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Chaotic chemical sensing : advances for improving the resolution of chaos-based sensorial systems

Index terms: *Non-linear dynamic system, chaos, chemical sensor, parameter space map.*

Abstract

In this paper we will advance a read-out technique allowing the estimation of the value of a measurand through a dynamics-based sensing device. The technique joins complex system theory to electronic design and data analysis, and provides higher resolution and accuracy than traditional approaches based on the read-out of static signals. The paper describes a simple sensor system in which we have implemented this technique.

1. Introduction

Read-out from a sensor is usually based on standard static procedures (i.e. measuring either the voltage between two nodes of the circuit or the current flowing in a branch). The technique described in this paper, on the other hand, is a refinement of the new approach based on the qualitative evaluation of the dynamic behaviour of the system containing the sensor device, as introduced by Davide et alii [5]. Accordingly, the sensor system is seen as a non-linear dynamic system, which is coupled with an evaluating device for identifying the dynamic behaviour of the former.

2. Refinement of the sensor read-out

Our read-out device adds a switching system to the previously mentioned components, as described in Fig. 1.

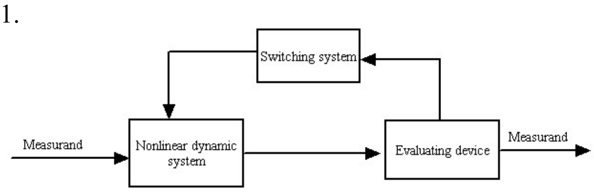

Fig. 1. System overview

The non-linear system, which the sensor is contained in, displays a variety of dynamic behaviors (cyclic behavior with different periods, convergence to a fixed point, chaotic behavior) depending on a set of system parameters: one at least chosen such as a monotonic function of the measurand. The goal of the evaluating device is to associate specific values of the measurand with specific patterns of dynamic behavior. The switching system introduces real-time variations in the values of certain system parameters said "switching parameters" because can be controlled in real time. The read-out device relies on a Map of the system dynamics in the parameter space. The Map is defined as a function of: 1) the "switching parameters, to be varied in real-time following a time-based rule; 2) the parameters whose values are monotonic functions of the measurands;

2.1 Non-linear dynamic system

As an example we have chosen a simple chaotic chemical system, consisting of a non-linear chemical sensor, a chem-FET connected in diode fashion [4] (with the drain and gate short-circuited) and a simple oscillator [5]. The state of the system can be described in terms of three voltages x, y, z that evolve in a periodic or chaotic fashion depending on the concentration of H_2 in the environment, which in turn affects the threshold voltage *L* for the chem-FET. The set of switching parameters reduces to the voltage reference *V* (placed at the leftmost lower corner in Fig. 2). The circuit shown in Fig. 2 can thus be modelled by the following equations [1]:

$$\begin{cases} \dot{x} = ax + by + cz \\ \dot{y} = dx + ey \\ \dot{z} = fg[h(x), L] + hz \end{cases} \tag{1}$$

$$\begin{cases} g[h(x), L] = g_m (h(x) - L)^2 U_{-1}(h(x) - L) \\ h(x) = \alpha x + (1-\alpha) V_{ref} \end{cases} \tag{2}$$

with $U_{-1}(\cdot)$ is the Heavyside function. The parameters in (1), (2) can be selected as in Table 1 to match with the circuit shown in Fig. 2.

$$a = -\frac{1}{C_x R_{10}}, \quad b = -\frac{1}{C_x R_9},$$
$$c = -\frac{1}{C_x R_{13}}, \quad d = \frac{R_5}{C_y R_6 R_4},$$
$$e = -\frac{1}{C_y R_7}\left(1 - \frac{R_5}{R_8}\frac{R_7}{R_6}\right),$$
$$f = \frac{R_1}{C_z R_{12}}, \quad h = -\frac{1}{C_z R_{12}}, \quad \alpha = \frac{R_2}{R_2 + R_3}$$

Table 1. Values of the constant system parameters

In Fig. 3, we report the system trajectories due to fixed specific value of the control parameter L (depending on the concentration of H_2 in the environment) [2]. The main difficulty with the approach described in [5] is in finding a simple way of detecting whether the system trajectories are periodic or chaotic and thus of measuring the concentration of H_2.

