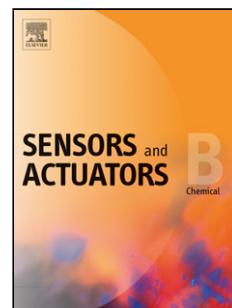


Accepted Manuscript



Title: Reservoir Computing compensates slow response of chemosensor arrays exposed to fast varying gas concentrations in continuous monitoring

Author: Jordi Fonollosa Sadique Sheik Ramón Huerta
Santiago Marco

PII: S0925-4005(15)00352-4

DOI: <http://dx.doi.org/doi:10.1016/j.snb.2015.03.028>

Reference: SNB 18221

To appear in: *Sensors and Actuators B*

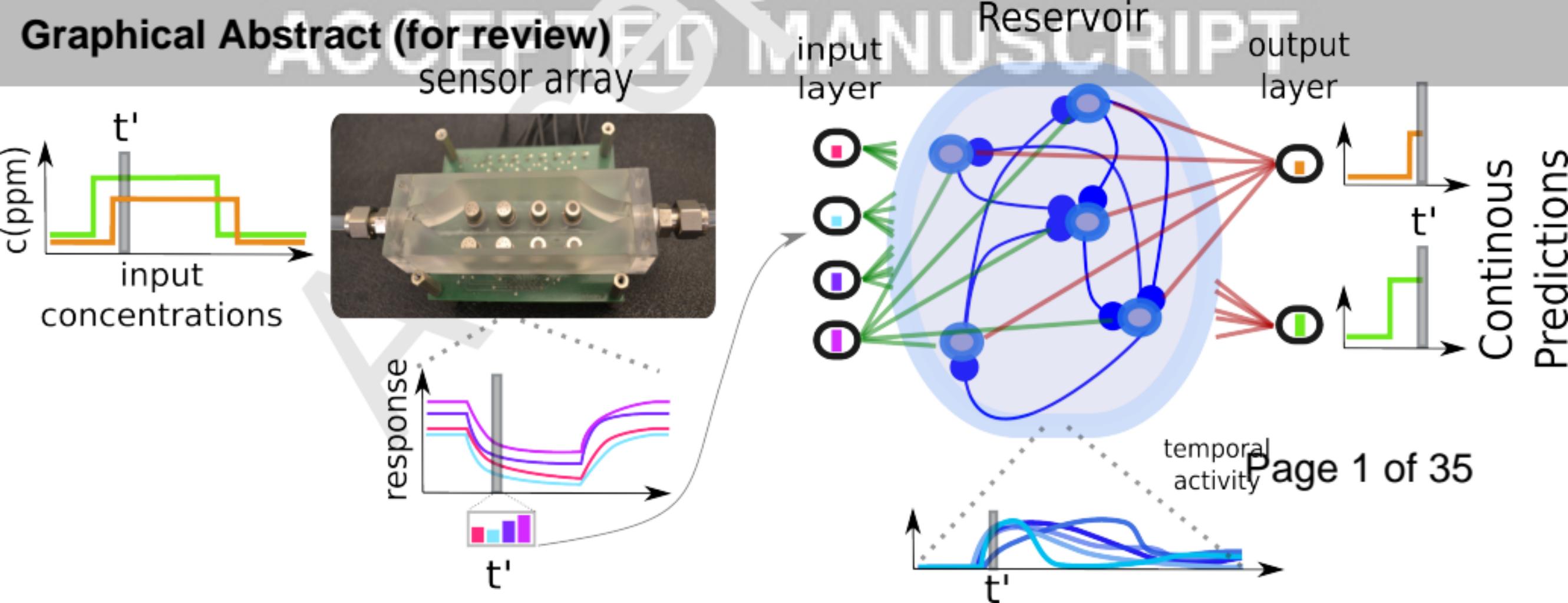
Received date: 31-10-2014

Revised date: 12-3-2015

Accepted date: 17-3-2015

Please cite this article as: Jordi Fonollosa, Sadique Sheik, Ramón Huerta, Santiago Marco, Reservoir Computing compensates slow response of chemosensor arrays exposed to fast varying gas concentrations in continuous monitoring, *Sensors & Actuators: B. Chemical* (2015), <http://dx.doi.org/10.1016/j.snb.2015.03.028>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



We applied Reservoir Computing (RC) algorithms to chemical gas sensor data

The RC approach improves the time response of the chemical sensory system

RC is able to provide accurate predictions in real time

RC is suitable for continuous monitoring applications and open sampling systems

Our approach was tested over two public datasets that include dynamic gas mixtures

Reservoir Computing compensates slow response of chemosensor arrays exposed to fast varying gas concentrations in continuous monitoring

Jordi Fonollosa^{a,b}, Sadique Sheik^a, Ramón Huerta^a, Santiago Marco^{b,c}

^a*BioCircuits Institute (BCI), University of California San Diego.
9500 Gilman Dr., La Jolla, CA 92093, USA*

^b*Signal and Information Processing for Sensing Systems, Institute for Bioengineering of Catalonia (IBEC).
Baldíri Reixac, 4-8, Barcelona, 08028, Spain*

^c*Departament d'Electrònica, Universitat de Barcelona.
Martí i Franquès, 1, Barcelona, 08028, Spain*

Abstract

Metal Oxide (MOX) gas sensors arrays are a predominant technological choice to perform fundamental tasks of chemical detection. Yet, their use has been mainly limited to relatively controlled instrument configurations where the sensor array is placed within a closed measurement chamber. Usually, the experimental protocol is defined beforehand and it includes three stages: the array is first exposed to a gas reference, then to the gas sample, and finally to the reference again to recover the initial state. Such sampling procedure requires signal acquisition during the complete experimental protocol and usually delays the output prediction until the predefined measurement duration is complete. Due to the slow time response of chemical sensors, the completion of the measurement typically requires minutes. In this paper we propose the use of Reservoir Computing (RC) algorithms to overcome the slow temporal dynamics of chemical sensor arrays, allowing identification and quantification of chemicals of interest continuously and reducing measurement delays. We generated two datasets to test the ability of RC algorithms to provide accurate and continuous prediction to fast varying gas concentrations in real time. Both datasets – one generated with synthetic data and the other acquired from actual gas sensors – provide time series of MOX sensors exposed to binary gas mixtures where concentration levels change randomly over time. Our results show that our approach improves the time response of the sensory system and pro-

Email address: fonollosa@ucsd.edu (Jordi Fonollosa)

vides accurate predictions in real time, making the system specifically suitable for online monitoring applications. Finally, the collected dataset and developed code are made publicly available to the research community for further studies.

Keywords: Electronic Nose, Chemical sensors, Reservoir Computing, Continuous gas prediction, Online detection, MOX sensors, time response, Real-time detection

1. Introduction

Chemo-resistive transducers, and MOX-based sensors in particular, are a predominant sensor choice to solve a wide variety of complex tasks due to their sensitivity, ease of use, low-cost, and fast response time compared to other technologies. The response of these sensors carries information about the presented stimulus in both the steady-state and the transient portions of the signals [1, 2, 3]. Hence, in order to capture the information contained in the dynamics of the sensors, usually, the sampling methodology is based on a fixed, predefined experimental protocol: Typically, before and after sample presentation, the sensor array is exposed to a gas reference (*clean air*) to capture the rising and decaying signal transients [4, 5]. Then, the complete set of acquired time series, or a set of features extracted from the time series [6, 7, 8, 9, 10], is used to train a calibration model [11, 12]. Therefore, such a calibration methodology requires the acquisition of the complete set of features to evaluate a new sample, making it necessary to capture the sensors' signals over a measurement time defined beforehand. As a result, the model prediction for a new sample can only be provided after the measurement is complete.

Experimental protocols based on the presentation of gas reference require complex delivery systems since it is necessary to alternate the gas sample with the reference baseline. Furthermore, the composition of the gas samples has to remain constant during the whole sample presentation, which assumes certain control on the samples. In many real world applications, one may not have control over the order of gas exposure, concentration of the volatiles present in the mixture or the duration of sample exposition. For example, in open sampling systems the sensor array is exposed directly to the environment with no measurement test chamber, making the system sensitive to flow turbulence, such as alarms for toxic and inflammable compounds and fire alarms based on chemical sensors [13]. Also, autonomous platforms designed for odor source localization, as they navigate towards the source, may cross the gas plume several times, experiencing sudden and rapid gas concentration transitions. A rapid detection of the concentration change is paramount for efficient gas source localization and preventing erratic robot behavior [14]. Hence, robotic navigation but also continuous monitoring and process control applications, are hindered by the slow time response of gas sensing systems that behave as non-linear low-pass filters. A method that is able to provide

continuous and accurate prediction according to the present and past states of the sensor array would be better suited for such applications.

The dynamic behavior of chemical sensor systems has been modeled in the past, remarking the need of dynamic non-linear models [15, 16]. The design of inverse filters or deconvolution algorithms for linear systems is well understood and limited by noise [17], but the nonlinearity of chemical sensors challenges the design of multivariate data processing algorithms for real-time prediction.

Only a few works have explored quantitative prediction algorithms for continuous gas concentration estimation with fast varying concentration inputs. In essence, they were based on a regressor with tapped-delayed input to provide a finite and fixed memory to the system. In particular, tapped-delay predictors have been explored with linear (Finite Impulse Response filters) and polynomial regressors (Wiener regressors)[18], neural networks [18, 19, 20, 21] or support vector regressors [20]. However, in such architectures the memory is fixed by the length of the chain (or duration of the delay) and has to be optimized in calibration phase.

In a different approach, Monroy et al., and more recently Di Lello et al., presented a model to provide continuous prediction in time. The model alternates two linear dynamical systems fitted to the rise/recovery phase dynamics of MOX sensors. From the sensors' responses, they estimate the probability of increasing/decreasing ethanol concentration, from where they select the corresponding linear inverse model based on Kalman Filtering approach [14, 22].

