On-line Calibration of Semiconductor Gas Sensors Based on Prediction Model

Fengchun Tian[1], Jingwei Feng[2] , Guorui Li[3], Lijun Dang[4], Xin Yin[5], Xiongwei Peng[6]

[1,2,3,4,5,6]College of Communication Engineering, Chongqing University, Chongqing, 400044, China

Email: Fengchuntian@cqu.edu.cn, cqufjw@cqu.edu.cn, liguorui1213@163.com, danglijunshasha@163.com, 358621786@qq.com, pxwtxxy@163.com

Abstract—In this study, an Electronic nose (Enose) instrument used indoor for monitoring formaldehyde is designed. In mass production of this instrument, because of the inherent variability in the sensor manufacturing process, the Enose instruments give different outputs. It is impossible to train an individual prediction model on each instrument to have uniform output. A new on-line calibration method based on prediction model without real master instrument is proposed. This method avoids the problem that if the real master instrument behaves drift, the calibration of the other batch of instruments would lose its effect. In this paper, the prediction model is radial basis function (RBF) neural network and particle swarm optimization (PSO) is used to determine the parameters in RBF. The results show that the responses of the same type sensors are uniform after calibration, and this new method is easy and robust.

Index Terms—on-line calibration; electronic nose; radial basis function neural network; particle swarm optimization

I. INTRODUCTION

Electronic nose (Enose), which is composed of semiconductor gas sensors, has been studied for many years and used in many fields [1-14].

Our project is devoted to design of Enose instrument used indoor for monitoring formaldehyde so that many these instruments should be produced for extensive users. However, inherent variability in the sensor manufacturing process leads to slight differences in the reactivity of the tin oxide substrate of individual sensors [15]. These slight differences will lead to different outputs of instruments. In mass production of Enose instruments, it is impossible to train an individual prediction model on each instrument to have uniform output. Some calibration transfer methods [16-21] are proposed for spectrophotometers instruments standardization. Because of the complexity and robustness, these methods are not very suitable for on-line using in our Enose instruments. An easy way to overcome this problem is to calibrate the same type sensor responses in different instruments. In Ref. [22], a simple and robust method is proposed for on-line calibration transfer among multiple Enose instruments. But this method always needs a master Enose instrument when calibration, if gas sensors in this master instrument behave drift, the calibration of the other batch of instruments would lose its effect. Moreover,

there is no effect method to detect and completely overcome drift.

In this paper, a new on-line calibration transfer method based on prediction model without real master instrument is proposed. For each sensor in master instrument, a concentration prediction model is built. A temporary master instrument is selected among new instruments that are need to be calibrated. Different batch of instruments are calibrated to master instrument by using this temporary master instrument and the prediction models of sensors in master instruments. Because of no real master instrument, there is no effect on calibration when the master instrument behaves drift.

II. MATERIALS AND EXPERIMENTS

In construction as a gas sensor array which is used in our instrument, three semiconductor gas sensors from Figaro Engineering Inc. are selected. They are TGS2620, TGS2602 and TGS2201 with two outputs named A and B (TGS2201A/TGS2201B). In addition, a module (SHT2230 of Sensirion in Switzerland) with two auxiliary sensors for temperature and humidity is also used. These sensors are mounted on a custom designed printed circuit board (PCB), along with associated electrical components. An analog-digital converter is used as interface between the FPGA processor and the sensors. A flash memory is added to save data which can be uploaded to a personal computer (PC) via the joint test action group (JTAG) cable.

All the experiments were performed in a Constant Temperature and Humidity chamber (LRH-150S) in which temperature and humidity can be effectively controlled in the range of 5-50℃ and 0-100%, respectively.

First, the dataset of master instrument is obtained. The master instrument should be exposed to formaldehyde in different concentrations and environment conditions. Totally, 125 samples named dataset 1 are obtained. These samples are measured through different combinations of target temperature of 15, 25, 30 and 35℃ and target humidity of 40, 60 and 80%. The total measurement cycle time for a single measurement was set to 10 min, i.e., 2 min for reference air (baseline) before formaldehyde was injected into

chamber, and then another 8 min for formaldehyde. Between each measurement, clean air was injected for more than 10 min to clean the chamber.

The second is calibration experiment. There are eleven other instruments that will be calibrated, named #1, #2, #3, #4, #5, #6, #7, #8, #9, #10 and #11. The instrument #11 is selected as temporary master instrument. The calibration experiment for these instruments is almost the same with the first experiment, but the concentrations of formaldehyde is unnecessary to be known. So the calibration experiment is very easy. It is worth noting that these eleven instruments, especially the temporary master instrument, would employ the experiments together at the same time in the chamber to ensure the condition of experiment is the same for these instruments. The dataset obtained from this experiment is named dataset 2.

