



## Brief Modeling Equation for Metal-Oxide; TGS Type Gas Sensors

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**Abstract.** The main aim of this research is to propose a mathematical equation in order to reduce the model parameters based on temperature, humidity and gas density variation in metal-oxide semi-conductive sensors. Also the Arduino based Designed E-nose with the capability to change the temperature and humidity is used to obtain the real sensor's response in various conditions. The sampling procedure consists of three sectors: fixed temperature and fixed humidity, variable temperature and fixed humidity, fixed temperature and variable humidity, which are stored in Excel software and analyzed with MATLAB. The output response is based on combination of First-Order Plus Dead Time (FOPDT) which has the Minimum Parameters system (MPS) to investigate the behavior of the sensors. Finally, after evaluating the models with the real sensor response and bi-sentence exponentials, it is suggested that the MPS model introduces fewer and simpler parameters, which helps to simulate the sensor's behavior more accurately and consequently in order to draw a better short response.

### 1. The first section

Gaseous sensors are vastly used in industries [1] and measuring their parameters are considered as a usual practical method in both industrial and academic domains [1-3]. We can categorize gas sensing technologies into two groups: The methods based on the variation of electrical properties and on other properties, as well [1]. Among different sensor classes, metal-oxides (MOX) are the major materials used in producing the sensors [1], which are based on electrical conducting in the presence of chemical substances [4], so not only have they an uncomplicated structure, reasonable price, short response and high accuracy [5-6], but also they are user-friendly and long-lasting [5,7]. Although their operations might be affected by temperature, humidity and high energy consumption [5-6, 8-9], they are used extensively in various applications like E-nose for gas detection, odor localizing, plume tracking, etc [3,5,10]. Gaseous sensors responses are varied and depend on density, temperature and humidity conditions [5-6] and the purpose of this study is to introduce a more efficient model for TGS sensors and to analyze the impact of temperature, humidity and gas density on the sensor's responses. As it is shown in Figure 1, responses are restricted to three sections: transient rise time, overshoot and steady state [5]. There are different methods to analyze the specifications of MOX gaseous sensors, which are based on electrical impedance caused by very small

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changes in temperature, biasing voltage and gas density [11].The famous models formula are shown in Equation 1 to 6.

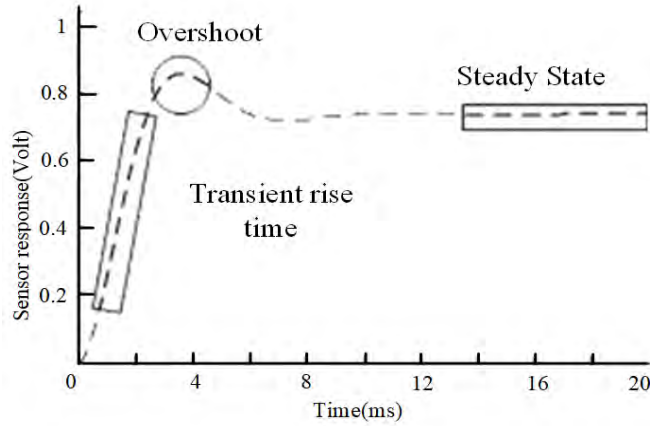


Fig. 1 Sample gas sensor response[5].

According to Equations(1) [15] in Table I,  $\sigma_l$  is conductivity coefficient before temperature changes,  $\sigma_f$  is conductivity coefficient at steady state in the new heating condition,  $\sigma_p$  is to regulate temperature changes and  $t$  time and  $\tau$  is a time constant.

$$\delta(t) = \delta_l e^{-\frac{t}{\tau}} + \delta_p e^{-\frac{t}{\tau}} (1 - e^{-\frac{t}{\tau}}) + \delta_f (1 - e^{-\frac{t}{\tau}}) \tag{1}$$

In Equations(2)[16]  $R$  is the sensor resistance,  $R_0$  is the sensor resistance in air,  $C_{gas}$  is the concentration of the target analyze,  $\beta$  is the power characteristic of the particular sensor and the proportionality constant  $K_{gas}$  depends on the analysis. Equations(1 and 2 ) indicate a reduced mathematical model for impedance changing.

$$\frac{R}{R_0} = (1 + K_{gas} \times C_{gas}) \tag{2}$$

The response regarding Equation 3 [17] occurs in the neighborhood nominal temperature, which includes important information that its parameters are hard to find (the models for the Equations: 2 and 3 are static).

$$Y = A_0 + A_1 X + A_2 X^2 + A_3 X^3 \tag{3}$$

$$Y = A_0 + A_1 e^{-\frac{t}{\tau_1}} + A_2 e^{-\frac{t}{\tau_2}} \tag{4}$$

Equations 3 and 4 [17] respectively display the sensor response in a polynomial and exponential mode in on and off mode. ON mode:  $Y$  is sensor value-baseline and  $X$  is the time from gas on to gas off. Off mode:  $Y$  Collect response and baseline-sensor value,  $X$  Collect time from gas on to gas off and 240 s.  $A_0, A_1, A_2, A_3$  coefficients in the fitted equations were then used as parameters to characterize each measurement. The parameter extraction and curve fitting were made on both the rising (test gas on) and the decreasing (test gas off) part of the response curves. Equations: 3 is one of the most satisfactory models [15], but it would be complicated to find the correct parameters [5,18]. Equation: 4 introduce the sensor reactions in the absorbing processes, though determined parameters are hard to calculate.