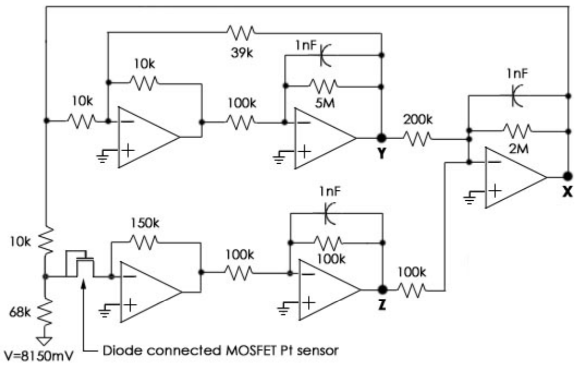

Fig. 2. The chaotic chemical sensor circuit. Note in the left bottom corner the reference voltage V and the square block representing the non-linear sensor device.

2.2. The Evaluating device

In order to evaluate the dynamic behaviour, after [5] we have to compute the map of the system dynamics in the system parameter space (the Map in the following). We also need an appropriately defined metric allowing the measurement of distances between different dynamics in the parameter space. Finally we have to evaluate the dynamic behaviour of the system, sampling its output and then correlating with and a reference. Thus the evaluating device is based on the Map, but it is not always able to associate specific values of the measurand with specific patterns of dynamic behaviour. In many cases all that it is possible to achieve is the identification of a set of non-contiguous intervals containing the value of the measurand. In general monotonic changes in the value of the control parameter for a non-linear system will produce a complex sequence of behaviors: on occasions the same behavior can be produced by non-contiguous values of the control parameter, as illustrated in Fig. 4 where "Period 2 behaviour" is displayed for non-contiguous values of the control parameter. As a result our knowledge of the measurand is necessarily ambiguous [2].

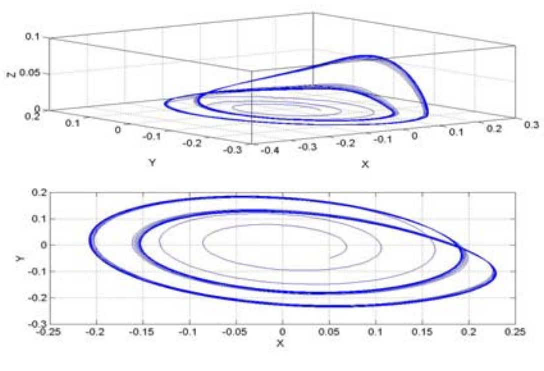

Fig. 3. System trajectories in the phase space

2.3 The switching system

The switching system introduced improves on the read-out technique eliminating ambiguous estimates and making it possible to refine estimates producing overall superior performance. The system uses a time-based rule to produce real time changes in one or more "switching parameters" – which are independent of the measurand.

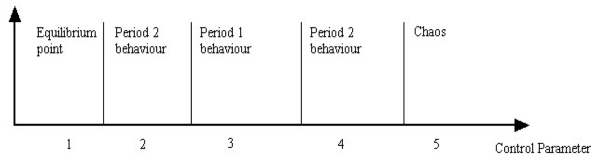

Fig. 4:System dynamics vs one parameter. Let us remark how two period 2 areas are present.

The behaviour transitions produced by these variations are used to generate an unambigous estimate of the measurand. Using the Map, the switching system makes it possible to characterize behaviors in quantitative terms and moreover to identify the relationship between changes in parameter values and transitions in the dynamic behavior they determine. The possibility of varying parameters (in our case switching parameters) in real-time is essential if a read-out technique based on the dynamic behavior of a chaotic system has to produce accurate estimates of the measurands. In fact, it has been proved that in general, where behavior is chaotic, there exists no monotonic function mapping an indicator of chaotic behavior (such as the Lyapunov exponent) onto the control parameter. It follows that there exists no general method capable of estimating the value of the measurands when the system is driven into the chaotic regime. In brief, in our technique the switching system makes it possible to control the value of the switching parameter in real time, allowing the testing of the system in those regions of parameter space where it is most sensitive to variations of the measurands.

