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Volatile Organic Compounds and Lung Cancer: Public Health Impacts, Biomarker Potential, and Artificial Intelligence Applications

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ABSTRACT

Volatile organic compounds (VOCs) are a class of widespread organic chemical compounds. They can act as both environmental pollutants and biomarkers of health conditions, such as lung cancer. The paper first provides an overview of the role of exogenous VOCs in lung cancer causation, and evaluates particular public policies that aim to reduce VOC emissions. By summarizing recent and past findings and research on VOCs and lung cancer, this literature then discusses the role of endogenous VOCs in lung cancer and their potential as a tool for lung cancer detection. The current applications of artificial intelligence (AI) in VOC research, as well as the performance of several algorithms trained to identify lung cancer and differentiate between its subtypes, are evaluated. The key findings of the paper highlight the need for stronger regulation and policies for VOCs, especially in underdeveloped industrial areas, the strong potential of VOCs as a non-invasive method for detecting lung cancer, and the promise of utilizing AI technologies in medical advancements that leverage VOC data to enhance lung cancer diagnostics. This paper highlights the potential of VOC-based and AI assisted breath analysis as a noninvasive approach for early lung cancer detection.

Keywords: *Volatile organic compounds (VOC), artificial intelligence (AI), lung cancer, public health, biomarkers, regulation, breath analysis, machine learning (ML), cancer detection, developing countries*

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INTRODUCTION

Volatile organic compounds (VOCs) are organic chemical compounds characterized by their increased volatility and mobility. Due to their unique properties, VOCs can easily vaporize and travel far distances. They are produced by both natural sources, like plants and forest fires, and anthropogenic sources from domestic and industrial processes, including traffic, chlorination, fertilizers and pesticides, burning of hydrocarbon fuels, etc. (David & Niculescu, 2021). VOCs are also released from the human body, most commonly from breath, sweat, skin, urine, faeces and vaginal secretions (Shirasu & Touhara, 2011). Given this, VOCs can provide crucial information regarding changes in metabolic processes and can serve as telling biomarkers for health conditions, such as lung cancer (Setlhare et al., 2025).

VOCs are primarily classified in two ways: volatility and chemical properties. The volatility classification can be divided into very volatile organic compounds (VVOCs), volatile organic compounds (VOCs), and semivolatile organic compounds (SVOCs) (David & Niculescu, 2021). VVOCs are a hazardous pollutant class, as these molecular substances are potentially extremely toxic even at very low concentrations. They have a boiling point range of 0 to 50-100℃. Common examples in this class are propane, butane, and methyl chloride. Similarly, VOCs are also dangerous, but can be found within household products and the environment. They have boiling points ranging from 50-100℃ to 240-260℃. Formaldehyde, acetone, alcohol, isopropyl, and hexanal are examples of the second category. SVOCs are substances characterized by a higher molecular weight and boiling point of 240-260℃ to 380-400℃, meaning that they are less likely to become vapors at room temperature. For instance, pesticides (chlordane), plasticizers (phthalates), and benzyl alcohol are well-known examples. Another classification of volatile organic compounds is based on their chemical properties (Janfaza et al., 2019) . For clarity within this paper, VOCs will be divided into three categories: aliphatic hydrocarbons, aromatic hydrocarbons, and functionalized VOCs. Aliphatic hydrocarbons consist of carbon and hydrogen atoms and include examples such as methane, ethane, and propane. Aromatic hydrocarbons are similar to aliphatic hydrocarbons, but have a ring structure with carbon and hydrogen. Examples include benzene and toluene. The final group includes functional VOCs, such as ketones, esters, alcohols, terpenes, and terpenoids, as well as aldehydes.

