Estimation of the parameters of SAW sensor's frequency shift: Application to odour recognition and concentration evaluation

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Abstract

In this paper, an approach to determine the time constants and the amplitudes of the mass loading effect and of the viscoelastic contribution of SAW sensor's frequency shift is proposed. This approach consists in optimizing a function of these parameters which is independent of the concentration profile. Then, we show that these values are suitable features for chemical compounds identification and concentration evaluation.
Keywords: SAW sensors, odour recognition, concentration evaluation.

1 Introduction

In this paper, we focus on a category of gas sensors called surfaces acoustic waves (SAW) sensors. These sensors are based on the propagation of mechanical waves produced by piezoelectric materials along a layer composed of a substrate covered by chemically interactive materials. Volatile compounds are absorbed onto the surface of the sensitive material, changing its properties and yielding to a measurable frequency shift of the mechanical waves. It was established that the frequency shift is the superposition of two main contributions (the electro-acoustic one can be neglected) [1]:

1. a viscoelastic contribution due to changes in the coating's Young modulus; and
2. a mass loading effect due to changes of the coating film's mass.

These contributions can be modelled by first order linear differential equations [1]:

$$\begin{cases} \tau_m \frac{\partial F_m}{\partial t} + F_m = K_m c \\ \tau_v \frac{\partial F_v}{\partial t} + F_v = K_v c \end{cases}$$

where F_m and F_v are respectively the frequency shift due to the mass loading effect and to the viscoelastic contribution, K_m and K_v are respectively their gains, τ_m and τ_v are their time constants and c is the concentration profile of the volatile compound. The total frequency shift is then given by $F = F_m + F_v$ [1]. Moreover, it was established that the mass loading effect involves a positive frequency shift i.e. $K_m < 0$. In this paper, we propose an approach to determine the gains and the time constants of the mass loading effect and to the viscoelastic contribution. We also show that these parameters are suitable features for chemical compounds identification and concentration evaluation. This work was motivated by the facts that these features are independent of the concentration profile c and belong to an higher dimension space than the traditional features (steady state amplitude of the response, rise time) used for compounds identification and hence should carry more information about them.

2 Problem formulation

The problem addressed in this paper is to determine the parameters of the sensors in a blind way, i.e. without any knowledge of the concentration profile. The discretization of the differential equations using the backward difference operator and the fact that such equations are linear and time invariant yield to: $F_i[n] = h_i[n] * c[n], \quad i \in \{m, v\}$, where h_i is the impulse response of the considered contribution. The impulse response of a dynamic system is its output when its input is the Dirac function. Thus, they are given by

$$h_i[n] = K_i \frac{T_s}{\tau_i + T_s} \left(\frac{\tau_i}{\tau_i + T_s} \right)^n, \quad i \in \{m, v\}.$$

Let's define the new variables for $i \in \{m, v\}$:

$$T_i = \frac{\tau_i}{\tau_i + T_s} \quad \text{or} \quad \tau_i = \frac{T_i T_s}{1 - T_i}; \quad \text{and} \tag{1}$$

$$A_i = K_i(1 - T_i) \quad \text{or} \quad K_i = \frac{A_i}{1 - T_i}. \tag{2}$$

to get a much simpler form of the impulse response: $F[n] = \left(A_m {T_m}^n + A_v {T_v}^n \right) * c[n]$. This relation shows that the parameters A_m and A_v can be identified up to a multiplicative constant $\alpha \neq 0$ since

$$F[n] = \left(\frac{A_m}{\alpha} {T_m}^n + \frac{A_v}{\alpha} {T_v}^n \right) * (\alpha c[n])$$

so without loss of generality we can assume that the amplitude of the concentration profile c^* is unitary

$$c^* = \frac{c}{c_{SS}} \quad \text{or} \quad c = c_{SS} c^*, \tag{3}$$

where c_{SS} is the steady state value of the concentration profile. It involves

$$F[n] = \left(A_m {T_m}^n + A_v {T_v}^n\right) * c^*[n]; \quad \text{and}$$

$$\frac{A_m}{1 - T_m} + \frac{A_v}{1 - T_v} = F_{SS},$$

F_{SS} is the steady state value of F. As the presence of the convolution product in the equations makes any further development arduous, we propose to transform them using a generating function.