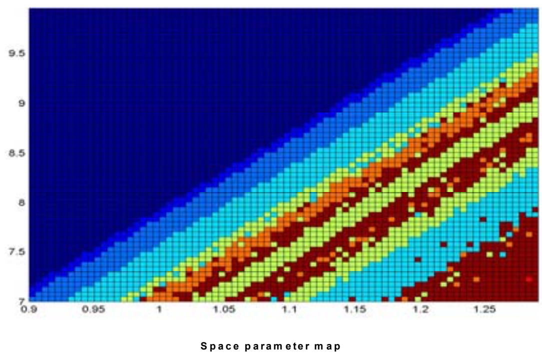

Fig. 5: Two-dimensional Space Parameter Map

3 Mathematical Model

We have evaluated through experiments and simulations the two-dimensional Map, shown in Fig. 5, as function of the switching parameter V and the measurand sensitive parameter L, considered over specific ranges. In the following we propose a simple but formal approach to the Map usage and to the read-out technique. Let us consider the orthogonal plane (L,V), in which each point $P=(l,v)$ is associated to the system dynamics $D(P)$. Let us define a family of straight lines $r_i = \{(V,L): V = \mu_i L + \nu_i\}$ as the boundaries of regions at the same dynamics (D constant). Note that in the case shown in Fig. 5: $\mu_i \cong \mu$ (the subscript can thus be ignored); there exists a monotonic decreasing sequence $\{v_i\}$, representing the intercepts between the straight lines $\{r_i\}$ and the V axis; thus regions at D constant R_i are stripes, each one having two intercepts at *V=0,* the smallest being v_i. Let us define $\overline{T}$, the *reference period*, as the smallest *period* computed among the cases when the system behaviour is periodic and the parameters vary along the Map. Within this framework, the system dynamics $D(P)$ can be characterized by the ratio π between the period T of the dynamics (where it is defined) and $\overline{T}$. Thus a π_i remains defined at any R_i: in our simple example it is an integer everywhere, eventually zero when it has a point attractor, and accidentally divergent when the system has a chaotic attractor. Let C be the set of the values $\{v_i\}$, and A the set of the values $\{\pi_i\}$, then the function $F: A \to C$ is non invertible in general, because the system dynamics can alternate in a non-monotonic fashion: in short there exist cases where $\pi_i = \pi_j, v_i \neq v_j$. As a result it is not always possible to identify a single interval L belongs to, even when π_i is known.

4 Read-out procedure

The procedure is simply the following. Let us start from a given value $\overline{V}$ of the voltage reference and decrease V applying the rule $V = \overline{V} - \alpha t$, (where α is the *measurement rate)* until time t_1 when the system jumps from state π_i to state π_{i+1}. In Fig. 6, we start with $\overline{V}$ equal to 8.5 and the evaluating device labeling the dynamic behavior of the system at $\pi = 2$. This implies that the value of that L may lie either in interval A or in interval B. Following the rule, and meeting a transition of the dynamics at V equal to 8.2, we face two possibilities: $\pi = 4$ or $\pi = 6$. In consequence we have a unique interval L can belong to, and a first level ambiguity in the estimation of the measurand is solved. There is a further refinement we can do exploiting the knowledge of the exact instant when the transition takes place.

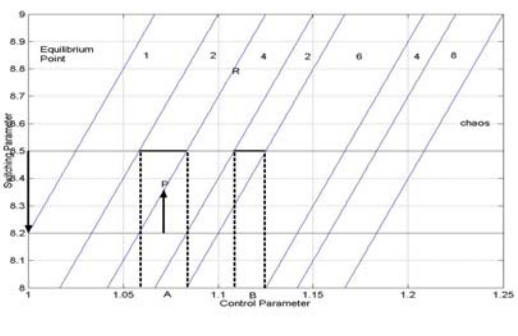

Fig. 6: Read out procedure in the LV plane

Let us suppose that the system has come to $\pi = 4$ and L is known to lie in interval A. The switching system can now increase V from 8.2 back to 8.5. The instant t_2 of the new dynamics transition allows for the placement of point P over the transition line *r*, being the estimate of L equal to the abscissa of P. This procedure provides for quantitative estimation intensive variables, such as continuous control parameters, starting from extensive knowledge, i.e. the dynamic behaviour. In addition it can be easily implemented in real-time. These characteristics make the proposed technique the only one, at authors' knowledge, being suitable for measurement techniques based on dynamic behaviors of a system.