To understand how VOCs act as carcinogens and affect public health, an overview of their exposure pathways and sources is needed. VOCs can originate from both natural and anthropogenic sources. They can occur naturally from plants or forest fires, but can also be a result of human activities, such as traffic-related pollution, industrial activities, or the release of household products (Michanowicz et al., 2022). Humans can be exposed to VOCs through ingestion, skin contact, and inhalation. Because VOCs can escape the respiratory tract's filtering and cleansing mechanisms, they can penetrate the alveoli, making the lung a primary target organ (Fischader et al., 2008; He et al., 2015).

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The primary goal of this paper is to examine the role of VOCs in lung cancer, specifically as a tool for lung cancer detection and classification of subtypes. For context and background information, the paper will first provide a comprehensive review of the impacts of exogenous, or external, VOCs on public health, with a particular focus on the burden on developing countries, and also examine potential policies that can better regulate VOC emissions to create a safer environment. Lastly, this review will analyze the current applications of artificial intelligence (AI) in VOC and lung cancer research and evaluate the success of specific models.

VOCs AND PUBLIC HEALTH IN DEVELOPING COUNTRIES

VOCs should be considered a threat to public health given their toxic characteristics. Given that they can easily evaporate into the air and some are especially harmful as carcinogens, it is important to evaluate their effects. The World Health Organization (WHO) and the U.S. Environmental Protection Agency (EPA) recognize VOCs as a health concern and note that they may cause adverse health effects (United States Environmental Protection Agency, 2024; World Health Organization, 2010). VOCs can hurt human health by causing direct DNA damage, DNA mutations, and activating carcinogenic pathways (Hussain et al., 2024). Some examples of common VOCs and their applications include polybrominated diphenyl ethers (PBDEs), which are additive flame retardants found in various consumer goods, such as textiles, furniture, and electronic devices (Duan et al., 2010). Phthalates are also present in various items, including paint, cleaning products, and building materials (Ataei et al., 2023).

VOCs can be a particularly detrimental source of pollution in developing countries. The scarcity of research conducted in developing countries makes this topic particularly important. In fact, pollution-related deaths totaled 6.7 million premature deaths in 2019, of which ambient air pollution caused 4.2 million deaths. Of that statistic, 89% of the premature deaths occurred within low and middle-income countries, disproportionately affecting Southeast Asia and Western Pacific regions (World Health Organization, 2024). VOCs are a key air pollutant due to their adverse impacts on human health and the environment. A study of VOCs within four different developing countries, including Ethiopia, Vietnam, the Philippines, and Bangladesh, found that in Bangladesh, high TVOC levels were a result of industrial processes and transportation, like two-stroke auto-rickshaws, which emit four to seven times the maximum permissible level (Schwela et al., 2012). Also in Bangladesh, the most dominant BTEX, a group of highly typical VOCs, was toluene, accounting for 28% of aromatic concentration levels in industrial campaigns (Do et al., 2015).

The effects of VOCs on people, specifically those inhabiting developing countries, should be a key focus. Within the study about VOCs in four developing countries, the carcinogenic risk (CCR) values ranged from 97 in Mekelle, Ethiopia, to approximately 300 in Dhaka, Bangladesh, both under urban campaigns (Do et al., 2015). However, it is essential to note that total volatile organic compound (TVOC) levels do not necessarily indicate a cancer risk. Cancer risk is based on which VOCs dominate, not just their quantity. This explains why, although TVOC levels in Manila and Laguna were the highest, their cancer risk was lower than in Dhaka (Do et al., 2015).

