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# **COMPUTER DESIGN OF A THERMOELECTRIC PULMONARY AIR CONDENSER FOR THE DIAGNOSTICS OF CORONAVIRUS AND OTHER DISEASES**

*The physical model of a thermoelectric device for collecting exhaled air condensate is considered. By means of computer simulation, the distribution of temperature and velocity of air movement in the working chamber of the device was determined depending on the temperature of the working chamber, as well as humidity, temperature and volume of exhaled air. The results of calculations of the cooling efficiency of thermoelectric modules, necessary to ensure the specified modes of operation of the device, are given. Bibl. 6, Fig. 9.* 

**Key words:** diagnostics, coronavirus, condensate, exhaled air, thermoelectric cooling.

#### **Introduction**

The coronavirus disease COVID-19, caused by the severe acute respiratory syndrome coronavirus SARS-CoV-2, is attracting the attention of doctors, researchers, politicians and communities around the world. COVID-19 is the third major outbreak of a coronavirus in the last two decades, with a greater global impact than the previous outbreaks of coronaviruses in 2003 (SARS-CoV) and 2012 - 2015 and 2020 (MERS-CoV). Transmission of SARS-CoV-2 could be enhanced by spread from individuals with asymptomatic and mildly symptomatic disease. Diagnostic testing plays a crucial role in overcoming the pandemic of the coronavirus disease COVID-19. Rapid and accurate diagnostic tests are essential for identification and treatment of infected individuals, contact tracing, epidemiologic characterization, and healthcare decision-making.

Modern diagnostic testing for the coronavirus disease COVID-19 is based on the detection of the SARS-CoV-2 coronavirus in swab samples from the nasopharynx by the reverse transcription polymerase chain reaction (RT-PCR) method. However, this test is associated with an increased risk of viral spread and environmental contamination and shows a relatively low sensitivity due to technical shortcomings of the sampling method. Given that COVID-19 is transmitted through aerosols and droplets exhaled by humans, the detection of SARS-CoV-2 in lung condensate may serve as a promising non-invasive diagnostic method. This method is proposed in the works of scientists from Japan, the USA, Ireland and other countries as a more sensitive and reliable method of detecting COVID-19 [1 – 4]. Usually, special devices are used to collect condensate - condensers, in which vapors from the air exhaled by a person condense at a temperature from 0 to -70 °C and are collected in a container for further research by the RT-PCR method [5].

It is important to ensure a controlled low temperature of the condenser, convenience, low cost and safety of using such a device. Lowering the condensation temperature makes it possible to speed up obtaining the amount of biological material required for research. At the same time, the operating temperatures of condensers that use ice at 0°C or compressor cooling down to -20 °C are not efficient enough and do not provide a high condensation rate. In addition, compressor condensers are complex, expensive, with insufficient control and maintenance of operating temperature, as well as the presence of dangerous refrigerants. There are attempts to make thermoelectric condensers of exhaled air, but their thermoelectric capabilities are not used to the maximum (the operating temperature level up to -20 °C). The temperature of -70 °С, which is achieved using dry ice (solid *СО*2), is excessive and extremely inconvenient for operation, which radically reduces the possibilities of using this method. Therefore, it is important to create a thermoelectric condenser with precisely controlled temperatures below -20 °С and close to -70 °С without using dry ice.

*The purpose of this work* is the computer design and development of the design of the thermoelectric pulmonary air condenser for the diagnostics of coronavirus and other diseases.

#### **Physical and computer models of thermoelectric pulmonary air condenser**

The thermoelectric device for collecting condensate from the air exhaled by a person contains a cooling unit, a power supply unit and a respiratory circuit. The physical model of its main element, the cooling unit, is shown in Fig. 1.



