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Application of machine learning for the diagnosis of some socially significant diseases from an exhaled human air by the infrared laser spectroscopy

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The infrared spectra of the air exhaled by several groups of volunteers were studied: those suffering from type 1 diabetes, bronchial asthma, and pneumonia. To record infrared spectra, a tunable quantum-cascade laser (QCL) was used. QCL emits in the wavelength range from 5.3 to 12.8 μm in a pulsed mode with a pulse width of 50 ns, a power of up to 150 mW, and a tuning step of 1 cm^{-1}. The laser is optically coupled to an astigmatic Herriot gas cell with an optical path length of 76 m. A difference was found in the intensity of selective lines of biomarker molecules in the spectra of exhaled air of healthy volunteers compared to similar indicators of volunteers suffering from a certain disease. For an example of methods such as the support vector machine (SVM), the k-nearest neighbors (k-NN) and the random forest algorithm (Random Forest), the possibility of classifying volunteers by the infrared spectra of their exhaled air is shown. In terms of the accuracy metric, the accuracy of disease classification improved to 98% by the use of dimensionality reduction techniques (PCA and t-SNE).

Keywords: infrared spectroscopy, quantum-cascade laser, diagnostics, exhaled air, type 1 diabetes, pneumonia, chronic disease, machine learning.

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1. Introduction

Socially significant diseases [1–3], such as diabetes mellitus, bronchial asthma, pneumonia require early diagnosis, which is especially important for timely therapy. Non-invasive examination methods are preferred due to the low impact on the patient's organism, which is especially important in cases where diagnostic tests need to be done throughout the entire patient's life. Modern methods of exhaled breath diagnosis allows detecting a wide range volatile organic compounds (VOC) emitted by the human body [4]. Changes in their concentrations are often associated with certain diseases [5] or metabolic disorders in general. It is promising to define VOCs as markers with prognostic significance for detecting the development of metabolic disorders, among which a specific place is held by the diabetes mellitus. The use of such predictors in the screening of large population groups and the formation of preventive measures on this basis is an important social and biomedical problem, especially when it comes to children's health. One of the promising volatile compounds associated with the peculiarities of metabolism is acetone. Variations in its content in exhaled breath or urine quite accurately reflect changes in lipid metabolism, in particular beta oxidation of lipids.

However, there is a need to identify more clearly the relevant gas-metabolic profiles in patients with diabetes mellitus, reflecting systemic changes in metabolism under normal and pathological conditions, because light hydrocarbons are intermediate products or by-products of many metabolic cycles [6]. Thus, for example, the formation of acetone is due to the involvement of fatty acids in energy metabolism [7] in the case of diabetes mellitus [8]. Also, the formation of acetone in the exhaled breath is possible during starvation [9], prolonged intense physical work [10], changes in the state of the enteric environment [11].

In recent years, allergic diseases of the respiratory tract have become of greater significance due to the high increase in their prevalence among the population, especially in the child population [12]. According to a report by the Global Asthma Network (GAN), about 339.4 million people suffer from this disease and approximately 14% of them are children. The Centers for Disease Control and Prevention (CDC) reports that in 2015 there were 24.6 million (7.8%) people in the USA diagnosed with asthma. 6.2 million (8.4%) of them were children: 4.7% diagnosed cases were in patients under the age of 4 years, 9.8% were in patients aged from 5 to 14 years, 9.8% were in patients aged from 15 to 17 years. It is known that more than half of the cases of bronchial asthma onset occur in early and preschool age, however, it is in these patients that diagnosis is particularly difficult [13]. The modern strategy for the treatment of bronchial asthma is aimed at preventing the development of pathology and stopping exacerbations. The development of new methods of early diagnosis and the study of development mechanisms of the disease will improve the quality of life of children and their parents. There are known methods for early diagnosis of bronchial asthma in infants by determining carbon monoxide (CO) in the exhaled breath. In infants with asthma, the threshold level of CO is more than 2 ppm, in healthy children the CO level is not more than 1 ppm. This method can be used as an additional non-invasive method for monitoring asthma and diagnosing asthma in infants [14]. Dynamic monitoring of FeNO is an effective indicator of inflammation of the respiratory tract and, therefore, is an important clinical tool for assessing the course of asthma [15], which concentration decreases in response to glucocorticosteroid therapy [16]. The statistical significance of the difference in the concentration of hydrogen peroxide in the exhaled breath condensate between patients with asthma and healthy patients (480 and 780 nmol, respectively) has been shown in [17].