The limited research on volatile organic compounds in developing countries highlights the need for effective regulations and policies. Air quality guidelines in developing countries, such as Ethiopia, Vietnam, the Philippines, and Bangladesh, are largely unregulated. Based on the study's findings, the benzene concentrations in Vietnam, the Philippines, and Bangladesh do not match the European directive limit of 5 $\mu g/m^3$ (European Commission, 2010). This suggests that there are still critical steps that need to be taken to strengthen VOC control in developing countries and create a safe environment. A study simulation by Zhang et al. evaluated the effectiveness of different VOC tax-based regulation policies within the context of Chinese provincial realities, setting four scenarios: business-as-usual (BAU) with no emission constraints, a uniform national policy (NP-VOC), and regionally differentiated policies (R1-VOC and R2-VOC). The study concluded that VOC tax policies generally result in both national and provincial reductions in VOC emissions. Specifically, by 2060 at the national level, NP-VOC, R1-VOC, and R2-VOC policy scenarios result in 16.9%, 17.88%, and 23.27% decreases in VOC emissions compared to the BAUE scenario, respectively. Moreover, the R2-VOC policy was found to be likely the most effective in reducing VOC emissions due to its incorporation of twenty provinces in the High area, or provinces with high energy intensity, suggesting that they are more polluting and industrialized areas (Zhang et al., 2023). In this study, the model shows that in those areas, VOC emissions are taxed at a higher rate, resulting in significantly fewer emissions. Based on these findings, tax-based environmental policies appear to have high potential for reducing VOC emissions, and may serve as a model to be referenced in government regulations.

VOCs AS BIOMARKERS FOR LUNG CANCER DETECTION

Lung cancer is the most commonly diagnosed cancer worldwide, accounting for 12.4% of total cancer cases. It is also the leading cause of cancer death, with an estimated 1.8 million deaths, 18.7% of all cancer-related deaths (Bray et al., 2024). Lung cancer can be classified into non-small cell lung cancer (NSCLC) and small cell lung cancer (SCLC). NSCLC is more common, representing approximately 87% of all lung cancer cases (American Cancer Society, 2023). NSCLC has three main histological subtypes: adenocarcinoma (ADC), with 39% of cases; squamous cell carcinoma (SCC), 25% of cases; and large cell carcinoma (LCC), approximately 8% of cases (World Health Organization, 2023).

VOCs have the potential to serve as a tool for detecting lung cancer. Within human bodies, VOCs are present in the exhaled breath, albeit in low concentrations. Given that metabolic processes in cells lead to the consumption and production of VOCs, and these metabolic byproducts can circulate within the blood and be exhaled through the lungs, the composition of VOCs in exhaled breath can reflect body metabolic activity (Mazzone et al., 2012). Therefore, if there are any changes in the body's metabolic processes, it could possibly be shown within unique breath VOC signatures. Moreover, the VOCs identified from exhaled air can provide information about oxidative stress, which is strongly related to cancer (Chan et al., 2010). There has been extensive research from various authors that proves breath samples have many different VOCs and that many VOCs have been identified from the breath of lung cancer patients (Poli et al., 2005). Accordingly, VOCs can be studied for their purpose in lung cancer detection. To further that basis, the potential of a VOC-based detection process for lung cancer is promising because the analysis of exhaled breath is noninvasive and has minimal risk. This offers a novel and more accessible option for first-line lung cancer detection.

To gain a more comprehensive understanding of current and past VOC applications in lung cancer detection, this review will conduct a thorough analysis of various experiments that utilize exhaled breath to analyze VOCs in relation to lung cancer. Beginning in 1985, Gordon et al. (1985) identified several alkanes in the exhaled air of lung cancer patients, and this research was further developed by Phillips et al. (1999), who used 22 VOCs to distinguish between lung cancer patients and healthy subjects. Kischkel et al. (2012) found significant differences in substances acetone, butane, pentane, cyclohexanone, and benzene between diseased and healthy lungs. This study was based on cancer patients undergoing lung resection, using alveolar breath samples from both healthy and diseased lungs, both prior to and after tumor resection, to identify VOCs through mass spectrometry. One key finding from this study was that exhaled butane and pentane concentrations decreased most between the diseased and healthy lungs, suggesting that butane and pentane may be potential biomarkers for lung tumor growth. A similar study by Poli et al. (2005) also used breath samples from NSCLC patients who underwent lung surgery. However, this study did not find a single biomarker or VOC that indicated lung cancer. Yet, because only the levels of isoprene and decane dropped significantly after the surgery, it can be a sign that these compounds are related to tumor metabolism.