*Fig. 1 – Physical model of the cooling unit of a thermoelectric device for collecting condensate from the air exhaled by a person: 1 – thermostat (device body); 2 – tube for collecting condensate; 3 – working chamber; 4 – thermoelectric modules; 5 – air heat exchangers; 6 –thermal insulation*

In Fig. 1:

*G*, *T*air, φair – flow rate, temperature and relative humidity of air exhaled by the patient;

 $Q_0$  – cooling capacity of thermoelectric modules;

 $Q_1$  – heat flow entering the tube for collecting condensate together with the air exhaled by the patient;

 $Q_2$  – heat flow removed from the test tube to the environment;

 $Q_3$  – the heat released in the test tube during the condensation of exhaled air vapours;

 $Q_4$  – heat flow transferred from the walls of the test tube to the cooling chamber;

 $Q_5$  – inflow of heat to the test tube from the environment through thermal insulation;

 $Q_6$  – inflow of heat to the test tube from the air heat exchangers through thermal insulation;

 $Q_7$  – heat flow removed from the air heat exchangers to the environment;

 $T_1$  – the temperature of the test tube walls;

 $T_c$  – the cold side temperature of thermoelectric module;

*Т*<sup>h</sup> – the hot side temperature of thermoelectric module;

 $T_2$  – the temperature of air heat exchangers;

 $T_0$  – the temperature of environment (device body).

A computer model of the device was built using the Comsol Multiphysics software package. In doing so, the following program modules were used.

1. *Turbulent Flow*. Allows simulating turbulent flow using a wide range of turbulence models, as well as Large Eddy Simulation (LES) and Detached Eddy Simulation (DES). The eight turbulence models differ in how they model flow near walls, the number of additional variables that are calculated, and what these variables represent. All these models supplement the Navier-Stokes equation with an additional eddy viscosity term of turbulence, but they differ in the way it is calculated.

2. *Heat Transfer in Solids*. Allows solving equation

$$
\rho C_p \left( \frac{\partial T}{\partial t} + {\bf u}_{\rm trans} \cdot \nabla T \right) + \nabla \cdot ({\bf q} + {\bf q}_{\rm r})\,=\,-\,\alpha T \cdot \frac{dS}{dt} + Q
$$

where:

- $\rho$  density (SI unit: kg/m<sup>3</sup>);
- $Cp$  specific heat capacity at constant pressure (SI unit:  $J/(kg·K)$ );
- $T$  absolute temperature (SI unit: K);
- **u**<sub>trans</sub> vector of translational speed (SI unit: m/s);
- $q$  heat flow due to thermal conductivity (SI unit:  $W/m^2$ );
- $q_r$  heat flow due to radiation (SI unit:  $W/m^2$ );
- $\alpha$  coefficient of thermal expansion (SI unit: 1/K);
- *S* the second Piol-Kirchhoff stress tensor (SI unit: Pa);
- $Q$  comprises additional sources of heat (SI unit:  $W/m<sup>3</sup>$ ).

For a stationary problem, the temperature does not change with time and conditions and derivatives disappear with time.

3. *Moisture Transfer in Air*. Interface of moisture transfer in air solves the equation

$$
M_{\mathbf{V}} \frac{\partial c_{\mathbf{V}}}{\partial t} + M_{\mathbf{V}} \mathbf{u} \cdot \nabla c_{\mathbf{V}} + \nabla \cdot \mathbf{g} = G
$$

in which the change in moisture content is expressed through the transfer of vapour concentration, which itself can be expressed as the product of the molar mass of water, the relative humidity, and the vapour saturation concentration:

$$
\mathbf{g} = -M_{\mathbf{v}} D \nabla c_{\mathbf{v}}
$$

$$
c_{\mathbf{v}} = \phi c_{\mathbf{sat}}
$$

with the following material properties, fields and source:

- $M_v$  (SI unit: kg/mole molar mass of water vapour;
- $\varphi$  (dimensionless) relative humidity;
- $c_{\text{sat}}$  (SI unit: mole/m<sup>3</sup>) vapour saturation concentration;
- *D* (SI unit:  $m^2/s$ ) coefficient of vapour diffusion in air;
- u (SI unit:  $m/s$ ) air velocity field;
- *G* (SI unit:  $kg/(m^3 \cdot s)$ ) moisture source (or absorber).

Transfer of vapour concentration occurs by convection and diffusion in moist air. It is assumed that moisture consists only of vapour. In other words, the concentration of the liquid is zero.

