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A time delay neural network for estimation of gas concentrations in a mixture

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Abstract

The problem of quantifying the concentrations of CO and NO_2 present in a mixture starting from the electrical response of a sensors array is addressed. A comparison between a traditional approach based on the steady state conductance and one using a time delay neural network is drawn.

Keywords: Neural network; Gas; Mixture

1. Introduction

Many successful attempts of distinguishing different single gas species and estimating their concentrations starting from the conductance variations of chemical sensors arrays are reported in the literature [3,6]. Much less frequent is the case in which the concentration of the components of a gas mixture is estimated [2]. In this contribution data from a five-sensors array exposed to different concentrations steps of the mixture $CO–NO_2$ were analyzed. We adopted two different approaches for estimating concentrations with artificial neural nets (ANN): a more classical one, using the ratio $R = (G_f)/(G_0)$ of the steady state to the baseline conductance, and one based on the temporal evolution of the conductance.

2. Experimental

An array of five tin oxide thin films have been deposited through the R.G.T.O. technique over alumina substrates [4]. A Pt thin film was deposited on the back of the substrate as a heater and temperature sensor. The experimental set-up used for the sensor characterization (measurements) has been described elsewhere [5]. The change of conductance has been monitored by a volt–amperometric technique at constant bias. In order to broaden the array response spectrum, ultra thin films of metal catalysts (Au and Pt) were deposited over the sensor surface. Before characterization, the sensors were aged for 2 weeks by keeping them at the operating temperature.

The array conductance response to nitrogen dioxide (0.2–0.6–2–4 ppm) and carbon monoxide (25–50–100–200 ppm) mixtures was examined. These values are close to the alarm levels for environmental protection in many European countries. During the characterization, relative humidity was set to rh = 30% at $T = 20$°C. Two runs of measurements — each constituted by 24 different concentration mixtures — were completed in order to verify the reproducibility of the array performance. Moreover, since tin oxide sensitivity to NO_2 is enhanced at lower temperature while CO one at higher values, the local operating temperature of two sensors was kept equal to 600 K (Pt, Au), while others were operated at 700 K (bare, Pt, Au).

3. Results and discussion

3.1. Gas responses

In Fig. 1, a typical sensor response to a concentration step is shown. It is known that NO_2 reduces the conduc-

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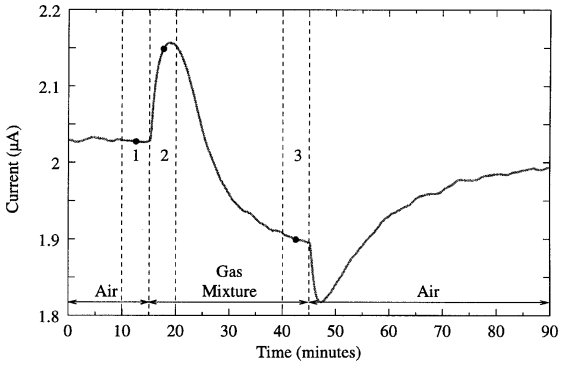

Fig. 1. A typical sensor response. The three zones are depicted in which the input points used in the dynamical method are taken. A particular input is also shown (full points).

tance, while CO produces the opposite effect. Moreover, CO reacts faster with the sensor surface than NO_2 when they are present as single gases. Therefore, one can interpret the response shape in the following way: the fast rise of conductance after the introduction of the mixture is given by the reaction of CO with the surface. After a few minutes, the absorption of NO_2 sets in and the conductivity decreases. Specularly, when the gas introduction is stopped, CO desorbs rapidly followed by NO_2 after circa 1 min.

3.2. Data analysis

We adopted two different approaches for estimating gas concentrations which differ in the way the feature extraction step is performed. In both cases, the first run was used for training and the second for testing.

3.2.1. Steady state approach

We used the ratio $R = (G_f)/(G_0)$ of the steady state to the baseline conductance. Features were extracted by computing the PCA on the training set. The three first principal components, which contain almost 100% of the total variance, were used as the inputs of the nets. We got the best results training two separate networks for the two gases, each with three input, three hidden and one output units. The results are shown in Fig. 2a.

