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Lung Cancer Diagnosis Based on the Analysis of Volatile Markers in Exhaled Breath

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ABSTRACT

Aim. To evaluate the diagnostic accuracy of a developed gas analysis sensor system combined with neural network algorithms for detecting lung cancer based on volatile organic compounds in exhaled breath.

Materials and methods. The study group included 53 exhaled breath samples from patients with morphologically confirmed stage I–IV lung cancer. The control group ($n = 47$) consisted of individuals with no history or prior diagnostic findings of cancers at the time of enrollment. The study was conducted using the developed Multisensory Gas Analysis System, comprising an array of semiconductor sensors and implementing neural network data processing algorithms.

Results. The experimental results of classifying lung cancer patients and healthy volunteers demonstrated distinct differences in the exhaled breath samples. The system achieved the accuracy of 95.8%, sensitivity of 98.1%, and specificity of 93.6%. In a series of experiments with balanced stage distribution (stages I–II vs. stages III–IV), the mean classification accuracy was 75%, with sensitivity and specificity ranging from 65 to 80%. Both prepped and non-prepped patients showed comparable results, confirming the reproducibility of the method. The accuracy level of 75% allowed for the differentiation between early- and late-stage disease samples.

Conclusion. The developed system demonstrates high diagnostic performance, surpassing existing methods, including low-dose computed tomography. The findings support the potential of this technology for both early detection and staging of lung cancer.

Keywords: lung cancer, exhaled breath, volatile organic compounds, sensory gas analysis system, non-invasive diagnosis, neural network

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Conformity with the principles of ethics. All study participants signed an informed consent to participate in

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the study. The study was approved by the local Ethics Committee at Cancer Research Institute, Tomsk National Research Medical Center, Russian Academy of Sciences (Minutes No. 3a dated March 25, 2020).

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Диагностика рака легкого на основе анализа летучих маркеров в выдыхаемом воздухе

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РЕЗЮМЕ

Цель. Определить диагностическую эффективность разработанного газоаналитического сенсорного комплекса в сочетании с алгоритмами искусственной нейронной сети для выявления рака легкого по маркерным летучим органическим соединениям в выдыхаемом воздухе.

Материалы и методы. В исследуемую группу включены 53 пробы выдыхаемого воздуха от пациентов с морфологически подтвержденным раком легкого I–IV стадий. Контрольная группа ($n = 47$) состояла из лиц, не имеющих на момент включения в исследование признаков онкологических заболеваний по данным анамнеза и (или) предшествующих диагностических мероприятий. Исследование проводилось с помощью разработанного мультисенсорного газоаналитического комплекса, состоящего из набора полупроводниковых сенсоров и реализующего алгоритмы нейро-сетевой обработки данных.

Результаты. Полученные при проведении экспериментов по классификации пациентов с раком легкого и здоровых добровольцев результаты показывают наличие явных признаков различия в пробах выдыхаемого воздуха. Точность составила 95,8 %, чувствительность – 98,1% и специфичность – 93,6%. В серии экспериментов с равным распределением стадий (I–II и III–IV) средняя точность классификации составила 75%, чувствительность и специфичность – 65–80%. Подготовленные и неподготовленные пациенты демонстрировали сопоставимые результаты, что подтверждает воспроизводимость метода. Уровень точности 75% позволяет различать пробы от пациентов с ранними и поздними стадиями заболевания.

Заключение. Разработанный комплекс демонстрирует высокую диагностическую эффективность, превосходящую существующие методы, включая низкодозную компьютерную томографию. Полученные данные подтверждают перспективность технологии как для раннего выявления, так и для стадирования рака легкого.

Ключевые слова: рак легкого, выдыхаемый воздух, летучие органические соединения, сенсорный газоаналитический комплекс, неинвазивная диагностика, нейронная сеть

Конфликт интересов. Авторы декларируют отсутствие явных и потенциальных конфликтов интересов, связанных с публикацией настоящей статьи.

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INTRODUCTION

Lung cancer remains a critical global public health burden, accounting for some of the highest incidence and mortality rates among all malignancies. These unfavorable outcomes are largely attributable to late-stage diagnosis, when curative treatment options are limited and prognosis is poor [1, 2].

