Extract Spatial Distribution of a Specific Gas from Mixed Gas Data Measured by the LSPR Gas Sensor

Zheng, Xiaofan
dept. Informatics (Graduate School of ISEE), Kyushu University

Matsuoka, Masato
dept. Electronics (Graduate School of ISEE), Kyushu University

Hayashi, Kenshi
dept. Electronics (Graduate School of ISEE), Kyushu University

Tomiura, Yoichi
dept. Informatics (Graduate School of ISEE), Kyushu University

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1st Xiaofan Zheng
dept. Informatics (Graduate School of ISEE)
Kyushu University
Fukuoka, Japan
zheng.xiaofan.413@s.kyushu-u.ac.jp

2nd Masato Matsuoka
dept. Electronics (Graduate School of ISEE)
Kyushu University
Fukuoka, Japan
matsuoka.masato.380@s.kyushu-u.ac.jp

3rd Kenshi Hayashi
dept. Electronics (Graduate School of ISEE)
Kyushu University
Fukuoka, Japan
hayashi@ed.kyushu-u.ac.jp

4th Yoichi Tomiura
dept. Informatics (Graduate School of ISEE)
Kyushu University
Fukuoka, Japan
tom@inf.kyushu-u.ac.jp

***Abstract*—Visualizing invisible gas molecules can be a great help to our lives. At present, gas sensors can already visualize the spatial distribution of gas mixture, however, the visualization of a specific gas requires further analysis of the measurement data. In this study, matrix decomposition is used to analyze the measurement data of localized surface plasmon resonance (LSPR) gas sensor. To satisfy the linear relationship between the concentration of gas and the output of the device required for applying matrix decomposition, we formulated a procedure for processing the measurement data instead of using them directly. To obtain the diffusion trace of a specific gas, we designed a method to obtain the characteristic output of the specific gas, then by using the characteristic output as the known information, the corresponding diffusion trace can be estimated better through the matrix decomposition algorithm. We used the designed method to analyze the measurement data, and the results show that our method can obtain the spatial distribution of some gas.**

***Index Terms*—gas sensor, trace visualization, matrix decomposition**

I. Introduction

Gas molecules diffused in the air can provide us with important information, and people are developing devices that can sense odors so that diffusion traces can be measured. Visualizing odor traces can be helpful in many aspects, such as human tracing and so on.

Two of our co-authors developed a localized surface plasmon resonance (LSPR) gas sensor for measuring the gas diffused in the air. The device uses metal nanoparticles with different light absorbance properties in different mediums to identify gas molecules in the environment. And the measurement result is recorded by a hyperspectral camera so that the diffusion traces can be visualization. The purpose of this study is to visualize the diffusion traces of a target gas by analyzing the data measured by the LSPR gas sensor, when multiple kinds of gas are mixed at the observation position.

Matrix decomposition [1] is an unsupervised learning algorithm, which decomposes a matrix into the product of two matrices. These two matrices obtained from the decomposition usually have practical significance, and they can be regarded as a characteristic matrix and a weight matrix respectively. Matrix decomposition has been applied in many aspects such as audio source decomposition [2], bioinformatics [3], etc. According to application requirements, matrix decomposition has more detailed classifications such as non-negative matrix decomposition (NMF) [4], orthogonal decomposition [5] and so on.

In this study, the feature matrix X is obtained by processing the data measured by the LSPR gas sensor, and X is decomposed as

$$X = AB, \tag{1}$$

where matrix A represents the concentration of each element gas at each position, matrix B represents the characteristics of each element gas and we call B as the profile matrix. To be specific, x_{ij} in matrix X is the feature value corresponding to the j-th wavelength at the i-th position. a_{ik} in matrix A represents the concentration of gas k at the i-th position, and b_{kj} in matrix B is the feature value corresponding to the j-th wavelength when we measure the unit concentration of gas k. Therefore, the k-th row B_k in B can be seen as the profile of gas k, and the k-th column A_k in A can be used to visualize the trace of gas k.