4. *Heat Transfer in Moist Air*. It is used to model heat transfer in moist air by convection and diffusion using thermodynamic properties defined as a function of the amount of vapour in moist air.

5. *Multiphysics. Nonisotermal Flow*. Non-isothermal flow refers to fluid flows with non-constant temperatures. When a liquid undergoes a change in temperature, its material properties, such as density and viscosity, change accordingly. In some situations, these changes are large enough to have a significant effect on the flow field. And since the liquid transfers heat, the temperature field, in turn, is affected by changes in the flow field.

6. *Multiphysics. Moisture Flow.*. The Moisture Flow multiphysics coupling is used to model fluid flows where fluid properties (density, viscosity) depend on moisture content. The Moisture Flow interface allows one to maintain vapour concentration, mass and momentum in the air. It synchronizes the functions of the moisture transport and fluid flow interfaces when a turbulent flow regime is defined.

7. *Multiphysics. Heat and Moisture*. This Multiphysics relationship is used to model coupled heat and moisture exchange processes in various environments, including moist air by modeling moisture transport by vapour diffusion and convection and heat transfer by conduction and convection. The thermodynamic properties of moist air depend on the moisture content, while the temperature is used to define the saturation conditions for vapor concentration. This module synchronizes the functions of heat transfer and moisture transport interfaces:

• determines the relative humidity  $φw$  (with appropriate temperature and pressure) to adjust the appropriate input to the Wet Air function of the heat transfer interface;

• defines the temperature to set the model input data in the functions of the moisture transport interface;

• calculates the latent heat source due to evaporation and condensation fluxes on surfaces and adds it to the heat transfer equation.

The geometry of the working chamber with a tube for collecting condensate, as well as the mesh of the finite element method used for calculations in Comsol Multiphysics are shown in Fig. 2.

The created computer model allows one to calculate temperature distributions in the working chamber and tube for collecting condensate from air exhaled by a person, the velocity of air movement in the tube, and determine the amount of condensate received.



*Fig. 2. A computer model of a thermoelectric device for collecting exhaled air condensate*

#### **Computer simulation results**

The used boundary conditions of the computer model correspond to the physical model shown in Fig. 1. In this case, the average consumption of incoming air is determined by the number of exhalations per minute and the volume of exhaled air. It is known from the literature that the typical number of exhalations per minute is between 12 and 21. In doing so, the volume of exhaled air is equal to 0.3 - 0.7 l. The work [7] shows the results of experimental studies of the temperature and relative humidity of the exhaled air: the temperature range of exhaled air is 31.4 - 35.4 °C for participants from Haifa and 31.4 - 34.8 °C for participants from Paris, and the exhaled air relative humidity range is 65.0 - 88.6 % and 41.9 - 91.0 % for Haifa and Paris. participants respectively. That is, the temperature of air exhaled by people is in the range of 34 - 35 °C, and the relative humidity of the air is high, 90 % and above, regardless of geographical location.

The above ranges of input parameters were used for calculations. Fig. 3 shows typical temperature and air velocity distributions in the working chamber and condensate collection tube. The following input parameters were used for this case: temperature of the working chamber – 263.15 K; temperature of the air exhaled by a person is 306.65 K; humidity of exhaled air  $-70\%$ ; the average air velocity at the entrance to the test tube is equivalent to 12 exhalations per minute with an air volume of 0.31 l.

The computer model makes it possible to obtain similar distributions for other values of the input parameters, to build the dependence of the amount of collected condensate and its temperature on these parameters, to determine the requirements for thermoelectric modules and to optimize the design and operating modes of the device.

Figs. 4, 5 give an example of the results of computer calculations of the condensate collection velocity  $V_K$  (in ml per minute) and the thermal power  $Q_0$  that must be removed from the working

chamber at different values of the temperature of the working chamber  $T_K$ , relative humidity of the exhaled air  $\varphi_{air}$ , temperature and exhaled air consumption.



