Calibration of MOX gas sensors in open sampling systems based on Gaussian Processes

Javier G. Monroy*, Achim Lilienthal†, Jose Luis Blanco‡, Javier González-Jimenez* and Marco Trincavelli†
*Dept. of System Engineering and Automation, University of Málaga, Spain
†AASS Research Centre, Örebro University, Sweden
‡Dept. of Civil Engineering, University of Málaga, Spain

Abstract— **Calibration of metal oxide (MOX) gas sensors for continuous monitoring is a complex problem due to the highly dynamic characteristics of the gas sensor signal when exposed to a natural environment in an Open Sampling System (OSS). This work presents a probabilistic approach to the calibration of MOX gas sensors using Gaussian Processes (GP). The proposed approach estimates for every sensor measurement a probability distribution of the corresponding gas concentration, which enables the calculation of confidence intervals for the predicted concentrations. Being able to predict the uncertainty about the concentration related to a particular sensor response is particularly advantageous in OSS applications where typically many sources of uncertainty exist. The proposed approach has been tested with an experimental setup where an array of MOX sensors and a Photo Ionization Detector (PID) are placed downwind with respect to the gas source. The PID is used to obtain ground truth concentration measurements. Comparison with standard calibration methods demonstrate the advantage of the proposed approach.**

I. INTRODUCTION

Gas sensing applications often require continuous and direct exposition of gas sensors to the environment to be analyzed, since it contains useful information about the nature of the gas plume that can be used e.g. to localize the source of the gas [1]. This configuration, to which we refer as open sampling system (OSS), is the preferred solution when limitations in dimension, payload or energy consumption do not allow the adoption of a sampling system where the sensors are hosted in a chamber with controlled airflow, temperature and humidity.

The most common gas sensing technology for OSS applications is metal oxide (MOX) gas sensors. The most prominent reasons for the selection of MOX sensors are their wide commercial availability, low price, and their higher sensitivity to the compounds of interest in comparison to most other sensing technologies. However, this technology presents among other drawbacks, an important lack of selectivity, does not provide calibrated concentration readings, suffers from long and short term drift and is rather slow [2], especially when recovering to the baseline, *i.e.* the steady output value given by a gas sensor when exposed to clean air.

The problem addressed in this paper is the estimation of gas concentration from the readings of a MOX sensor deployed in an OSS. This is a crucial step for some real applications of gas sensing since legal requirements and regulations are expressed in terms of absolute gas concentration, toxicity levels, etc. The main difference compared to gas quantification with sensors within a sensing chamber (where controlled conditions can be imposed), are that several additional sources of uncertainty are present in OSS. The most relevant is the exposition of the sensors to the turbulent airflow that brings the chemical compound in contact with the sensors. Indeed, given the slow dynamics of MOX gas sensors and the rapid fluctuations in concentration due to turbulent airflow, the sensors never reach a steady state (see Fig. 1).

In this paper we propose an approach for sensor calibration that calculates a posterior distribution of the concentration using a Gaussian Process (GP) model [3], which provides an estimation of the uncertainty (as a variance) that can be used to calculate confidence intervals for the predictions.

The structure of this article is as follows. After a discussion of related works in Section II, we introduce in Section III the basics of Gaussian processes regression for gas quantification. Then, Section IV presents the experimental setup and comparative results for different types of MOX sensors.

II. RELATED WORKS

Traditionally, research has been mostly focused on the calibration of MOX gas sensors enclosed inside a chamber, where environmental conditions, gas exposure times and concentrations are known and controlled. This setup allows the measurement of steady state values, which are used in a regression process.