The third is the experiment of temporary master instrument. This experiment is the same with the first experiment, 6 samples named dataset 3 are obtained with different concentrations of formaldehyde. In this experiment, the concentrations of formaldehyde should be known.

III. CALIBRATION TRANSFER

Fig. 1 shows the correlation between TGS2620 in instrument 01 (#01) and instrument 11 (#11). From Fig. 1, we can see that the correlation between the same type gas sensors is approximately linear except some divergent points that stay away from most of the points when they are in the same condition. These divergent points in Fig. 1 are the points in the adsorption slope of gas sensor which is a short stage (less than 40s) and have very little effect on calibration.
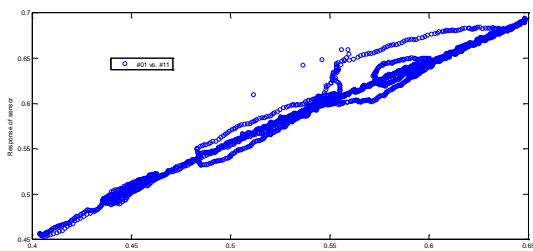

Figure 1. The correlation of TGS2620 between instrument 01 (#01) and instrument 11 (#11).

From Fig. 1, the calibration model can be described by linear relationship and it is shown as follow,

$$y = ax + b, \qquad (1)$$

where x denote the response of one sensor measured on the other instrument, and y is the calibrated response from x to the master instrument, a and b are the calibration transfer coefficients.

The problem in the above calibration model is that if gas sensors in master instrument behave drift, the calibration of the other batch of instruments would lose its effect. A new on-line calibration method based on prediction model is proposed. The details on this method are given as follows.

Step 1:
The first experiment for mater instrument is performed and dataset 1 is obtained.
Step 2:
Radial basis function (RBF) [23-24] neural network is trained as concentration prediction model of master instrument using dataset 1. The temperature, humidity and response of sensor are used as inputs of RBF, and the concentrations of formaldehyde are used as outputs. Two-thirds of dataset 1 is used as train dataset, and the rest is used as test dataset. The parameters in RBF are optimized by using PSO. Finally, four prediction models for TGS2620, TGS2602, TGS2201A and TGS2201B are obtained.
Step 3:
A temporary master instrument is selected among new instruments that are need to be calibrated.
Step 4:
The second experiment, namely, calibration experiment, is performed and dataset 2 is obtained.
Step 5:
The same batch instruments are calibrated to temporary master instrument by using (1) based dataset 2. Because the condition of experiment of same batch instruments is the same with temporary master instrument, so (1) can be used.
Step 6:
Repeat steps 4-5 until all batch instruments are calibrated.
Step 7:
The third experiment is performed and dataset 3 is obtained.
Step 8:
Based on dataset 3, the temperature, humidity, and concentrations of formaldehyde are used to calculate the responses of sensors in master instrument by using the prediction models in step 1. The calculated master instrument responses are in the same condition with temporary master instrument. Because of computation complexity, PSO is used to search the responses instead of straight calculation. The particle in PSO is the response of one sensor in master instrument. The value of particle, temperature and humidity are inputted to corresponding prediction model. The absolute value of the difference between the output of prediction model and real concentration is used as the fitness value of PSO. Thus, PSO can find the response of each sensor in master instrument by minimizing the fitness value.
Step 9:
The temporary master instrument is calibrated to calculated responses (master instrument) by using (1).
Step 10:
The other instruments are calibrated to master instrument according to the temporary master instrument.

IV. RESULTS AND DISCUSSION

For concentration prediction, absolute value of mean relative error (AMRE) is used. AMRE is defined as follow:

$$AMRE = \frac{1}{n} \sum_{i=1}^{n} \frac{|y_i^{pred} - y_i^{true}|}{y_i^{true}} \qquad (2)$$

where y_i^{pred} is the predicted concentration, y_i^{true} is the actual concentration, n is the number of samples .

The AMRE of four models for TGS2620, TGS2602, TGS2201A and TGS2201B are shown is TABLE Ⅰ.

TABLE Ⅰ
AMRE OF FOUR MODELS FOR TGS2620, TGS2602, TGS2201A AND TGS2201B

	TGS2620	TGS2602	TGS2201A	TGS2201B
AMRE (%)	41.33	183.04	126.93	58.56

Because of only one sensor, the results of each model in TABLE Ⅰ are not very good. But, We have tried our best to give the best prediction model for each sensor.

