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MODELING THE ENTRY OF AIR CONTAMINANTS INTO A ROOM

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Abstract: A mathematical model of air contaminant (products of human activity) inflow into the isolated air space has been developed. On the basis of the formula modified by us the simulation of human respiration with carbon dioxide, water vapor and heat emission is implemented. The model also takes into account the heat input from the human body through clothing.

Applying numerical modelling ANSYS CFD (Computational Fluid Dynamics) on the basis of continuity equations and Reynolds-Averaged Navier-Stokes equations "RANS" (Reynolds-Averaged Navier-Stokes) the following results on air medium state change in the isolated space were obtained:

- the human respiratory cycle is modelled at simultaneous heat transfer from the body surface through clothes into the studied air space;

- the exponential equation of the trend line of CO_2 concentration to observation time was obtained;

- monitoring and rendering (visualization) of changes in CO_2 concentration, temperature and relative humidity in the space under study by time along the room height was performed.

These results and regularities served as initial data for solving a number of model non-stationary problems on aerodynamics and heat and mass transfer in the room. The inverse problem of general exchange ventilation was to be solved. Changes in the state of the air environment initially contaminated with carbon dioxide, heat and water vapors were studied when people were in the studied space and the supply and exhaust ventilation was operating.

Of the four air change schemes planned for the study, the results for one schemes are presented in this publication. The dynamics of assimilation of excess heat, humidity and carbon dioxide (CO_2) made it possible to assess the efficiency of ventilation systems and to predict improvements in their energy efficiency when air parameters are brought up to standard values.

Keywords: mathematical model, air contaminant, aerodynamics, computational fluid dynamics, air change scheme, relative humidity, temperature, carbon dioxide concentration, room working area, rebranding, supply and exhaust ventilation.

МОДЕЛЮВАННЯ НАДХОДЖЕННЯ «ШКІДЛИВОСТЕЙ» У ПРИМІЩЕННЯ

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Анотація: Розроблено математичну модель надходження «шкідливостей» (продуктів життєдіяльності людини) до ізольованого повітряного простору. На основі модифікованої нами формули реалізовано імітацію дихання людини з виділення діоксиду вуглецю, водяної пари та тепла. Моделью враховується так само надходження тепла від тіла через одяг.

Застосувавши чисельне моделювання ANSYS CFD (Computational Fluid Dynamics – обчислювальна гідрогазодинаміка) на основі рівнянь нерозривності та усереднених за

Рейнольдсом рівнянь Нав'є-Стокса «RANS» (Reynolds-Averaged Navier-Stokes) отримані результати зміни

- змодельований дихальний цикл людини при одночасному перенесенні тепла з поверхні тіла через одяг у повітряний простір, що досліджується;
- одержано експоненційне рівняння лінії тренду концентрації CO_2 до часу спостереження;
- виконано моніторинг та рендеринг (візуалізація) по висоті приміщення зміни концентрації CO_2, температури, вмісту вологи та швидкості повітря в досліджуваному просторі за часом.

Ці результати і закономірності послужили вихідними даними на вирішення низки модельних нестаціонарних завдань з аеродинаміці і тепломасобміну у приміщенні. Вирішенню підлягало зворотне завдання загальнообмінної вентиляції. Досліджувалося зміна стану повітряного середовища спочатку забрудненої діоксидом вуглецю, теплом та водяними парами при знаходженні в досліджуваному просторі людей та роботі припливно-витяжної вентиляції. З чотирьох запланованих схем повітрообміну результати досліджень однієї схеми представлені у цій публікації. Динаміка асиміляції надлишків теплоти, вологи та діоксиду вуглецю (CO_2) дала можливість оцінити ефективність роботи систем вентиляції, спрогнозувати підвищення їхньої енергоефективності при доведенні параметрів повітря до нормативних значень.

Ключові слова: математична модель, «шкідливості», аеродинаміка, обчислювальна гідрогазодинаміка, схема повітрообміну, відносна вологість, температура, концентрація діоксиду вуглецю, робоча зона приміщення, ребрендинг, припливно-витяжна вентиляція.

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1 INTRODUCTION

Tasks related to the design, installation, adjustment and control of supply and exhaust ventilation systems require careful monitoring of changes in the air environment. This is due to both the implementation of the requirements of the legislative framework of Ukraine and its harmonization with the standards of the European Union [1, 2], and the solution of problems to prevent the spread of pandemics that are currently haunting humanity [3].

Changes in the air environment are typical for rooms with mechanical supply and exhaust ventilation (flow classrooms of educational institutions, classrooms of schools, group rooms of kindergartens, conference rooms, offices). The main air contaminants that are released in this case are carbon dioxide, water vapor and heat.

Based on the patterns of distribution of air contaminants in the volume of isolated air space, it became possible to solve the inverse problem of supply and exhaust ventilation. The change in the state of the air environment initially polluted with carbon dioxide, heat and water vapor was studied when people were in the space and the supply and exhaust ventilation was operating. A study of the efficiency of four generally accepted indoor air change schemes has been conducted:

Scheme A "air supply from above – removal from below";
Scheme B "air supply from above – removal from above";
Scheme C "air supply from above – removal of air from two zones above and below";
Scheme D "air supply from below – removal from above" (displacement ventilation).

The results for Scheme A (change in carbon dioxide concentration) are presented in this publication.

2 LITERATURE REVIEW AND PROBLEM STATEMENT

Creating a comfortable indoor microclimate involves meeting a number of restrictions related to:

- temperature;
- relative humidity in the working area (WA) of the room;
- velocity of the stream entering the WA from the air distributor;
- temperature difference between the air in the WA and the stream from the air distributor entering the space under study.

The content of carbon dioxide, water vapor, sensible and total heat, as well as other air , if any, in the indoor air must also be monitored.

In the practice of calculating changes in the state of the air environment in rooms for various purposes, different methods and approaches were used [4-11]. Examples of successful solutions to applied ventilation problems do not remove the question of the accuracy of the results obtained using mathematical modeling. Currently, mathematical modeling methods are used in engineering calculations, which provide an estimate of flow parameters based on the numerical solution of the Reynolds equations of stationary or non-stationary Navier-Stokes equations. (English RANS/URANS: Steady/Unsteady Reynolds Averaged Navier-Stokes) [7].

The above-mentioned works do not consider in aggregate the issues of interaction of air pollution from people, occurring during moderate work, in ventilated rooms with different air change schemes.

3 THE AIM AND OBJECTIVES OF THE STUDY

The aim of the study is to develop a mathematical model that determines the processes of heat and mass exchange between humans and the environment. Based on this model, it is possible to solve applied problems related to the creation of a comfortable microclimate in rooms, increasing the energy efficiency of systems that provide air change.

4 RESEARCH RESULTS

4.1 Study of the entry of air contaminants into an isolated space

Initial conditions:

- isolated space (see Fig. 1), with a volume of $12\ m^3$, at a rate of $2\ \mathrm{m}^2/\mathrm{person}$, according to the requirements of [1];
- number of people in the isolated space: 2 people;

Air parameters in the isolated space:

- air temperature: $t = 22°$;
- initial level of CO_2 concentration: $350\ ppm$;
- atmospheric pressure: $\mathrm{P_b} = 101325\ \mathrm{Pa}$;
- relative humidity: $\varphi = 50\,\%$;
- humidity content: $\mathrm{d} = 8{,}2\ \mathrm{g/kg}$;
- average body surface temperature of a dressed person: $\mathrm{t_h} = 27°$.

Air parameters exhaled by a person [4]:

- CO_2 content in exhaled air – $4{,}0\%(40000\ ppm)$;
- air temperature: $34°$;
- relative humidity: $\varphi = 91\%$;
- humidity content: $\mathrm{d} = 31{,}2\ \mathrm{g/kg}$.

Modeling of the release of air contaminants into an isolated space is presented in the research scheme in Fig. 1.