2.1 Generating functions

The generating function of a sequence $a_0, a_1, ..., a_n$ is

$$G(a[n], x) = \sum_{n \geq 0} a[n] x^n, \tag{4}$$

the main advantage of generating functions is their property to transform a convolution product into a scalar product [2]:

$$G(a[n] * b[n], x) = G(a[n], x) G(b[n], x).$$

Generating functions are defined only for the x where the sum (Eq. 4) converges. The region of convergence (ROC) of a generating function is the set

$$\text{ROC } = \left\{ x \ : \ \sum_{n \geq 0} a[n] x^n \text{ converges} \right\}.$$

It can be shown that the generating function associated with the impulse response $h[n] = h_m[n] + h_v[n]$ is

$$G(h[n], x) = \frac{A_m}{1 - T_m x} + \frac{A_v}{1 - T_v x}$$

and its ROC is

$$ROC(G(h[n], x)) = \left\{ x : |x| < min(\frac{1}{T_m}, \frac{1}{T_v}) \right\}.$$

Moreover, we can easily prove the properties:

- $\{x : |x| < 1\} \subset ROC(G(c^*[n], x))$; and
- $\{x : |x| < 1\} \subset ROC(G(F[n], x))$.

In practice, the generating function of a digitalized signal F of length N can be approximated with high precision for $|x| < 10^{\frac{\epsilon}{N}}$ where ϵ is the machine precision if x belongs to the ROC of F.

2.2 Optimization problem formulation

Since SAW sensor based electronic noses are composed of an array of sensors, they can be modelled as a single input multiple outputs system. The e-nose is driven by a single input sequence $c[n]$ and yields to M output sequences $F_i[n]$. Computing the associated generating functions yields to the set of equations $i = 1..M$:

$$G(F_i[n], x) = \left(\frac{A_{i,m}}{1 - T_{i,m}x} + \frac{A_{i,v}}{1 - T_{i,v}x} \right) G(c^*[n], x). \tag{5}$$

One can determine $G(c^*[n], x)$ using the equation associated with the first sensor ($i = 1$)

$$G(c^*[n], x) = \frac{G(F_1[n], x)}{\frac{A_{1,m}}{1-T_{1,m}x} + \frac{A_{1,v}}{1-T_{1,v}x}}$$

and substitute it to the others ones ($i = 2..M$)

$$G(F_i[n], x) = \left(\frac{A_{i,m}}{1 - T_{i,m}x} + \frac{A_{i,v}}{1 - T_{i,v}x} \right) \frac{G(F_1[n], x)}{\frac{A_{1,m}}{1-T_{1,m}x} + \frac{A_{1,v}}{1-T_{1,v}x}}. \tag{6}$$

So, by construction, the parameters A and T can be estimated by solving the following optimization problem:

$$\begin{cases} \text{argmin} & \sum_{x \in X} \left\| GH(x) \frac{GF(F_1,x)}{\frac{A_{m,1}}{1-T_{m,1}x} + \frac{A_{v,1}}{1-T_{v,1}x}} - F(x) \right\|_2^2 \\ \text{subject to :} & \\ & \forall i \quad T_{i,m} \in]0..1[\text{ and } T_{i,v} \in]0..1[\\ & \forall i \quad A_{i,m} < 0 \\ & \forall i \quad \frac{A_{m,i}}{1-T_{m,i}} + \frac{A_{v,i}}{1-T_{v,i}} = SS_i \end{cases}$$

where $GH(x) = \begin{pmatrix} \frac{A_{m,2}}{1-T_{m,2}x} + \frac{A_{v,2}}{1-T_{v,2}x} \\ \vdots \\ \frac{A_{m,N}}{1-T_{m,N}x} + \frac{A_{v,N}}{1-T_{v,N}x} \end{pmatrix}$,

$F(x) = \begin{pmatrix} GF(F_2, x) \\ \vdots \\ GF(F_N, x) \end{pmatrix}$ and X is a finite subset of $[-10^{\frac{\epsilon}{N}}, 10^{\frac{\epsilon}{N}}]$.

3 Application to odours recognition and concentration evaluation

In this section, we show that the estimates of the parameters of the impulse response of the SAW sensors (K_m, K_v, τ_m, τ_v) are suitable features for odours recognitions and concentration evaluation.

3.1 Outline of the electronic nose and of the optimization process

The selected electronic nose system is based on an array of six functionalized nano-diamond coated SAW sensors each with a fundamental frequency of 433.9 MHz [3]. The sensors were exposed to five different gases (NH_3, SO_2, H_2S, CH_3OH and C_7H_8) at a concentration of 10 ppm, 8 ppm, 6 ppm, 4 ppm and 2 ppm. Nitrogen was used as the reference and carrier gas to transport the volatile chemical compounds through the gas cell containing the sensors. The temperature of the sensors (22^o C) and the flow rate (200 ml/min) above them were kept constant. Data acquisition was carried out at 10 Hz using the SAGAS instrument [4]. Several cycles exposition (15 sec) - purge (30 sec) were done for each gas at each concentration. The optimization problem was solved using the particle swarm optimization algorithm [5], its parameters were set empirically, its inertia weight was set to 0.729, its social and cognitive acceleration coefficient were set to 1.49445. 100 particles were used. The algorithm was run for 250 iterations. The parameters K_m, K_v, τ_m, τ_v were then retrieved using Eq. 1 and Eq. 2.