3.2.2. Dynamical approach

In this case, we considered as input of two ANN, for every time t, the conductance G at that time and at some past times — in order to capture the sensors memory effects. The quantity to be estimated is the concentration present at the same time t. The point was now how many delayed time points and what time delay to use. We started with the prescriptions arising from dynamical system theory (Takens–Mane theorem [1]): the number of delayed points should be at least equal to the system's embedding dimension, which is two for our non-chaotic signals, and the time delay comparable to the first zero of the autocorrelation function, which turned out to be 28 min. Moreover, we took account of the physical information contained in the initial peak with which the sensor responds to the concentration step: the peak seems to depend on the relative concentrations of the components. Therefore, we used a third point lying in this zone. The input patterns for every concentration step are — setting $i = 0$ at the gas introduction — $(G(i-50),\ G(i),\ G(i+250))$; $i \in \{1,2,\ldots,50\}$ (see Fig. 1); i is the sample index and the sampling rate is one sample every 6 s. The output is $C(i+250)$, which is constant (on a concentration step) for the teaching output but varies for the predicted output (see Fig. 3). We consequently trained two neural nets, each

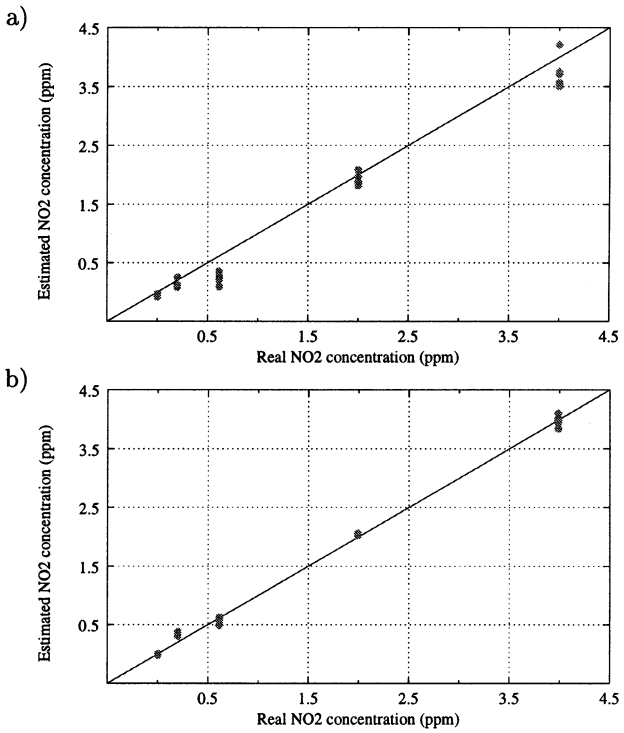

Fig. 2. Comparison between the results of the steady state approach (a) and of the dynamical approach (b) for NO_2.

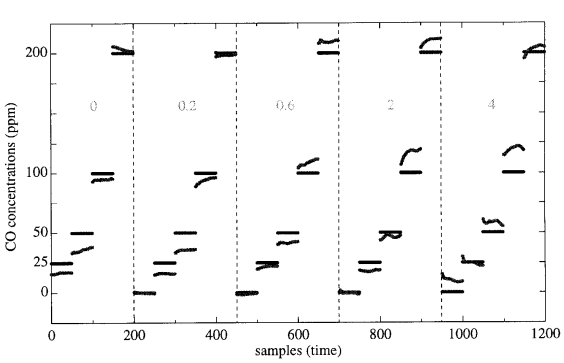

Fig. 3. Dynamical method. Predicted (curved segments) and real concentration (horizontal segments) for CO at the output of the ANN (before the postprocessing). Only the last 50 points of every concentration step are shown. The NO_2 concentrations are displayed in light digits.

with 15 input, 20 hidden and one output units. The post-processing consists in the time average over the 50 predicted concentrations belonging to the same concentration step in order to have one predicted concentration value. The results obtained with the dynamical approach are shown in Fig. 2b. We see that in comparison to the steady state approach, the prediction of NO_2 is sensibly improved. The results for CO are similar for both approaches. We now have that for NO_2, the relative error on 80% of the test patterns is under 5%.

4. Conclusions

In this contribution, a comparison was drawn between an approach which uses steady state data as input of the data analysis and one which uses the information present in the dynamical evolution of the sensor conductivity when exposed to a concentration step. We showed that the prediction of the NO_2 concentration is enhanced with the second procedure. The relative error of the resulting estimation is always less than 20% and in the majority of cases less than 10% for CO and of 5% for NO_2.

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