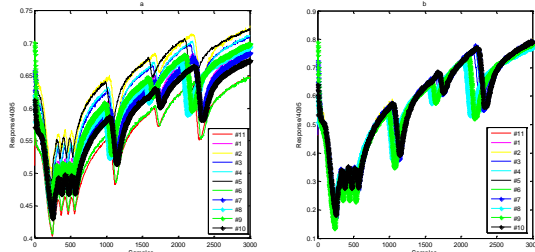The calibration results are shown in Fig. 2 - 5.

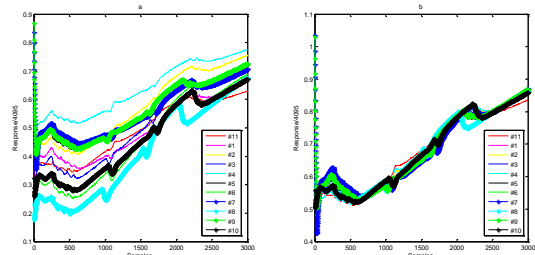Figure 2. Response of TGS2620 before (a) and after (b) calibration.

Figure 3. Response of TGS2602 before (a) and after (b) calibration.
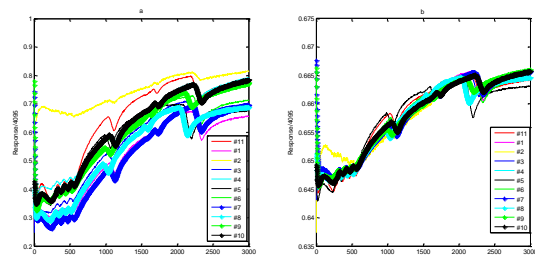

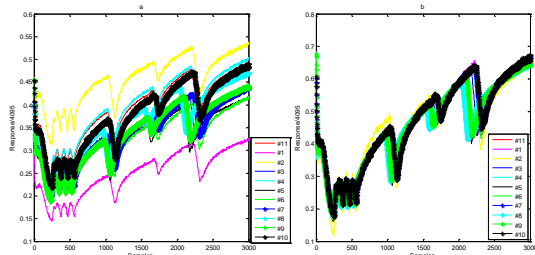Figure 4. Response of TGS2201A before (a) and after (b) calibration.

Figure 5. Response of TGS2201B before (a) and after (b) calibration.

The absolute value of mean relative distance (AMRD) of each sensor is used to evaluate the effect of the proposed calibration method.

$$AMRD = \frac{1}{M-1} \sum_{i=1}^{M-1} \frac{1}{N} \sum_{j=1}^{N} \left| \frac{\mathbf{x}_{i,j} - \mathbf{x}_{i,11}}{\mathbf{x}_{i,11}} \right|. \qquad (3)$$

Where, N is the number of samples, M is the number of instruments, $\mathbf{x}_{i,j}$ is the ith sample of jth instrument, $\mathbf{x}_{i,11}$ is the ith sample of #11 instrument. Because of no real master instrument, we calculate the AMRD between temporary master instrument and other instruments. The AMRD of each sensor is given in TABLE Ⅱ.

TABLE Ⅱ
AMRD OF EACH SENSOR

sensor	AMRD	
	Before calibration	After calibration
TGS2620	0.0989	0.0334
TGS2602	0.1457	0.0278
TGS2201A	0.1290	0.0017
TGS2201B	0.1442	0.0373

From Fig. 2-5 and TABLE Ⅱ, we can see that the responses of the same sensors in different instruments become uniform. This calibration method is effective. The temporary master instrument does not have to be selected. If the temporary master instrument dose not be selected, the third experiment is directly performed and the concentration of formaldehyde should be known. In mass production, this experiment should be performed many times, and this is very time-consuming and complicated. So it is best to select a temporary master instrument, and the third experiment is only performed one time.

In this method, we just keep the prediction models of master instruments instead of real master instrument, and other instruments are calibrated to master instruments according these prediction models. We do not use real master instruments, so there is no effect on these prediction models if the master instrument behaves drift.