Different methods have been proposed for such regression process like Principal Component Regression (PCR) or Partial Least Squares Regression (PLSR) [4], [5], [6]. Alternatively, non-linear methods like Artificial Neural Networks (ANN) or more recently kernel methods, have also drawn significant interest [7], [8], [9]. Among those, Support Vector Regression
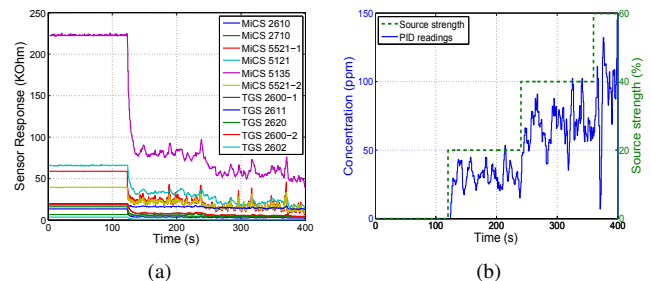

Fig. 1. Instantaneous sensor response of metal oxide gas sensors (a) and PID measurements (b) for a standard open sampling system experiment.

(SVR) has probably received most attention in chemometric applications [10].

Unfortunately, all these approaches make calibration to rely on steady state measurements of the sensor, which are not immediately applicable to OSS because steady state values are almost never reached [11].

The scope of this work is towards applications in which the sensors are deployed in a highly dynamic environment, being frequently exposed to intermittent patches of gas, like for example in robotics applications. In this field, traditionally most of the works on olfaction directly obviate this problem, working directly with the conductance readings of the sensors as an approximate measure of the gas concentration. An exception is [12], where Ishida et al. proposes sensor calibration based on steady state values as a rough approximation.

It must be noticed that all mentioned methods ignore the uncertainty in the calibration while, if we work with OSS, measurements of MOX conductance are always affected by a high uncertainty due to the above mentioned gas transport mechanisms, the inherent sensor dynamics and environmental factors [13] as temperature or humidity (environmental factors are not addressed in this work). Due to these uncertainties, it is preferable to provide confidence information together with the gas concentration predicted at any time. The GP-based method proposed in this paper generates an estimate of the uncertainty (as a variance) which can be used to calculate confidence intervals for the predictions.

III. THE ALGORITHM FOR ESTIMATION OF GAS CONCENTRATION.

This section details our proposal for the concentration estimation in OSS, summarizing the theory behind Gaussian Process regression for the particular case of gas quantification. Additionally, two different loss functions are proposed for evaluating the results.

A. Gaussian Process Regression for Gas Concentration Estimation

GPs can be seen as a generalization of the Gaussian probability distribution to distributions over functions [3]. That is, they perform inference directly in the space of functions, starting with a prior distribution over all possible functions and subsequently learning the target function from data samples. In our case, the relationship to be inferred is $f : r_t \longmapsto c_t$, where r_t is the sensor resistance and c_t the gas concentration at time t.

A GP is completely specified by its mean and covariance functions, $m(r_t) = \mathbb{E}[f(r_t)]$ and $k(r_t, r_{t'}) = cov(f(r_t), f(r_{t'}))$ respectively. We denote the GP as:

$$f(r_t) \sim \mathcal{GP}(m(r_t), k(r_t, r_{t'})) \qquad (1)$$

Moreover, to account for noise in the sensor it is assumed that the observed concentration values c_t are corrupted with an additive i.i.d Gaussian noise with zero mean and variance σ_n^2, that is:

$$c_t = f(r_t) + \varepsilon \qquad (2)$$
$$\varepsilon \sim \mathcal{N}(0, \sigma_n^2)$$

The selection of the mean and covariance functions of the GP, as well as the values of their hyper-parameters, determines the prior over the functions (informally, the "shape" of the functions) considered in the inference process [3]. In our case of study we consider GPs with zero mean function and the commonly used squared exponential (SE) covariance function, that is:

$$m(r_t) = 0 \qquad (3)$$
$$k(r_t, r_{t'}) = \sigma_f^2 \exp\left(-\frac{1}{2}\frac{\| r_t - r_{t'} \|^2}{\ell^2}\right) \qquad (4)$$

where σ_f^2 is the overall variance hyper-parameter and ℓ is the characteristic length scale (distance in the input space for the function values to become uncorrelated).

The obtained regression model depends on the selection of the hyper-parameters, which can be grouped in a vector $\boldsymbol{\theta} = (\ell^2, \sigma_f^2, \sigma_n^2)$. The optimal hyper-parameters are found by maximizing the marginal likelihood function $p(\mathbf{c}|\mathbf{r}, \boldsymbol{\theta})$, where $\mathbf{c}$ is a vector of training concentration values, $\mathbf{r}$ the vector containing the sensor measurements, and $\boldsymbol{\theta}$ is the vector of unknown parameters.