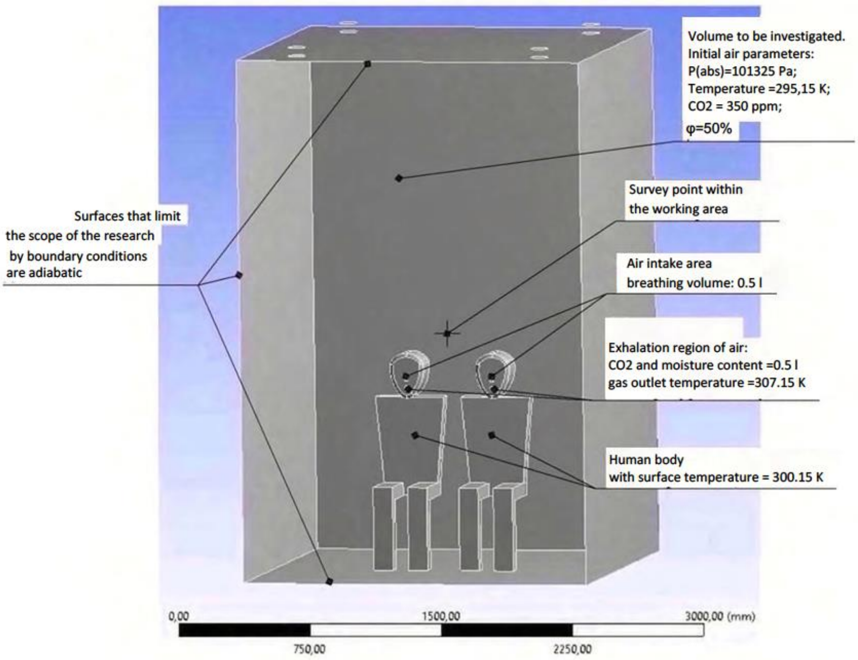


Fig. 1. Schematic representation of air contaminants entering an insulated room

Using the ANSYS CFD (Computational Fluid Dynamics) computational hydrodynamics simulation complex, a human breathing cycle function was mathematically created, which generally simulates the flow of air contaminants (water vapor, relative humidity, carbon dioxide, air mass temperature) into the study space. At the same time, the flow of heat from the human body through clothing into the study space is also simulated.

The breathing cycle was modeled by a sinusoidal function with a period of 4 seconds and a respiratory volume of air $V_t = 0,5l$, which corresponds to breathing at rest [5]. The breathing function is defined in the boundary conditions of the "EXHAIL" outlet, with a diameter of $20\,mm$, which corresponds to the diameter of the human trachea. The function is given by equation

$$Q(t) = \frac{\pi M t}{T} \cdot \sin\left(\frac{2\pi}{T} t\right),$$

where $Q(t)$ – mass flow rate, kg/s, $M(t)$ – mass of air exhaled by a person $\left(\rho V_t\right)$, kg, T – period s, t – time step, s. One respiratory cycle takes $4s$, and the time step for the calculation was set at $0,2s$, which is of fundamental importance according to the Courant number [6].

Visualization of breathing by time is presented in the graphs of Fig. 2 and 3, for which, according to the function $Q(t)$, 16 respiratory cycles were realized within 1 minute.

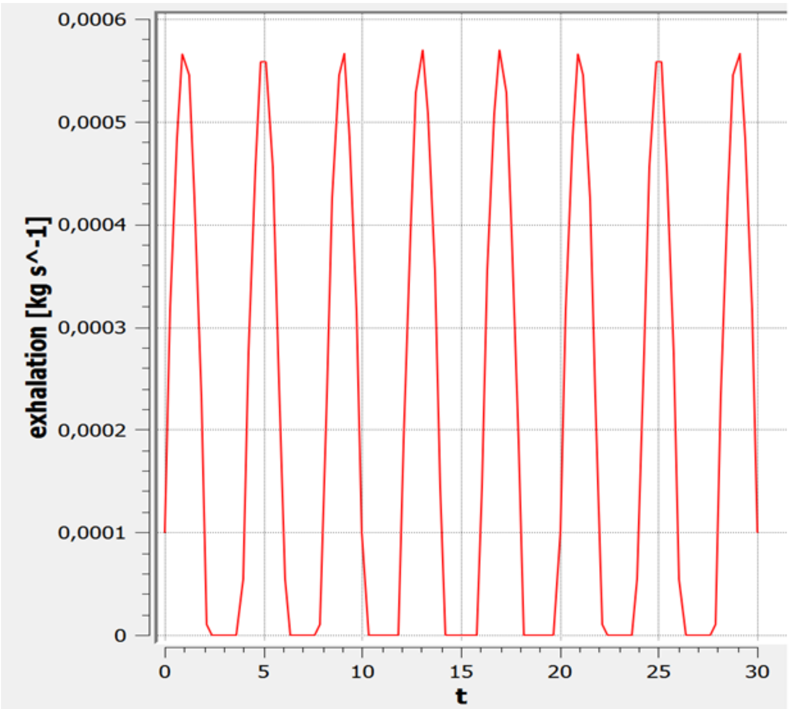


Fig. 2 Graph of the respiratory function $Q(t)$

The modeling of carbon dioxide, heat and humidity emissions from humans was performed in the ANSYS CFX software package under non-stationary conditions in a multi-component air environment, in which the monitoring of the air contaminants into the work area was performed, geometrically located at a distance of $1,0-1,2\,m$, that is, the rooms where sedentary activity predominates were considered. The model series of non-stationary problems considered in this work are based on the mathematical analysis and interpretation of physical processes of heat and mass transfer and hydrogasdynamics. Mathematical modeling is based on the continuity equations averaged by Reynolds, the Navier-Stokes equations "RANS" (Reynolds-Averaged Navier-Stokes), which is an abbreviated form of the general

Navier-Stokes equations and the equations of the k-ε turbulence model (two-equation standard model) [6-8].

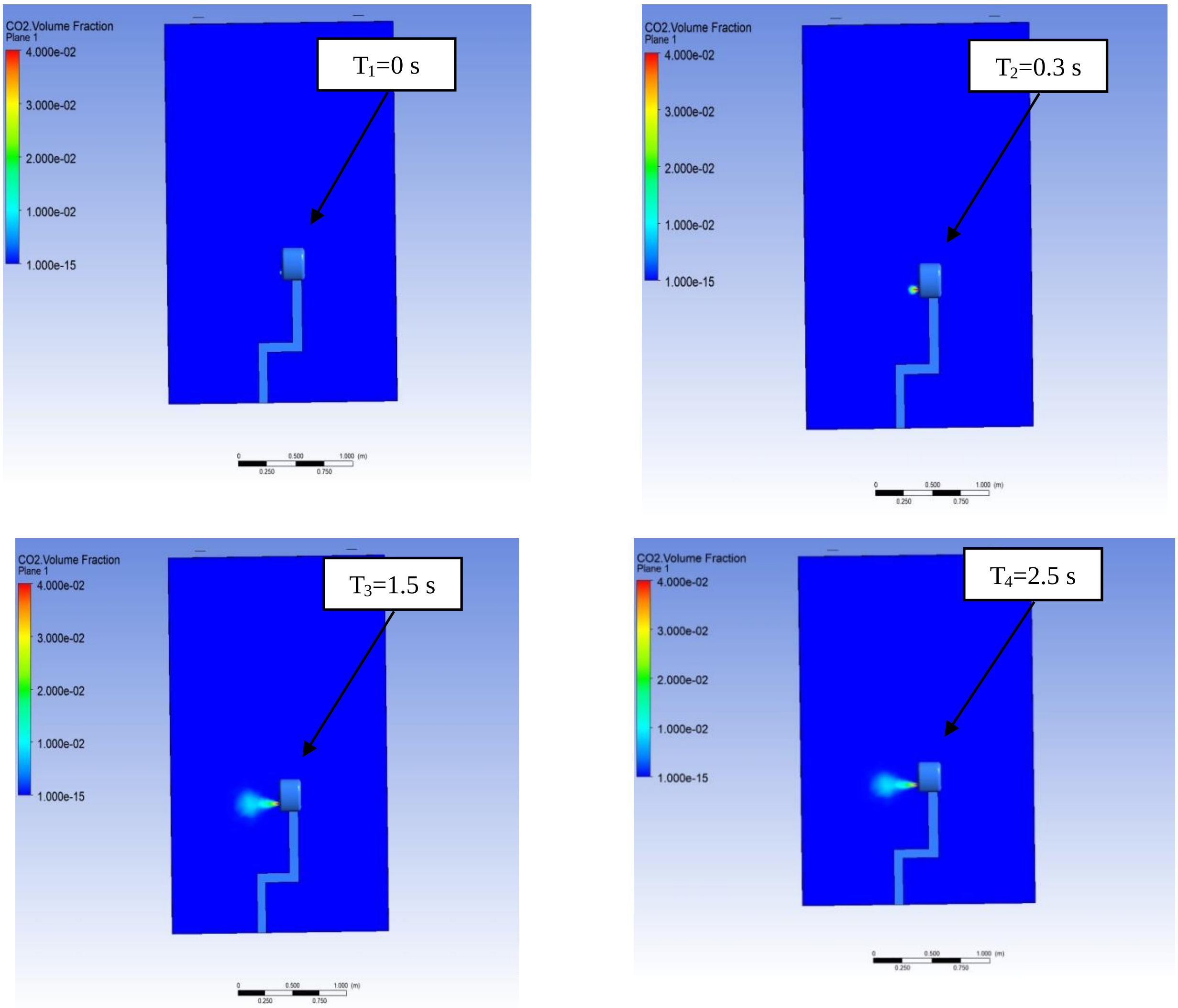


Fig. 3 Simulation of the human respiratory cycle

Continuity equation

$$\frac{d\rho}{dt} + \nabla(\rho u) = 0,$$

where ρ – air density, u – flow velocity, ∇ – Nabla operator.