5 Measurement Theory

From the switching law we have:

$$\overline{V} - \alpha t_1 = \mu L + v_{i+1} \tag{3}$$

with t_1 the instant of the first dynamics transition. Thus, in absence of any impairment we have the actual value of L expressed as:

$$L = \frac{1}{\mu}\left(\overline{V} - \alpha t_1 - v_{i+1}\right) \tag{4}$$

The error sources given by the imperfect knowledge of the dynamics map are independent of the real time operation of the read out technique, therefore they can be considered static errors. In practice there are an error Δv_i on the estimate of v_i and an error on μ that is an order of magnitude lower and can be neglected. During the real time operation the technique is affected by a dynamic error on t_1 that can be expressed as the sum of two finite delays: one, τ_T, for the transition completion, the other, τ_O, for observing the dynamics until the change is unequivocally recognized. Therefore we have both an estimate of the transition instant $\hat{t}_1 = t_1 + \tau_T + \tau_O$ and an estimate of the i-th intercept $\hat{v}_i = v_i + \Delta v_i$ where τ_T, τ_O and Δv_i are random variables. Considering the preceding error sources from eqn.3, we have $\overline{V} - \alpha\left(\hat{t}_1 - \tau_T - \tau_O\right) = \mu L + \hat{v}_{i+1} - \Delta v_{i+1}$ and finally:

$$L = \frac{1}{\mu}\left(\overline{V} - \alpha\hat{t}_1 - \hat{v}_{i+1}\right) + \frac{1}{\mu}\left(\alpha\tau_t + \alpha\tau_o - \Delta v_{i+1}\right) = \hat{L} + \Delta L \tag{5}$$

being $\hat{L} = \frac{1}{\mu}\left(\overline{V} - \alpha\hat{t}_1 - \hat{v}_{i+1}\right)$ the estimate of *L,* and $\Delta L = \frac{1}{\mu}\left(\alpha\tau_T + \alpha\tau_O + \Delta v_{i+1}\right)$ its error. To progress further on ΔL some notes arerequired. The mean length of the discovery phase, during which eqn 3 holds, is $T_d = \langle v_i - v_{i+1}\rangle / 2\alpha$, with $\langle\cdot\rangle$ the average operator. If it is expressed in terms of multiple d of the reference period, we have $\alpha = \langle v_i - v_{i+1}\rangle / 2d\overline{T}$. Delay τ_T is strictly dependent on the system structure, whereas τ_O is due to the read out implementation. We can assume they have the same order of magnitude, and their sum be expressed as $(\tau_T + \tau_O) = 2\sigma\overline{T}$ with σ the number of reference periods required for observation. Characterization of $\Delta\nu_i$ can take benefit from a rich theoretical framework given by the bifurcation theory. In our case, where a period doubling cascade is met around many r_i, we can simply note that the map model is coarse grained, so that doublings over a certain order are confused with a fat boundary of the transition to chaos. $\Delta\nu_i$ is nothing else that the length of this boundary, when projected along the V axis. Introducing the Feigenbaum universal constant δ=4.669…, we have at the left side of certain i-th boundaries: $(\nu_i - \nu_{i+1} + \Delta\nu_{i+1}) \propto \delta^{-i}$, then using together the (i+1)-th condition we have $(\nu_i - \nu_{i+1} + \Delta\nu_{i+1})/\Delta\nu_{i+1} = \delta$ and $\Delta\nu_{i+1} = (\nu_i - \nu_{i+1})/(\delta - 1) \leq \langle \nu_i - \nu_{i+1}\rangle/(\delta - 1)$ where the equality holds as much as higher the order of the bifurcation at r_i and locally restricted the average. Finally we have:

(6) $$\Delta L \leq \frac{\langle \nu_i - \nu_{i+1}\rangle}{\mu}\left(\frac{\sigma}{d} + \frac{1}{\delta - 1}\right)$$

It is worthwhile noting that $\langle \nu_i - \nu_{i+1}\rangle/\mu$ has the meaning of the map resolution ΔL_M, i.e. the mean length of the interval L belongs to, as can be determined after the approach in [5], relying only on the knowledge of the dynamic regime, and holding only when the interval remains univocally determined. Under these hypotheses, the improvement of the proposed read out technique in terms of resolution can be expressed as:

(7) $$\frac{\Delta L_M}{\Delta L} \geq \frac{d}{\sigma + d/(\delta - 1)}$$

Actually an improvement of 10dB has been experimentally measured with the set up in Fig. 2, where the requirements and the system design choices give: $m = 340$, $\sigma \approx 4$. This is in excellent agreement with eqn 7. In terms of average resolution over the estimate of $[H_2]$, this means moving from 15.0ppm to 3.2ppm. (considering the non linear dependency between L and $[H_2]$). Last remarks are about the limit behaviour of eqn. 7:

- $\sigma/d \to 0$, $\frac{\Delta L_M}{\Delta L} \geq (\delta - 1) = 11.29dB$ that has the physical meaning of imposing as a requirement over the system a short observation and recognition time, when a transition is met, in comparison with a much longer time spent on map exploration: the gain is the most significant possible, and implies an ideal observation mechanism.
- $\sigma/d \to 1$, $\frac{\Delta L_M}{\Delta L} \geq \left(\frac{\delta - 1}{\delta}\right) = -2.09dB$ that has the physical meaning of exploring the D constant region at comparatively high speed, loosing any benefit because of the dynamics changes, on average, before the observation is completed. This introduces a methodical dynamic error that makes the proposed approach inconvenient;
- $\sigma/d \to \frac{\delta - 2}{\delta - 1} = 0.724...$, $\frac{\Delta L_M}{\Delta L} \geq 0dB$ that has the physical meaning of null trade off between knowledge gained from π_i only (according to [5] and applicable when the interval is univocally determined) and additionally from transition to π_{i+1} with an intrinsic dynamic error. $(\delta - 2)/(\delta - 1)$ is a limit value under these considerations, and must be taken as the rightmost boundary of the working zone.

It is interesting to remark that the improvement at $\sigma/d \to 0$ depends on a universal constant; thus it cannot be over performed because of the intrinsic structure of the dynamics map. Further the boundary $(\delta - 2)/(\delta - 1)$ is still universal and independent of technology implementation. Therefore the reign of technology improvement results to be well framed: to try to compress the ratio σ/d below the boundary and correspondingly to approach the maximum gain.

6. Conclusions

To sum up the original technique, together with the proposed refinement, confirms to have some important characteristics which make it a very useful approach to chemical sensing and dynamical sensorial systems:

- first of all the read out is in general faster than with traditional chemical sensing because the transitions between different behaviours are in general quicker than saturation of any other chemically driven electrical phenomenon [5];
- the system joins together quickness with accuracy, because, on the opposite of other dynamics-based read out techniques, it refines the measurement controlling suitable system parameters;
- finally, the system performance can be easily predicted in terms of universal constants and straightforward figures of merit.

Further research will be devoted to the last point in order to conceive and evaluate a wide family of dynamics-based read out techniques for sensorial systems.

7. References

[1] L.O. Chua, C.A. Desoer and E.S. Kuh, Linear and Nonlinear Circuits, New York, McGraw Hill 1987.
[2] Yu.A. Kutsetsov, Chapter V, in Elements of Applied Bifurcation Theory, Berlin, Springer, 1998.
[3] I. Lundström, et alii, “From hydrogen sensors to olfactory images-twenty years with catalytic field effect devices”, Sens. and Act. B13-14, 16-23, 1993.
[4] I. Lundström, et alii, “Recent developments in field-effect gas sensors”, Sens. and Act. B23, 127-133, 1995.
[5] F. Davide, M. Andersson, M. Holmberg, I. Lundström, “Chaotic Chemical Sensing”, IEEE Sensors, in press.