About 150 million cases of pneumonia in preschool children are registered annually in the world. Severe pneumonia occurs in 7–13% of cases and accounts for up to 11–20 million hospitalizations annually. It has been shown in [18] that the main substances found in the exhaled breath of patients with pneumonia were pentane and isoprene. Isoprene is the main hydrocarbon present in alveolar gas and is formed from isopentenyl pyrophosphate and dimethylallyl pyrophosphate, which are products of the conversion of mevalonate to cholesterol. The production of mevalonate is a step in the biosynthesis of tissue cholesterol. Isoprene is a by-product of sterol synthesis, and any change in the rate of cholesterol synthesis will cause comparable changes in the amount of isoprene in the exhaled breath.

Thus, from the point of view of physiology, it is possible to determine some relationships between the breathing profile and the state of human health. However, it is often impossible to isolate one specific chemical compound and determine reference values, which necessitates the analysis of composition of the exhaled breath as a whole. Infrared spectroscopy in the mid-infrared range (the „fingerprint" range) makes it possible to simultaneously record the characteristic spectral lines of a number of chemical compounds, which allows developing a method for diagnosing a number of diseases by analyzing the exhaled breath. For example, in [19] the possibilities of using a quantum-cascade laser tunable in the range of 1150–1250 cm^{-1} for the analysis of acetone in the exhaled air have been shown. In [20], the possibility has been shown to detect about 60 ppt NO at a wavelength of 5.6 μm using a tunable infrared laser. However, the significant overlap of a number of selective lines for the components of exhaled breath makes it very difficult to solve the inverse problem of spectroscopy.

Machine learning methods have been widely used in various fields of science and technology, as well as in

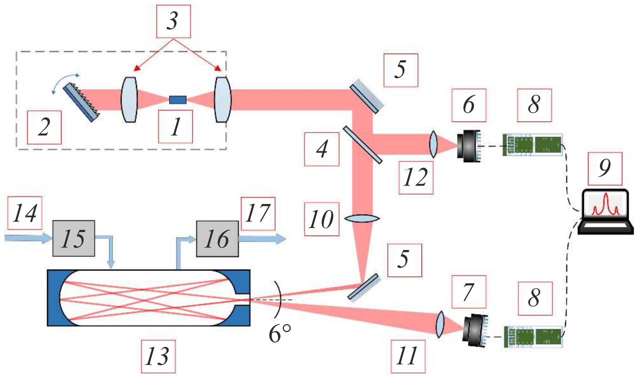

Figure 1. Schematic diagram of the experimental setup.

healthcare [21], which allows solving diagnostic problems in various fields, such as medical data imaging, cancer diagnosis, on-chip systems, etc. [22]. Machine learning is used to study important clinical parameters such as extracting medical information, predicting diseases and developmental stages. Thus, it helps in planning and maintaining the status of the patient. In addition, it provides effective health monitoring that helps to analyze data and send timely alerts [23]. For a machine learning system to be useful in solving medical diagnostic problems, the following characteristics are required: high execution speed, the ability to properly handle missing data and noisy data, the transparency of diagnostic knowledge, the ability to explain solutions, and the ability of the algorithm to reduce the number of tests needed to obtain a reliable diagnosis. Machine learning algorithms are actively used in automated diagnostic applications. Such algorithms help medical staff in predicting diseases, as well as improve the accuracy of disease diagnosing [24, 25].