The main contributions of this study are: (1) designed a method to extract a diffusion trace of the target gas from the data measured by the LSPR gas sensor; (2) analyzed the data measured in the laboratory by the LSPR gas sensor and visualize diffusion traces individually.

II. Method

A. Processing Measurement Data

Fig. 1 shows a schematic diagram of using an LSPR substrate to measure gas molecules in the laboratory, please refer to [7] for details. And the actual placement of 4 gas source liquid on the well plate is also shown in Fig. 1. The

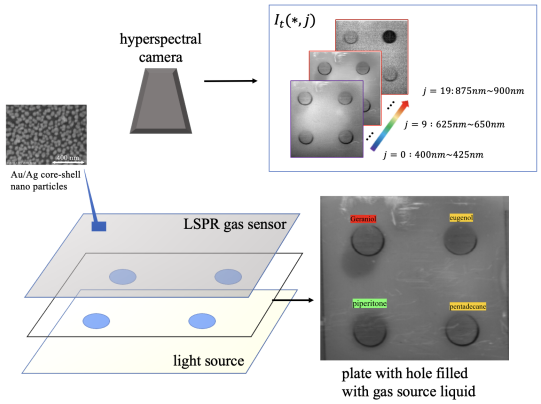

Fig. 1. A schematic diagram of measuring experimental data in the laboratory.

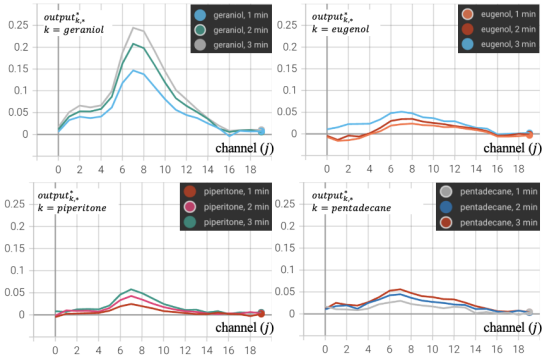

Fig. 2. The changes of $output^t_{k,j}$ with time. The horizontal axis represents channel, the vertical axis represents $output^t_{k,j}$

wavelength range of the measurement data is 400 nm ˜900 nm, images are taken for each 5 nm. Therefore, for each measurement, a total of 101 images that record the transmitted light intensity spatial distribution of 101 different wavelengths is obtained. For the measurement data used in this study, pictures are taken every minute within 10 minutes after the plate filled with gas source liquid was placed. Therefore, the measurement data include 11 groups (including the pictures at 0 minutes) of 101 images. In order to alleviate the impact caused by measurement errors during shooting photos, we used the first 100 of 101 images and compressed the raw data by taking the median value of each 5 images and each 5*5 pixel. In this study, we analyze these compressed 11 groups of 20 images. 20 images of each group represent the measurement result of different wavelength ranges, and we call these 20 different wavelength ranges as 20 channels.

We use $I_t(i,j)$ to represent the light intensity of the j-th channel on the i-th position at t minutes, and use $I_e(i,j)$ to represent the intensity of source light of the j-th channel on the i-th position. The element x^t_{ij} in X^t, the feature matrix at t minutes, is defined by the difference in the absorbance between t minutes and 0 minutes as shown in (2).

$$\begin{aligned} x^t_{ij} &= -\log\frac{I_t(i,j)}{I_e(i,j)} - (-\log\frac{I_0(i,j)}{I_e(i,j)}) \\ &= -\log\frac{I_t(i,j)}{I_0(i,j)} \end{aligned} \tag{2}$$

For each gas source liquid k, we convert the measurement value on the area near the k-th gas source liquid (i.e. four positions $i^k_{top}, i^k_{bottom}, i^k_{left}, i^k_{right}$ are located at the top, bottom, left, and right of gas source liquid k) at from 1 to 3 minutes to corresponding x^t_{ij}, and compute

$$output^t_{k,j} = \frac{1}{4}\sum_{i\in\{i^k_{top},i^k_{bottom},i^k_{left},i^k_{right}\}} x^t_{ij}.$$