In this work we propose the use of RC algorithms to estimate gas concentrations in dynamic mixtures due to their ability to provide continuous prediction in time with implicit memory and to cope with the nonlinearities present in MOX gas sensors. To the best of our knowledge, only Muezzinoglu et al. have explored a signal conditioning scheme that can be considered as a mathematical image of RC algorithms for chemical gas data [23, 24]. They addressed a three-class classification problem. However, their experimental protocol required a gas reference before the volatile was introduced, keeping the sample onset always at the same time. Moreover, gas class was kept constant (both, analyte and concentration) during the whole data acquisition, sensors' baselines were corrected for each measurement, and time was scaled. In contrast, we evaluated the use of RC algorithms in a regression task using a synthetic dataset and a dataset acquired with MOX sensors exposed to dynamic

gas mixtures¹. The datasets provide time-series from MOX sensors and were generated by exposing the gas sensors to binary mixtures of gases, the concentration of which changed to random levels at arbitrary times. Our results show that by means of RC algorithms, it is possible to estimate the concentration levels in dynamic gas mixtures in real-time, without the restriction of defining a fixed duration for the measurement or waiting until the sensors recover the baseline (see Fig. 1). Hence, our approach is sensitive to changes in sample composition that happen at random times, making it specifically suitable for monitoring and navigation applications. The remainder of the paper is organized as follows. We review the general working principles of RC algorithms (Section 2). Then, we present the methodology to generate the datasets (Section 3), followed by the results (Section 4) and the conclusions of this work (Section 5).

2. Reservoir Computing algorithm

In this paper we show the feasibility of RC algorithms to predict the concentration of dynamic gas mixtures in real-time. Reservoir Computing [25, 26] approach employs a large network of recurrent randomly connected non-linear units, e.g. neurons, to transform temporally varying input signals to a higher dimension. The output of such a network is then used by simple linear units that can be trained to operate as regressors or classifiers. An important feature of this algorithm is that the recurrent non-linear dynamic units are not trained, being trained only the output linear layer.

In addition to the nonlinearity of neurons, RC algorithms rely on two key strategies to efficiently classify its inputs [27, 28]:

Projection to a higher dimension. The random connections from input to the recurrent network enable projection of input to a large population of neurons. This organization allows for linear separation of two classes that were not linearly separable in the input space. It has also been shown theoretically that such random projections enable “mixed selectivity” in the neuron’s response properties, which are very critical for classification of complex inputs and for performance of complex cognitive tasks [29].

¹The generated dataset is made publicly available to the research community at [weblink]. The code is provided in the Supplementary Material

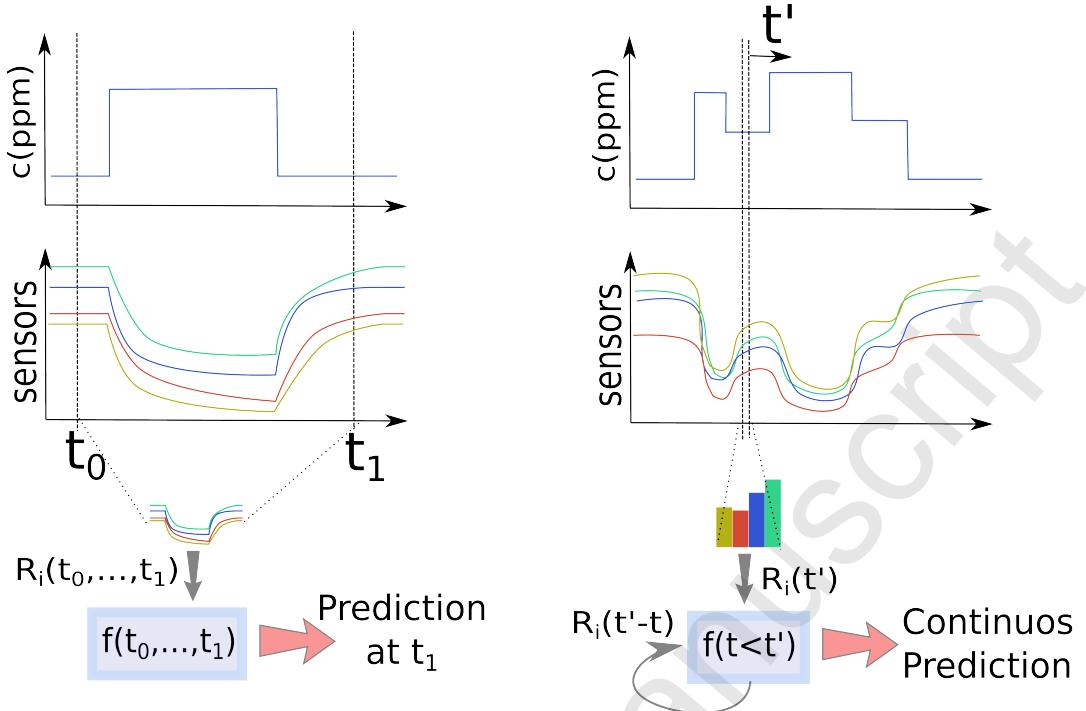


Figure 1: Experimental protocols are designed to capture the information contained in the dynamics of the chemical sensors. Typically, the sensors are exposed to a gas reference before and after sample presentation, while the sensors' signals are continuously acquired. The acquired time series S_{data} , or a set of extracted features, are used to build a predictor. In order to evaluate new samples, the complete set of features needs to be supplied to the classifier, making it necessary to wait until the end of the measurement defined in the experimental protocol (left panel). For a real-time system that deals with time varying input signals, a more dynamic protocol that relies on acquiring instantaneous activity to make continuous predictions would be more suitable (right panel).

Induce memory. In addition to the random feed forward projections from the inputs to a large pool of neurons, a reservoir consists of *recurrent* connections within this pool. Such recurrent connections impart dynamics to the pool, which allows transfer of temporal information over time. This configuration, in essence, provides diversity of time constants to the network about its inputs in the recent past, thereby converting temporal information into spatial information. The relevant dynamics for the modeling task are selected only by the weights of the output linear layer.

Because of these properties, the response of the reservoir is easily classifiable with any linear classifier/regressors, only using spatial information ie. instantaneous activity of the reser-

voir. Unlike the traditional approach, where the classifiers are directly trained on the inputs, the linear classifiers/regressors here are trained on the activity of the reservoir in response to the inputs. In terms of the underlying neural network, only the weights of projections from the reservoir to the classifier are modified during the training process (see Fig. 2). All other weights remain constant during the training and testing period.

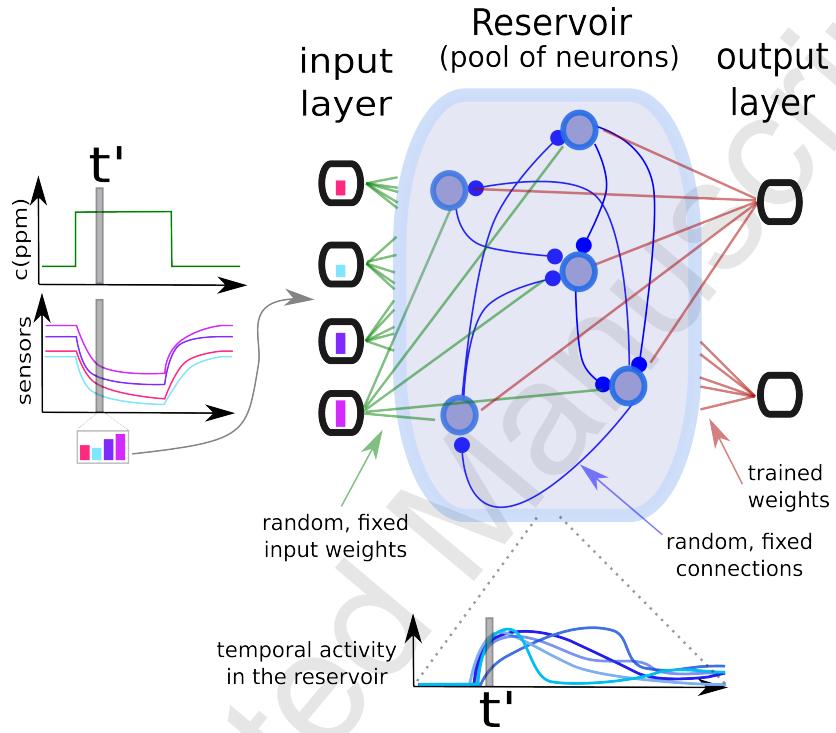


Figure 2: Reservoir of recurrently connected neurons receiving inputs from sensors. The inputs are connected to all the neurons of the intermediate layer. The random connections between neurons generate internal dynamics in the network that carry temporal information in the network. The neurons are connected to the output layer such that the weights are adapted to assign one output to each class. This configuration corresponds to a classical RC scheme [30]. The sensors in the array respond to the gas with a temporally changing response profile. The instantaneous sensor responses are fed into the reservoir at every time step through random projections. The recurrently connected neurons in the reservoir transform the input to a higher dimensional temporally varying activity signal. The higher dimensional activity signals of the neurons are used to train the output layer consisting of classifiers or regressors to make predictions on the presented gas concentrations.

The non-linear elements in the reservoir are randomly interconnected, such that they capture the dynamical properties of the input. The connectivity is defined by two scalar parameters namely “input scaling” and “spectral radius”. On the one hand, the “input scaling” effects the input weight matrix that connects inputs to the reservoir. The input

weight matrix (σ) is generated from a uniform distribution with weights in the interval $[-1, +1]$. This weight matrix is then rescaled by multiplying it by the “input scaling”. The value of “input scaling” is chosen such that the input activity can induce sufficient activity in the reservoir.

On the other hand, the “spectral radius” is the magnitude of the largest eigen vector of the connectivity matrix of the reservoir. The weights of the connectivity matrix of the reservoir (ρ) are initialized from a Gaussian distribution, with mean 0 and variance 1. The matrix is multiplied by a scalar number so that the magnitude of its largest eigen vector is equal to the desired “spectral radius”. This parameter is chosen to ensure that the resultant activity of the reservoir on presentation of the input is sufficiently diverse for different classes of inputs.