V. CONCLUSIONS

In mass production of Enose instruments, calibration is quite necessary. One of the main disadvantages of calibration using real master instrument is that if the sensors in the master instrument behave drift, the calibration of the other batch of instruments would lose its effect. In this paper, a new on-line calibration method is proposed. Using this method, the real master instrument is not needed, so there is no need to care about the drift. This new calibration method is robust. It is worth noting that the prediction model used in this paper is RBF, other prediction models with good accuracy and generalization can also be used. The gas used in calibration is formaldehyde, but we believe that the calibration coefficients also work in other gases like benzene, carbon monoxide, alcohol etc. The main reason is that the features we used in this calibration method are steady state responses of semiconductor gas sensors, but

it still needs a further research to prove it.

REFERENCES

[1] C. Di Natale, A. Macagnano, A. Mantini, F. Davide, A. D'Amico, R. Paolesse, T. Boschi, M. Faccio, and G. Ferri, "Advances in food analysis by electronic nose," in *Industrial Electronics, 1997. ISIE '97., Proceedings of the IEEE International Symposium on*, 1997, pp. SS122-SS127 vol.1.

[2] Y. B. C. Man, H. L. Gan, I. NorAini, S. A. H. Nazimah, and C. P. Tan, "Detection of lard adulteration in RBD palm olein using an electronic nose," *Food Chemistry,* vol. 90, pp. 829-835, 2005.

[3] E. R. Thaler and C. W. Hanson, "Use of an electronic nose to diagnose bacterial sinusitis," *American Journal of Rhinology,* vol. 20, pp. 170-172, 2006.

[4] S. Dragonieri, R. Schot, B. J. A. Mertens, S. Le Cessie, S. A. Gauw, A. Spanevello, O. Resta, N. P. Willard, T. J. Vink, K. F. Rabe, E. H. Bel, and P. J. Sterk, "An electronic nose in the discrimination of patients with asthma and controls," *Journal of Allergy and Clinical Immunology,* vol. 120, pp. 856-862, 2007.

[5] N. H. Beltran, M. A. Duarte-Mermoud, V. A. S. Vicencio, S. A. Salah, and M. A. Bustos, "Chilean Wine Classification Using Volatile Organic Compounds Data Obtained With a Fast GC Analyzer," *IEEE Transactions on Instrumentation and Measurement,* vol. 57, pp. 2421-2436, 2008.

[6] A. D'Amico, R. Bono, G. Pennazza, M. Santonico, G. Mantini, M. Bernabei, M. Zarlenga, C. Roscioni, E. Martinelli, R. Paolesse, and C. Di Natale, "Identification of melanoma with a gas sensor array," *Skin Research and Technology,* vol. 14, pp. 226-236, 2008.

[7] F. De Cesare, S. Pantalei, E. Zampetti, and A. Macagnano, "Electronic nose and SPME techniques to monitor phenanthrene biodegradation in soil," *Sensors and Actuators B: Chemical,* vol. 131, pp. 63-70, 2008.

[8] S. De Vito, E. Massera, M. Piga, L. Martinotto, and G. Di Francia, "On field calibration of an electronic nose for benzene estimation in an urban pollution monitoring scenario," *Sensors and Actuators B: Chemical,* vol. 129, pp. 750-757, 2008.

[9] A. Lamagna, S. Reich, D. Rodríguez, A. Boselli, and D. Cicerone, "The use of an electronic nose to characterize emissions from a highly polluted river," *Sensors and Actuators B: Chemical,* vol. 131, pp. 121-124, 2008.

[10] S. Dragonieri, J. T. Annema, R. Schot, M. P. C. van der Schee, A. Spanevello, P. Carratu, O. Resta, K. F. Rabe, and P. J. Sterk, "An electronic nose in the discrimination of patients with non-small cell lung cancer and COPD," *Lung Cancer,* vol. 64, pp. 166-170, 2009.

[11] V. H. Tran, C. Hiang Ping, M. Thurston, P. Jackson, C. Lewis, D. Yates, G. Bell, and P. S. Thomas, "Breath Analysis of Lung Cancer Patients Using an Electronic Nose Detection System," *IEEE Sensors Journal,* pp. 1514-18, 2010.

[12] C. Cevoli, L. Cerretani, A. Gori, M. F. Caboni, T. Gallina Toschi, and A. Fabbri, "Classification of Pecorino cheeses using electronic nose combined with artificial neural network and comparison with GC–MS analysis of volatile compounds," *Food Chemistry,* vol. 129, pp. 1315-1319,

2011.

[13] T. García-Martínez, A. Bellincontro, M. d. l. N. L. de Lerma, R. A. Peinado, J. C. Mauricio, F. Mencarelli, and J. J. Moreno, "Discrimination of sweet wines partially fermented by two osmo-ethanol-tolerant yeasts by gas chromatographic analysis and electronic nose," *Food Chemistry,* vol. 127, pp. 1391-1396, 2011.