Conventional imaging modalities, although indispensable, often lack the sensitivity required for the detection of early-stage disease. This limitation underscores the pressing need for non-invasive, rapid, and cost-effective screening strategies capable of facilitating earlier diagnosis and, ultimately, improving clinical outcomes.

Exhaled breath analysis has emerged as a promising non-invasive diagnostic modality. It is based on the qualitative and quantitative characterization of volatile organic compounds (VOCs) present in exhaled breath, which collectively reflect the underlying metabolic state of the body. The rationale for this approach lies in the premise that a wide range of VOCs are generated during physiological and pathological metabolic processes, and that alterations in their composition and concentration may serve as surrogate markers of disease [3]. In lung cancer, these metabolic perturbations are predominantly driven by heightened oxidative stress, chronic inflammation, and lipid peroxidation, which result in elevated levels of alkanes, aldehydes, ketones, and alcohols. Such compounds are considered to be potential biomarkers that may not only enable differentiation between malignant and benign processes but also contribute to disease staging [4, 5]. Nonetheless, robust analytical and clinical validation of these candidate biomarkers remains essential prior to their incorporation into routine clinical practice, particularly given the influence of genetic, environmental, and behavioral variables on VOC profiles across populations.

Established analytical techniques, including gas chromatography and mass spectrometry, offer high specificity for VOC detection but are constrained by prohibitive costs and lengthy processing times. By contrast, electronic nose (eNose) technologies allow for a real-time and pattern-recognition-based assessment of composite VOC signatures, thereby providing a practical and scalable solution for clinical deployment. This technology is particularly suited for point-of-care use, as it integrates rapid analysis with the capacity to detect early-stage pathological changes through unique “metabolic fingerprints” of exhaled breath [6].

The aim of the present study was to evaluate the diagnostic accuracy of a novel gas analysis sensor platform combined with artificial neural network-based algorithms for the detection of lung cancer through the analysis of VOC biomarkers in exhaled breath.

MATERIALS AND METHODS

This prospective study was conducted between 2023 and 2025 and aimed to classify individuals with lung cancer and healthy volunteers using exhaled breath analysis. A total of 100 validated breath samples were analyzed, selected from an initial pool of more than 250 samples. All participants (aged 35–80 years) were stratified into two groups: the study (lung cancer) group and the control group.

The study protocol was reviewed and approved by the Bioethics Committee of the Cancer Research Institute, a branch of Tomsk National Research Medical Center of the Russian Academy of Sciences (Minutes No. 3a dated March 25, 2020). A written informed consent was obtained from all participants.

The study group comprised 53 samples obtained from patients with morphologically confirmed

primary lung cancer, spanning clinical stages I–IV (T1–4N0–3M0–1). The control group ($n = 47$) consisted of individuals with no prior, clinical, and laboratory evidence of malignant disease at the time of inclusion. Both groups contained samples from prepared and unprepared patients in approximately equal proportions (50:50). Efforts were made to ensure balanced distribution of samples by age, sex, preparation status, and tumor stage (in the study group).

Inclusion criteria were: lung cancer in the medical history (for the study group), absence of decompensated somatic-symptom comorbidities, and age ≥ 18 years. Exclusion criteria were: refusal to participate in the study, prior history of malignant disease (for the control group), age < 18 years, acute infectious disease, antibiotic therapy within the preceding 30 days, decompensated comorbidities, pregnancy, or lactation.

All patients in the study group underwent comprehensive cancer staging in accordance with the national clinical guidelines for lung cancer [7]. Exhaled breath was collected as the primary biological sample using previously validated standardized protocols [8]. The samples were obtained in sterile 5-l polymer collection bags using two modalities. For prepared samples, participants abstained from food (except water), smoking, oral hygiene, and the use of perfumes or personal care products for at least 6 hours prior to sample collection. These samples were collected in the morning immediately after awakening. Unprepared samples were collected in the afternoon without any restrictions to diet, hygiene, or activity.

Breath analysis was performed using a multisensory gas analysis platform comprising 24 semiconductor gas sensors and a humidity sensor. The platform incorporated artificial neural network (ANN) algorithms capable of recognizing molecular signatures in exhaled breath from individuals with lung cancer and distinguishing them from those of healthy individuals.