The dynamics of the reservoir can be described as:

$$\dot{X} = \text{Sigm}(\sigma \cdot u + \rho \cdot X) \quad (1)$$

where X is a vector representing the state of neurons in the reservoir and whose connectivity weight matrix is given by ρ . σ is the weight matrix for connections from inputs $u(t)$ to the reservoir. In the case where sensor data is used as inputs, $u(t) = S_{\text{data}}(t)$, the sigmoid activation function $\text{Sigm}(x)$ of each neuron is defined by:

$$\text{Sigm}(x) = \frac{1}{1 + e^{-x}} \quad (2)$$

To sum up, the ability of reservoir computing algorithms to carry temporal information makes them suitable for real-time gas concentration prediction. The input to the reservoir is the instantaneous activation levels acquired from the sensors, which generate the dynamics in the internal layer of the reservoir. When the weights of the connections between the neurons and the outputs are properly defined after a training phase, the system is able to provide predictions in real time.

We used the open-source Python library Oger [31] for the implementation of the algorithms developed to predict gas concentration levels. The developed code is available in the Supplementary Material of this paper.

3. Benchmark Datasets

We generated two datasets to explore the ability of RC algorithms to identify and quantify the presence of chemicals in dynamic gas mixtures in real time. We focused the study on MOX sensors since they are a common choice in machine olfaction. The first dataset is based on sensor models that simulate sensor conductivity when exposed to gas mixtures, whereas the second dataset was acquired from actual MOX sensors exposed to mixtures of volatiles. Both datasets were generated using binary gas mixtures at random concentration levels. Hence, different temporal dynamics in the sensors induced by different input transitions were included in the datasets.

3.1. Synthetic dataset

The sensitive layer of a MOX sensor and the chemical sample exchange oxygen/electrons between each other, producing a change in the sensor conductivity. The composition of the sensing layer and the operating temperature of the sensor, which is usually controlled with a built-in heater, determine the sensor sensitivity to the different gas samples.

Based on experimental observations, Clifford-Tuma introduced a model to describe the sensor conductivity (G_S) as a function of the gas concentration (c) and the sensor conductivity in air (G_0). The model can be described by the equation:

$$\frac{G_S}{G_0} = (1 + b \cdot c)^\beta \quad (3)$$

where b and β are parameters that depend on the gas sample under test and the sensor's operating temperature [32, 33]. Correct fitting of the Clifford-Tuma model in the steady-state and at different temperatures was confirmed with experimental data [34, 35, 36]. Equation 3 can be extended to binary mixtures of gases:

$$\frac{G_S}{G_0} = \left(1 + b_1 \cdot \left(c_1 + \frac{\left((1 + b_2 \cdot c_2)^{\beta_2} \right)^{1/\beta_1}}{b_1} \right) \right)^{\beta_1} \quad (4)$$

where b_1 , β_1 and b_2 , β_2 are the coefficients of the sensor for the two gases present in the mixture, at concentrations c_1 and c_2 respectively [37]. Hence, from the sensor behavior when the sensor is exposed to pure compounds, the model predicts sensor response when it is exposed to gas mixtures.

We utilized the model presented in Eq. 4 to generate synthetic data from an heterogeneous sensor array exposed to binary gas mixtures. In particular, the array included models for the following commercially available MOX sensors: SB-11, SB-30, SB-31, SB-95, SB-2, SB-3, SP-11, SP-41, SP-42a, SP-53, SP-AQ2 (FIS Inc., Hyogo Japan). Models' coefficients were fitted from mixtures of Carbon Monoxide (CO) and Methane in air based on experimental measurements. More details on the sensors' models and the parameter fitting can be found in Ref. [38].

Using the fitted sensor models, we simulated the resistance change of 11 MOX sensors when exposed to changing mixtures of CO and Methane in air. The concentration levels changed randomly in the range of 15 – 60 ppm, in intervals of 60 s. The signals were acquired with a 16-bit ADC sampling at a constant frequency of 100 Hz. The gas sample was simulated to flow constantly at 300 ml/min through a 100 ml measurement test chamber. The dynamics of the test chamber was simulated by means of a second order low pass filter with 20 s time constant. For a more realistic scenario, thermal noise equivalent to 1 ppm was introduced in the system. During the whole simulation, the operating temperature of the sensors was kept constant at 375 °C. The total duration of the simulation was 6000 s, thereby generating 100 different binary combinations of concentration levels.

3.2. Hardware recordings

In addition to the simulated data, we also measured sensor responses from a real MOX sensor array in response to dynamic gas mixtures.

3.2.1. Experimental setup

We built a chemical sensing system to measure the conductivities of a MOX sensor array exposed to different gas conditions. The complete system consists of a data acquisition platform, a power control module, and a chemical delivery system. For an accurate and reproducible data generation, the system was fully operated by a computerized environment (see Fig. 3).

The developed chemical detection platform included 16 off-the-shelf chemical sensors (Figaro Inc., US). In particular, the sensor array was composed of 4 different types of sensors: TGS-2600, TGS-2602, TGS-2610, TGS-2620 (4 units of each type). The sensors were integrated with customized signal conditioning and control electronics. The operating voltage of

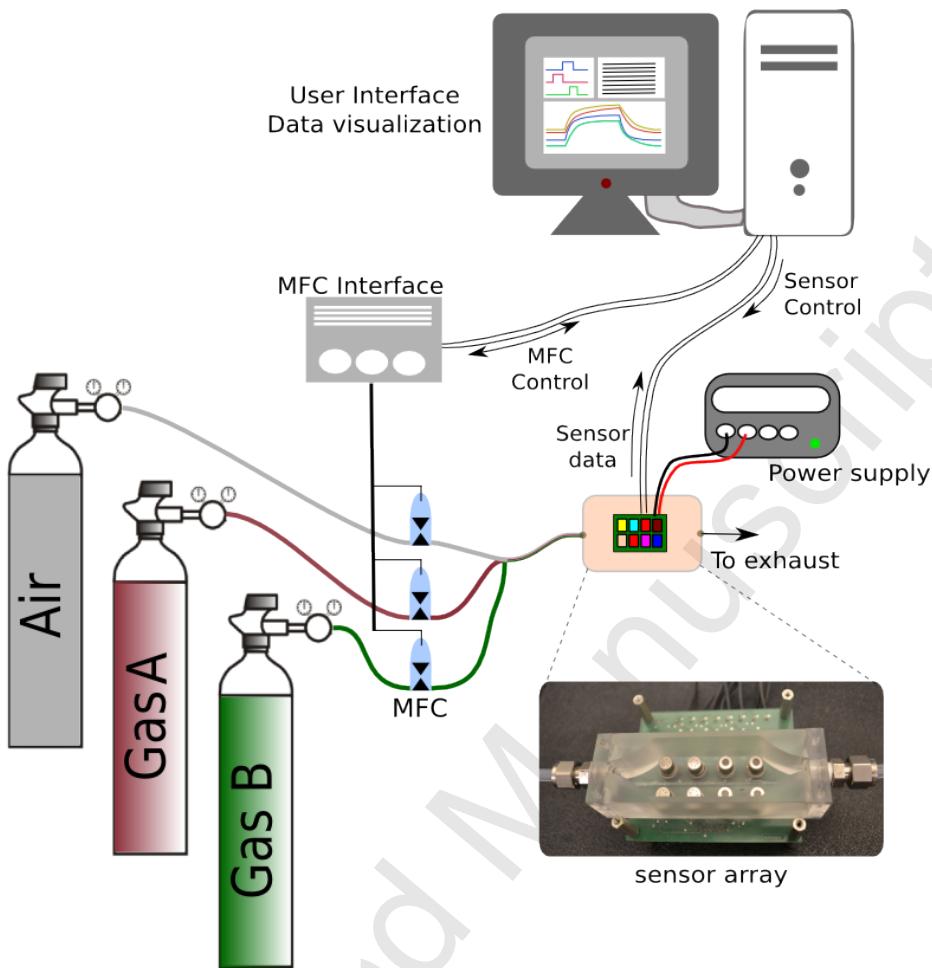


Figure 3: The gas sensor array was integrated with signal conditioning and control electronics. The time series generated by the sensors when exposed to changing gas conditions were acquired continuously. By means of a set of Mass Flow Controllers the total flow was kept constant, while changing the gas concentration in the measurement chamber.

the sensors, which controls the sensors' operating temperature, was kept constant at 5 V for the whole duration of the experiments. The sensors' conductivities were acquired continuously at 100 Hz by means of a computer with a data acquisition board (PCI-6023E, National Instruments).

The sensor array was placed in a 60 ml measurement chamber, where the gas sample was injected at a constant flow of 300 ml/min. The flow control system was based on three different branches made of Polyethylene (inner diameter 3/16", outer diameter: 1/4"). To control individually the gas flow of each branch while keeping the total flow constant, each branch was connected to a different pressurized gas cylinder through a Mass Flow

Controller (MFC) system. The first fluidic branch was used to control the flow of dry air supplied by Airgas Inc. in a pressurized gas cylinder. The other two branches were free to be connected to any pressurized gas cylinder. The three branches met together to obtain the desired gas mixture. Finally, the resulting mixture circulated continuously through the measurement chamber and was collected by the exhaust system.

Hence, by means of the set of MFCs and the acquisition system, the sensor array was exposed to controlled and changing gas conditions while the sensors' signals were recorded. At the end of the measurement, we acquired 16 time-series that were indicative of the presented gas conditions.

3.2.2. Experimental protocol

Using the experimental setup described previously, we exposed the chemical sensors to dynamic mixtures at random concentration levels. In particular, we generated gas mixtures of Ethylene with Methane or CO. To the best of our knowledge, it is the first experimental protocol in which gas mixtures are controlled such that the concentration levels can change to random values at random time intervals.

The dataset includes a continuous measurement in which mixtures of Ethylene and Methane in air were generated, and another measurement for the mixture of Ethylene and CO in air. Each measurement was constructed by the continuous acquisition of the 16-sensor array signals for a duration of about 12 hours without interruption. While we describe the methodology to set the concentration levels for the generated mixtures of Ethylene and Methane in air, we followed the same methodology to acquire data for mixtures of Ethylene and CO.

