Prediction of Acetone Levels in Gas Mixtures with High Ethanol Concentration: Investigating its Relevance for Diabetes Detection in Exhaled Air

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Currently, the number of people with diabetes is growing rapidly, and early diagnosis and monitoring of the disease plays a key role in its treatment. Research on non-invasive determination of blood glucose levels on the basis of exhaled air is still underway. Previous studies do not take into account the influence of interfering factors on the response of gas sensors. One of them is ethanol, which shows a similar response mechanism of semiconductor gas sensors as acetone, which is a known biomarker of diabetes. As part of laboratory studies, we examined the effect of the presence of ethanol in gas mixtures that mimic human breath on the ability to predict the concentration of acetone in gas mixtures. The results showed that in mixtures without ethanol, the e-nose composed of gas sensors and the use of machine learning algorithms mean absolute error of predicting the acetone concentration was 0.25 ppm, and in the case of the presence of ethanol in the mixture, the error increased to 0.36 ppm. The conducted research emphasizes the importance of identifying influencing factors and examining their impact on the operation of e-nose-based systems. Recognizing and understanding these factors can improve the quality and reliability of breath analysis as a diagnostic tool.

METHODS

The water bubbler was used to simulate the relative humidity of the gas mixture to mimic human exhaled air. The measurement system is shown in Figure 1. Acetone in the mixtures was in the range of 0-2.5 ppm [1]. The average RH of the mixtures was 75% to best mimic human breathing. Sensor signal acquisition was performed using DAQ970A (Keysight Technologies, Santa Rosa, CA, USA).