This allows us to predict gas concentration values $\mathbf{c}_*$ for arbitrary sensor resistances $\mathbf{r}_*$, even for values not seen in the training set thanks to what we learned from the training data about the latent function. The posterior distribution over functions (our prediction) is also a Gaussian, and is obtained by conditioning the joint prior on the training samples:

$$\mathbf{c}_*|\mathbf{r}, \mathbf{c}, \mathbf{r}_* \sim \mathcal{N}(\bar{\mathbf{c}}_*, cov(\mathbf{c}_*)), \text{where} \qquad (5)$$
$$\bar{\mathbf{c}}_* \triangleq \mathbb{E}[\mathbf{c}_*|\mathbf{r}, \mathbf{c}, \mathbf{r}_*] = \mathbf{K}(\mathbf{r}_*, \mathbf{r})[\mathbf{K}(\mathbf{r}, \mathbf{r}) + \sigma_n^2\mathbf{I}]^{-1}\mathbf{c}$$
$$cov(\mathbf{c}_*) = \mathbf{K}(\mathbf{r}_*, \mathbf{r}_*) - \mathbf{K}(\mathbf{r}_*, \mathbf{r})[\mathbf{K}(\mathbf{r}, \mathbf{r}) + \sigma_n^2\mathbf{I}]^{-1}\mathbf{K}(\mathbf{r}, \mathbf{r}_*)$$

Note that the predictive distribution is based on a mean value $\bar{\mathbf{c}}_*$ (our best estimation for $\mathbf{c}_*$), which is a linear combination of the observed values $\mathbf{c}$, and a variance value $cov(\mathbf{c}_*)$ which denotes the uncertainty in our estimation, and does not depend on the observed targets but only on the inputs.

B. Evaluation of the Predictions

In this section we propose two performance measures in order to compare the results of the gas quantification based on GP for different sensor types, and to compare the results with other methods previously proposed in literature:

Root Mean Squared Error (RMSE): The RMSE is calculated as the difference between the ground-truth concentration (obtained with the readings from the PID) and the expected value of the predictive distribution (see (5)).

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(c_i - \bar{c}_{*i})^2} \qquad (6)$$

Notice that the RMSE takes only into account the predictive mean, while it ignores its uncertainty. However, this indicator

allows us to compare the prediction of the proposed GP with other regression methods, like Partial Least Squares Regression (PLSR) or Support Vector Regression (SVR), that do not provide any estimation of the prediction uncertainty.

Negative Log Predictive Density (NLPD): The NLPD is a standard criterion to evaluate probabilistic models:

$$NLPD = -\frac{1}{n}\sum_{i=1}^{n}\log(p(c_i|\mathbf{r_i})) = \qquad (7)$$

$$= \frac{\log(2\pi)}{2} + \frac{1}{2N}\sum_{i=1}^{n}\left[\log(\sigma^2(c_i)) + \frac{(c_i - \mu(c_i))^2}{\sigma^2(c_i)}\right]$$

where c_i is the ground truth gas concentration, $\sigma(c_i)$ is the predictive standard deviation, and $\mu(c_i)$ the predictive mean.

It is worth noting that the NLPD considers the whole posterior distribution and not only its expected value. In general, smaller NLPD values indicate better predictions with a small uncertainty.

IV. RESULTS

In this section we present the experimental setup and results for the gas quantification based on GP. We start describing the composition of the experimental dataset, and how samples are selected from training and validation of the GP. Then, results for different scenarios are presented and a comparison is performed between the different sensors types available. Finally, the average results of the gas quantification with GP is compared with traditionally regression methods.

To test the proposed GP based gas quantification, an induced artificial airflow of approximately 0.1 m/s is generated to spread the gas released from an odour blender, a device described in [14] that enables rapid switch of compound and concentration, allowing the generation of rapidly changing controlled signals. The outlet of the olfactory blender is placed on the floor $0.5\ m$ upwind with respect to an array of 11 MOX gas sensors (5 Figaro TGS and 6 e2V MiCS) and a PID[1]. The compound selected for this experiment is ethanol which is heavier than air and, consequently, forms plumes at ground level.