In order to set the concentration profiles for Ethylene and Methane respectively, we defined 4 different states. Each state defined a measurement block. The measurement blocks were concatenated to complete 12 hours of acquisition. Figure 4a shows the four states that defined the complete profile of concentrations. The first state was aimed to perform random variations of Methane concentration while Ethylene concentration was kept constant. To do so, we first chose the duration of the block randomly in the interval $800 - 1000\text{ s}$, and we set the Ethylene concentration for the entire block. Then, the concentration level of Methane was selected such that 50% of the times was set to 0 ppm . The duration of the Methane

concentration was randomly chosen from the interval $80 - 120\text{ s}$. The Methane concentration was changed in the specified time intervals until the total duration reached the block duration. Similarly, the second state aimed at measuring changes produced by variations in the Ethylene concentration while Methane levels remained unchanged. The procedure to define Methane/Ethylene concentration profiles was analogous as the one explained for the first state. The third state defined transitions of different Ethylene concentrations to air and no Methane was released. For a period of time included in the interval $800 - 1000\text{ s}$, Ethylene concentration was changed randomly every $80 - 120\text{ s}$. To ensure transitions to and from the baseline, Ethylene levels were set to 0 ppm randomly 50% of the times. Finally, the fourth state intended to measure the system reaction to pure Methane transitions, using the experimental procedure analogous to the third state. The mixtures of Ethylene with CO were generated following the same methodology, changing only the concentration levels (see Fig. 4b).

At the beginning, ending, and approximately every 10000 s , we inserted additional predefined concentration patterns with pure gas mixtures. The purpose of the predefined pattern was twofold. On the one hand, it was used to control the measurement and verify its correct execution. On the other hand, the repetition of the same pattern along a long measurement will allow further study of short-term drift or baseline deviations in MOX sensors.

The concentration ranges for Ethylene, Methane, and CO were selected based on previous studies with similar experimental setups [39, 40, 41]. We selected the concentration levels such that the induced magnitudes of the sensor responses were similar. Moreover, for gas mixtures, lower concentration levels were favored. Therefore, the multivariate response of the sensors to the presented set of stimuli is challenging since none of the configurations (single gas or mixture presentation) can be easily identified from the magnitude of sensors' responses. Figure 5 shows a portion of the acquired signals with the corresponding gas concentration levels and the map of measured concentration levels.

Hence, in contrast to traditional experimental protocols, we were able to acquire the sensors' responses to complex transitions that are usually not considered, such as changing (increasing, decreasing, or setting to zero) the concentration of one volatile while the concentration of the other volatile is kept constant.

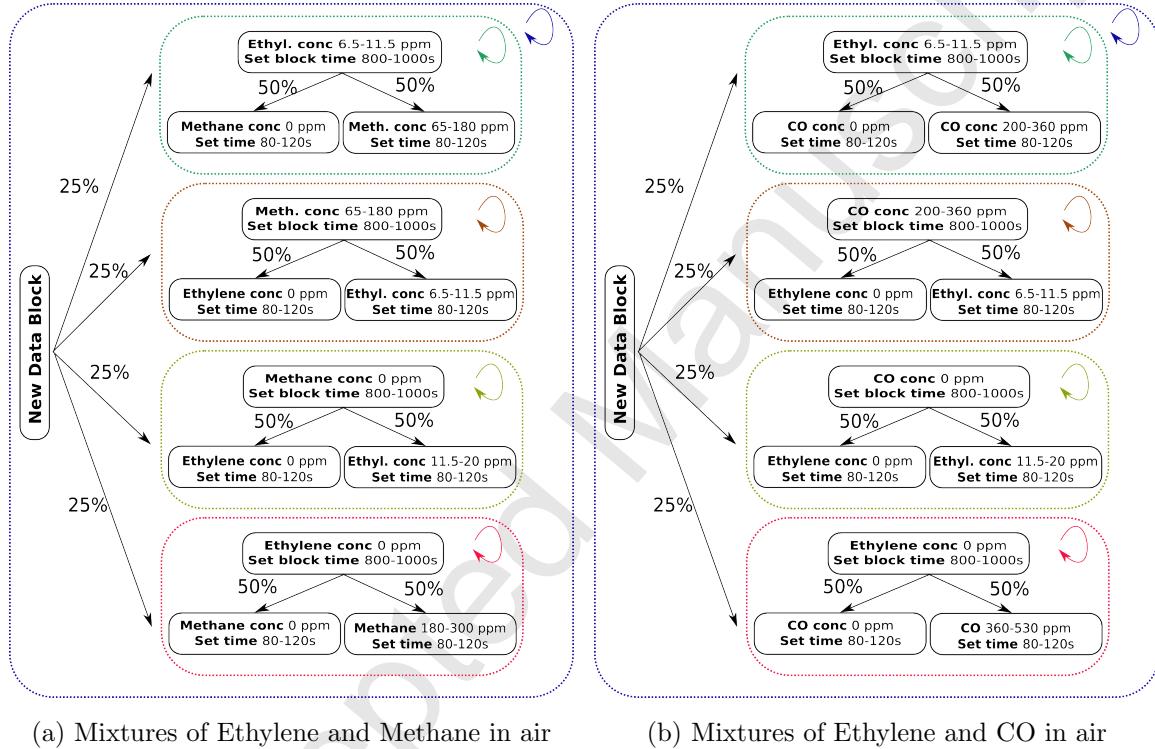


Figure 4: We followed the same methodology to generate the mixtures of (a) Ethylene with Methane and (b) Ethylene with CO, changing only the concentration levels. The complete profile of concentration levels was set by the concatenation of measurement blocks. Each block was defined by four equally probable states. To induce responses of similar magnitude and make the dataset more challenging for the classifiers, lower concentration levels were favored for gas mixtures.

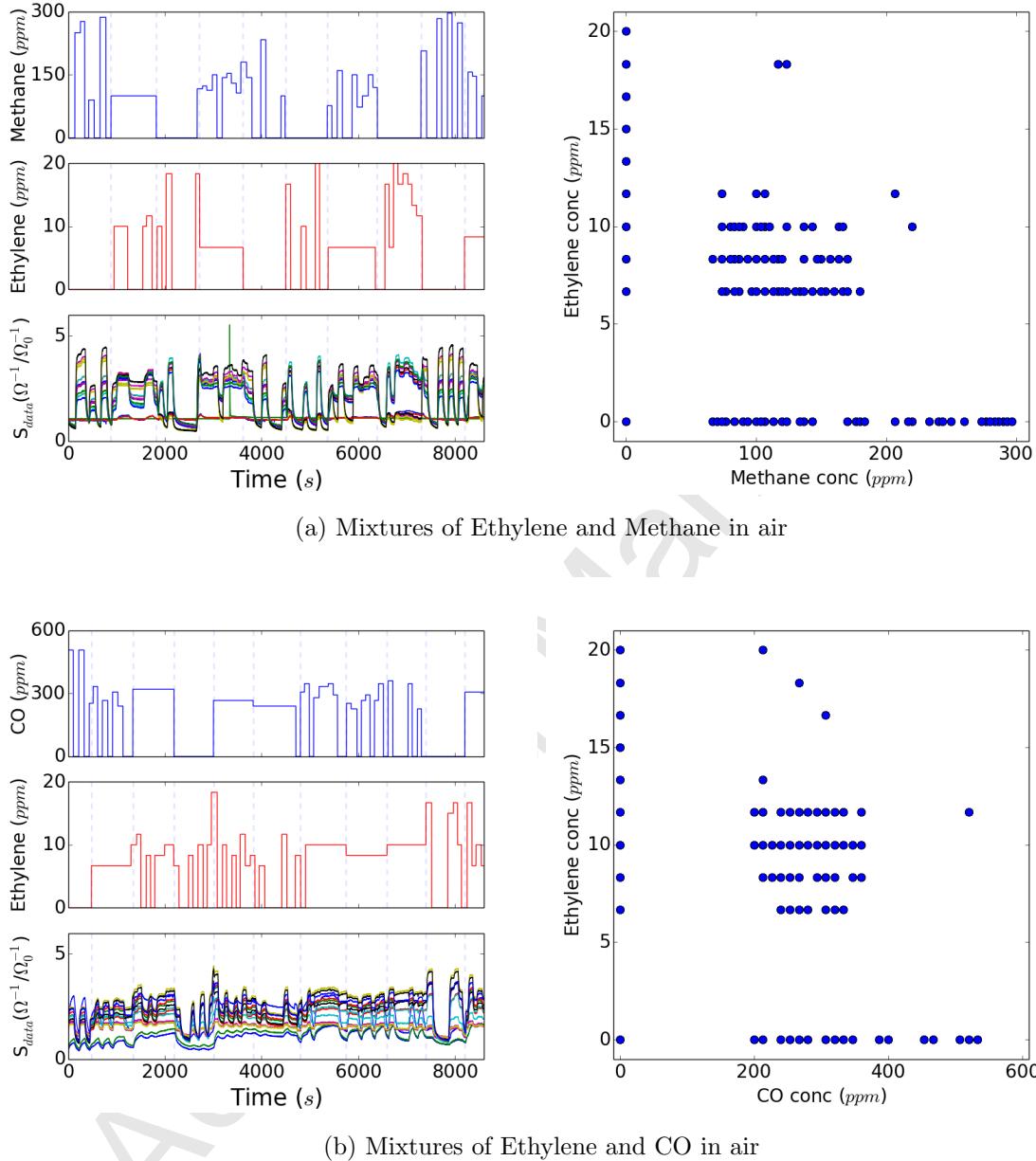


Figure 5: (a) (left) Portion of the acquired signals S_{data} (bottom) with the corresponding concentration levels of Ethylene and Methane (upper panels). Auxiliary vertical lines indicate transition between measurement blocks. Note that due to the experiment protocol, in which transition times are set randomly, concentration transitions of both volatiles may not happen simultaneously at the end of each measurement block. (right) Map of the measured concentration points. For gas mixtures, lower concentration levels are favored to induce similar magnitude change in the sensors' signals. (b) Idem for the mixture of CO and Ethylene in air.

4. Results

We aimed at applying reservoir computing algorithms to a practical and challenging scenario in which gas sensors are exposed to gas mixtures with varying concentration levels changing at arbitrary times. In order to simulate this scenario, we produced two datasets, one set of simulated signals from a 11-sensor array and a second set of time-series data acquired from a 16-sensor array. In this section we describe the obtained results with both datasets.