The changes of $output^t_{k,j}$ with time are shown in Fig. 2. It can be seen from Fig. 2 that the gas concentrations and $output^t_{k,j}$ are approximately proportional. Since the gas is dilute, it can be considered as an ideal gas, and it can be assumed that there is no interaction between different gas molecules, and the effects of individual gases can be added. Therefore, (1) can be considered to hold approximately, and we can get the concentration matrix by decomposing X^t. In this study, only the data from channel 0 to channel 14 (wavelength 400˜ 775) is used to conduct analyzing.

B. Matrix Decomposition

The matrix X is decomposed into the product of a concentration matrix A and a profile matrix B with an algorithm of matrix decomposition. In our case, it is necessary to constrain the estimated matrix $\hat{A}$ to positive values. In this study, we used the semi-NMF algorithm proposed by [6] which satisfies the constraint of $\hat{A}$.

In practice, there is a case that we may already know a specific gas k that we intend to trace and thus we only interest the concentration distribution $\hat{A}_k$ ($\hat{A}_k$ is the k-th column in $\hat{A}$). In this case, the concentration distribution $\hat{A}_k$ of gas k can be obtained by matrix decomposition given the profile B_k of gas k. In this experiment, we assume that only gas k and air exist above the area near gas source liquid k at 1 minute, and regard $[output^1_{k,0}, output^1_{k,1}, \cdots, output^1_{k,14}]$ as the profile of gas k. With the measurement data used in this study, the correlation coefficients between the computed profiles of four kinds of gas ranged from 0.58 to 0.98.

III. Result and Discussion

We first decomposed X^t by assuming that profiles of all gas are known information to reduce the difficulty of matrix decomposition. The visualization result of $\hat{A}$ is shown in Fig. 3. For geraniol, we can see that the gas has diffused on the area around the corresponding hole at 0 minutes, this may be caused by a slight overflow of the gas source liquid from the hole. Even though we can't observe noticeable diffusion traces over time, the visualization shows that the concentration of geraniol increases with time. For pentadecane, we can see the clear diffusion trace over time, and the visualization result also shows that gas pentadecane can be distinguished from other gas. For eugenol and piperitone, we cannot see the diffusion