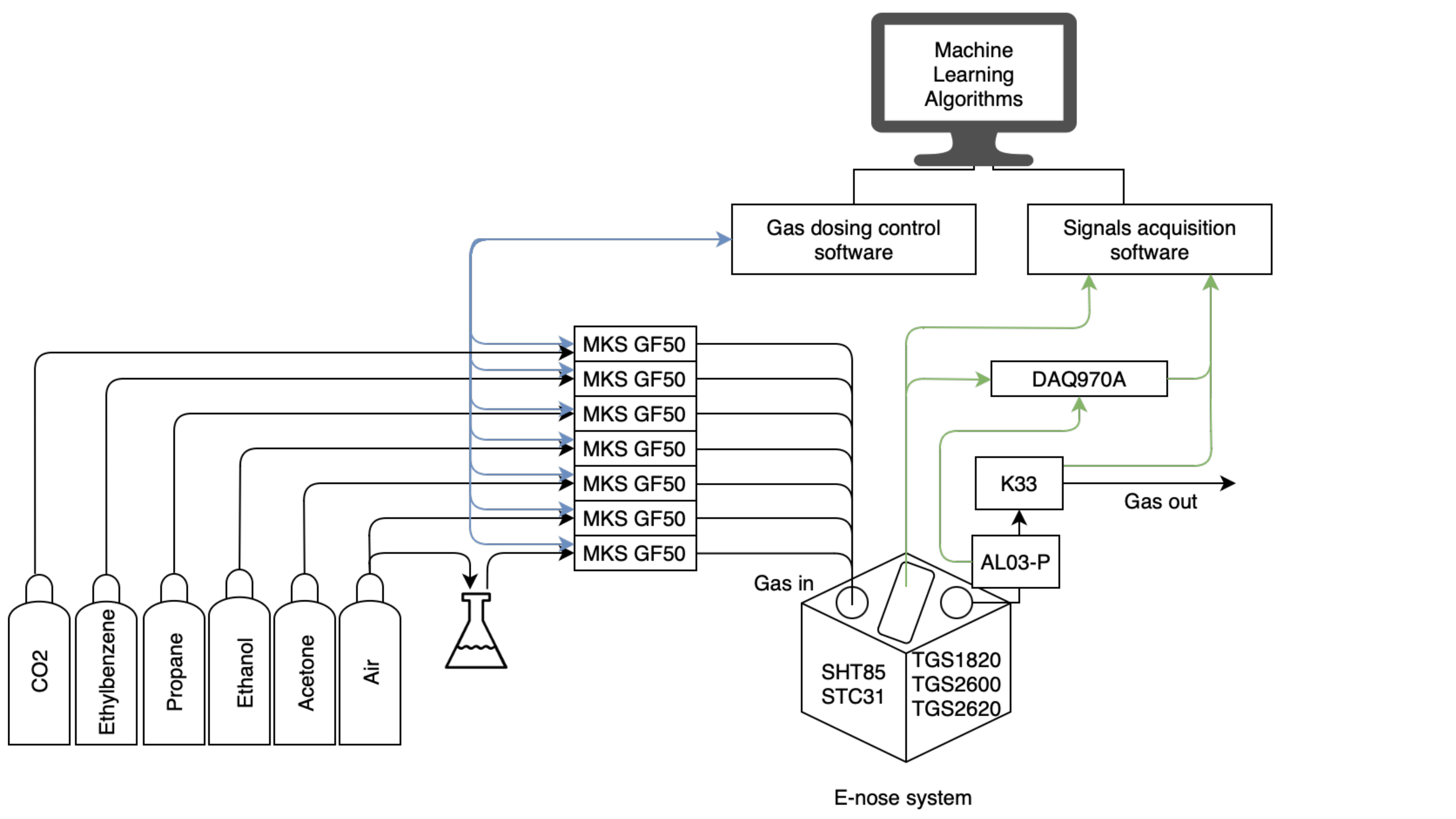


Figure 1. Measurement setup

As input data from sensors, raw sensor responses R_G and sensitivity S values given by:

$$S = R_g - R_0,$$

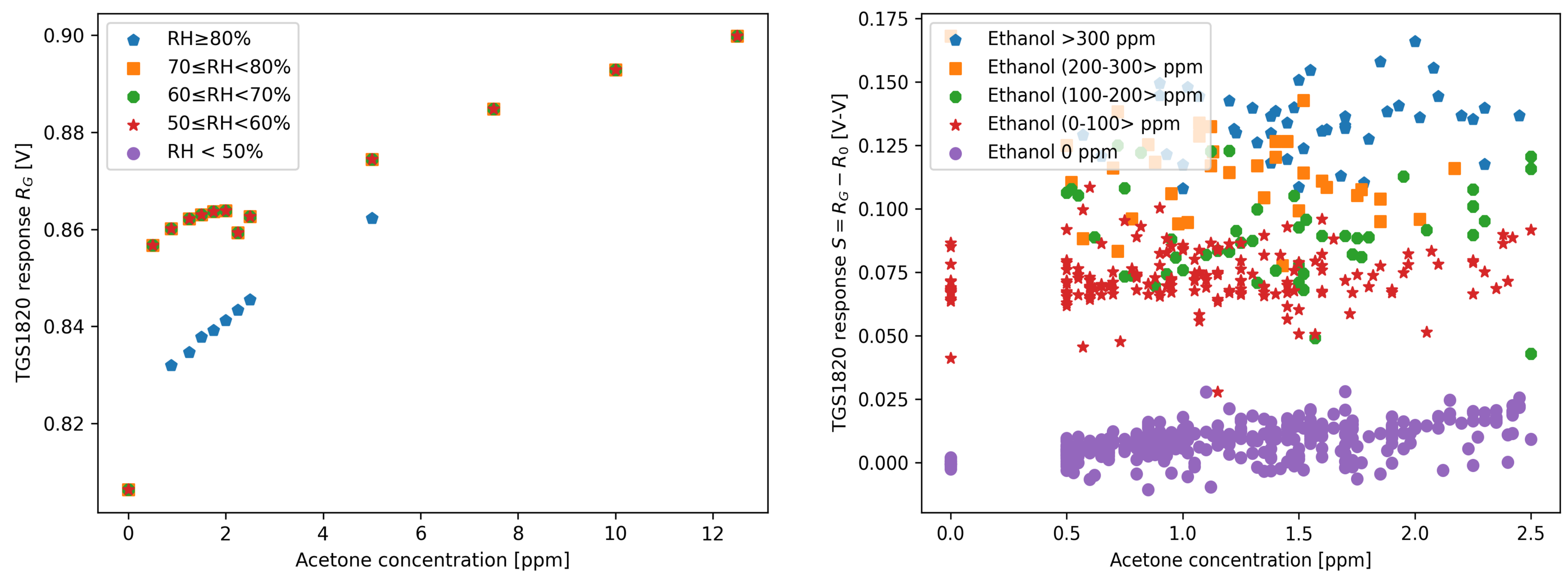
where:

- S – sensor sensitivity,
- R_g – sensor exposed to the gas mixture exposure,
- R_0 – sensor exposed to the synthetic air and RH exposure.

The relationship between breath alcohol concentration (BrAC) and blood alcohol concentration (BAC) is not a linear one and varies depending on factors such as age, sex, weight, and metabolism. In order to estimate the potential concentration of ethanol in human breath, we assumed a maximum of 2‰ BAC, which is equivalent to 0.95 mg/l of BrAC (conversion factor of 2100:1 for BAC to BrAC [2]). Assuming a breath temperature of 36°C and a measurement pressure of 1013 hPa, the 0.95 mg/l BrAC translates to 522 ppm [3].