4.1. Synthetic dataset

The simulated time-series follow the concentration set points, and the sensors show different sensitivities to the presented volatiles (see Section 3.1 for details on data generation). Figure 6 shows the simulated sensors' responses (top panel) exposed to varying concentration levels of CO and Methane, which are shown in the third and fourth panels. The sensors' signals do not reach the steady state since the dynamics of the sensor system are slower than the changes in the gas concentrations, making the prediction more challenging for the regressors.

The generated dataset was divided in a training phase and a test phase, in which the accuracy of the model was evaluated. In particular, the model was trained utilizing the initial 3600 s ie. 60% of the complete dataset. Using only the training dataset, we trained two linear regressors on the reservoir activity while the reservoir is being exposed to synthetic data for gas mixtures of Methane and CO. We used “spectral radius” = 0.9 and “input scaling” = 10^{-6} as parameter values to train the reservoir. We utilized a reservoir composed of 200 neurons randomly interconnected, which is sufficiently larger than the input dimension. The integration time step used for the simulations was 10 ms which was the same as the sampling frequency. The reservoir states evolve according to the sensors' responses (see Fig. 6, second panel). The output of the classifiers after training are presented in the lower panels of the same figure, showing that the predicted values follow the input concentrations and that the built model can be used to estimate the presented gas mixture. To quantify the accuracy of the models, we computed the root mean square (RMS) error of the estimated gas concentrations, being 7.5 ppm for CO and 3.3 ppm for Methane. These absolute errors correspond to 11.4% and 5.7% errors (relative to the maximum concentration levels presented) in CO and Methane respectively.

We also trained two linear regressors without the RC to evaluate the benefits of our approach. Table 1 shows a comparison of the prediction errors with the reservoir approach and the linear regressors. The noise introduced in the gas concentrations during the generation of simulated data is also included in the table since it provides a limit for the performance. Considering the noise in the simulated data, the classifiers trained with the reservoir were able to approximate and faithfully follow the concentration of both gases based on simulated sensor data. It is also interesting to note that the training algorithm was trained with the noisy gas concentrations as opposed to the set point values. This leads to the reservoir also trying to model the noise in the system.

Algorithm	Methane (ppm)	CO (ppm)
Simulation noise	1.0	1.0
Linear regressor	9.2	7.7
Reservoir	7.5	3.3

Table 1: Comparison of simulation induced noise to prediction errors obtained with a linear regressor and Reservoir computing. The reservoir approach performs significantly better than a simple linear regressor.

4.2. Recordings from real MOX sensors

Encouraging results from experiments with synthetic data led us to extend the same approach to real MOX sensor recorded data. A sensor array of 16 MOX sensors was exposed to two different sets of dynamic gas mixtures - Methane with Ethylene and CO with Ethylene - to acquire two sets of data (see Section 3.2.2 for more details on data acquisition).

Acquired data was divided in training and test sub sets. Likewise the simulated data from sensors, the initial 60% of data was used to train the network and the residual 40% was then used to test the prediction accuracy. The training subsets were used as input to the reservoir, with linear regressors being trained on the reservoir activity to estimate the underlying gas concentrations. We used “spectral radius” = 0.1 and “input scaling” = 10^{-5} for training a reservoir of 100 units. The different values of the parameters compared to the synthetic dataset are due to the different ranges of the input data. However, as shown in Supplementary Material Fig S.1, the performance of the predictor remains stable for wide range of parameters.

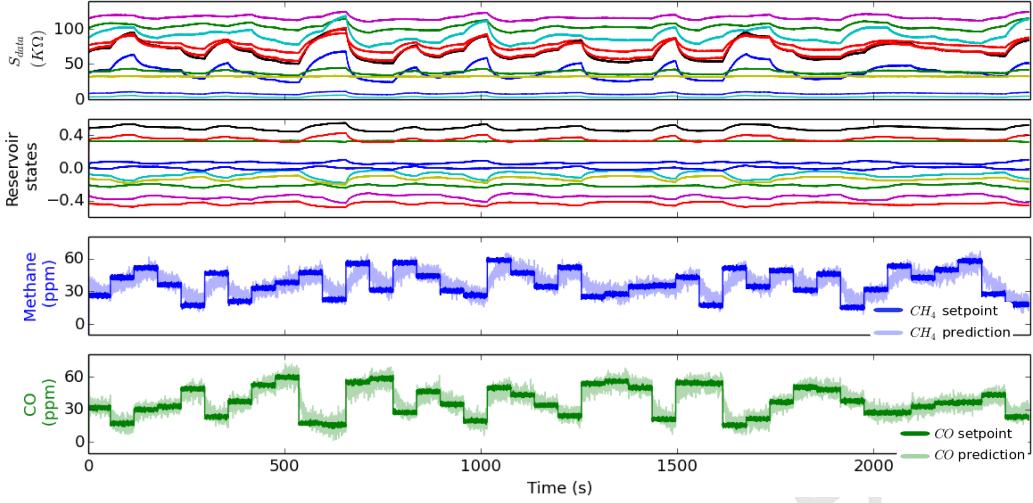


Figure 6: Response of the system to the presentation of varying concentrations of Methane and Carbon Monoxide simultaneously. The upper plot shows the response S_{data} of 11 sensors to mixtures of Methane and CO in air. The second panel shows the activity in the reservoir over time (for visualization purposes, only 10 randomly selected neurons out of 200 are shown). The lower panels show the predicted concentrations along with the corresponding setpoints.

The prediction performance of RC algorithms was evaluated for both mixtures. In the case where Ethylene and Methane were simultaneously presented (Fig. 7a), the RMS error of the estimated gas concentrations for Ethylene is 7.2% and for Methane is 4.5%, relative to the corresponding maximum presented concentrations. These errors correspond to 1.3 ppm and 12.5 ppm RMS errors in Ethylene and Methane respectively. In the case where Ethylene and CO were simultaneously presented (Fig. 7b), the RMS error of the estimated gas concentrations for Ethylene is 8.3% and for CO is 8.5% with respect to the maximum concentration values, corresponding to 1.7 ppm and 45.9 ppm RMS errors in Ethylene and CO respectively.

We also evaluated the performance of a linear regressor and a nonlinear support vector regression that had already been tested with MOX data to identify volatiles and quantify their concentration levels [42]. Both models operated directly on the raw sensor data. We compared the accuracy of the regressors with and without RC. We also considered the experimental error, which was estimated for each volatile from the errors introduced by the MFCs, that result in uncertainty in the gas flows, and the tolerance in the nominal gas concentration in the pressurized cylinders. Table 2 shows the RMS error in ppm for the regressors along with the experimental errors. The obtained errors are in accordance with the experimental errors

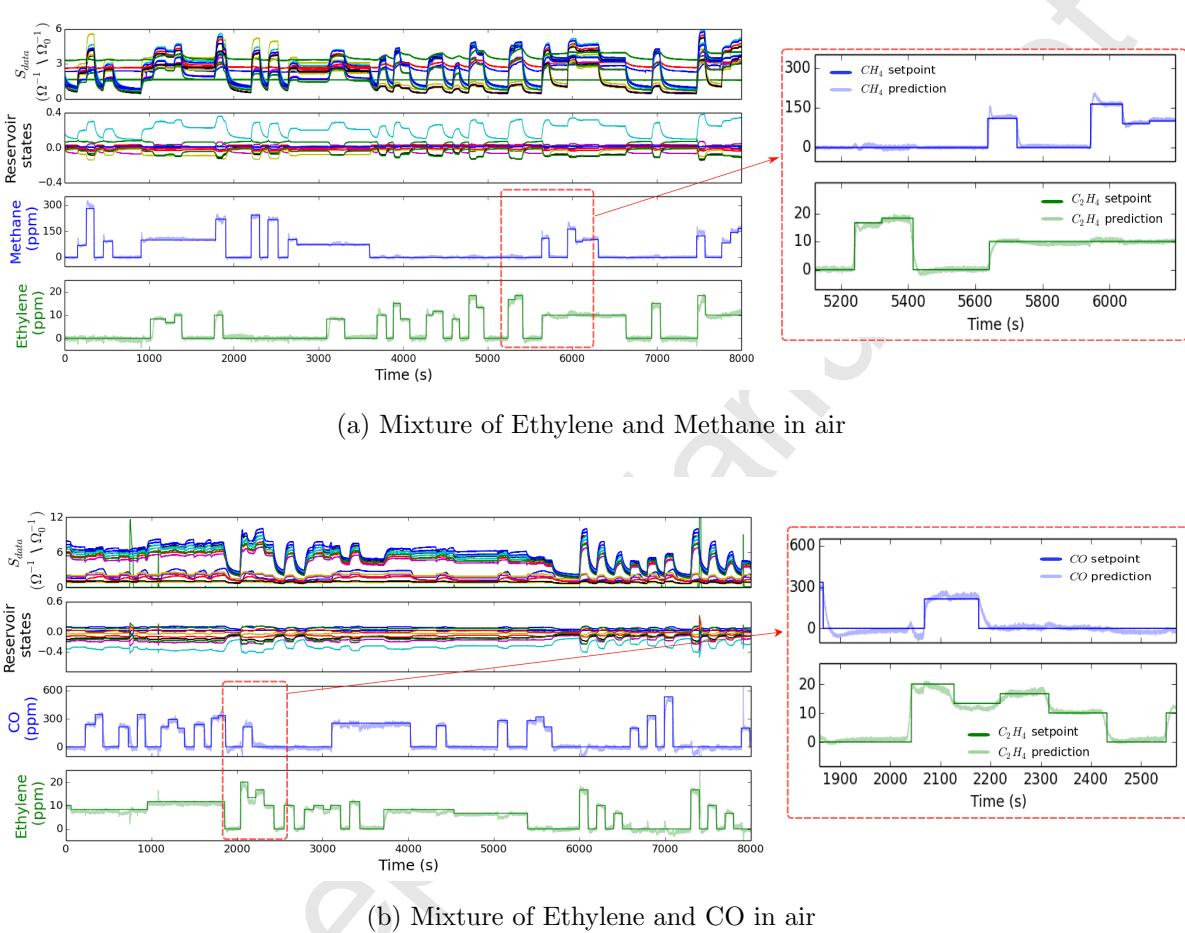


Figure 7: Response of the system to the presentation of varying mixtures of Ethylene and Methane in air (a) and Ethylene and CO in air (b). (a) The first panel shows normalized conductivities of 16 sensors, S_{data} , when the sensors are exposed to the concentration mixtures defined by the setpoints. The second plot shows the activity of 10 of the 100 neurons of the reservoir over time. Third panel shows predicted concentration levels of Methane along with the corresponding setpoints. The lower panel shows the predicted concentrations and setpoints of Ethylene. (b) Idem for the mixture of Ethylene and CO in air. Closer views of predictions and setpoints confirm that predictions follow accurately concentration setpoints (right-hand side panels).

introduced in the experimental setup, which limit the accuracy of the predictions. In all the tested gas mixtures, the RC improves the accuracy of the regressors. The performance increase is significantly higher (35% for Methane and CO) when the prediction error of linear system is far from the experimental error.