A multilayer perceptron ANN architecture was employed. Input data consisted of digitized signals from the gas sensors, categorized according to the participant groups. Raw sensor outputs were initially stored in the XML (eXtensible Markup Language) format, with each file representing one exhaled breath sample. Each XML file contained integer analog-to-digital converter (ADC) values (0–1023) for all sensors.

Given the large volume of raw data, preprocessing was performed to optimize computational efficiency without compromising classification accuracy. XML data were converted into consolidated text files containing metadata (group composition, ANN input and output layer dimensions) and signal matrices. Signals were expressed as the ratio of the tenth thermal cycle to the first thermal cycle for each sensor, repeated across all sensors and participants. Larger datasets prolonged ANN training and testing times; therefore, input arrays were downsampled five-fold, reducing the input layer dimensionality without loss of performance.

The final ANN input layer comprised 432 nodes (18 values per sensor for 24 sensors), and the output layer contained two nodes corresponding to the two classification outcomes: (1, 0) indicating a healthy volunteer and (0, 1) indicating a participant with lung cancer [8]. Each ANN configuration underwent at least 10 independent training experiments with parameter optimization.

Multidimensional data visualization and clustering were performed using the t-distributed stochastic neighbor embedding (t-SNE) algorithm [9], which projects high-dimensional data into a two-dimensional space while preserving topological relationships: similar samples were projected as proximate clusters, whereas dissimilar samples were separated by greater distances.

The diagnostic performance of the ANN classifier was evaluated by the receiver operating characteristic (ROC) analysis, providing an objective measure of the discriminative ability of the proposed approach.

RESULTS

During neural network training experiments, we identified an architecture and set of hyperparameters that enabled classification of exhaled breath samples across two datasets with the mean accuracy of 92%. In selected experiments, the model achieved sensitivity and specificity values of 98 and 96%, respectively. Preliminary analysis of the datasets using the t-SNE algorithm revealed significant differences between the two subgroups (lung cancer and healthy volunteers), as visualized by scatter plots (Fig. 1).

In a series of 50 independent experiments aimed at differentiating the two subgroups, the mean area under the ROC curve (AUC) exceeded 0.9, with ROC curves approaching 1.0 (Fig. 2), indicating robust discriminative performance of the ANN-based classifier.

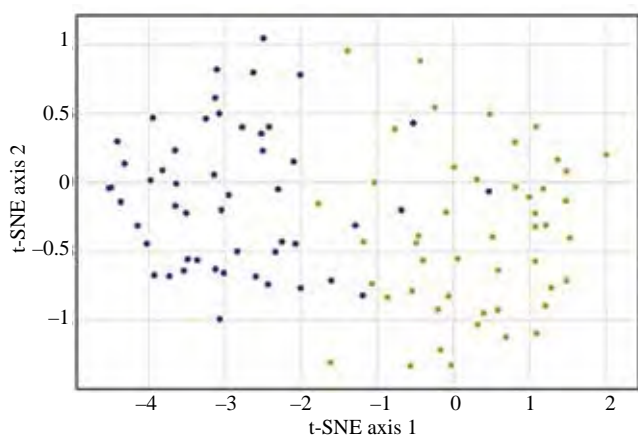


Fig. 1. The t-SNE distribution plot of exhaled breath samples from healthy volunteers and patients with lung cancer, illustrating subgroup differentiation based on dimensionality reduction

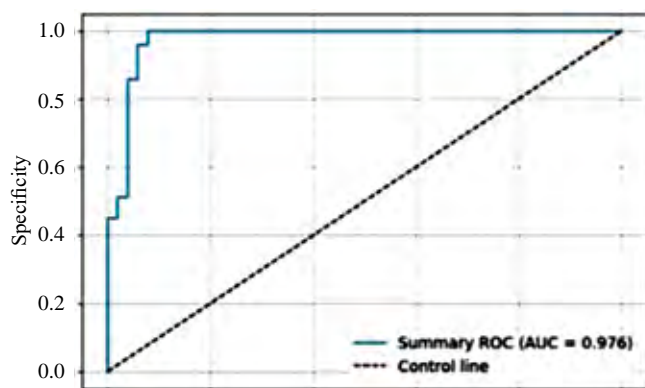


Fig. 2. ROC curve for neural network classifier performance in differentiating exhaled breath samples from healthy volunteers and patients with lung cancer.