Navier – Stokes equation:

$$\frac{\partial}{\partial x_j}\left(\rho \bar{u}_i \bar{u}_j\right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \bar{u}_i}{\partial x_i}\right)\right) - \delta_{i3}\rho g + \frac{\partial}{\partial x_j} - \left(\rho \bar{u}_i \bar{u}_j\right),$$

$$-\rho\overline{u_i'}\,\overline{u_j'} = \mu_t\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) - \frac{2}{3}\left(\rho k + \mu_t \frac{\partial \bar{u}}{\partial x_j}\right)\delta_{ij},$$

where p – pressure; Pa, μ – dynamic viscosity, $\mathrm{kg/ms}$; μ_t – turbulent dynamic viscosity, $\mathrm{kg/ms}$; g – acceleration of gravity, m/s^2; k – kinetic energy of turbulence,

m^2/s^2, $j=1,2,3.$; δ_{ij} – Kronecker symbol.

According to the Boussinesq approximation [7], the linear relationship between turbulent and Reynolds stress and mean velocity is expressed as follows

$$\tau_{ij}=\rho\overline{u_i'}\overline{u_j'}=\frac{2}{3}\rho k\delta_{ij}-\mu_t\left(\frac{\partial\bar{u}_i}{\partial x_j}+\frac{\partial\bar{u}_j}{\partial x_i}\right)$$

Turbulent kinetic energy

$$k=\frac{1}{2}\overline{u_i'}\overline{u_i'}=\frac{1}{2}\left(\overline{u_1^2}+\overline{u_2^2}+\overline{u_3^2}\right)$$

The RANS k-ε two-equation standard model is the definition of two transport equations for two turbulent properties: the turbulent kinetic energy and the other turbulent properties, which are the dissipation rate of the turbulent kinetic energy or the specific dissipation rate [7]. Thus, the turbulent viscosity equation is defined using k and ω:

$$\mu_t=\frac{\rho k}{\omega},$$

$$\omega=\max\left\{\omega,\quad C_{\lim}\sqrt{\frac{2\bar{S}_{ij}\bar{S}_{ij}}{\beta^*}}\right\},\quad \bar{S}_{ij}=\bar{S}_{ij}-\frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ki},\quad C_{\lim}=\frac{7}{8},$$

The transport of turbulent kinetic energy (k) according to the standard $k-\varepsilon$ model is determined by the equation

$$\frac{\partial}{\partial_t}(\rho k)+\frac{\partial}{\partial x_j}(\rho u_j k)=\rho\tau_{ij}\frac{\partial u_i}{\partial x_i}-\beta^*\rho k\omega+\left[\left(\mu+\sigma^*\frac{\rho k}{\omega}\right)\frac{\partial k}{\partial x_j}\right]$$

The specific dissipation rate ω according to the equation:

$$\frac{\partial}{\partial_t}(\rho\omega)+\frac{\partial}{\partial x_j}(\rho u_j\omega)=\alpha\frac{\omega}{k}\rho\tau_{ij}\frac{\partial u_i}{\partial x_j}-\beta^*\rho\omega^2+$$

$$+\sigma_d\frac{\rho}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial\omega}{\partial x_j}+\frac{\partial}{\partial x_j}\left[\left(\mu+\sigma^*\frac{\rho k}{\omega}\right)\frac{\partial\omega}{\partial x_j}\right]$$

The closing coefficients of the $k-\omega$ model:

$$\alpha=0,52;\beta=\beta_0 f_\beta;\beta^*=0,09;$$

$$\sigma=0,5;\sigma^*=0,6;\sigma_{d0}=0,125,$$

$$\sigma_d=\begin{cases}0, & \dfrac{\partial k}{\partial x_j}\dfrac{\partial\omega}{\partial x_j}\le 0,\\ \sigma_{d0}, & \dfrac{\partial k}{\partial x_j}\dfrac{\partial\omega}{\partial x_j}>0,\end{cases}\qquad f_\beta=\frac{1+85\chi_\omega}{1+100\chi_\omega},$$

$$\chi_\omega=\left|\frac{\Omega_{ij}\Omega_{ik}S_{ki}}{(\beta^*\omega)^3}\right|,\quad S_{ki}=S_{ki}-\frac{1}{2}\frac{\partial u_m}{\partial x_m}\delta_{ki}$$

$$\Omega_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} - \frac{\partial \overline{u}_j}{\partial x_i}\right),$$

where $C_{\lim}$ – force limiting the stress [9]; τ_{ij} – Reynolds stress tensor, f_β – vortex stretching function, χ_ω – dimensionless vortex stretching parameter, S_{ki} and S_k – function of the undesirable effect of flow compression, Ω_{ij} – mean rotation tensor.

Another commonly accepted $k-\varepsilon$ recommended model of turbulent viscosity [6, 10], is calculated using k and ε (13)

$$\mu_t = c_\mu \frac{k^2}{\varepsilon}.$$

The transport equation for the standard $k-\varepsilon$: model is determined by the equation:

$$\frac{\partial}{\partial_t}(\rho k) + \frac{\partial}{\partial x_j}(\rho u_j k) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] - \rho\overline{u_i'u_j'}\frac{\partial u_i}{\partial x_j} - \rho\varepsilon;$$

$$\frac{\partial}{\partial_t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(\rho u_j \varepsilon) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] - c_{1\varepsilon}\frac{\varepsilon}{k}\rho\overline{u_i'u_j'}\frac{\partial u_j}{\partial x_{ji}} - c_{2\varepsilon}\rho\frac{\varepsilon^2}{k}.$$

The coefficients of the model are constants:

$$c_{1\varepsilon} = 1,44,\ \ c_{2\varepsilon} = 1,92,\ \ c_\mu = 0,09,\ \ \sigma_k = 1,0,\ \ \sigma_\varepsilon = 1,3.$$

First of all, in an isolated volume, the change in CO_2 concentration over the observation time is determined, the source of which is the physiology of human respiration. The graph of the change in CO_2 concentration is shown in Fig. 4. Geometrically, the monitoring point is a point located in the WA at a distance of $1,0-1,2\,m$ from the floor level. The contours (planes) of air contaminants distribution in the room volume were also used to display the results of the study.

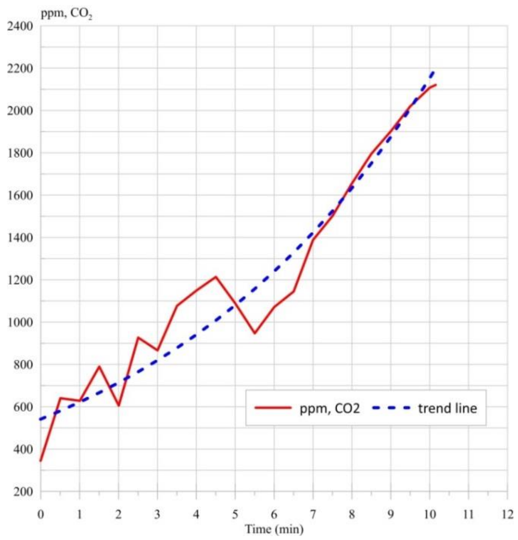


Fig. 4 Graph of CO_2 concentration (ppm) by observation time

Regression analysis of CO_2 inflows indicates that the growing line of CO_2 concentration (ppm) acquires a linear-broken character at small concentration values $(< 900\ ppm)$, which is due to the convective properties of the environment and an exponential character at concentrations above $900\ ppm$.

