EVALUATION OF FLOW-INDUCED VOLTAGE FLUCTUATIONS OF GAS CHEMIRESISTORS BY PARAMETRIC EMPIRICAL MODEL

Filip Mivalt

Master Degree Programme (1), FEEC BUT

E-mail: xmival00@stud.feec.vutbr.cz

Supervised by: Petr Sedlak

E-mail: sedlakp@feec.vutbr.cz

Abstract: Analyses of voltage or current fluctuations in gas chemical sensors provide precise evaluation metrics for non-flowing gases. Automatic analysis of sensed flowing gas fluctuations is challenging task. The signal is a superposition of more stochastic processes. The presented paper proposes a machine learning empirical model for further automated parametrical analysis of voltage fluctuations produced by a gas sensor and flowing air.

Keywords: Analytical fluctuations, machine learning model, gas sensor

1 INTRODUCTION

In signal theory, a noise is considered as a redundant part of signals. Noise suppression , i.e. increase of signal-to-noise ratio (SNR) is necessary or required for almost all applications. But in some cases, noise might be considered as a useful part of signals. This paper deals with stochastic ergodic processes, which are measured macroscopically as voltage fluctuations (VF). Thanks to analysis of VF, the description of processes generating VFs is available. These descriptions are optional for electrical components non-destructive analysis and/or manufacturing process analysis and optimization. Stochastic behaviour also becomes increasingly dominant characteristics of electrochemical processes [1], [2]. Fluctuations of physical and chemical processes occur on all electrochemical interfaces. Thus, electrochemical sensors evaluation through VFs analysis is possible way to increase the sensitivity and resolution of sensing system from 10 to 100 times compared to conventional methods [3], [4]. The electrochemical sensors evaluation methods rest in 1/f noise analysis and are developed for equilibrium conditions as temperature, humidity and zero flow rate.

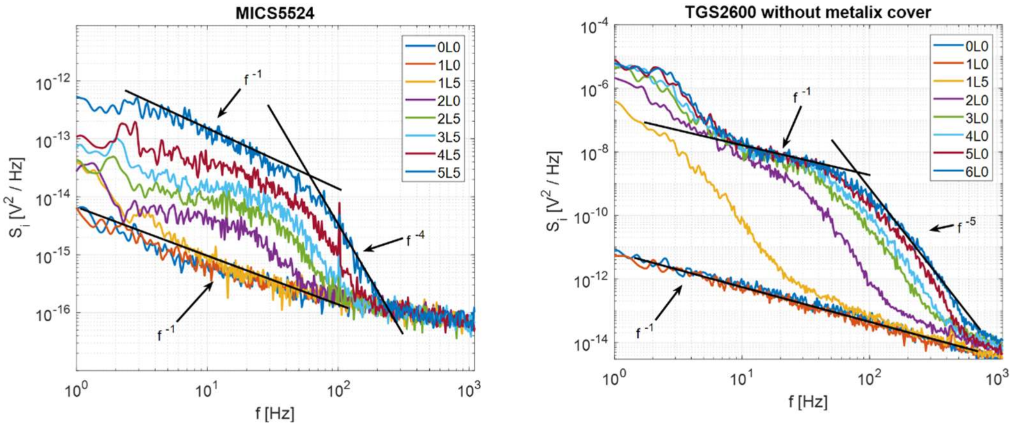

Figure 1: Spectral densities estimation for constant temperature, humidity and sensed gas concentration for different flow rates for conductometric sensors MICS 5524 and TGS 2600

When the gas flows through the chamber, where the sensor is placed, an unexpected noise component arises in a signal spectrum. According to well-established theory, this noise source is probably a result of two mutual influencing stochastic processes: adsorption-desorption noise and noise arising from turbulent/laminar flow around the sensor (partial pressure fluctuations). Two conductometric sensors, MICS 5524 and TGS 2600 were placed in the same position at gas chamber under almost same fluidic conditions. Figure 1 shows how the spectral densities of voltage fluctuations evolve as flow rate of analyzed gas increases through the chamber. This paper proposes machine learning approach for the automated analysis of estimated spectral densities for different flow rates through the chamber.

2 PARAMETRIC EMPIRICAL MODEL DESIGN

Empirical mathematical model structure comes out of the needs of analysis. Three parts of estimated spectral density are analysed as lines (on logarithmic scale) by conventional methods. Example of analysed data you can see below in Figure 2. The parameter of a slope of a line a and also bias parameter b of each line equation $log(Y) = a \cdot log(f) + b$ for model Y are evaluated in the following analysis. Variable f denotes frequency as x-axis variable. The proposed model is designed to combine all sub models A, B and C in one equation. The model has 4 parts. First and third part, A and C, are straight lines on the logarithmic scale or exponential on linear scale $y = 10^b \cdot f^a$. The part B comes out from transition characteristics of high pass RC filter $H(\omega) = \left|\frac{X_C}{X_C + R}\right|$ where X_C is capacitance and R is resistance of a filter. The R is set to 1 to ensure unit transition on pass frequencies of the filter. Thus, time constant of the filter depends only on the parameter C. The model Y_B of the part B is then as:

$$Y_B = \left|\frac{\frac{-1}{j2\pi fC}}{\frac{-1}{j2\pi fC}+1}\right| = \left|\frac{1}{1-j2\pi fC}\right| = \sqrt{\frac{1}{1+(2\pi fC)^2}} \tag{1}$$