*Fig. 3. Typical distributions of temperature (a) and air velocity (b) in the working chamber of the device for collecting exhaled air condensate*



*Fig. 4. Dependences of the condensate collection velocity*  $V_K$  *on the temperature in the working chamber T*<sup>K</sup> *for different values of the relative humidity of the exhaled air (the temperature of the exhaled air is 33.5 °С; the air consumption is equivalent to 18 exhalations per minute with an exhalation volume of 0.5 l)*



*Fig. 5. Dependences of the thermal power Q*<sup>0</sup> *which must be removed from the working chamber, on the temperature in the working chamber*  $T_K$  *for different values of the relative humidity of the exhaled air (the temperature of the exhaled air is 33.5 °C; the air consumption is equivalent to 18 exhalations per minute with an exhalation volume of 0.5 l)*

Fig. 6 shows the dependence of the condensate collection velocity  $V_K$  on the exhaled air consumption G for different temperature values of the working chamber  $T_K$  (at the exhaled air temperature of 33.5 °C and its relative humidity of 90 %). It can be seen that lowering the temperature of the working chamber from -10 ℃ to -50 ℃ allows you to increase the velocity of condensate collection by 1.5 times. Fig. 7 shows the dependence of the thermal power  $Q_0$ , which must be removed from the working chamber to ensure such operating modes.



*Fig. 6. Dependences of the condensate collection velocity*  $V<sub>K</sub>$  *on the exhaled air consumption G for different values of the temperature of the working chamber*  $T_K$  *(at the temperature of the exhaled air 33.5 °С and its relative humidity 90 %)*



*Fig. 7. Dependences of the thermal power Q*0*, which must be removed from the working chamber, on the exhaled air consumption G for different temperature values of the working chamber*  $T_K$ *(at the temperature of the exhaled air 33.5 °C and its relative humidity 90 %)*

Based on the results of computer simulation, to ensure the necessary operating modes of a thermoelectric device for collecting condensate from the air exhaled by a person, one module, for example, Altec-2 type produced by the Institute of Thermoelectricity, is sufficient to maintain the temperature of the working chamber at the specified cooling capacity of the module.

Using computer simulation in Comsol Multiphysics for the physical model shown above in Fig. 1, the values of heat inflow from the environment  $Q_{inflow}$  are calculated, consisting of heat  $Q_5$  – heat inflow into the test tube from the environment through thermal insulation) and  $Q_6$  – heat inflow into the test tube from air heat exchangers through thermal insulation. The calculation results are shown in Fig. 8.



*Fig. 8. Dependences of heat inflow from the environment Qinflow. on the temperature of the working chamber*  $T_K$  *for different hot side temperatures of the thermoelectric module*

Taking into account the maximum values of the thermal power *Q*0,, which must be removed from the working chamber for different values of its temperature  $T<sub>K</sub>$ , the dependence of the total cooling capacity of the thermoelectric module  $Q_{0total}$  on the temperature of the working chamber for different hot side temperature values of the module was obtained (Fig. 9).



*Fig. 9. Dependences of the cooling capacity of the thermoelectric module*  $Q_{\text{total}}$ *. on the temperature of the working chamber*  $T_K$  *for different hot side temperature values of the thermoelectric module*

Thus, in order to ensure the necessary modes of the working chamber of the device (temperature below -20 ℃) with a power consumption of the Altec-2 thermoelectric module of about 145 W and a cooling capacity of up to 20 W, a heat exchange system is required, which will remove about 165 W of heat with a temperature difference relative to the environment above 15 ℃.

The presented results are the basis for the further development of the design of a thermoelectric device for collecting exhaled air condensate.

## **Conclusions**

- 1. A physical and computer model of a thermoelectric device was built for collecting condensate of exhaled pulmonary air to determine the distributions of temperature and air velocity in the working chamber of the device, to establish the patterns of heat transfer in such a device and to determine the conditions that ensure the achievement of the required level of operating temperatures and improvement of the efficiency of condensate collection.
- 2. The dependences of the distributions of temperature and air velocity in the working chamber of the device on the temperature of the working chamber, humidity, temperature and volume of exhaled air, and the amount of heat inflow from the environment are calculated. It has been established that lowering the temperature of the working chamber from -10 ℃ to -50 ℃ makes it possible to increase the velocity of condensate collection by a factor of 1.5.
- 3. It was established that to ensure the necessary operating modes of the device, namely, the temperature of the working chamber below -20 ℃, the cooling capacity of thermoelectric modules should be 15 - 20 W.