The exponential trend line model has the following equation, $ppm(t)$

$$ppm(t) = 541{,}53\exp(0{,}138t).$$

Monitoring the distribution of CO_2 concentration (Fig. 5) along the vertical line H, (by room height, m) includes observations: at the beginning – $ppm(0\,s)$; during – $ppm(150\,s)$ and at the end – $ppm(600\,s)$.

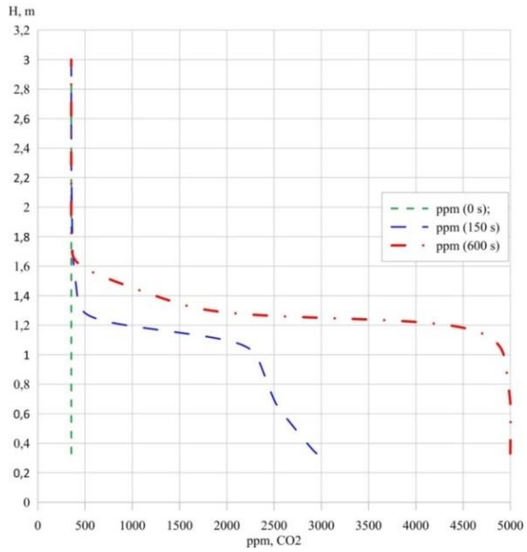
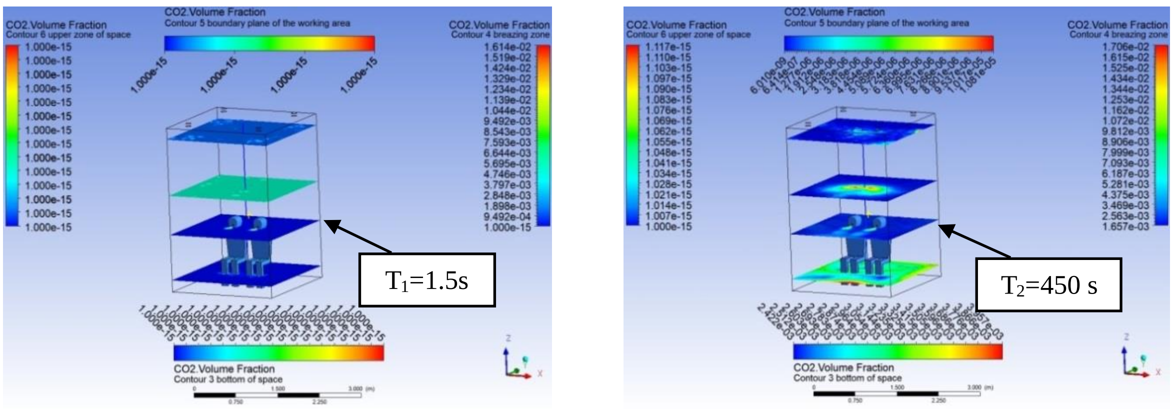


Fig. 5 Monitoring the distribution of CO_2 concentration by the height of the study space

Monitoring the CO_2 concentration on the vertical scale shows that in a homogeneous air environment, under the influence of gravitational forces, the highest CO_2 concentration is concentrated closer to the floor. The straightness of the lines (Fig. 5) at the beginning of the observations is due to the principle of detailed equilibrium of the system [11].

Visualization of the results of the process of CO_2 inflow into the study volume over a 15-minute period is presented in Fig. 6.



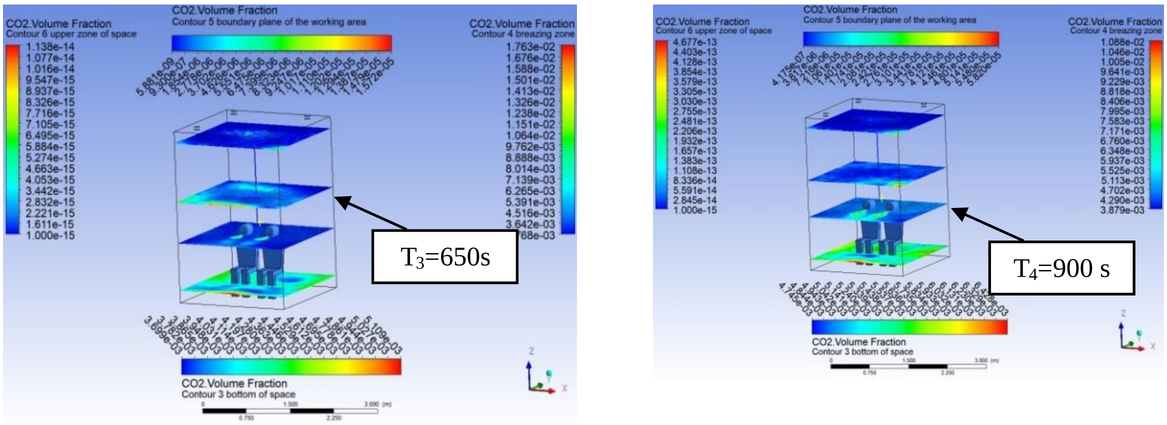


Fig. 6 Change in CO_2 concentration by the height and time of the isolated space

Secondly, observations were made on changes in temperature and relative humidity in the isolated volume (Fig. 7) over time, in connection with breathing and heat loss from the surface of the human body in clothing.

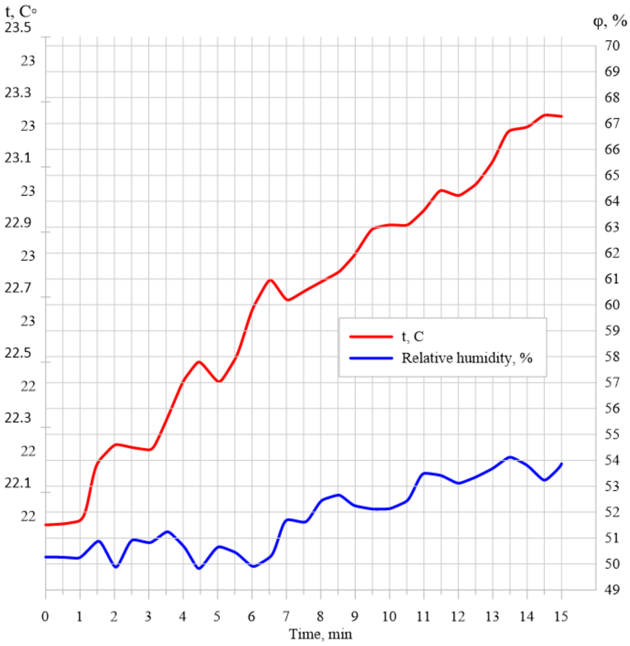


Fig. 7 Graph of changes in temperature and relative humidity

Fig. 8 shows a visualization of changes in temperature and humidity that occur over a 15-minute period. The simultaneous increase in temperature and humidity causes the process of increasing the enthalpy of air in rooms where humans are primarily the source of pollution.