In order to create a dataset that contains many different changes of concentration for the training of the GP, four different odour emitting strategies have been used. In all strategies the gas source starts emitting clean air for two minutes, time enough for us to assume that the sensors response is baseline. Fig. 2 depicts the source strength profile of the four emitting strategies. In the fourth and last emitting strategy, after the first 2 minutes in which the source emits clean air, the intensity of the source is chosen randomly in among 20%, 40%, 60%, 80%, 100%. Every two minutes the concentration is switched to another random value. After 10 switches the source emits clean air for two minutes and the experiment finishes. Overall, the dataset includes a total of 18 experiments, three repetitions of each strategy, plus six additional repetitions of the random strategy.

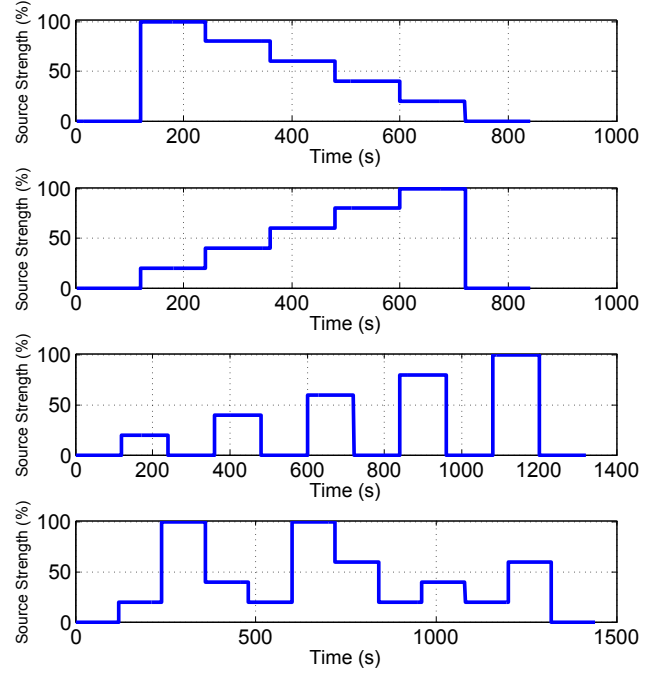[1]PID model ppbRAE2000 from RAESystem with a 10.6 eV UV lamp

Fig. 2. Source strength profile of the four emitting strategies employed in the generation of the experimental dataset. The bottom subfigure depicts an instance of the fourth strategy (random profile).

For the training and posterior evaluation of the GP, a cross validation procedure at experiment level has been used to provide significance to the results. This means that if samples from an experiment have been used during the training procedure, no sample from that experiment will be used for calculating the performance indexes. This is done in order to take into account variations in the sensor response caused by short term drift and changing environmental conditions. Furthermore, due to the computational complexity of the training algorithm of the GP (which is dominated by the inversion of the kernel matrix, to be performed at every step of the maximization of the marginal likelihood) a subset of 1000 samples from the experiments considered for the training set, is randomly selected for training the GP.

Fig. 3 depicts the gas concentration estimation for two different experiments. In order to compare the proposed methodology with others previously proposed for gas quantification, we provide for each scenario the results using Partial Least Squares Regression (PLSR) and Support Vector Machine Regression (SVR). Additionally, in Fig. 4 the NLPD and RMSE for each sensor in the array are plotted using a box-plot format to enable a comparison between the different sensors types. According to these results, sensors *TGS-2611* and *MiCS-5121* can be considered as the most advisable sensors in the array for this specific configuration and target gas (ethanol) for measuring the gas concentration.