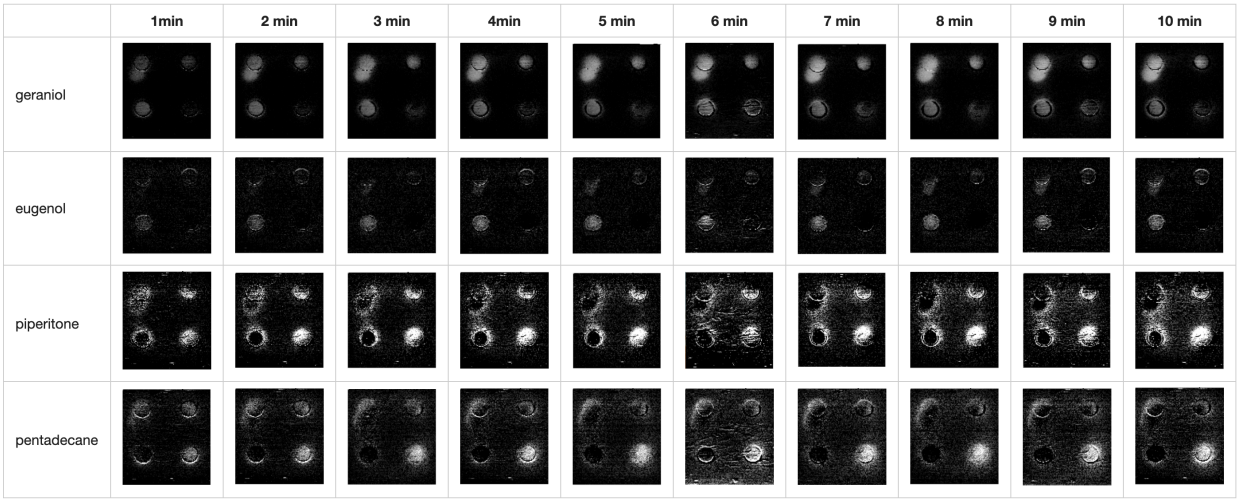

Fig. 3. Visualization results when profiles of all kind of gas is known.

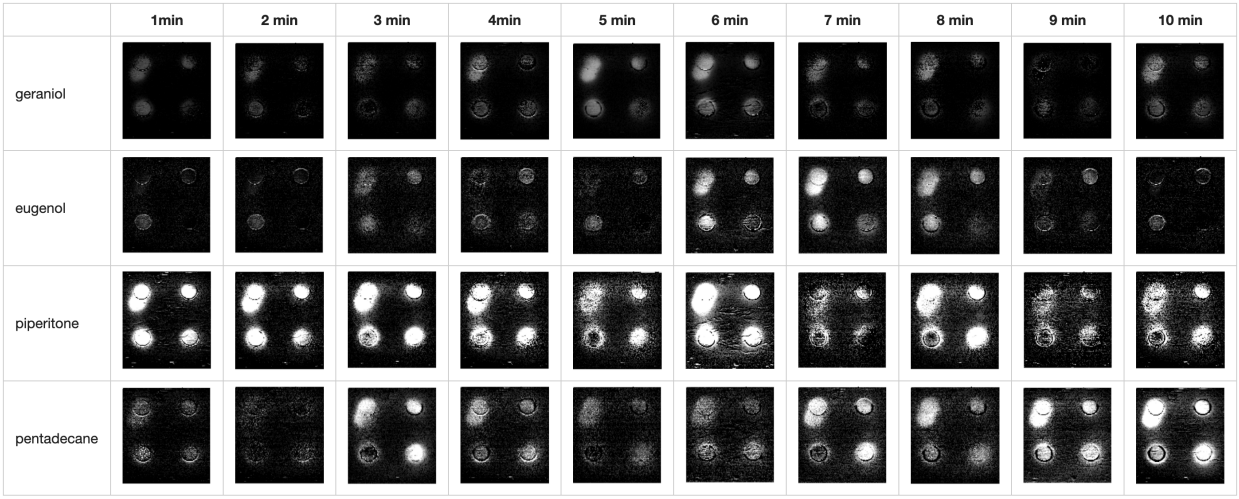

Fig. 4. Visualization results A_k when profile B_k is known.

trace expanding with time, and the target gas also can not be distinguished from other gases.

Then we decomposed X^t by assuming only the profile of target gas B_k is known, and visualized the corresponding concentration distribution $\hat{A}_k$. Fig. 4 shows a visualization of the concentration distribution of the target gas when we used each of the four gases as the target gas and obtained $\hat{A}$ by decomposing X^t. Even if the result is worse than Fig. 3 in general, we can observe the diffusion trace over time from the results of pentadecane.

According to Fig. 3, the visualization of pentadecane shows that analyzing the measurement data with matrix decomposition can successfully visualize the trace of pentadecane. The correlation coefficient between profiles of different gas shows that the response of the device to different gas is not distinguished from each other sufficiently, which may cause the difficulty of matrix decomposition when assuming only one profile of gas is known. We expect to achieve a better visualization result when the response of the LSPR gas sensor is more distinguishable for different gas.

IV. Conclusion

In this study, we designed an analysis method for data measured by an LSPR gas sensor which is developed by our co-authors, so that the spatial distribution of a specific gas can be visualized. We applied the designed method to one experimental data, and the visualization results show that our designed method can visualize the diffusion trends of some gas molecules.

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