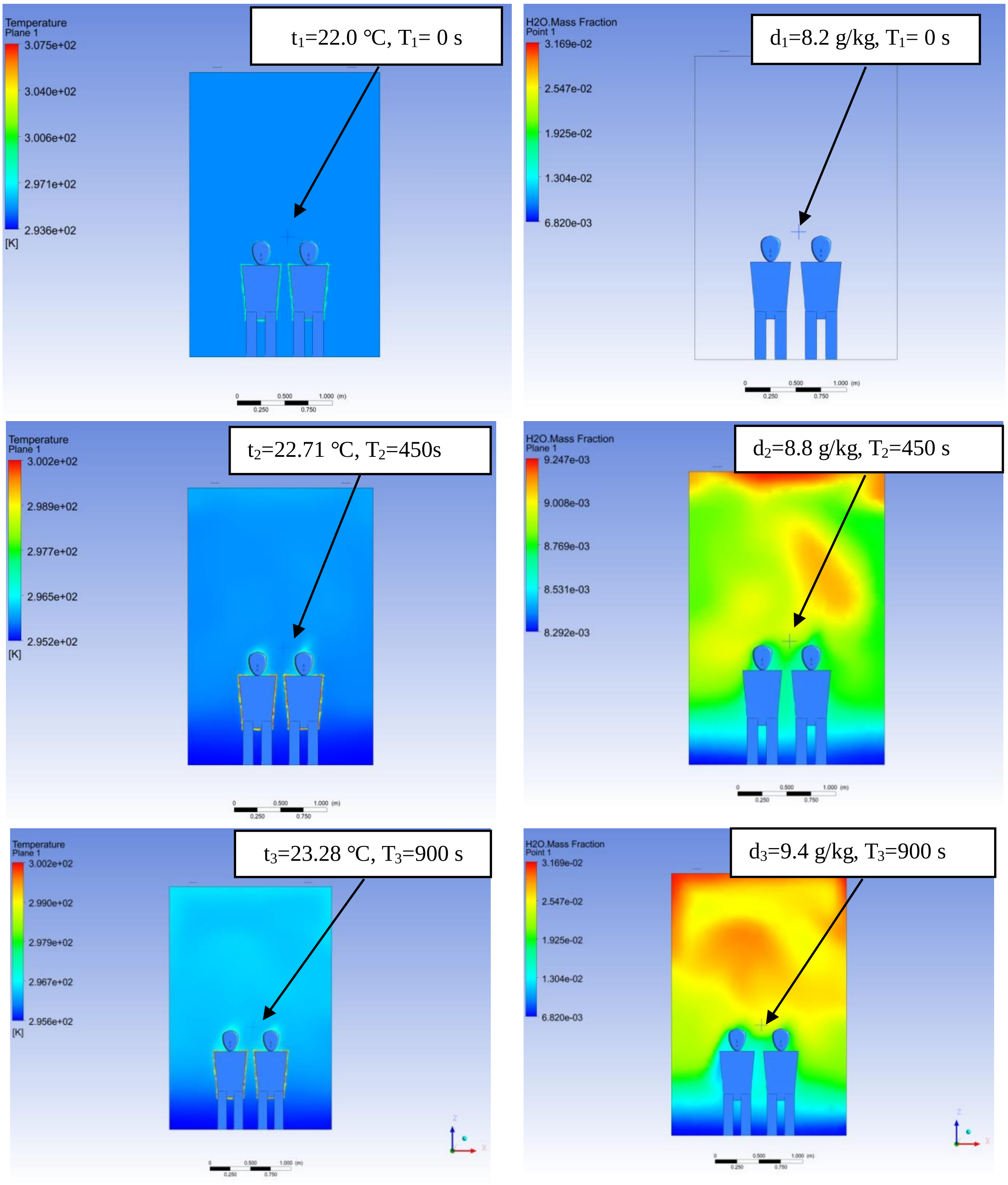


Fig. 8 Rendering of temperature and humidity content relative to the research point over time

Figs. 9-11 represent the planes of the distribution of the height of the studied space over time:

- humidity content;
- temperature;
- air velocity.

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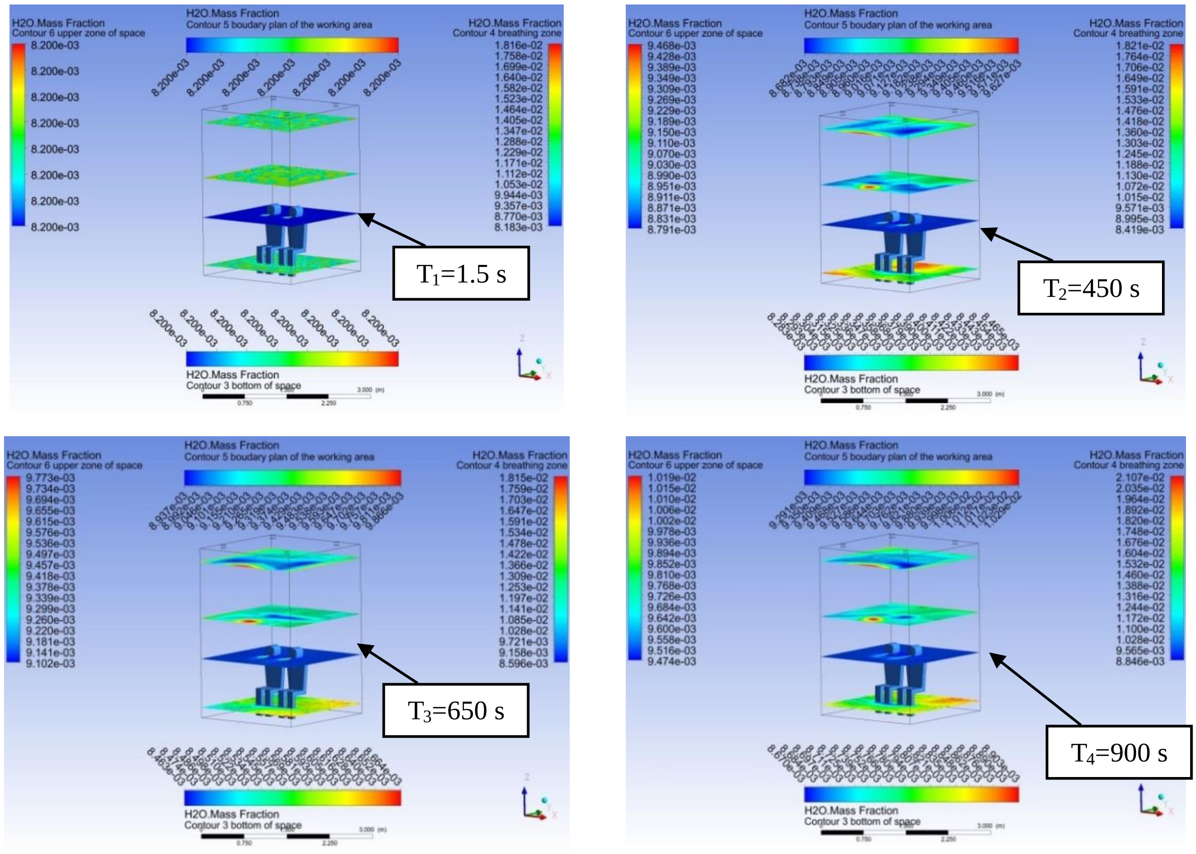

Fig. 9 Changes in humidity content along the height of the isolated space over time