Cross-validation analysis determined an optimal classification threshold of 0.24, which provided a balanced trade-off between false-positive and false-negative results across varying subgroup sample sizes. The corresponding distribution of exhaled breath samples after cross-validation is presented in Fig. 3.

Overall, classification of exhaled breath samples from patients with lung cancer versus healthy volunteers yielded diagnostic accuracy of 95.8%, sensitivity of 98.1%, and specificity of 93.6%. These results demonstrate strong evidence of subgroup differentiation and underscore the potential of this approach for clinical application in lung cancer diagnosis.

We further investigated the ability of the model to differentiate between prepared ($n = 55$) and unprepared ($n = 54$) breath samples from patients with lung cancer. In 50 experiments, the mean AUC reached 0.7, with

ROC curves tending toward 1.0 (Fig. 4). The mean classification accuracy for this subgroup analysis was 65%, with sensitivity and specificity ranging from 60 to 72%. These findings suggest only minor compositional differences in VOC profiles between prepared and unprepared samples from patients with lung cancer. While patient preparation may marginally improve classification accuracy, its implementation would inevitably complicate the sampling procedure.

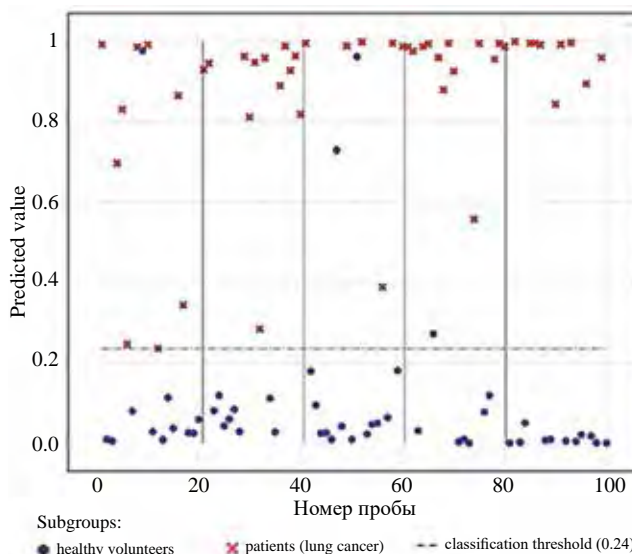


Fig. 3. Distribution plot of exhaled breath samples from the study subgroups following cross-validation

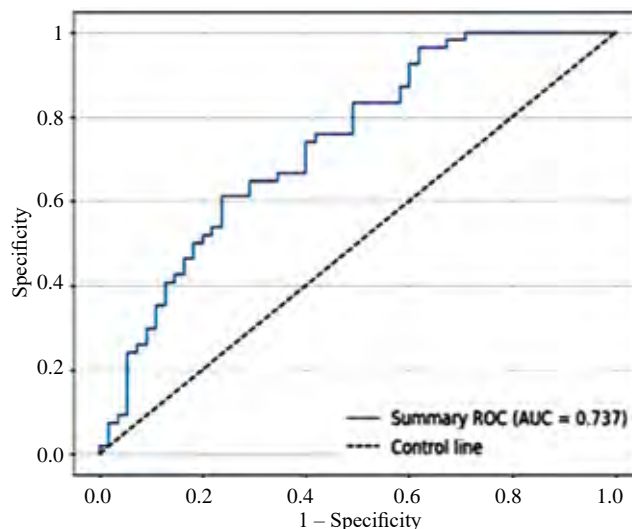


Fig. 4. ROC curve for ANN classifier performance in differentiating exhaled breath samples from prepared versus unprepared lung cancer patients.