CatBoost is an open-source supervised machine learning framework based on Gradient Boosted Decision Tree (GBDT) commonly used in medical machine learning tasks, especially with heterogeneous data. CatBoost supports categorical features and deals with gradient bias, which leads to reducing overfitting [4].

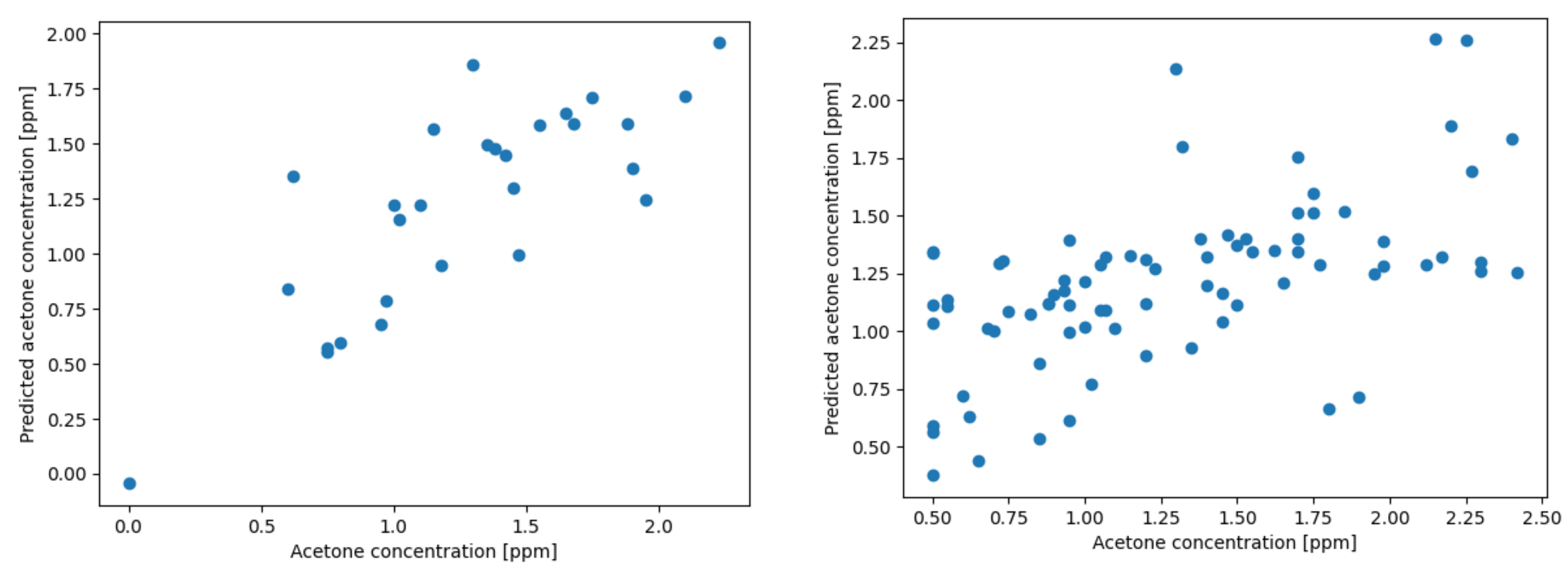
RESULTS



a) b)

Figure 2. a) TGS1820 response to acetone concentration; **b)** TGS1820 response to acetone concentration in ethanol environment.

Figure 2a and Figure 2b show how the sensor's response changes with different acetone concentrations in the mixtures depending on presence of ethanol. When trying to predict acetone concentration, using only one TGS1820 sensor designed for acetone detection was not enough because this sensor's sensitivity could be affected by high levels of ethanol.



a) b)

Figure 3. a) Prediction of acetone concentration in mixtures without ethanol; **b)** Prediction of acetone concentration in mixtures with ethanol.

CatBoost Regressor algorithm was used for acetone concentration prediction. The findings revealed that when ethanol was absent in the mixtures, employing an e-nose consisting of gas sensors and machine learning algorithms yielded a mean absolute error of 0.25 ppm in predicting acetone concentration. However, when ethanol was present in the mixture, this error rose to 0.36 ppm.

CONCLUSIONS

The early diagnosis of diabetes plays a significant role in its further treatment and reduction of its complications. Therefore, it is important to conduct research and develop a device for non-invasive disease detection. The device based on breath measurements consists of gas sensors, but due to low concentrations of VOCs and poor selectivity of the sensors, it is necessary to use an array of sensors and machine learning algorithms. The next step in the research on the development of noninvasive devices should be to test the system using human breaths and to develop algorithms to predict blood glucose levels that can be used both for the detection of diabetes and its subsequent monitoring.

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References

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