Other studies developed models to attempt to predict lung cancer using exhaled breath VOCs. Wang et al. (2024) employed a lung cancer screening strategy to develop the ensemble text and breath analysis (ETBA), which combines radiology report text analysis and breath analysis. The 22 VOCs in exhaled breath helped serve as predictors for developing the ETBA and breath analysis (BA) model. The study revealed that the BA model actually performed better than the text analysis (TA) model, with a specificity of 63.6% and a sensitivity of 88.6%. The ETBA model, which combines both methods, showed the best performance, achieving a specificity of 86.4% and a sensitivity of 91.4%. This data is important as it shows that all models performed better than the radiologist's diagnosis. Likewise, Mazzone et al. (2012) created a breath biosignature for lung cancer using the exhaled breath from patients and a colorimetric sensor array. The model that performed better was the one focused on only one histology, achieving a concordance statistic (C-statistic) of 0.825-0.890. The data also demonstrated that the model could distinguish between individuals with different histologies, with a C-statistic of 0.889 between adenocarcinoma and squamous cell carcinoma. This suggests that breath VOC fingerprints can be used to classify lung cancer and even distinguish between subtypes. Another model trained an electronic nose using the exhaled breath of healthy controls and individuals with bronchogenic carcinoma. The findings concluded that the model could correctly identify 330 out of 388 exhaled breath samples, an accuracy of 85%. Moreover, it had 71.6% cross-validation results, 71.4% sensitivity, and 91.9% specificity. Politi et al. (2021), in a study, used alveolar air of patients with squamous cell lung cancer, lung adenocarcinoma, or colon cancer. It created a prediction model through least absolute shrinkage and selection operator (LASSO) logistic regression (LLR) to select the most relevant VOCs. It found 5 shared compounds identified in ADC and SCC: acetic acid, ammonia, ethylenimine, acetaldehyde, and M48. This can suggest VOCs associated with common lung cancer biology. However, the two lung cancers also had 10 other VOCs that behaved differently. Across the three cancers examined in the study, only acetic acid and ethylenimine showed consistent changes. The model also achieved an 86% sensitivity and 84% specificity for ADC and 88% sensitivity and 84% specificity for SCC. Numerous studies implementing this model have shown that exhaled breath VOC analysis is a promising tool for lung cancer detection and subtype classification.

AI APPLICATIONS IN VOC-BASED LUNG CANCER DETECTION

Artificial intelligence (AI) is a technology that enables computational systems to simulate and perform tasks that typically require human intelligence. Machine learning (ML) is a subset of AI that focuses on the development of algorithms that help machines and computers learn from patterns and make predictions. Both AI and ML have been a major hotspot in the medical world. Its growing influence and usage in everyday life make an undeniable presence, especially in healthcare. The rapidly improving technology opens up new opportunities for advancements in the medical field, potentially being used to enhance certain clinical processes and create novel solutions. Because one of the most promising developments from AI in healthcare is its ability to diagnose and detect health concerns, it can be beneficial to analyze recent uses of AI in relation to VOCs to improve lung cancer detection.

Several studies have explored the role of AI in enabling lung cancer detection by analyzing exhaled breath. Vinhas et al. (2024) created several models using the data of 203 participants. Using machine learning to construct various classification models, specifically neural networks (NN), a type of machine learning model. The study included GoogleNet Inception V1, Visual Geometry Group VGG-11, Residual Network ResNet-18, the first optimized convolutional neural network (CNN1), and the second optimized convolutional neural network (CNN2). The best-performing model, based on 5-fold cross-validation, utilized the GoogLeNet Inception V1 deep neural network, achieving an average precision rate of 84%, an average accuracy of 0.47, and an average loss of 0.47. The CNN models also performed very well, achieving nearly identical performance to GoogLeNet in cross-validation, with an average accuracy of 82% and an average loss of 0.56. However, after model optimization, CNN1 was able to outperform GoogLeNet, reaching a weighted F1 score of 0.94 and an area under the curve (AUC) of 0.96. This suggests that this approach can outperform the typical well-known architectures. The study also proposes that an agonistic screening approach, instead of using specific compounds, could be an alternative.