In [26], a method is proposed for diagnosing acute myocardial infarction by the exhaled breath using machine learning methods. The reference group included 30 people and the healthy group included 42 people. Data clustering was performed by the PCA method based on six biomarkers of acute myocardial infarction (C_5H_{12}, N_2O, NO_2, C_2H_4, CO, CO_2) with further classification by support vector machine. The achieved sensitivity and specificity were 0.82 and 0.93. In [27], the possibility has been studied to use artificial intelligence and machine learning methods in the diagnosis of respiratory diseases, such as asthma and chronic obstructive pulmonary disease. In [28], the use of these methods has been shown for the analysis of the condition of patients suffering from lung cancer and chronic obstructive pulmonary disease on the basis of infrared photoacoustic spectroscopy data. In [29, 30], machine learning methods have been used to analyze multicomponent gas mixtures. In [31, 32], the possibilities have been shown to use machine learning and deep learning to analyze the human exhaled breath.

Table 1. Gender-age distribution (people) of healthy volunteers and volunteers with an established disease

	Female, under 14 years	Female, over 14 years	Male, under 14 years	Male, over 14 years	Sum
Type 1 diabetes	10	12	18	20	60
Bronchial asthma	6	2	13	11	32
Community-acquired pneumonia	4	0	1	0	5
Healthy volunteers	14	9	15	22	60

Experimental setup

Fig. 1 shows schematic diagram of the laboratory setup used in this study.

The setup consists of a quantum-cascade laser (*1*) emitting in the wavelength range of $5.8-12.3\,\mu$m in a pulsed mode with a pulse length of 50 ns and a power of up to 150 mW. The laser is built in accordance with the Littrow configuration: (*2*) — diffraction grating, (*3*) — aspherical lenses. The infrared radiation passes through the system of mirrors (*5*) and enters the beam splitter (*4*) and part of the beam enters the reference photodetector (*6*) through the matching optics (*12*) . Then, the radiation is directed to the lens (*10*) with a focal length of $f \sim 350$ mm located so as to focus the beam inside the volume of the gas cell at a distance of $1/3-1/2$ of its length. The Herriott-type gas cell (*13*) makes it possible to obtain 238 laser beam reflections and an optical path of 76 m. The outgoing beam is focused by the matching optics (*11*) on the signal photodetector (*7*). Photodetectors (*6*) and (*7*) were implemented as cadmium−mercury−tellurium photodetectors cooled by a cascade of Peltier cells with a detectivity D^* equal to $\sim (6-8) \cdot 10^9\,\mathrm{cm}\sqrt{\mathrm{Hz}}/\mathrm{W}$. The signal from both photodetectors is read by the 18-bit analog-to-digital converter (*8*), after which the reference spectrum and the signal spectrum are transferred to the computer (*9*). The analyzed sample (*14*) through the dryer (*15*) enters the multipass cell (*13*). The concentration of water vapor after drying is about $1\,\mathrm{g/m^3}$. The vacuum pump (*16*) is installed at the cell outlet, which maintains the pre-defined pressure and pumps out the sample (*17*).

Fig. 2 below shows the characteristic spectra of the exhaled breath of a healthy volunteer, a patient with an established diagnosis of type 1 diabetes, and a patient with a diagnosis of bronchial asthma, as well as the spectra of acetone and nitrogen monoxide as characteristic biomarkers of diabetes and asthma, respectively.

In Fig. 2, the regions of the spectrum are highlighted with the most explicit differences corresponding to the absorption of biomarker molecules. However, it should be noted that the exhaled breath spectrum contains several hundred components, some of which have their spectra significantly overlapped, so it is impossible to assert that only one substance affects the characteristic absorption line. Thus, a sufficiently wide region of the infrared spectrum is used for the analysis.