3.2 Chemical compounds identification

To perform odours recognition, large margin nearest neighbour (LMNN) [6] was implemented. We compared the performances obtained by using the amplitudes (K_m and K_v) of the two contributions as features versus the signal amplitude during the steady state. The mean of the relative classification performance obtain during a 5-fold cross-validation process were respectively 96.8% and 94.5%. These results show that the amplitudes of the two contributions are suitable features to perform odours recognition.

3.3 Chemical compound concentration evaluation

The sensor's response, $F_i(n)$, is given by

$$F_i[n] = h_i[0]c^*[n] + h_i[1]c^*[n-1] + ... + h_i[N]c^*[n-N].$$

This equation can be written as $F_i = \mathbf{H_i}c^*$ where

$$\mathbf{H_i} = \begin{pmatrix} h_i[0] & 0 & \cdots & \cdots & 0 \\ h_i[1] & h_i[0] & 0 & & \vdots \\ h_i[2] & h_i[1] & h_i[0] & 0 & \vdots \\ \vdots & & & \ddots & \ddots \\ h_i[N] & & & & h_i[0] \end{pmatrix}.$$

Stacking this equation for each sensor of the nose yield to:

$$\begin{pmatrix} F_1 \\ F_2 \\ \vdots \\ F_M \end{pmatrix} = \begin{pmatrix} \mathbf{H_1} \\ \mathbf{H_2} \\ \vdots \\ \mathbf{H_M} \end{pmatrix} c^* \text{ or } F = \mathbf{H}c^*$$

and $c^* = (\mathbf{H^T H})^{-1}\mathbf{H^T}F$. However, the measured data F are noisy. In this case the previous equation generally produces a noisy estimate of the concentration profile. To improve the deconvolution, one can minimize the energy of the second-order derivative of the concentration profile. Moreover, in some situation, it may be interesting to add prior knowledge about the concentration profile, for instance $c^*[0] = 0$ i.e. $sc^* = 0$ where $s = [1\ 0..0]$. So c^* can be estimated by solving the problem:

$$\begin{cases} \text{argmin} & ||F - \mathbf{H}c^*||_2^2 + k||\mathbf{D}c^*||_2^2 \\ \text{subject to :} & \\ & sc^* = 0 \end{cases}$$

where $\mathbf{D}$ is the second-order derivative matrix:

$$\mathbf{D} = \begin{pmatrix} 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & 1 & -2 & 1 \end{pmatrix}.$$

Building the Lagrangian, computing its gradient and nullifying it yields to:

$$\begin{pmatrix} c^* \\ \lambda \end{pmatrix} = \begin{pmatrix} 2\mathbf{H^T H} + 2k\mathbf{D^T D} & s^T \\ s & 0 \end{pmatrix}^{-1} \begin{pmatrix} 2\mathbf{H^T}F \\ 0 \end{pmatrix},$$

where λ is the Lagrange's multiplier. To obtain the real concentration profile, we must determine the coefficient c_{ss} (see Eq. 3). This is a traditional regression problem. To solve it, we implemented the metric learning for kernel regression algorithm (MLKR) [7] algorithm which gave a relative error of 17%. Fig. 1 shows the result of the concentration profile estimation process: the true concentration is 8 ppm (estimated 8.2 ppm) from 0 to 10 sec and 4 ppm (estimated 3.74) from 10 to 15 sec, (k was set to 10^6).

4 Conclusion

The optimization problem developed in this study enables the determination of the parameters of the mass loading effect and oh the viscoelastic contribution to SAW sensor's frequency shift. This work was motivated by the facts that these features are independent of the concentration profile c and belong to an higher

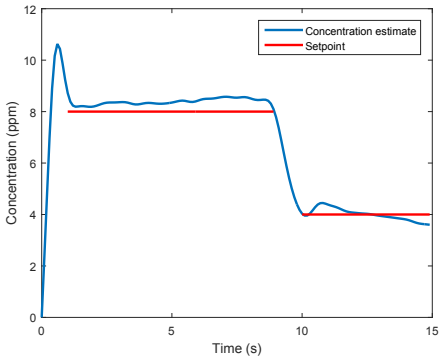

Figure 1: Concentration setpoint and concentration profile estimate

dimension space than the traditional features used for compounds identification and hence should carry more information about them. This assumption was verified experimentally by comparing the classification rate obtained with these features and the one obtained with the steady state amplitude. Moreover we showed that the features we introduced, make possible the determination of the temporal profile of the concentration by performing a deconvolution.

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