To observe the distribution of the error along the different concentration levels, the predicted measurements were compared to the concentration set points from the above experiments across all the tested concentrations (see Fig. 8). As it can be seen from the plots, the data points remain close to the diagonal signifying that the predicted values follow the actual concentrations very efficiently.

Finally, to validate the robustness of the results we generated 20 new partitions of the collected datasets. The datasets were divided in training/test sets including the same number of training/test points as in the original partition (60/40% respectively). However, for this new evaluation, the time series were closed in a cyclic loop such that the first sample was concatenated after the last sample of the captured strings. We selected one random point for each partition that represented the initial measurement, and selected the following 60% of samples for training and the last 40% for test, rolling around from the last sample to the beginning of the collected data to complete the sets.

The methodology based on RC consistently provided better results than the SVR and the linear regressor when evaluated on the reorganized datasets. Figure 9 compares the accuracy provided by the three tested regressors. The approach based on RC resulted in more accurate predictions than the linear regressors and provided smaller prediction error than SVR for most of the data partitions. The nonparametric Wilcoxon signed-rank test for paired data was used to test whether the distribution of prediction errors provided by the RC approach differs from the errors obtained with linear regressors or SVR (ie the tested approaches have significantly different prediction ability). A one-sided test provided p-values of 4×10^{-5} for the linear regressor versus RC, for both Methane and CO. Similarly, the test resulted in p-values of 4×10^{-5} and 2×10^{-3} for SVR versus RC, for CO and Methane respectively. Hence, one can conclude that the errors provided with the approach based on RC are statistically significantly lower than the errors obtained by means of the other tested approaches. Moreover, it is important to note that while such random partitions let us evaluate performance error under different training/test conditions, it includes a discontinuity

Algorithm	Ethylene (ppm)	Methane (ppm)	Ethylene (ppm)	CO (ppm)
Experimental error	1.4	7.0	1.4	26
Linear regressor	1.7	19.6	1.9	69.8
SVR	1.4	15.9	2.8	59.4
Reservoir	1.3	12.5	1.7	45.9

Table 2: Comparison of experimental errors to prediction errors when utilizing linear regressors, Support Vector Regression and Reservoir computing. The first two columns show errors for the data acquired with mixtures of Ethylene with Methane and the last two columns show the errors for mixtures of Ethylene and CO. The reservoir approach performs almost 35% better than a simple linear regressor when the volatiles are far from the limit that represents the experimental error. RC provides better accuracy in the predictions than SVR due to the ability of RC to obtain information from the sensors’ dynamics. The performance is bounded by the experimental errors.

in the time series and breaks the acquired temporal dynamics of the sensors in the return point. Temporal discontinuities lower prediction accuracy of RC algorithms since they rely on temporal properties of the presented data. Despite such limitation, RC still outperforms the other two tested regressors.

The above results indicate that classifiers trained with the reservoir outperform other classifiers in the accuracy predictions due to the ability of RC to include in the prediction information contained in the sensors’ dynamics. Hence, RC are able to quantify the concentration of the components present in a gas mixture when long-time effects and drift are not significant.

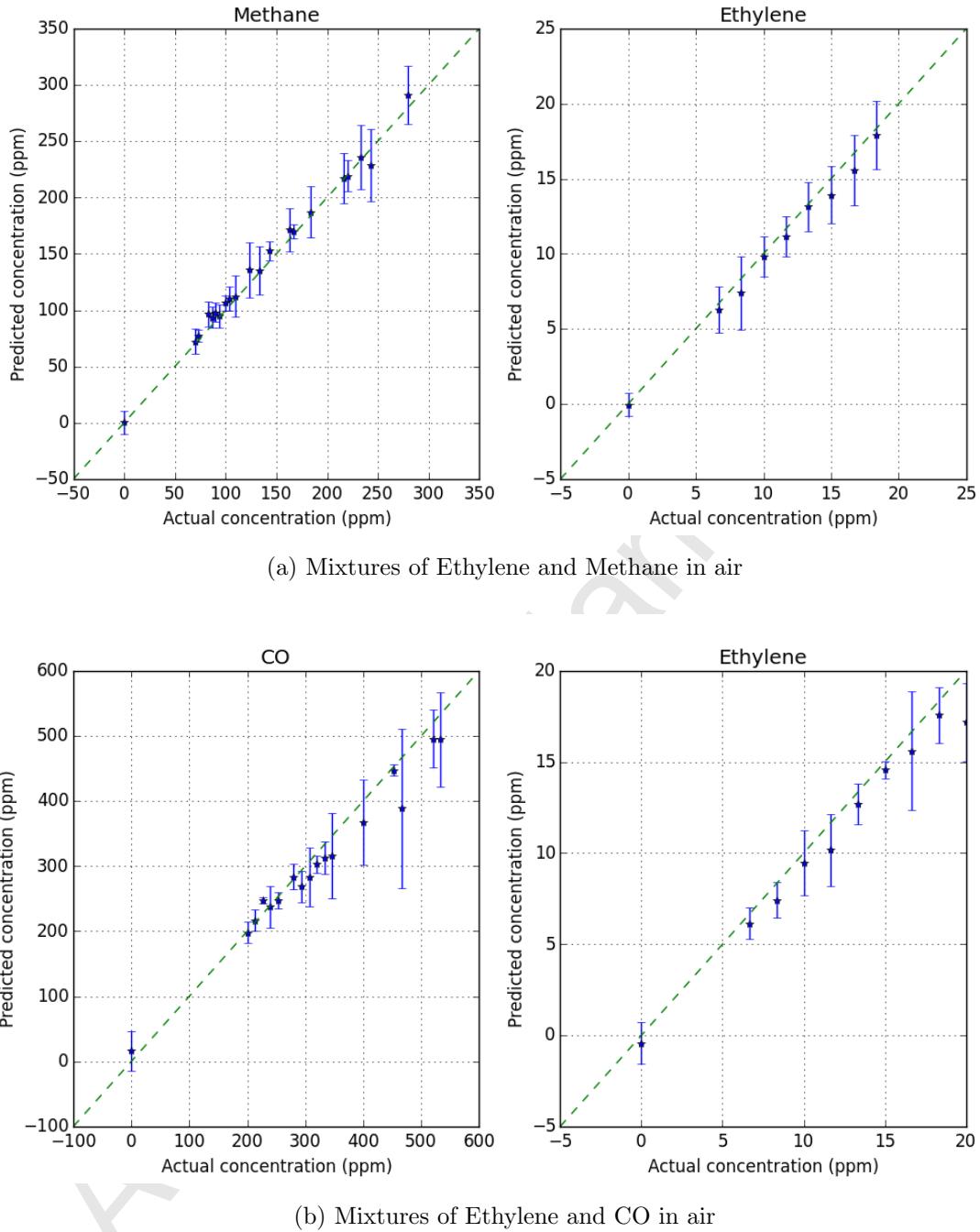


Figure 8: Predicted concentrations compared to the actual concentration set points for (a) mixture of Ethylene with Methane and (b) mixture of Ethylene with CO. The mean and standard deviation of the predicted concentrations are plotted across the concentration set points during the experiments. Although negative concentration levels are not realistic, we employed generic linear regressors that were not constrained to positive values. The prediction errors resulting from this generalization can be observed at zero concentration values, as shown in the plots. The errorbars at zero concentration show that the methodology does not provide large negative concentration values that may limit predictions at low concentrations.

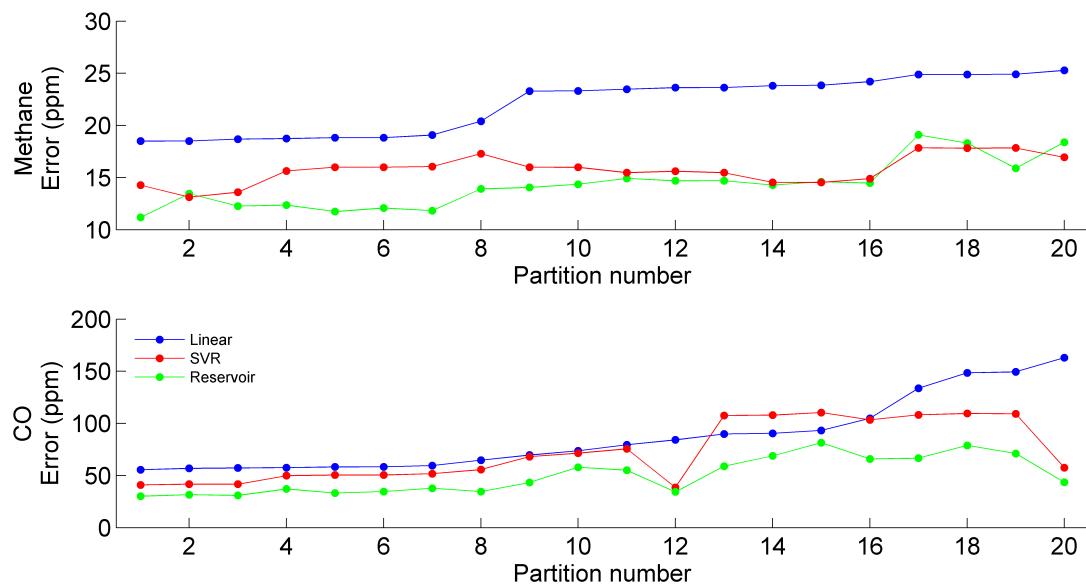


Figure 9: Prediction error provided by RC (green), SVR (red), and linear regressor (blue) for Methane (top) and CO (bottom) after 20 random data partitions. Both gases are presented in mixtures of Ethylene. Ethylene predictions are not presented since concentration errors are close to the experimental error and the benefits of using RC algorithms to predict concentration levels are not noticeable. Partitions are rearranged to increasing error provided by the linear regressor. Despite discontinuities introduced in the temporal dynamics of the sensors' time series, RC still outperforms the other two tested regressors.