### **References**

- 1. John Hunt. (2007). Exhaled breath condensate an overview. *Immunol Allergy Clin North Am*., 27 (4). 587 - 596.
- 2. Hunt J. (2002). Exhaled breath condensate: An evolving tool for noninvasive evaluation of lung disease. *J Allergy Clin Immunol*, 110(1):28 – 34.
- 3. Horvath I., Hunt J. and Barnes P.J. (2005). Exhaled breath condensate: methodological recommendations and unresolved questions. *Eur Respir J*, 26: 523 – 548.
- 4. Reinhold P, Langenberg A, Becher G, Rothe M. (1999). Breath condensate a medium obtained by a noninvasive method for the detection of inflammation mediators of the lung. *Berl Munch Tierarztl Wochenschr*, 254 – 259.
- 5. Efstathia M. Konstantinidi, Andreas S. Lappas, Anna S. Tzortzi, and Panagiotis K. Behrakis. Exhaled breath condensate: technical and diagnostic aspects (2015). *Scientific World Journal*. V 2015, Article ID 435160, 25 pages.
- 6. Mansour, Elias & Vishinkin, Rotem & Rihet, Stéphane & Saliba, Walaa & Fish, Falk & Sarfati, Patrice & Haick, Hossam. (2019). Measurement of temperature and relative humidity in exhaled breath. *Sensors and Actuators B Chemical*. 127371. 10.1016/j.snb.2019.127371.

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# **КОМП'ЮТЕРНЕ ПРОЄКТУВАННЯ ТЕРМОЕЛЕКТРИЧНОГО КОНДЕНСАТОРА ЛЕГЕНЕВОГО ПОВІТРЯ ДЛЯ ДІАГНОСТИКИ КОРОНАВІРУСНИХ ТА ІНШИХ ЗАХВОРЮВАНЬ**

*Розглянуто фізичну модель термоелектричного приладу для збирання конденсату з повітря, що видихається людиною. Шляхом комп'ютерного моделювання визначено розподіли температури та швидкості руху повітря у робочій камері приладу в залежності від температури робочої камери, а також вологості, температури та об'єму видихуваного повітря. Наведено результати розрахунків холодопродуктивності термоелектричних модулів, необхідної для забезпечення заданих режимів роботи приладу. Бібл. 6, рис. 9.* 

**Ключові слова:** діагностика, коронавірус, конденсат, видихуване повітря, термоелектричне охолодження.

## **References**

- 1. John Hunt. (2007). Exhaled breath condensate an overview. *Immunol Allergy Clin North Am*., 27  $(4)$ . 587 – 596.
- 2. Hunt J. (2002). Exhaled breath condensate: An evolving tool for noninvasive evaluation of lung disease. *J Allergy Clin Immunol*, 110(1):28 – 34.
- 3. Horvath I., Hunt J. and Barnes P.J. (2005). Exhaled breath condensate: methodological recommendations and unresolved questions. *Eur Respir J*, 26: 523 – 548.
- 4. Reinhold P, Langenberg A, Becher G, Rothe M. (1999). Breath condensate a medium obtained by a noninvasive method for the detection of inflammation mediators of the lung. *Berl Munch Tierarztl Wochenschr*, 254 – 259.
- 5. Efstathia M. Konstantinidi, Andreas S. Lappas, Anna S. Tzortzi, and Panagiotis K. Behrakis. Exhaled breath condensate: technical and diagnostic aspects (2015). *Scientific World Journal*. V 2015, Article ID 435160, 25 pages.
- 6. Mansour, Elias & Vishinkin, Rotem & Rihet, Stéphane & Saliba, Walaa & Fish, Falk & Sarfati, Patrice & Haick, Hossam. (2019). Measurement of temperature and relative humidity in exhaled breath. *Sensors and Actuators B Chemical*. 127371. 10.1016/j.snb.2019.127371.

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