Groups under the Study

Four groups of people were selected for clinical trials, which is a total of 157 people. The first group included 60 healthy volunteers (Table 1). The second group included patients suffering from community-acquired pneumonia (5 people). The third group was formed of patients with a confirmed diagnosis of type 1 diabetes (60 people) and the fourth group were patients with bronchial asthma (32 people).

The study was conducted according to the guidelines of the Declaration of Helsinki, and approved by the Ethics Committee of the Morozov Children.s Clinical Hospital State Budgetary Healthcare Institution of Moscow Healthcare Department (Moscow, Russia). Protocol code 174 on 18 January 2022. All participants were informed about details of the research and signed „Informed agreement“ for the actions carried out.

Results and discussions

The main challenge in this study was to classify volunteers by infrared spectra of their exhaled breath into 4 groups: volunteers without diagnosed abnormalities (healthy), patients with type 1 diabetes, patients with diagnosed asthma, and patients with community-acquired pneumonia. During the experiment, 100 spectra were obtained from each patient, which were subsequently averaged. The classification was preceded by data preprocessing. For the obtained transmission spectra, the baseline correction was carried out followed by spectra normalization so that each spectrum had a mean value equal to 0 and a standard deviation equal to 1, which allows bringing the data to a single scale.

During the studies, 204 spectra were recorded (for some patients, the samples were repeated), of which 71 were taken from healthy volunteers, 77 were taken

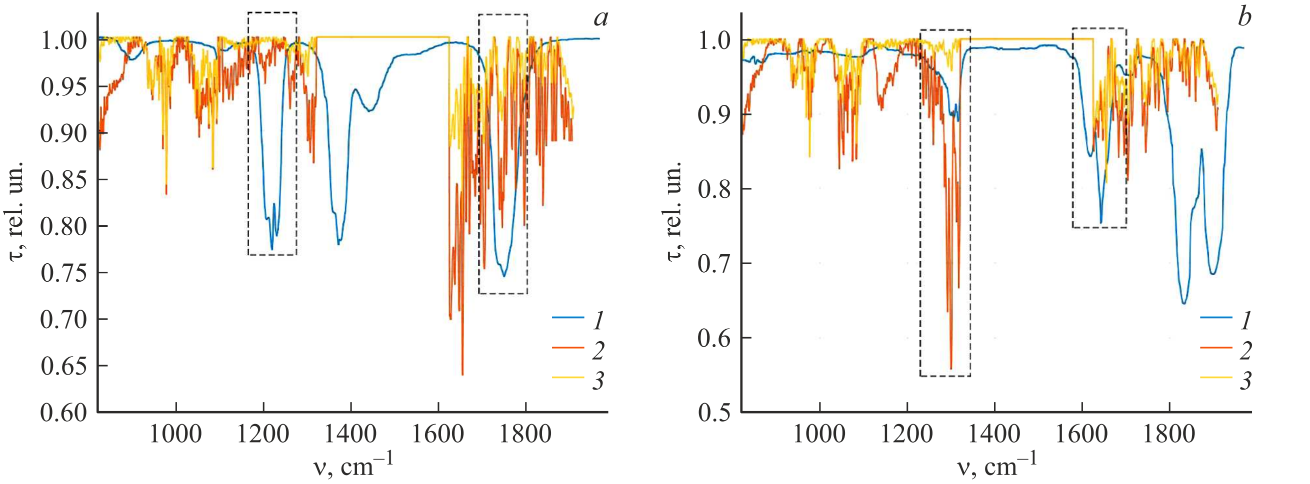

Figure 2. (*a*) Spectrum of acetone [33] (*1*), spectra of exhaled breath of a patient with type 1 diabetes (*2*) and a healthy volunteer (*3*); (*b*) spectrum of NO [33] (*1*), spectra of exhaled breath of a patient suffering from bronchial asthma (*2*) and a healthy volunteer (*3*).