5. Discussion and Conclusions

We proposed the use of Reservoir Computing (RC) algorithms to identify and quantify volatiles of interest continuously in real-time. We tested our approach with two datasets: a synthetic dataset based on sensors' models and a second dataset generated from data acquired from gas sensors. The datasets provided time-series of MOX gas sensors exposed to binary gas mixtures, the concentrations of which changed randomly over time. Our results show the feasibility of RC algorithms to predict and correctly identify volatiles in addition to estimating their actual concentrations.

Previously proposed algorithms for continuous gas concentration estimation were based on linear models or tapped-delayed networks. However, the capacity of memory in tapped-delayed networks is limited by the duration of the defined delay. Simple linear models only consider the value of the sensor after it reached the steady-state [43, 44, 45, 46]. Such a feature extraction procedure assumes that the gas composition remains constant until the sensor reaches the steady-state and discards any information contained in the sensor's dynamics. A system based on RC algorithms, owing to their nonlinearity and implicit memory, overcomes these limitations and successfully predicts the concentration of gases in mixtures. Hence, our approach is suitable for applications where abrupt concentration changes may occur, such as continuous monitoring applications or chemical source localization.

A very important aspect of real-time sensing is the ability to detect varying concentration of unstable gas mixtures. This feature is hindered by the slow response of gas sensors. Instrument configurations where the sensors are located within a gas chamber tend to be even slower. These systems are generally unable to follow rapid changes in gas concentration within a mixture. Moreover, algorithms based on batch, sequential measurements typically require very constrained experimental setups with fixed concentrations and fixed time length measurements. The complete measurement is required to provide a new prediction, and the system output can only be provided when the predefined measurement duration is complete. Furthermore, they require precise control of the gas concentration during the measurement since the sample onset always happens after the same time interval from the start of the measurement. Therefore, these algorithms cannot be directly applied to continuous sensing scenarios. Such scenarios demand methods and algorithms that can operate on streams of

measurements and incorporate information contained on the sensors' dynamics such as RC algorithms, overcoming the requirement of traditional experimental protocols that delay the system prediction until the measurement is finished. Therefore, algorithms based on RC are better suited for open sampling systems, in which the sensors are exposed directly to gas plumes in a turbulent environment, or continuous monitoring and alarm applications, in which large number of volatiles are expected to fluctuate irregularly [47, 48]. Previous experimental protocols in open sampling systems also assume control of the gas onset, which happens at specific times from the beginning of the measurement [49, 50]. A calibration model based on RC would be sensitive to changes in the sample composition at all times and to turbulence. Hence, it would provide a better representation of the spatio-temporal structure of the gas plume, which contains information on the position of the gas source [51].

Other appealing features of the approach presented here are that RC is very robust to moderate variations in the hyperparameters and that training the reservoir is extremely fast since it only requires the estimation of a linear regressor. Moreover, with increasing reservoir size, the performance of the reservoir is shown to improve [28]. It must be noted that the objective of this paper was to propose reservoir computing as a viable estimation method that incorporates information contained on the gas sensors' transients to the prediction, and not to find the most optimized set of parameters, especially since the parameters are dependent on the data set or specific set of sensors in use. Lukosevicius [28] elaborately discusses the techniques and recommendations for successfully applying reservoir computing (in particular echo state machines) to maximize system performance. Finally, RC requires no preprocessing and works on raw data acquired directly from the sensor array. This feature makes the implementation of an online system easier by not relying on explicit external memory to save the measurement time series.

Our results indicate that a gas detection system based on Reservoir Computing algorithms is capable of correctly identifying the variations in the gases by observing the sensors' time series in response to the changes in the composition of a gas sample in real time. However, there are several challenges that are posed while working with MOX sensors, such as drift of response over time, dependence on environmental conditions and variability across different "identical" sensors. In our future work, we will explore the plausibility of RC algorithms to tackle some of these challenges in chemical sensing. Furthermore, we made the collected data

and developed code available to the community for further development and benchmark of other approaches.

Acknowledgments

This work has been supported by the U.S. Office of Naval Research (ONR) (Grant # N00014-13-1-0205), by the California Institute for Telecommunications and Information Technology (CALIT2) (Grant # 2014CSRO 136), by the National Institute on Deafness and Other Communication Disorders (Grant # R01 DC011422), by ENIAC Joint Undertaking Programme (Grant # ENIAC JU 621272), and by the Spanish project PCIN-2013-195. JF and SM are members of the consolidated research group SGR2014-1445 by the Generalitat de Catalunya. JF acknowledges the support of the Secretary for Universities and Research of the Ministry of Economy and Knowledge of the Government of Catalonia and the COFUND programme of the Marie Curie Actions of the 7th *R&D* Framework Programme of the European Union, 2013 BP-B 00190. We thank Brenton Maisel for proof-reading the manuscript.

References

- [1] J. Samitier, J. Lopez-Villegas, S. Marco, L. Camara, A. Pardo, O. Ruiz, J. Morante, A new method to analyse signal transients in chemical sensors, *Sensors and Actuators B: Chemical* 18 (1) (1994) 308–312.
- [2] C. Di Natale, S. Marco, F. Davide, A. D'Amico, Sensor-array calibration time reduction by dynamic modelling, *Sensors and Actuators B: Chemical* 25 (1) (1995) 578–583.
- [3] E. Llobet, J. Brezmes, X. Vilanova, J. E. Sueiras, X. Correig, Qualitative and quantitative analysis of volatile organic compounds using transient and steady-state responses of a thick-film tin oxide gas sensor array, *Sensors and Actuators B: Chemical* 41 (1) (1997) 13–21.
- [4] S. Marco, A. Gutiérrez-Gálvez, Signal and data processing for machine olfaction and chemical sensing: a review, *Sensors Journal, IEEE* 12 (11) (2012) 3189–3214.
- [5] M. Trincavelli, S. Coradeschi, A. Loutfi, Odour classification system for continuous monitoring applications, *Sensors and Actuators B: Chemical* 139 (2) (2009) 265–273.
- [6] A. Perera, T. Yamanaka, A. Gutiérrez-Gálvez, B. Raman, R. Gutiérrez-Osuna, A dimensionality-reduction technique inspired by receptor convergence in the olfactory system, *Sensors and Actuators B: Chemical* 116 (1) (2006) 17–22.
- [7] E. Llobet, O. Gualdrón, M. Vinaixa, N. El-Barbri, J. Brezmes, X. Vilanova, B. Bouchikhi, R. Gómez, J. Carrasco, X. Correig, Efficient feature selection for mass spectrometry based electronic nose applications, *Chemometrics and Intelligent Laboratory Systems* 85 (2) (2007) 253 – 261.
- [8] F. Röck, N. Barsan, U. Weimar, Electronic nose: current status and future trends, *Chemical reviews* 108 (2) (2008) 705–725.
- [9] I. Rodriguez-Lujan, R. Huerta, C. Elkan, C. S. Cruz, Quadratic programming feature selection, *The Journal of Machine Learning Research* 11 (2010) 1491–1516.

- [10] J. S. Murguía, A. Vergara, C. Vargas-Olmos, T. J. Wong, J. Fonollosa, R. Huerta, Two-dimensional wavelet transform feature extraction for porous silicon chemical sensors, *Analytica chimica acta* 785 (2013) 1–15.
- [11] R. Gutierrez-Osuna, Pattern analysis for machine olfaction: a review, *Sensors Journal, IEEE* 2 (3) (2002) 189–202.
- [12] M. K. Muezzinoglu, A. Vergara, R. Huerta, N. Rulkov, M. I. Rabinovich, A. Selverston, H. D. Abarbanel, Acceleration of chemo-sensory information processing using transient features, *Sensors and Actuators B: Chemical* 137 (2) (2009) 507 – 512.
- [13] S.-J. Chen, D. C. Hovde, K. A. Peterson, A. W. Marshall, Fire detection using smoke and gas sensors, *Fire Safety Journal* 42 (8) (2007) 507–515.
- [14] J. G. Monroy, J. González-Jiménez, J. L. Blanco, Overcoming the slow recovery of MOX gas sensors through a system modeling approach, *Sensors* 12 (10) (2012) 13664–13680.
- [15] F. A. Davide, C. D. Natale, A. D'Amico, A. Hierlemann, J. Mitrovics, M. Schweizer, U. Weimar, W. Göpel, S. Marco, A. Pardo, Dynamic calibration of qmb polymer-coated sensors by wiener kernel estimation, *Sensors and Actuators B: Chemical* 27 (1) (1995) 275–285.
- [16] S. Marco, A. Pardo, F. A. Davide, C. D. Natale, A. D'Amico, A. Hierlemann, J. Mitrovics, M. Schweizer, U. Weimar, W. Göpel, Different strategies for the identification of gas sensing systems, *Sensors and Actuators B: Chemical* 34 (1) (1996) 213–223.
- [17] A. Bennia, S. M. Riad, Filtering capabilities and convergence of the van-cittert deconvolution technique, *Instrumentation and Measurement, IEEE Transactions on* 41 (2) (1992) 246–250.
- [18] A. Pardo, S. Marco, J. Samitier, Nonlinear inverse dynamic models of gas sensing systems based on chemical sensor arrays for quantitative measurements, *Instrumentation and Measurement, IEEE Transactions on* 47 (3) (1998) 644–651.
- [19] M. Pardo, G. Faglia, G. Sberveglieri, M. Corte, F. Masulli, M. Riani, A time delay

neural network for estimation of gas concentrations in a mixture, Sensors and Actuators B: Chemical 65 (1) (2000) 267–269.