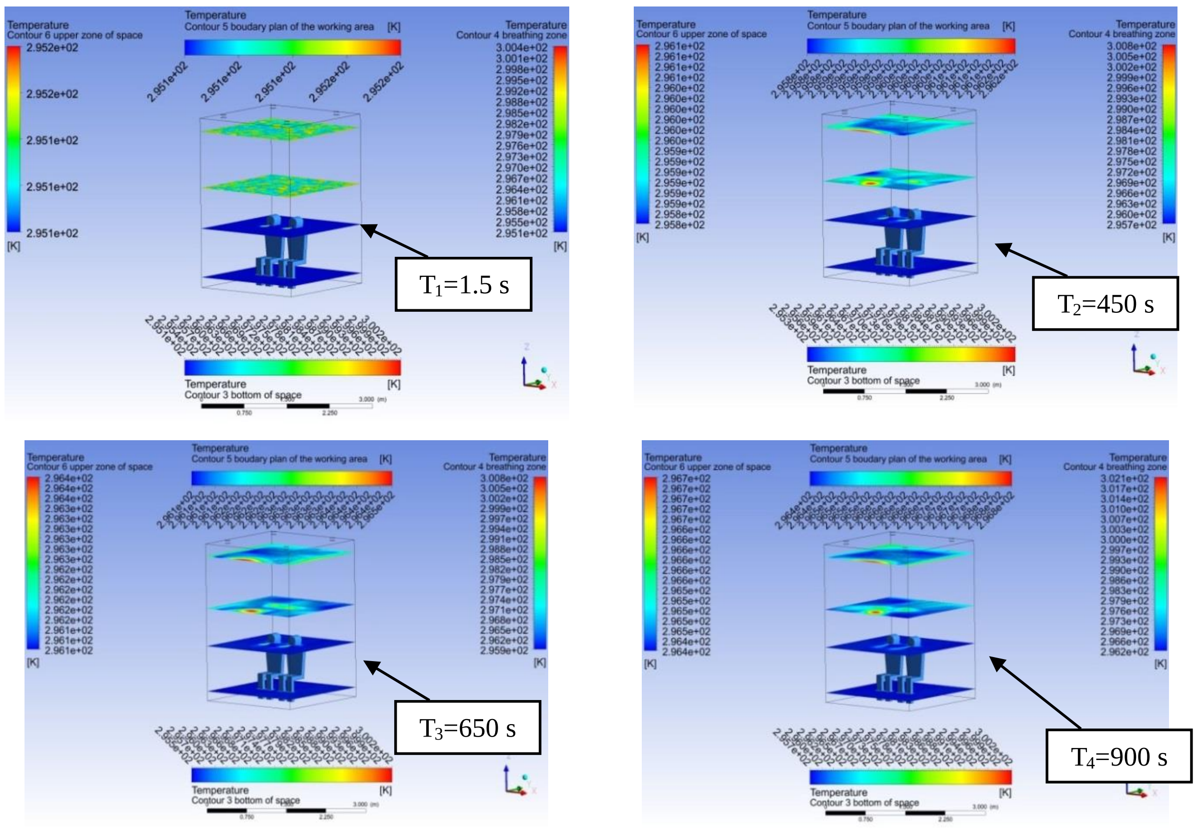

Fig. 10 Change in temperature along the height of the isolated space over time

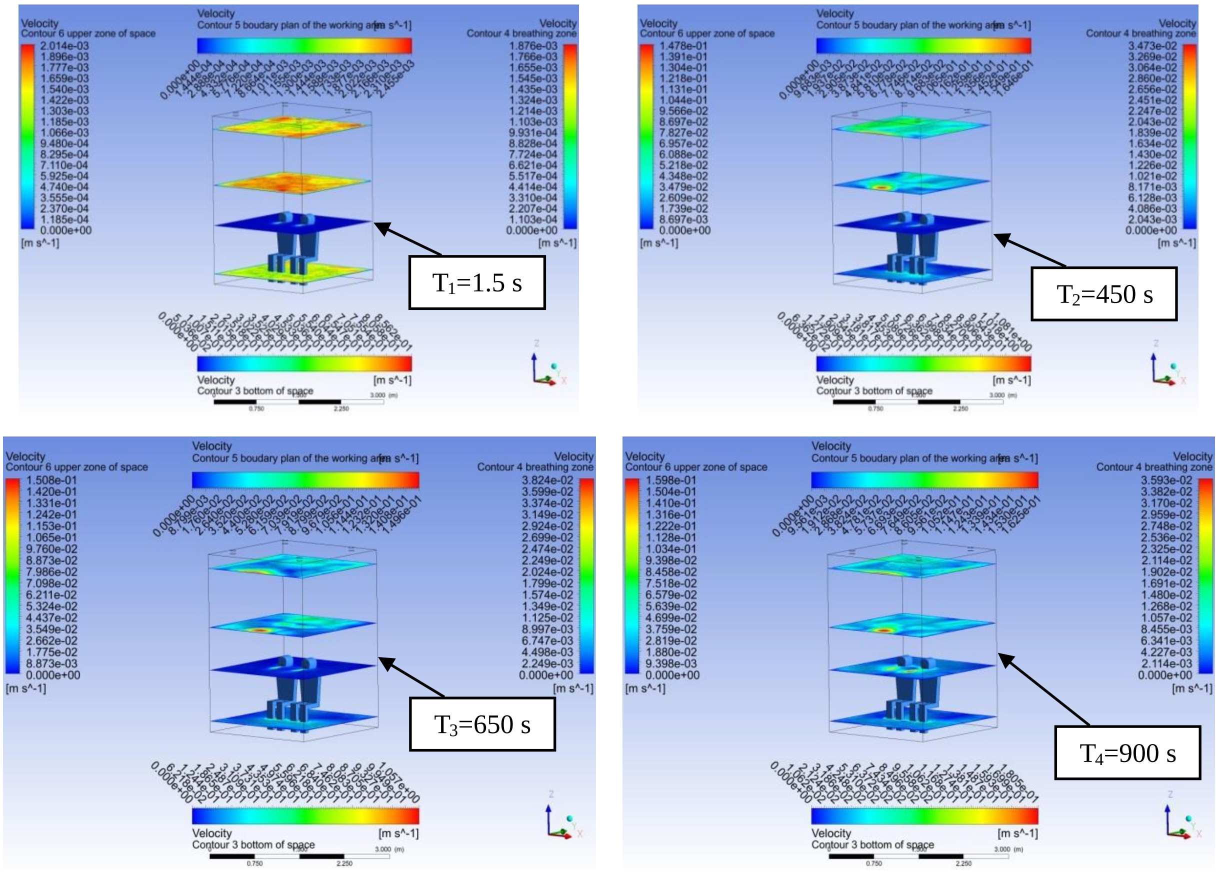

Fig. 11 Variation of velocity along the height of an isolated space over time

4.2 Modeling of air contaminant intake, scheme A

The assimilation of excess heat, humidity and carbon dioxide (CO_2) in the research space is organized according to variable schemes, which allows to assess the efficiency of ventilation systems with various design solutions taking into account constant air flow.

The air contaminant parameters, which are later assimilated by ventilation systems for all schemes, are adopted as follows:

- air temperature: $24°$;
- initial level of CO_2 concentration: $2100\ ppm$;
- atmospheric pressure: $101325\ Pa$;
- relative humidity: $\phi = 65\%$;
- average surface temperature of a clothed person: $27°$.

Results of studies of the "air contaminant" assimilation according to scheme A.

Scheme A (Fig. 12) provides the following constructive conditions for ventilation functioning:

- air supply from above using a static chamber and a ceiling diffuser with a working diameter of Ø150 mm;
- consumption of supply and exhaust air: $120\,m^3 / hour$;
- exhaust ventilation is organized in the lower part of the wall using a ventilation grid.

First of all, it is reasonable to consider the time required to bring the microclimate of the room to the normative state during CO_2 assimilation. In turn, preliminary studies have established that the highest concentration is concentrated in the working zone, which is due to the physical properties of carbon dioxide compared to the surrounding air.

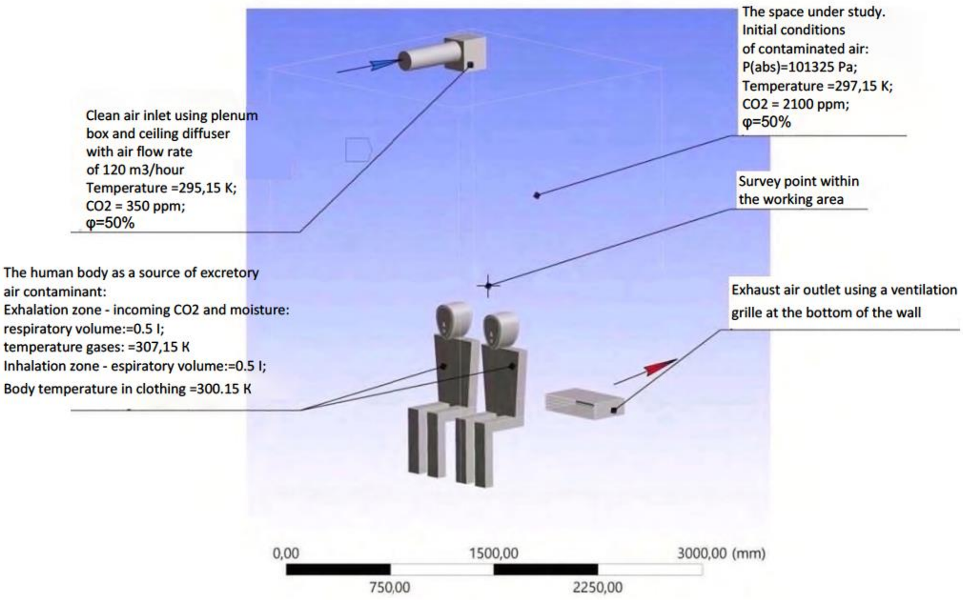

Fig. 12 Initial data for modeling and research according to scheme A

There is an interest in the organization of exhaust ventilation in the lower plane of the working area, where the extraction of polluted air has the shortest path and the possibility of repeated ascent of carbon dioxide into the human breathing zone is excluded. The dynamics of changes in CO_2 concentration at the monitoring point in a 9-minute period is presented in Fig. 13.