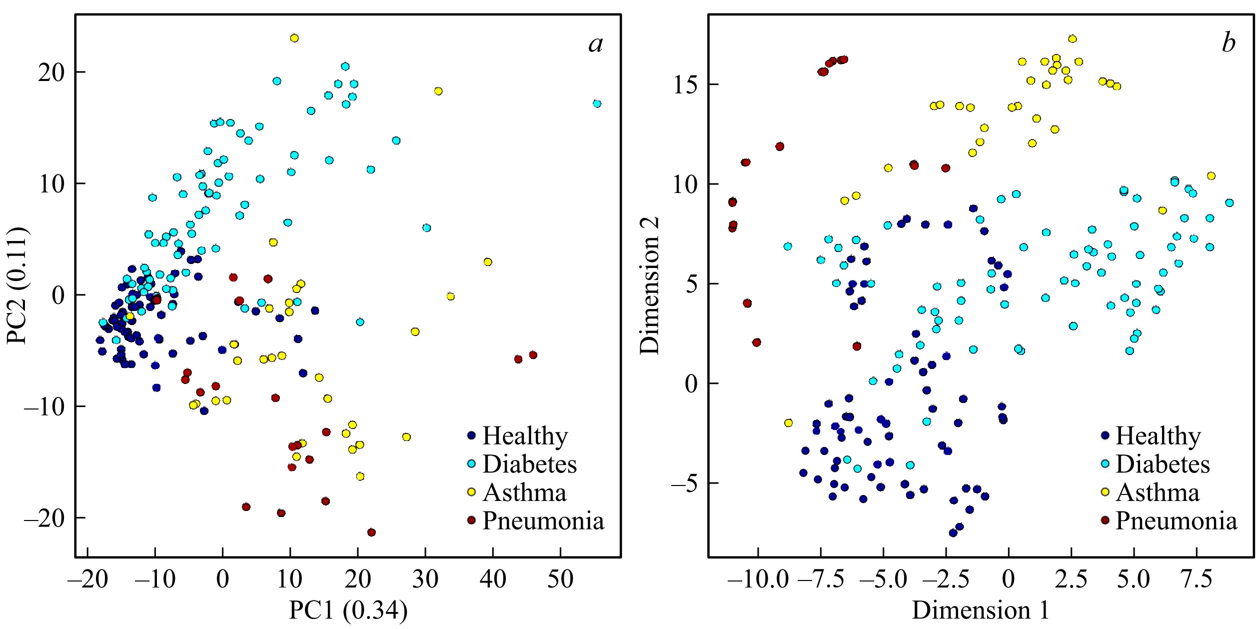

Figure 3. Data classification imaging using (*a*) PCA and (*b*) *t*-SNE methods.

from patients with type 1 diabetes, 32 were taken from patients with bronchial asthma, 24 were taken from patients with community-acquired pneumonia. The test sample was 20% of the presented dataset. Validation was carried out on the basis of the accuracy metric. For data imaging, the principal component analysis (PCA) and the *t*-distributed stochastic neighbor embedding (*t*-SNE) methods were used, the results of which are shown in Fig. 3.

Based on the data presented in Fig. 3, the principal possibility of classifying experimental data is shown. Fig. 3 for the PCA method shows 2 dimensions (for clarity), however, the explained variance is 0.45, although visually it can be seen that the groups can be separable. Data with ten features covers 90% of the explained variance [34], which is sufficient for reliable classification.