Finally, Table I summarizes a performance comparison between the proposed calibration method based in GP to that of PLSR and SVR. In general, and since only the RMSE can be used to compare between these regression methods, we can say that the PLSR approach is slightly worse than SVR, while the latter behaves as well as the GP approach.
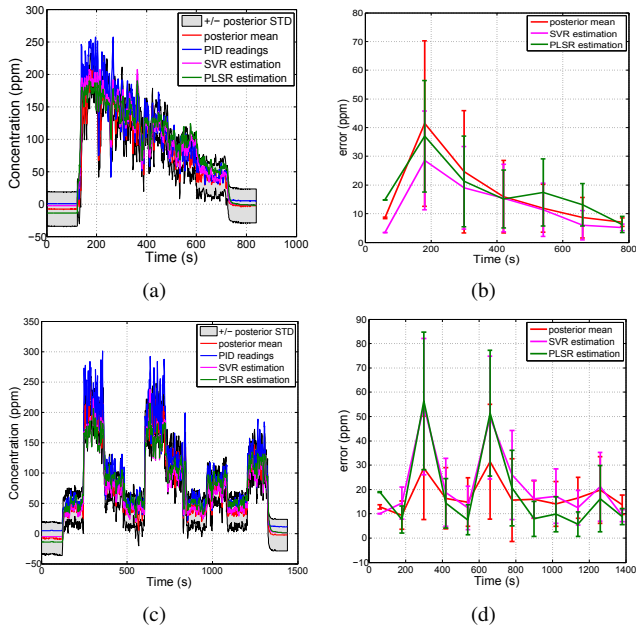
Fig. 3. Estimation of the gas concentration for two different gas emitting strategies (rows), obtained after the calibration of sensor *TGS-2611*. Left column outline the gas concentration profile, containing the ground truth (blue line), the estimation provided by the GP calibration (red line is the posterior mean while the shaded grey region represents the confidence interval $\pm 1\sigma$), the estimation provided by PLSR (green line), and the SVR estimation (magenta line). Right column plots for each scenario the error between the different estimations (in the case of GPs only the mean value is taken into account) and the ground truth.
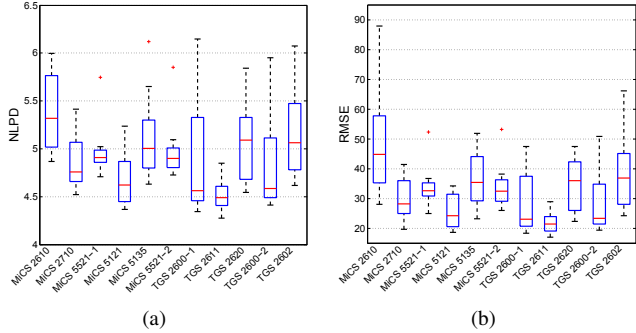

Fig. 4. NLPD and RMSE box-plot for the case of one-sensor GP calibration. For both indicators, as lower the value the better calibration. On each box, the central red mark is the median, the edges of the box are the 25th and 75th percentiles, the whiskers extend to the most extreme data points not considered outliers, and outliers are plotted individually as red crosses.

V. Conclusion and Future Works

In this paper we have proposed a new approach for metal oxide (MOX) gas sensors calibration when used in Open Sampling Systems (OSS). We approached the problem from a probabilistic perspective, employing Gaussian Processes to obtain an estimate of a posterior distribution over the gas concentration given the response of a MOX sensor. This has the advantage of enabling not only predictions of the expected value of gas concentration but also predictions of the uncertainty of the estimation. This advantage is particularly relevant for OSS applications where typically many sources of uncertainty exist.

Future works may include the use of the whole array in the estimation process in order to produce more accurate gas

TABLE I

Sensor Model	GPs	PLSR	SVR
MiCS 2610	43.81 ± 22.88	44.79 ± 14.26	46.01 ± 19.44
MiCS 2710	30.38 ± 7.83	31.89 ± 6.13	29.71 ± 6.42
MiCS 5521-1	33.64 ± 9.02	34.26 ± 7.03	34.09 ± 7.56
MiCS 5121	**23.84 ± 5.58**	**25.44 ± 4.20**	**24.18 ± 5.91**
MiCS 5135	32.09 ± 12.00	35.61 ± 8.21	33.37 ± 12.31
MiCS 5521-2	31.11 ± 8.01	32.37 ± 7.47	31.80 ± 8.09
TGS 2600-1	26.05 ± 10.08	31.10 ± 5.42	25.71 ± 8.79
TGS 2611	**21.46 ± 3.54**	**26.27 ± 3.59**	**21.57 ± 3.14**
TGS 2620	34.16 ± 24.02	35.41 ± 7.08	29.61 ± 8.38
TGS 2600-2	28.96 ± 15.13	32.43 ± 5.98	27.23 ± 9.92
TGS 2602	44.64 ± 15.58	41.87 ± 8.21	37.12 ± 12.69
OVERALL	**31.17 ± 6.27**	**33.77 ± 5.77**	**30.94 ± 6.78**