- [20] S. De Vito, A. Castaldo, F. Loffredo, E. Massera, T. Polichetti, I. Nasti, P. Vacca, L. Quercia, G. Di Francia, Gas concentration estimation in ternary mixtures with room temperature operating sensor array using tapped delay architectures, Sensors and Actuators B: Chemical 124 (2) (2007) 309–316.
- [21] S. De Vito, E. Massera, M. Piga, L. Martinotto, G. Di Francia, On field calibration of an electronic nose for benzene estimation in an urban pollution monitoring scenario, Sensors and Actuators B: Chemical 129 (2) (2008) 750–757.
- [22] E. Di Lello, M. Trincavelli, H. Bruyninckx, T. De Laet, Augmented switching linear dynamical system model for gas concentration estimation with MOX sensors in an open sampling system, Sensors 14 (7) (2014) 12533–12559.
- [23] M. K. Muezzinoglu, A. Vergara, R. Huerta, T. Nowotny, N. Rulkov, H. Abarbanel, A. Selverston, M. Rabinovich, Artificial olfactory brain for mixture identification, in: Advances in Neural Information Processing Systems, 2009, pp. 1121–1128.
- [24] M. K. Muezzinoglu, R. Huerta, H. D. Abarbanel, M. A. Ryan, M. I. Rabinovich, Chemosensor-driven artificial antennal lobe transient dynamics enable fast recognition and working memory, Neural computation 21 (4) (2009) 1018–1037.
- [25] T. Natschläger, W. Maass, H. Markram, The “liquid computer”: A novel strategy for real-time computing on time series, Special issue on Foundations of Information Processing of TELEMATIK 8 (LNMC-ARTICLE-2002-005) (2002) 39–43.
- [26] H. Jaeger, The echo state approach to analysing and training recurrent neural networks—with an erratum note, Bonn, Germany: German National Research Center for Information Technology GMD Technical Report 148 (2001) 34.
- [27] H. Jaeger, Echo state network 2 (9) (2007) 2330.
- [28] M. Lukoševičius, A practical guide to applying echo state networks, in: Neural Networks: Tricks of the Trade, Springer, 2012, pp. 659–686.

- [29] M. Rigotti, O. Barak, M. R. Warden, X.-J. Wang, N. D. Daw, E. K. Miller, S. Fusi, The importance of mixed selectivity in complex cognitive tasks, *Nature* 497 (7451) (2013) 585–590.
- [30] L. Appeltant, M. C. Soriano, G. Van der Sande, J. Danckaert, S. Massar, J. Dambre, B. Schrauwen, C. R. Mirasso, I. Fischer, Information processing using a single dynamical node as complex system, *Nature communications* 2 (2011) 468.
- [31] D. Verstraeten, B. Schrauwen, S. Dieleman, P. Brakel, P. Buteneers, D. Pecevski, Oger: modular learning architectures for large-scale sequential processing, *The Journal of Machine Learning Research* 13 (1) (2012) 2995–2998.
- [32] P. Clifford, D. Tuma, Characteristics of semiconductor gas sensors i. steady state gas response, *Sensors and Actuators* 3 (0) (19821983) 233 – 254.
- [33] P. Clifford, D. Tuma, Characteristics of semiconductor gas sensors ii. transient response to temperature change, *Sensors and Actuators* 3 (1983) 255–281.
- [34] Z. Szklarski, K. Zakrzewska, M. Rkas, Thin oxide films as gas sensors, *Thin Solid Films* 174 (1989) 269–275.
- [35] X. Vilanova, E. Llobet, R. Alcubilla, J. E. Sueiras, X. Correig, Analysis of the conductance transient in thick-film tin oxide gas sensors, *Sensors and Actuators B: Chemical* 31 (3) (1996) 175–180.
- [36] J. Fonollosa, L. Fernández, R. Huerta, A. Gutiérrez-Gálvez, S. Marco, Temperature optimization of metal oxide sensor arrays using mutual information, *Sensors and Actuators B: Chemical* 187 (2013) 331–339.
- [37] A. Chaiyboun, R. Traute, O. Kiesewetter, S. Ahlers, G. Müller, T. Doll, Modular analytical multicomponent analysis in gas sensor arrays, *Sensors* 6 (4) (2006) 270–283.
- [38] I. Montoliu, R. Tauler, M. Padilla, A. Pardo, S. Marco, Multivariate curve resolution applied to temperature-modulated metal oxide gas sensors, *Sensors and Actuators B: Chemical* 145 (1) (2010) 464–473.

- [39] A. Vergara, S. Vembu, T. Ayhan, M. A. Ryan, M. L. Homer, R. Huerta, Chemical gas sensor drift compensation using classifier ensembles, *Sensors and Actuators B: Chemical* 166 (2012) 320–329.
- [40] J. Fonollosa, A. Vergara, R. Huerta, Algorithmic mitigation of sensor failure: Is sensor replacement really necessary?, *Sensors and Actuators B: Chemical* 183 (2013) 211–221.
- [41] I. Rodriguez-Lujan, J. Fonollosa, A. Vergara, M. Homer, R. Huerta, On the calibration of sensor arrays for pattern recognition using the minimal number of experiments, *Chemometrics and Intelligent Laboratory Systems* 130 (2014) 123–134.
- [42] M. K. Muezzinoglu, A. Vergara, R. Huerta, A unified framework for volatile organic compound classification and regression, in: *Neural Networks (IJCNN), The 2010 International Joint Conference on*, IEEE, 2010, pp. 1–7.
- [43] P. Althainz, J. Goschnick, S. Ehrmann, H. Ache, Multisensor microsystem for contaminants in air, *Sensors and Actuators B: Chemical* 33 (1) (1996) 72–76.
- [44] L. Zhang, F. Tian, H. Nie, L. Dang, G. Li, Q. Ye, C. Kadri, Classification of multiple indoor air contaminants by an electronic nose and a hybrid support vector machine, *Sensors and Actuators B: Chemical* 174 (2012) 114–125.
- [45] L. Zhang, F. Tian, S. Liu, J. Guo, B. Hu, Q. Ye, L. Dang, X. Peng, C. Kadri, J. Feng, Chaos based neural network optimization for concentration estimation of indoor air contaminants by an electronic nose, *Sensors and Actuators A: Physical* 189 (2013) 161–167.
- [46] M. Mead, O. Popoola, G. Stewart, P. Landshoff, M. Calleja, M. Hayes, J. Baldovi, M. McLeod, T. Hodgson, J. Dicks, et al., The use of electrochemical sensors for monitoring urban air quality in low-cost, high-density networks, *Atmospheric Environment* 70 (2013) 186–203.
- [47] J. Kneer, A. Eberhardt, P. Walden, A. O. Pérez, J. Wöllensteiner, S. Palzer, Apparatus to characterize gas sensor response under real-world conditions in the lab, *Review of Scientific Instruments* 85 (5) (2014) 055006.

- [48] J. Fonollosa, I. Rodriguez-Lujan, A. V. Shevade, M. L. Homer, M. A. Ryan, R. Huerta, Human activity monitoring using gas sensor arrays, Sensors and Actuators B: Chemical 199 (2014) 398–402.
- [49] A. Vergara, J. Fonollosa, J. Mahiques, M. Trincavelli, N. Rulkov, R. Huerta, On the performance of gas sensor arrays in open sampling systems using inhibitory support vector machines, Sensors and Actuators B: Chemical 185 (2013) 462–477.
- [50] J. Fonollosa, I. Rodríguez-Luján, M. Trincavelli, A. Vergara, R. Huerta, Chemical discrimination in turbulent gas mixtures with MOX sensors validated by gas chromatography-mass spectrometry, Sensors 14 (10) (2014) 19336–19353.
- [51] A. J. Lilienthal, T. Duckett, H. Ishida, F. Werner, Indicators of gas source proximity using metal oxide sensors in a turbulent environment, in: Biomedical Robotics and Biomechatronics, 2006. BioRob 2006. The First IEEE/RAS-EMBS International Conference on, IEEE, 2006, pp. 733–738.

Author Biographies

Jordi Fonollosa received his Ph.D. in Electronic Engineering from the University of Barcelona in 2009. His research is focused on gas sensor array robustness and optimization, support vector machines, and Information Theory applied to chemical sensing. Other strong interests include biologically inspired algorithms, signal recovery systems, and infrared sensing technologies.

Sadique Sheik received his Ph.D. from ETH Zurich in 2013. He is a Postdoctoral Researcher at the BioCircuits Institute, UC San Diego. His research is at the intersection of Machine Learning with biological systems modelling. Other strong interest include neuromorphic engineering, role of stochasticity in learning, and large scale neuromorphic systems.

Ramón Huerta received his Ph.D. from Universidad Autónoma de Madrid in 1994. He is a Research Scientist at the BioCircuits Institute, UC San Diego. Prior his current appointment, he was Associate Professor at the Universidad Autónoma de Madrid (Spain). His areas of expertise include dynamic systems, artificial intelligence, and Neuroscience. His work deals with the development algorithms for the discrimination and quantification of complex multidimensional time series, model building to understand the information processing in the brain, and chemical sensing and machine olfaction applications based on bio-inspired technology. Dr. Huerta's research work gathers in a publication record of over 100 articles in peer-reviewed journals at the intersection of computer science, physics, and biology.

Santiago Marco (Ph.D., 1993 – University of Barcelona) is Associate Professor at the University of Barcelona and head of the Signal and Information Processing for Sensor Systems Lab at the Institute for Bioengineering of Catalonia, Barcelona, Spain. His research concerns the development of signal/data processing algorithmic solutions for smart chemical sensing based in sensor arrays or microspectrometers integrated typically using microsystem technologies. Dr. Marco research has produced over 100 articles in peer-reviewed archival journals. More at <http://www.ibecbarcelona.eu/research-groups/signal-and-information-processing-for-sensing-systems/>