[14] H. Li, D. Wang, and Y. Zhang, "Knowledge-based genetic algorithms data fusion and its application in mine mixed-gas detection," *Journal of Software,* vol. 7, pp. 303-307, 2012.

[15] E. J. Wolfrum, R. M. Meglen, D. Peterson, and J. Sluiter, "Calibration Transfer Among Sensor Arrays Designed for Monitoring Volatile Organic Compounds in Indoor Air Quality," *Sensors Journal, IEEE,* vol. 6, pp. 1638-1643, 2006.

[16] X. Liu, L. J. Han, and Z. L. Yang, "Transfer of near infrared spectrometric models for silage crude protein detection between different instruments," *Journal of Dairy Science,* vol. 94, pp. 5599-5610, 2011.

[17] E. L. Bergman, H. Brage, M. Josefson, O. Svensson, and A. Sparen, "Transfer of NIR calibrations for pharmaceutical formulations between different instruments," *Journal of Pharmaceutical and Biomedical Analysis,* vol. 41, pp. 89-98, Apr 2006.

[18] K.-S. Park, Y.-H. Ko, H. Lee, C.-H. Jun, H. Chung, and M.-S. Ku, "Near-infrared spectral data transfer using independent standardization samples: a case study on the trans-alkylation process," *Chemometrics and Intelligent Laboratory Systems,* vol. 55, pp. 53-65, 2001.

[19] J. Sjöblom, O. Svensson, M. Josefson, H. Kullberg, and S. Wold, "An evaluation of orthogonal signal correction applied to calibration transfer of near infrared spectra," *Chemometrics and Intelligent Laboratory Systems,* vol. 44, pp. 229-244, 1998.

[20] B. Walczak, E. Bouveresse, and D. L. Massart, "Standardization of near-infrared spectra in the wavelet domain," *Chemometrics and Intelligent Laboratory Systems,* vol. 36, pp. 41-51, 1997.

[21] E. Bouveresse and D. L. Massart, "Standardisation of near-infrared spectrometric instruments: A review," *Vibrational Spectroscopy,* vol. 11, pp. 3-15, 1996.

[22] L. Zhang, F. Tian, C. Kadri, B. Xiao, H. Li, L. Pan, and H. Zhou, "On-line sensor calibration transfer among electronic nose instruments for monitoring volatile organic chemicals in indoor air quality," *Sensors and Actuators B: Chemical,* vol. 160, pp. 899-909, 2011.

[23] Q. Luan and C. Zhu, "Surface Water Quality Evaluation Using BP and RBF Neural Network," *Journal of Software,* vol. 6, pp. 2528-2534, 2011.

[24] Y. Gu, Y. Shi, and J. Wang, "Efficient Intrusion Detection Based on Multiple Neural Network Classifiers with Improved Genetic Algorithm," *Journal of Software,* vol. 7, pp. 1641-1648, 2012.

Fengchun Tian received the BS degree in Wireless, the MS degree in Biomedical Instrumentation and the phD degree in Theoretical Electrotechnics from Chongqing University, Chongqing, China in 1984,1989 and 1996, respectively. He is currently professor of College of Communication Engineering in Chongqing University. His research projects have included signal and information processing and communication and information system. He has a strong interest in electronic nose. Several related papers have been published in international journals in recent years.

Jingwei Feng received the BS degree in Communication from Chongqing University, Chongqing, China in 2009. He is currently pursuing the Direct phD degree in the same university. His research interests include signal processing pattern recognition techniques applied to machine olfaction. He is currently working in the air quality monitor and wound infection detection by electronic nose.

Guorui Li is currently pursuing the MS degree in Chongqing University, Chongqing, China. His research interests include signal processing pattern recognition techniques applied to machine olfaction. He is currently working in the air quality monitor by electronic nose.

Lijun Dang is currently pursuing the MS degree in Chongqing University, Chongqing, China. Her research interests include signal processing pattern recognition techniques applied to machine olfaction. She is currently working in the air quality monitor by electronic nose.

Xin Yin is currently pursuing the MS degree in Chongqing University, Chongqing, China. His research interests include signal processing pattern recognition techniques applied to machine olfaction. He is currently working in the air quality monitor by electronic nose.

Xiongwei Peng is currently pursuing the MS degree in Chongqing University, Chongqing, China. His research interests include signal processing pattern recognition techniques applied to machine olfaction. He is currently working in the air quality monitor by electronic nose.