concentration estimates, the exploration of kernels for time series like the Autoregressive (AR) kernel, or the use of sparse GPs like the Relevance Vector Machine (RVM) or the Informative Vector Machine (IVM).

References

[1] M. Trincavelli, "Gas discrimination for mobile robots," *Künstliche Intelligenz*, vol. 25, no. 4, pp. 351 – 354, 2011.

[2] J. Gonzalez-Jimenez, J. G. Monroy, and J. L. Blanco, "The multi-chamber electronic nose - an improved olfaction sensor for mobile robotics," *Sensors*, vol. 11, no. 6, pp. 6145–6164, 2011.

[3] C. Rasmussen and C. Williams, *Gaussian processes for machine learning*, ser. Adaptive computation and machine learning. MIT Press, 2006.

[4] P. J. Gemperline, J. R. Long, and V. G. Gregoriou, "Nonlinear multi-variate calibration using principal components regression and artificial neural networks," *Analytical Chemistry*, vol. 63, no. 20, pp. 2313–2323, 1991.

[5] H. Sundgren, F. Winquist, I. Lukkari, and I. Lundstrom, "Artificial neural networks and gas sensor arrays: Quantification of individual components in a gas mixture," *Measurement Science and Technology*, vol. 2, no. 5, pp. 464–469, 1991.

[6] K. Domansk, D. L. Baldwin, J. W. Grate, T. B. Hall, J. Li, M. Josowicz, and J. Janata, "Development and calibration of field-effect transistor-based sensor array for measurement of hydrogen and ammonia gas mixtures in humid air," *Analytical Chemistry*, vol. 70, no. 3, pp. 473–481, 1998.

[7] L. Hadjiiski, P. Geladi, and P. Hopke, "A comparison of modeling non-linear systems with artificial neural networks and partial least squares," *Chemometrics and Intelligent Laboratory Systems*, vol. 49, no. 1, pp. 91–103, 1999.

[8] M. Blanco, J. Coello, H. Iturriaga, S. Maspoch, and J. Pags, "Calibration in non-linear near infrared reflectance spectroscopy: A comparison of several methods," *Analytica Chimica Acta*, vol. 384, no. 2, pp. 207–214, 1999.

[9] R. P. Cogdill and P. Dardenne, "Least-squares support vector machines for chemometrics: An introduction and evaluation," *Journal of Near Infrared Spectroscopy*, vol. 12, no. 2, pp. 93–100, 2004.

[10] A. Shmilovici, G. Bakir, S. Marco, and A. Perera, "Finding the best calibration points for a gas sensor array with support vector regression," in *Intelligent Systems, 2004*, vol. 1, june 2004, pp. 174 – 177 Vol.1.

[11] M. Trincavelli, S. Coradeschi, and A. Loutfi, "Odour classification system for continuous monitoring applications," *Sensors and Actuators B: Chemical*, vol. 58, pp. 265 – 273, 2009.

[12] H. Ishida, T. Nakamoto, and T. Moriizumi, "Remote sensing of gas/odor source location and concentration distribution using mobile system," *Sensors and Actuators B: Chemical*, vol. 49, no. 1-2, pp. 52 – 57, 1998.

[13] M. Trincavelli and A. Loutfi, "Feature selection for gas identification with a mobile robot," in *Proceedings of the IEEE International Conference on Robotics and Automation (ICRA)*, 2010, pp. 2852 – 2857.

[14] T. Nakamoto and K. Yoshikawa, "Movie with scents generated by olfactory display using solenoid valves," in *Virtual Reality Conference, 2006*, March 2006, pp. 291 – 292.