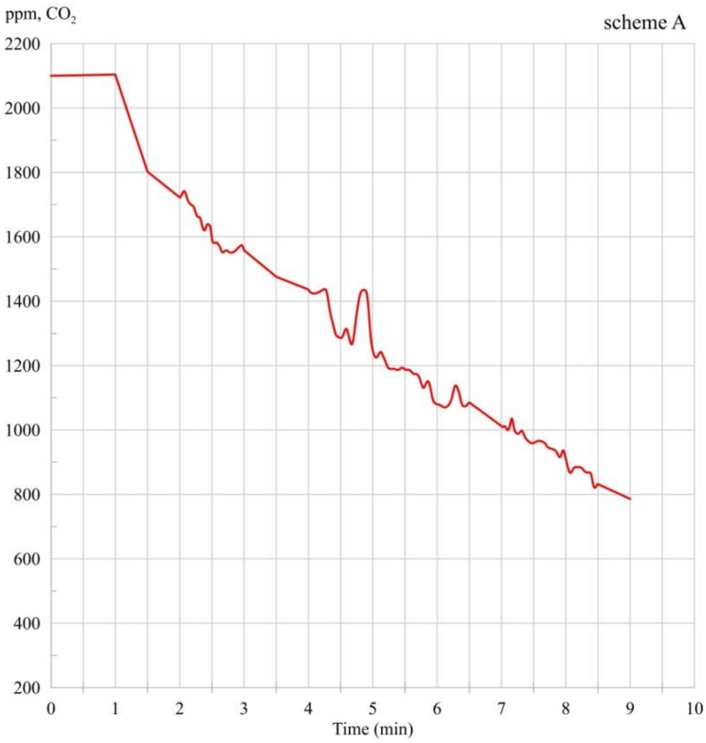

Fig. 13 Dynamics of changes in CO_2 concentration over the time of observation

The value of carbon dioxide on a vertical scale during the functioning of the ventilation system (Fig. 14) is distributed with a fluctuation within $200\,ppm$, which indicates uniform assimilation of polluted air in the study area over the time of observation.

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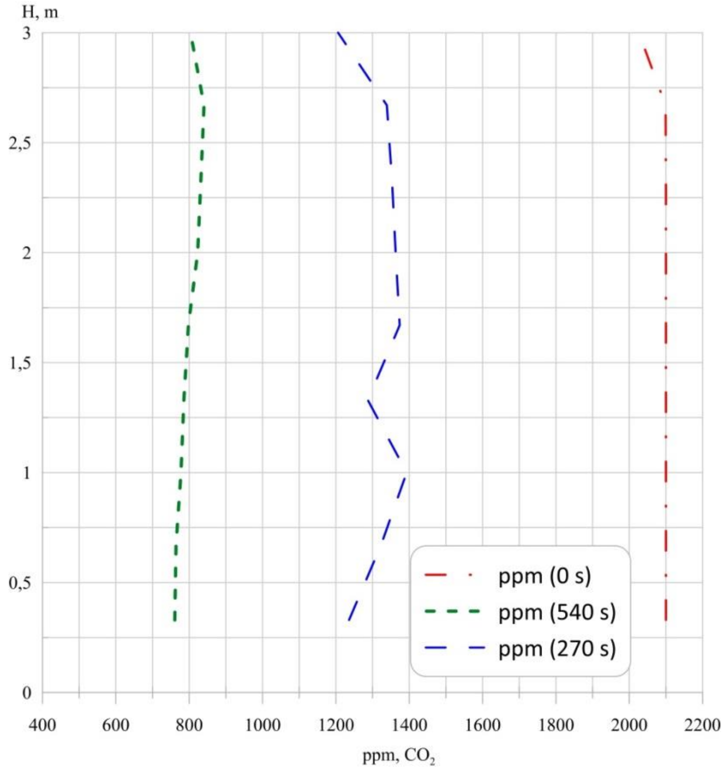

Fig. 14 Monitoring the distribution of CO_2 concentration on a vertical scale

Volumetric visualization of changes in the carbon dioxide content over a 9-minute period of time is shown in Fig. 15

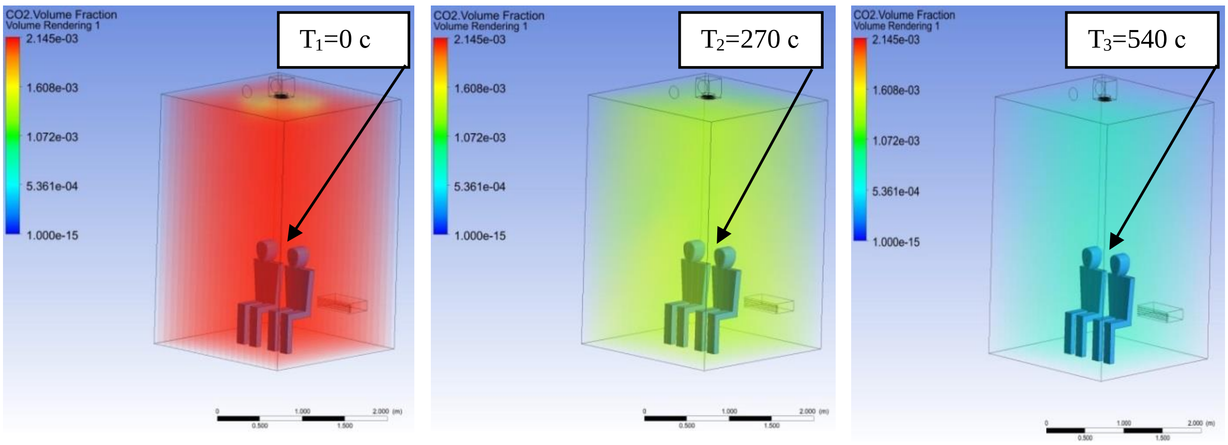

Fig. 15 Volumetric CO_2 rendering over time relative to the observation point

The formation of a uniform distribution of air is due to the geometric properties of the ceiling diffuser (Fig. 16), which forms stream lines of a cyclic nature along the adiabatic walls of the study space. The analysis of the jet (stream line) acquires a stable character, where the velocity vector of the supply air coincides with its direction. That is, the use of static pressure chambers in supply devices of air supply systems has advantages in terms of hydrodynamics and acoustics.

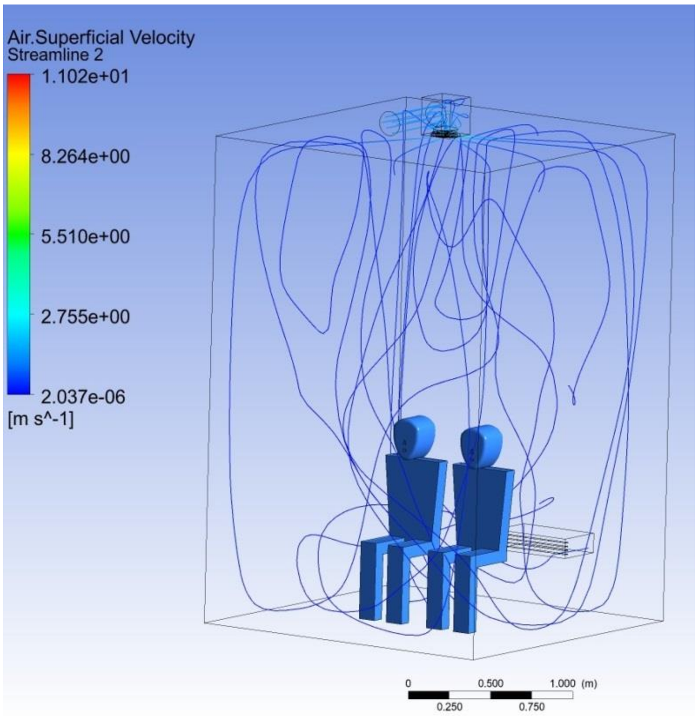

Fig. 16 Stream lines

The distribution of carbon dioxide concentration in different horizontal planes of the investigated volume by both height and time is presented in Fig. 17