Finally, we assessed the classifier's ability to differentiate exhaled breath samples from patients with early-stage (I–II) versus advanced-stage (III–IV)

lung cancer. This analysis was conducted separately for prepared and unprepared patients, with the same sample ratio in each subgroup (31:24). Across 50 experiments, the mean classification accuracy reached 75%, with sensitivity and specificity values ranging from 65 to 80%. Comparable results were observed for both prepared and unprepared cohorts. Achieving the mean accuracy of 75% highlights significant VOC profile differences between early- and advanced-stage disease, suggesting that the ANN-based approach may eventually enable not only early detection of lung cancer but also disease staging when applied sequentially with multiple classifiers.

DISCUSSION

Standard methods for early detection of lung cancer include chest radiography and low-dose computed tomography (LDCT). However, chest radiography — often employed for screening — has low sensitivity and a high false-negative rate due to its limited image resolution. LDCT provides superior anatomical detail and has proven high diagnostic value [10]. Current American Cancer Society guidelines recommend annual LDCT screening for high-risk individuals (current or former smokers aged 50–80 years with a ≥ 20 pack-year history), a strategy associated with a 20% reduction in lung cancer-related mortality compared to radiography [11].

Despite its proven efficacy, LDCT carries important limitations, including overdiagnosis (detection of clinically indolent lesions), high false-positive rates leading to unnecessary invasive procedures, and the need for multidisciplinary teams to interpret findings. Moreover, limited equipment availability, high cost, and the requirement for highly trained personnel restrict the scalability of LDCT-based screening programs, even in well-resourced health care systems [12].

Exhaled breath analysis of VOCs has emerged as a promising, non-invasive alternative for early lung cancer detection. Electronic nose (eNose) technologies have demonstrated consistently favorable results, even in populations with low to intermediate disease prevalence (5.4–22%) [13]. Across studies of non-small-cell and small-cell lung cancer, reported sensitivity and specificity have varied greatly, ranging from 71 to 99% and from 13 to 100%, respectively [6]. Integration of artificial intelligence (AI) has further enhanced eNose performance, enabling real-time data analysis and predictive assessment of tumor presence [14]. Nevertheless, the combination of AI and biosensory platforms for lung cancer screening

remains underexplored, with issues of reproducibility, sensor drift, and environmental interference limiting their clinical application.

Our multisensory gas analysis platform, which integrates semiconductor-based biosensors with AI-driven data processing modules, demonstrated diagnostic performance that surpassed existing eNose systems and LDCT. In this study, the platform achieved sensitivity and specificity of 98.1 and 93.6%, respectively, outperforming LDCT (sensitivity $\sim 93\%$, specificity $\sim 73\%$).

Compared with LDCT, the platform offers several clinical advantages: it is entirely non-invasive, free from ionizing radiation exposure, rapid, low-cost per test, and suitable for large-scale population screening. Its portability and ease of use further allow for deployment in outpatient and primary care settings, including resource-limited regions.

A key strength of the platform lies in high selectivity of its multilayer sensor array, which can discriminate subtle variations in VOC composition. AI-driven data processing ensures robustness against noise and artifacts and adapts to inter-individual variability in breath signatures related to age, smoking status, or comorbid conditions. Validation experiments evaluating prepared and unprepared samples confirmed the reproducibility and low inter-series variability of the system.

CONCLUSION

Exhaled breath analysis is emerging as a powerful diagnostic modality for the early detection and monitoring of lung cancer, particularly at its initial stages. The newly developed multisensory gas analysis platform demonstrated clinically meaningful superiority over existing screening approaches, including LDCT.

The combination of high diagnostic accuracy, scalability, and operational simplicity positions this platform as a promising tool for integration into lung cancer screening programs and personalized diagnostic pathways. Its ability to provide rapid, non-invasive, and reproducible results could transform current approaches to early lung cancer detection and population-level screening.

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Author Contribution

Rodionov E.O. – analysis and interpretation of the data, processing of the materials, drafting of the manuscript. Podolko D.V., Kulbakin D.E., Miller S.V. – collection of the material, processing of the results. Obkhodskaya E.V., Obkhodskiy A.V. – hardware platform development and technical design, interpretation of the results. Sachkov V.I., Chernov V.I. – scientific analysis, critical revision of the manuscript for important intellectual content. Popov A.S. – hardware platform development and technical design, interpretation of the results. Lakonkin V.S. – analysis and interpretation of the data.

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