A similar study by Binson and Subramoniam (2021) aimed to develop an AI-based electronic nose system that could distinguish between the exhaled breath of healthy individuals and individuals with lung cancer. The data enabled the drawing of important conclusions about the different VOC compounds examined and suggested specific compounds as potential lung cancer biomarkers. The e-nose model was developed using five different metal oxide semiconductor (MOS) gas sensors to detect various VOC compounds, such as ethanol and acetone. Using this information, the authors tested two ML models: random forest and logistic regression. The random forest classification algorithm achieved an accuracy of 85.38% and a mean AUC (area under the curve) of 0.87 for differentiating between lung cancer and healthy patients. Similarly, the model using logistic regression had an accuracy of 83.59% and a mean AUC of 0.86. This suggests that the model performed moderately well in classifying patients into the two groups.

Raimundo et al. (2025) aimed to further non-invasive lung detection through VOC and AI by testing various MOS gas sensors on VOC profiles from exhaled breath. The study incorporated ML algorithms to classify samples and distinguish between the healthy controls and lung cancer patients. The three tested AI supervised learning algorithms —support vector machines (SVM), multilayer perceptron (MLP), and K-nearest neighbor (KNN) —all performed similarly, with no statistically significant difference among the models, given that the p-values were uniformly higher than 0.05. The results showed that the three models demonstrated high specificity and negative predictive value (NPV) for lung cancer stage IA, the earliest stage of lung cancer, as well as for all stages of lung cancer detection. However, they had significantly lower performance for histological classifications. The models achieved a sensitivity of 75%-87%, specificity of 90%-94%, and an overall accuracy of approximately 90% for lung cancer stage IA. For LC all stages, models had a sensitivity of 84%-88%, specificity of 86%-92%, and accuracy of 87%-90%. In terms of histology, the models ranged from 71% to 77% sensitivity, 72% to 78% specificity, and an accuracy of 71% to 77% (Raimundo et al., 2025). This data reveals how well current models with AI algorithms perform in different aspects of lung cancer detection.

A fourth study evaluated AI models for VOC analysis by training several models: neural network, SVM, Convolutional Neural Network (CNN), Recurrent Neural Network (RNN), and XGBoost model (Hamilton, 2025). The study showed that XGBoost had the highest accuracy at 86%, compared to SVM's 80% accuracy and Neural Network's 77% accuracy. By using a Random Forest Model, the research also identifies key VOCs in lung cancer that could serve as markers of cancerous lung tumors, including butanal, heptanal, pentanal, decanal, nonanal, octanal, and tridecanal. Key diagnostic targets, such as 1-tridecanol, Butyric acid, butyraldehyde, cyclohexylmethanone, and 2-pentanone, were also identified in the same study. These various studies on the application of AI to improve lung cancer detection propose the future potential use of VOCs as a first-line, non-invasive method.

CONCLUSION AND FUTURE DIRECTIONS

This review highlights the significance of VOCs as a threat to public health and provides an overview of past and current research on volatile organic compounds in relation to lung cancer detection. It further provides an outline of current applications of artificial intelligence models for improving VOC lung cancer detection. Some limitations of this review to note include its inability to capture the entirety of all related research done; thus, there is, to some extent, a lack of breadth and scope. Moreover, some studies analyzed are not conclusive on the effectiveness of VOCs for lung cancer detection, but rather suggest further research to explore potential future applications. For future directions, VOCs can be considered more in lung cancer diagnosis, possibly serving as a form of non-invasive, cost-effective, and accessible detection method. AI applications have a strong ability to improve the research of VOC effectiveness. Additionally, training algorithms can greatly enhance the efficiency of lung cancer detection and possibly other health conditions.

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