52$ for the last bronchi. Flow expansion by a factor of two at the last bifurcations significantly reduces the effect of viscosity on the flow pressure drop. The air and thermoheliox breathing at the gas flow rate $Q = 100$ l/min is compared in Fig. 4. In this case, the pressure, temperature, and humidity reveal the same behavior.

The thermal conductivity of helium is 4.5 times higher than that of air (the heat capacity of helium is 2.3 times higher than that of air). Therefore, the bronchi are not thermally injured by breathing a heated helium–oxygen mixture. The temperature distributions of breathing with air heated to 96°C and the helium–oxygen mixture are shown in Fig. 4b. The calculations show that the temperature drop in the helium–oxygen mixture occurs much faster than that in heated air. Cooling of the heated gases (air and helium–oxygen mixture) occurs in the upper parts of

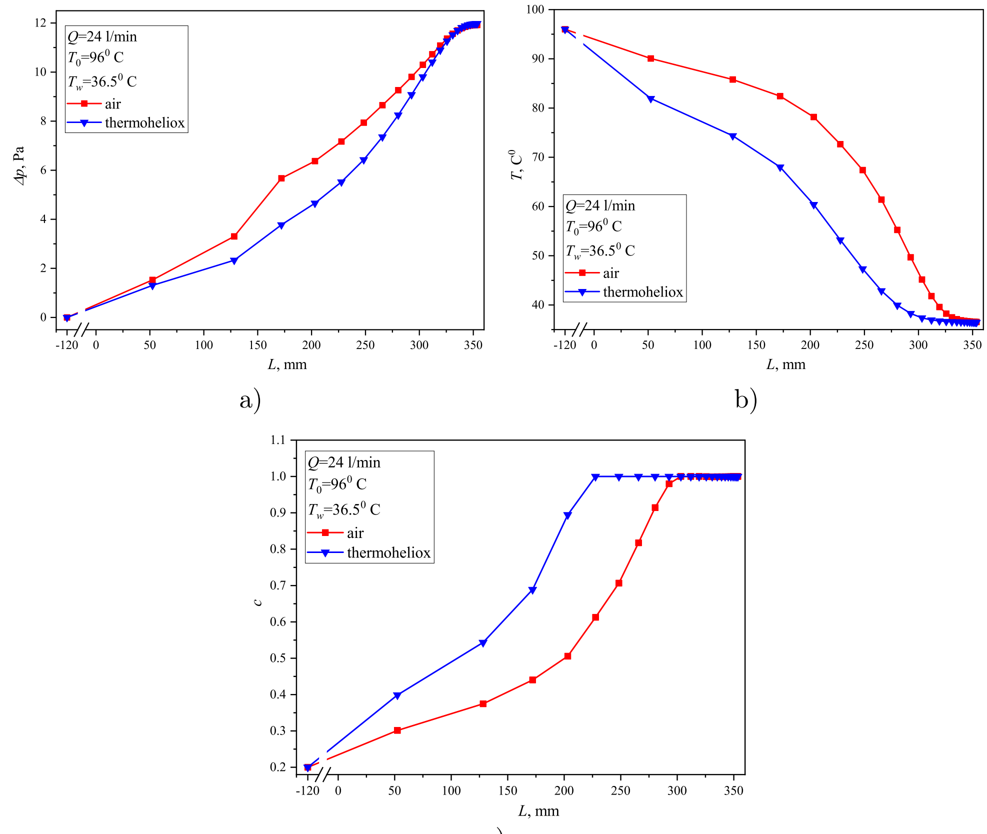


Fig. 4. Comparison of breathing with air and thermoheliox versus the length of the bronchial tree branch at the gas flow rate $Q = 24$ l/min. The inhaled gas temperature is $T_0 = 96$ °C, and the bronchial wall temperature is $T_0 = 36.5$ °C at the relative humidity $c_0 = 0.2$. Comparisons of the relative pressure (a), temperature (b), and relative humidity (c) are presented

the bronchi: in 300 mm of the branch length, the temperature of the heated gases is equalized with the temperature of the human body. Thus, the thermal effect of the heated helium–oxygen mixture "works" only in the upper parts of the bronchi and does not reach the alveoli. The humidity of the helium–oxygen mixture reaches saturation much faster than that of air (Fig. 4c).

Conclusions

Numerical calculations of heat and moisture transfer in human lungs were performed. The calculations were based on the bronchial tree construction method developed earlier by the authors and on the method of stage–by–stage calculation of the flow in the bronchi [?, ?, ?]. These methodologies allow for sequential calculations of the flow, heat, and moisture transfer from one bronchus to the next bronchus. Rather simple equations (3) and (4) were taken as heat and moisture transfer models. In these equations, the processes of heat and moisture transfer do not affect the dynamics of air motion through the bronchi; moreover, these processes are independent of each other. These assumptions can be made because the flow velocities, temperature, and vapor concentrations are rather small. The accuracy of calculations of heat and moisture transfer is significantly affected by the heat transfer and mass transfer coefficients.

Due to the lack of the values of these coefficients for the bronchial walls, we took the coefficients for water–wetted bent round tubes. However, even in such a simple formulation, our numerical solutions agree quite accurately with experimental data on heat transfer in human lungs (Figs. 2 and 3).

Three-dimensional numerical calculations of the air flow, thermal helium–oxygen mixture, and drops of medical aerosol in the complete (up to the alveoli) human bronchial tree were carried out. The available calculations were limited to the 15-th bifurcation (out of 23 lung bifurcations) [18]. To calculate the deposition of drug aerosols, a calculation up to the terminal alveoli of the human lung is necessary, because the deposition of drug aerosols occurs mostly up to the 21-st or 22-nd bifurcation. Breathing of a heated helium–oxygen mixture was calculated. It was shown that the patient needs to spend 15% less effort for breathing the thermal helium–oxygen mixture (compared to breathing of air). It was shown that the thermal effect (excess of the human body temperature) of the heated helium–oxygen mixture is observed only in the upper part of the bronchi (up to the 9-th bronchial bifurcation).

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Трехмерное моделирование теплообмена и влагообмена в бронхиальном дереве человека

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Аннотация. Разработана математическая модель тепломассопереноса в дыхательных путях человека. Проведены трехмерные расчеты распределения тепла и влажности вдыхаемого воздуха в бронхиальном дереве человека. Моделирование проводилось на основе разработанной ранее авторами аналитической модели полного бронхиального дерева по численной методике поэтапного расчета. Сравнение с экспериментальными данными по теплообмену в легких показало, что модель достаточно хорошо описывает изменение температуры воздуха по длине бронхиальной ветки. Рассмотрен процесс дыхания разогретой гелий–кислородной смесью. Эта смесь используется для лечения больных с бронхиальной астмой и COVID–19. Показано, что понижение температуры разогретой гелий–кислородной смеси в легких человека происходит быстрее, чем для разогретого воздуха. Полученные результаты показали, что термический эффект наблюдается не во всем бронхиальном дереве человека, а только в верхних дыхательных путях.

Ключевые слова: бронхиальное дерево, математическое моделирование, легкие человека, тепло– и влагообмен, термогелиокс, термическая гелиево–кислородная смесь.