The transmission spectra were classified using three machine learning methods: the support vector machine (SVM), the *k*-nearest neighbors (*k*-NN), the Random Forest. Table 2 shows the results of classification of full dimension data (without dimension reduction). The *Precision*, *Recall* and $F1$ are used as metrics, which can be described by the following formulae:

$$Precision = \frac{TP}{TP + FP},$$

$$Recall = \frac{TP}{TP + FN},$$

Table 2. Classification efficiency evaluation for full dimension data

Method	Groups	Precision	Recall	$F1$
SVM	Healthy	0.87	0.93	0.90
	Diabetes	0.93	0.88	0.90
	Asthma	1.00	1.00	1.00
	Pneumonia	1.00	1.00	1.00
k-NN	Healthy	0.72	0.93	0.81
	Diabetes	0.88	0.88	0.88
	Asthma	1.00	1.00	1.00
	Pneumonia	1.00	0.20	0.33
Random Forest	Healthy	0.77	0.91	0.83
	Diabetes	0.94	0.94	0.94
	Asthma	1.00	0.88	0.93
	Pneumonia	1.00	0.50	0.67

Table 3. Classification results for reduced dimension data

Method	Groups	Precision	Recall	$F1$
SVM	Healthy	0.93	1.00	0.97
	Diabetes of type 1	1.00	0.94	0.97
	Asthma	1.00	1.00	1.00
	Pneumonia	1.00	1.00	1.00
k-NN	Healthy	0.93	0.93	0.93
	Diabetes of type 1	0.94	0.94	0.94
	Asthma	0.86	1.00	0.92
	Pneumonia	1.00	0.80	0.89
Random Forest	Healthy	0.92	0.86	0.89
	Diabetes of type 1	0.88	0.94	0.91
	Asthma	1.00	1.00	1.00
	Pneumonia	1.00	1.00	1.00

$$F1 = 2\frac{Precision \times Recall}{Precision + Recall},$$

where TP is true-positive, FP is false-positive result, TN is true-negative result, FN is false-negative result.

Table 4. Accuracy calculation results for the obtained classifiers

Data	SVM	k-NN	Random Forest
Full dimension data	0.93	0.83	0.93
Reduced dimension data	0.98	0.93	0.93

Table 3 shows the results of classification of the experimental sample based on reduced-dimension data (10 features).

To determine the optimal method for classification, the algorithms were evaluated on a test sample on the basis of the accuracy metric. The result is shown in Table 4.

The obtained results show that the machine learning models for a given sample of volunteers and the spectrum registration technique allow classifying groups of people according to their infrared breathing spectra with *Precision* and *Recall* metrics of at least 0.8. The support vector machine showed the best result for classifying the diseases described in the study by infrared spectra of the human exhaled breath. Dimension reduction increases the accuracy of classification by highlighting the most significant features, and also allows a considerable increase in the speed of calculations. The number of significant features was chosen on the basis of the condition of achieving 90% of the explained variance.

Conclusions

The infrared spectra of exhaled breath were analyzed for four groups of volunteers: healthy people, patients suffering from type 1 diabetes, bronchial asthma and pneumonia. Infrared spectra were recorded using a tunable quantum-cascade laser emitting in the wavelength range from 5.3 to 12.8 μm. The laser was operated in a pulsed mode emission, with a pulse width of 50 ns and a power of up to 150 mW, with a tuning step of 1 cm^{-1}. The laser was optically coupled to an astigmatic gas cell of the Herriott type with an optical path length of 76 m. For healthy volunteers and volunteers suffering from diabetes or asthma, a difference was found in the intensity of the transmission spectra at wavelengths corresponding to biomarker substances (acetone and nitrogen monoxide).

To diagnose the disease by infrared spectrum, the following classification methods were used: SVM, k-NN and Random Forest. With the help of PCA and t-SNE methods, it is shown that the reduction of the dimension to the 10 most significant features covers 90% of the explained variance. Reducing the dimension of infrared spectra allows improvement of the classification accuracy. The method of support vector machine made it possible to obtain the *accuracy* value of at least 98%

when classifying the described sample of volunteers into 4 health classes, taking into account the reduction in the dimension of the experimental spectra of exhaled breath to 10 features. The method described in this study for analyzing the infrared spectra of exhaled breath makes it possible to develop devices for express diagnostics of the state of human health for further use in medical diagnostics.

Conflict of interest

The authors declare that they have no conflict of interest.

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