As shown in equation (2) we denote $K = 4\pi^2C^2$ and exponent parameter as d. The parameter d changes the slope of Y_B curve. Analogically to an ideal RC filter order.

$$Y_B = (1 + (2\pi fC)^2)^{-0.5} = (1 + K \cdot f^2)^d \tag{2}$$

The fourth part of the model is a bias parameter m. This parameter characterizes thermal noise of measured circuit marked as D in figure 2. Proposed empirical mathematical model is shown in equation (3).

$$\hat{Y} = (a \cdot f^b) \cdot (1 + K \cdot f^2)^d + (g \cdot f^h) + m \tag{3}$$

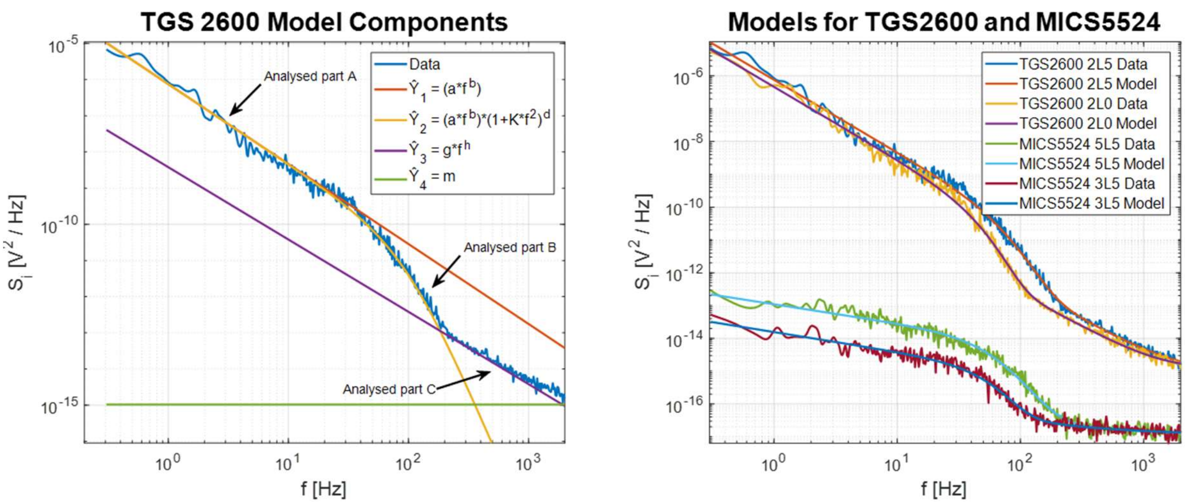

Figure 2: Parts of the model for TGS2600 sensor and flow rate 2.5 l/min (left); Models for MICS5524 and TGS2600 sensors experimental data for different flow rates(right)

3 PARAMETERS ESTIMATION METHOD

Curve fitting represents an optimization problem. Optimization process minimizes the value of cost function $J(\boldsymbol{\theta})$ where $\boldsymbol{\theta}$ is a vector of parameters. For proposed model, $\boldsymbol{\theta}$ is a vector of scalar parameters from equation (3). An optimization process is challenging task because the model is highly nonlinear. The cost function is showed in equation (4).

$$J(\boldsymbol{\theta}) = \frac{1}{2M}\sum_{i=1}^{M}\left(log(Y_i) - log(\hat{Y}_i)\right)^2 \tag{4}$$

Accurate initial estimation for the proposed method is essential. Especially for exponential coefficients. It is possible to estimate initial values of vector θ with multiple methods [5]. The following method for precise estimation is based on bisection method. For proposed method is necessary to define another one cost function (5).

$$J_2(\boldsymbol{\theta}) = \frac{1}{M}\sum_{i=1}^{M}\frac{Y_i - \hat{Y}_i}{Y_i}$$

The method iteratively computes cost function value for 5 values of $\boldsymbol{\theta_k}$ where $\boldsymbol{k}$ iterates over all $\boldsymbol{\theta}$ coefficients. The first point is set to a current value of $\boldsymbol{\theta_k}$. Next 2 points are given as $\boldsymbol{\theta_k} \mp r \cdot \boldsymbol{\theta_k}$ where $\boldsymbol{r}$ is chosen parameter of the method. And $\boldsymbol{r}$ is decreasing with iterations, so it increases the accuracy of final model estimation. Last two points lie in the middle of the intervals between mentioned three points. The decisive system chooses an optimal value using following conditions. When all signs of $J_2(\boldsymbol{\theta})$ are the same, the system chooses the parameter with the smallest $J(\boldsymbol{\theta})$. If there is a sign change, in $J_2(\boldsymbol{\theta})$, following $\boldsymbol{\theta_k}$ value is chosen in the middle of the interval defined by points with the sign change.

4 CONCLUSION

This paper proposes machine learning approach for the automatic parametric analysis of conductometric chemical sensors. Mean absolute percentage error of logarithms of the model and the reference curve was lower than 1.6 % for all experimental data evaluated by proposed model. The main advantage of the proposed model is a compact parametric description of spectral density estimations of analytical fluctuations measured across the sensors. Automatic estimation of model parameters, also proposed in this paper, enables fast and accurate evaluation of the big amount of measured data. Application of this method for other types of gas sensors is also possible. The disadvantage is the high demand for initial model parameters estimation and fact that the model is a mathematical not physical. Despite mentioned disadvantages, the model helps in a research of methodology of flowing gas concentration estimation.

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