

Mixture quantification based on active sensing using frequency shifts and resistance changes of QCM harmonics

Odors are usually composed of multiple volatile organic compounds (VOCs). While most existing odor sensing systems focus on **distinguishing** among different odors, being able to **quantify** odor components is equally important, as it forms the basis for accurately recording and reproducing odors. However, quantification is challenging because gas sensors often show cross-sensitivity and collinearity. As a result, most previous studies are

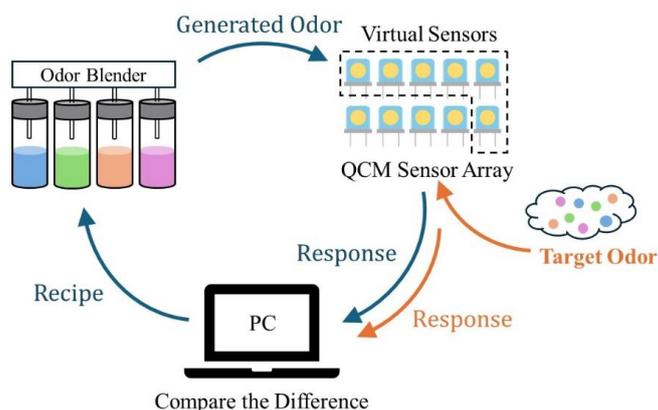


Figure 1. Overview of system

limited to binary or ternary mixtures.

In this study, we aim to enhance our previously developed active sensing-based odor sensing system (Fig. 1) in order to quantify **quaternary** mixtures. We used a vector network analyzer (VNA) to measure both frequency shifts and resistance changes of each QCM sensor from the 1st to the 11th odd harmonics, which serves as virtual sensors, effectively increasing the selectivity of the sensor array.

For the quantification, we selected **10 selected responses** from 4 QCM sensors, which is equal to using only fundamental responses from 10 sensors, to quantify varying gas mixtures composed of 4 main ingredients in apply flavor. Figure 2 shows the response patterns of the four ingredients using 10 selected responses and only the 4 fundamental

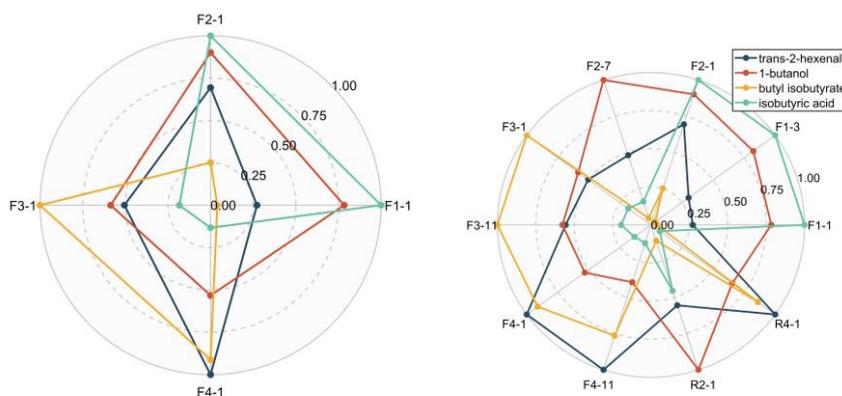


Figure 2. Response patterns of 4 ingredients with 4 fundamental frequency responses (left) and 10 selected additional responses (right). F_{i-j} means the i -th sensor frequency shift in j -th harmonic. R_{a-b} means the a -th sensor resistance response in b -th harmonic.

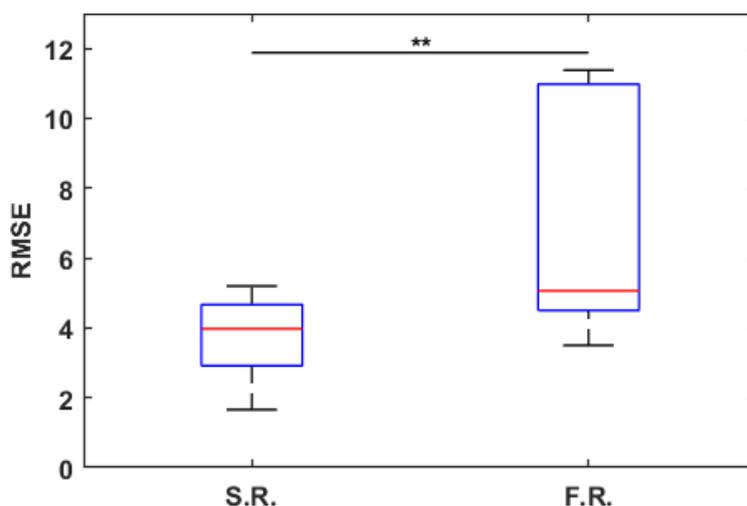


Figure 3. Box plot of the RMSE of total 20 experiments and comparison between selected 10 responses (S.R.) and fundamental ones (F.R.). In all of the boxplots, the red lines in the middle of the box represent the median, the box represents the 75th and 25th percentiles, the whiskers represent the maximum and minimum values, and the red crosses represent the outliers that are 1.5 times above or below the box. The two asterisks represent the significance with p -value below 0.01.

responses.

The quantification results are shown in Fig. 3. When only 4 fundamental responses were used, the average measurement RMSE was 7.12. After introducing the selected frequency and resistance responses from harmonics, the RMSE decreased to 3.74. A paired t-test ($p = 0.0070$) confirms that this improvement is statistically significant.

In summary, adding harmonic responses effectively contributes to a higher-accuracy quantification of multi-component gas mixtures.

Reference:

- [1] Z. Bao, M. Aleixandre, S. Hasegawa and T. Nakamoto, "A Robust Odor Mixture Quantification Method Based on Active Sensing Using Both QCM Frequency Shifts and Resistance Changes of Multiple Harmonics," *IEEE Sensors J.*, vol. 25, no. 23, pp. 42482-42489, 1 Dec.1, 2025.
- [2] S. N. Songkhla and T. Nakamoto, "Signal processing of vector network analyzer measurement for quartz crystal microbalance with viscous damping," *IEEE Sensors J.*, vol. 19, no. 22, pp. 10386–10392, Nov. 2019.
- [3] N. C. Speller, N. Siraj, B. P. Regmi, H. Marzoughi, C. Neal, and I. M. Warner, "Rational design of QCM-D virtual sensor arrays based on film thickness, viscoelasticity, and harmonics for vapor discrimination," *Anal. Chem.*, vol. 87, no. 10, pp. 5156–5166, May 2015.
- [4] I. Reviakine, D. Johannsmann, and R. P. Richter, "Hearing what you cannot see and visualizing what you hear: Interpreting quartz crystal microbalance data from solvated interfaces," *Anal. Chem.*, vol. 83, no. 23, pp. 8838–8848, Dec. 2011.
- [5] T. Yamanaka, R. Matsumoto, and T. Nakamoto, "Study of recording apple flavor using odor recorder with five components," *Sens. Actuators B, Chem.*, vol. 89, no. 1–2, pp. 112-119, Mar. 2003.