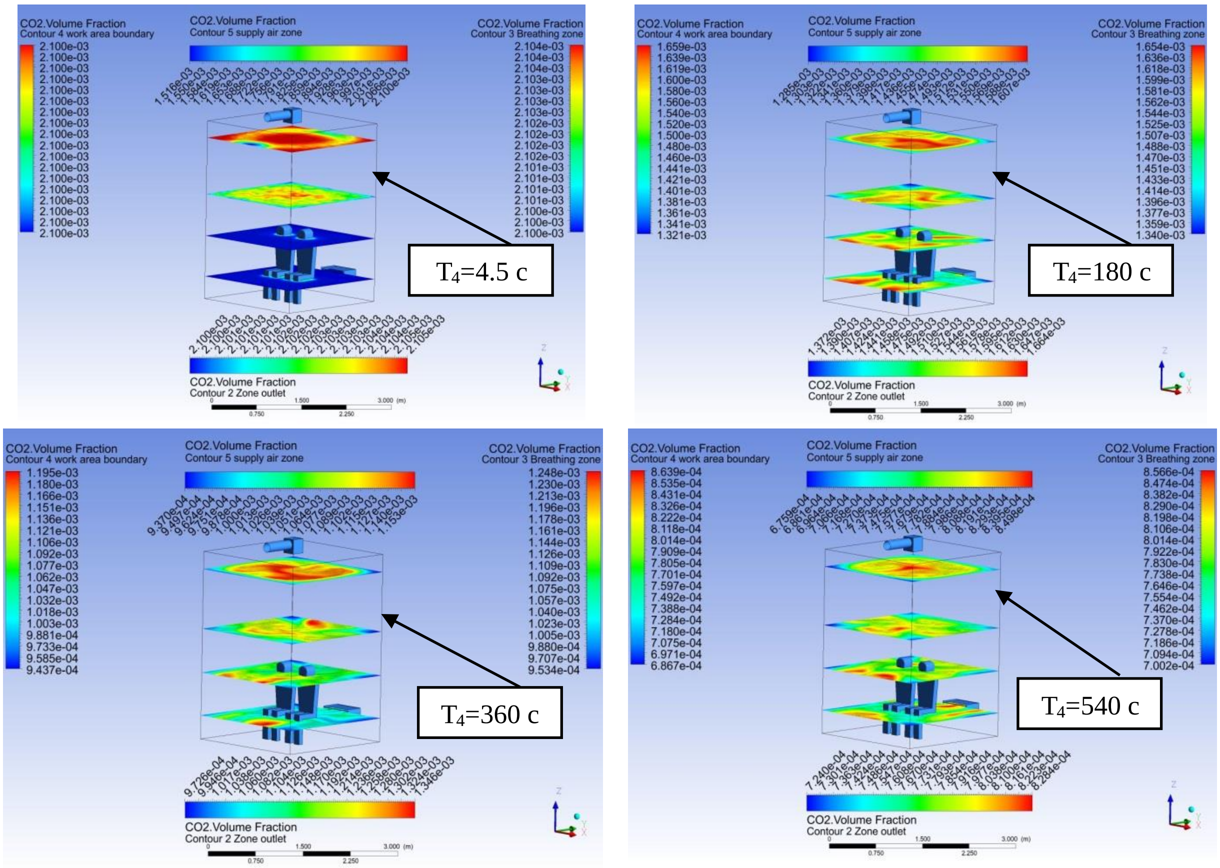

Fig. 17 Variation of CO_2 concentration by height and time, scheme A

5 DISCUSSION OF RESEARCH RESULTS

On the basis of the developed mathematical model, it became possible to solve such problems using the ANSYS software complex as:

• Human air contaminant intake in an isolated space;

• Modeling of the change in the concentration of carbon dioxide, scheme A.

The ANSYS mathematical apparatus allows analyzing the operation of air handling unit to redistribute and remove the main air contaminants from the room (carbon dioxide, heat, water vapor) and monitor temperature, humidity, relative humidity, enthalpy and air velocity parameters

In particular, based on the contour distribution of carbon dioxide (see Fig. 18), it can be concluded that after nine minutes of operation of the air handling unit according to scheme A, the CO_2 content decreased from $2100\,ppm$ to $600-800\,ppm$. The optimal parameters at the inlet of the stream into the working area of the room [1, 2] for this indicator are $400-600\,ppm$.

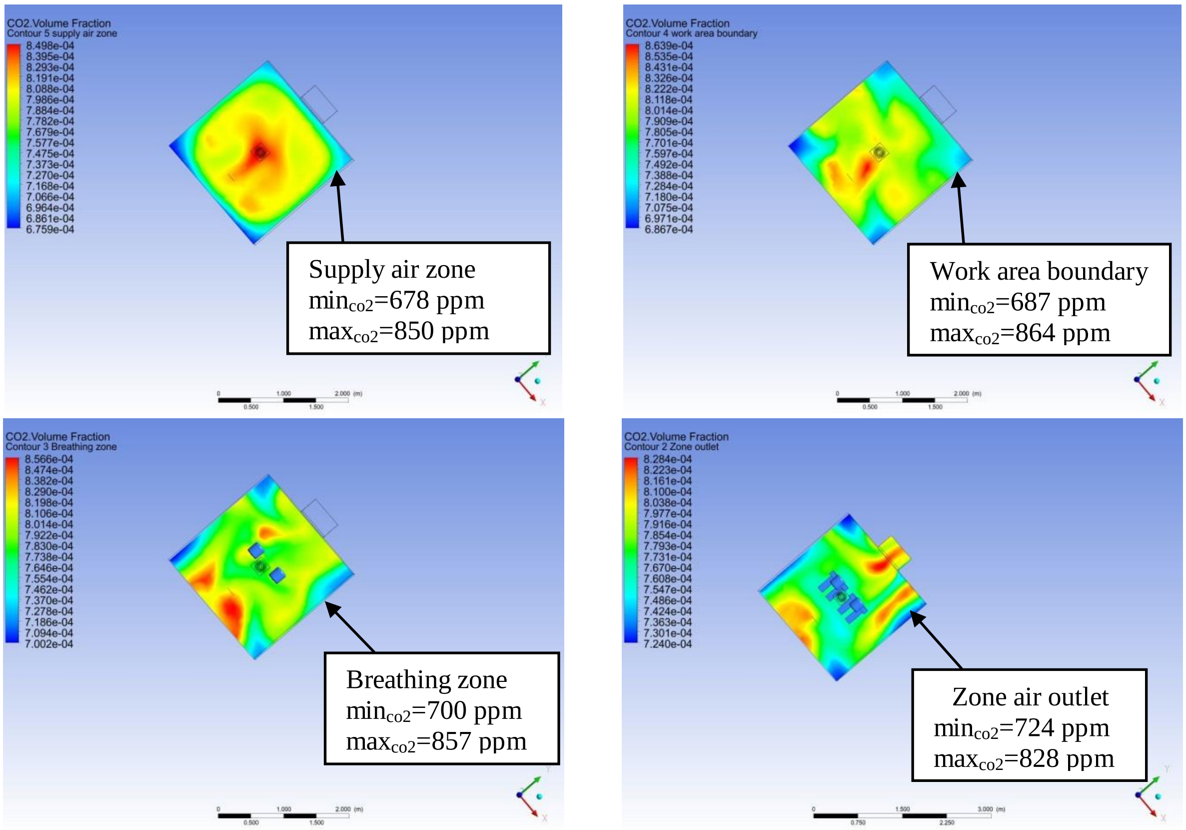

Fig. 18 Variation of CO_2 concentration by height and time, scheme A. Time 540 s

6 CONCLUSIONS

With the use of the ANSYS software package, mathematical modeling of processes of changing the state of the air environment has become possible. The above approach and method provided an opportunity:

- processes of heat and mass exchange and hydrogas dynamics during the interaction of systems (human and air handling unit operating according to various air change schemes);

- obtain intermediate results of the efficiency of various air change schemes in the room.

Subsequent publications will allow a comprehensive assessment and comparison of the efficiency of all four air change schemes we have chosen, when solving the inverse problem (bringing the parameters of the polluted air environment of the room to optimal standard parameters by means of general exchange ventilation).

7 ETHICAL DECLARATIONS

The authors have no relevant financial or non-financial interests to report.

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