$$f(t) = \sum_{i=1}^n G_i e^{-\frac{t}{\tau_i}} \tag{5}$$

Equation: 5 [18-19] where  $G_i$  is sample data,  $n$  is the number of exponential sentences and  $\tau_i$  the time constant.

$$G(T, N_2) = G_0 e^{-\frac{q^2 N_2^2}{2KT N_1 \epsilon + \epsilon_0}} + G_1 \tag{6}$$

Equation: 6 [10,20-21]  $G$  is the sensor conductance,  $G_0$  is conductivity sensor,  $T$  is the absolute temperature,  $N_z$  is the density of surface charge,  $k$  is Boltzmann's constant,  $q$  is electrical charge,  $N_d$  is the density of ionized,  $\epsilon\epsilon_0$  is permittivity constant and  $G_1$  is a constant term is more common, but its parameters are many and complex. The new model, which has been introduced recently, is based on the output response of sensors, trying to use just 3 parameters instead of multiple parameters [5]. As a result, the mentioned Equations illustrate that it is difficult to use many complex parameters in the simulation software. Thus, having the short form of gas sensor equation with the least number of parameters is essential. In section 2, the brief description of the Enose hardware and sampling procedure will be discussed. The MPS model is proposed as a novel model in section 3. Section 4 contains the results and evaluations and finally, the conclusions can be observed in section 5.

## 2. E-NOSE HARDWARE AND SAMPLING PROCEDURE

In order to extract the sensor behavior, Arduino based E-nose is designed to be used [22] (Figure 2). As it is shown in Figure 2, the E-nose structure consists of TGS26XX sensor arrays, a signal processor, data gathering by Arduino, and data analyzing by MATLAB [22]. Sensor arrays are installed in a tube with an air pump, temperature and humidity sensors, power supply and a DC fan to clean the space.

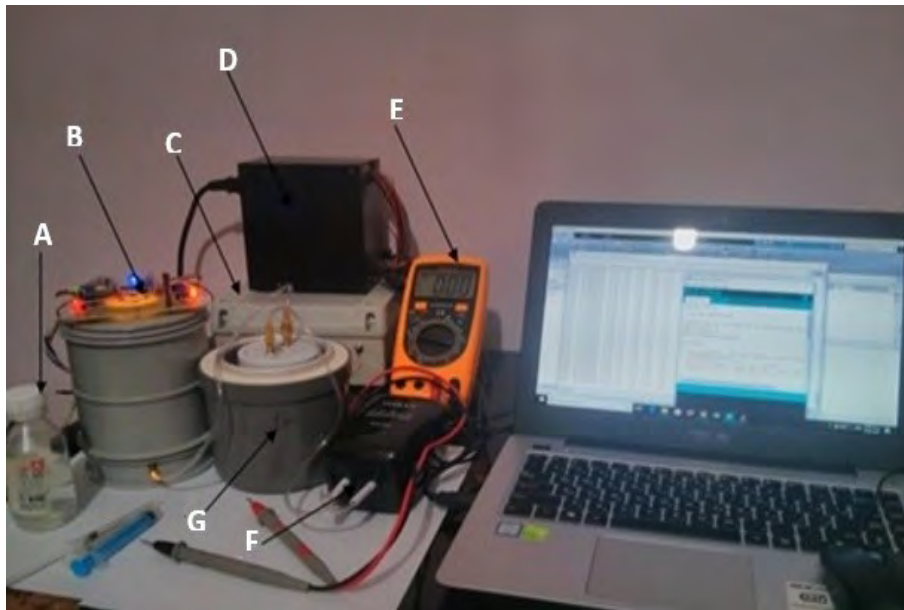


Fig. 2 Overview Of Hardware Electronic Nose With Arduino. A: Ethanol 96%, B: Array Sensor, C: Circuit Box, D: Power, E: Multimeters, F: Sampling Chamber, G: Air Pump

The main tube is made of PVC materials with a fan in one end and an electrical board at the other end and includes an SHT10 sensor [22-23] to sense the temperature and humidity, continuously. The sampling tube is made of glass with a pump on the one side and the other side is connected to the main tube for clearing the main tube with 3.5 liters per minute output. According to repeated calculation and comparison of models, designed in GUI, sensor outputs are reloading in an Excel file and attention to sensor's behavior, SYSTEM IDENT is chosen to find out the second transfer function which is not used here because of the low rate of proportion. So, it is calculated using a second-order polynomial Exponential function (CFTOOL) And MPS model (FOPDT) [23]. According to metal-oxide-semiconductor status, the structure of designed E-nose responses rapidly affected by temperature and humidity. But, it is restricted to the accurate amount of Ethanol. Based on the mentioned existence restrictions, the sensor's output is regulated each time before locating the accurate amount of Ethanol in the tube. After that by using DUE Arduino controller with 9600

bit/sec serial speed, the outputs would be demonstrated in Excel software. Finally, data are analyzed by repeating samples and comparing models by designing the GUI in MATLAB (Figure 3).

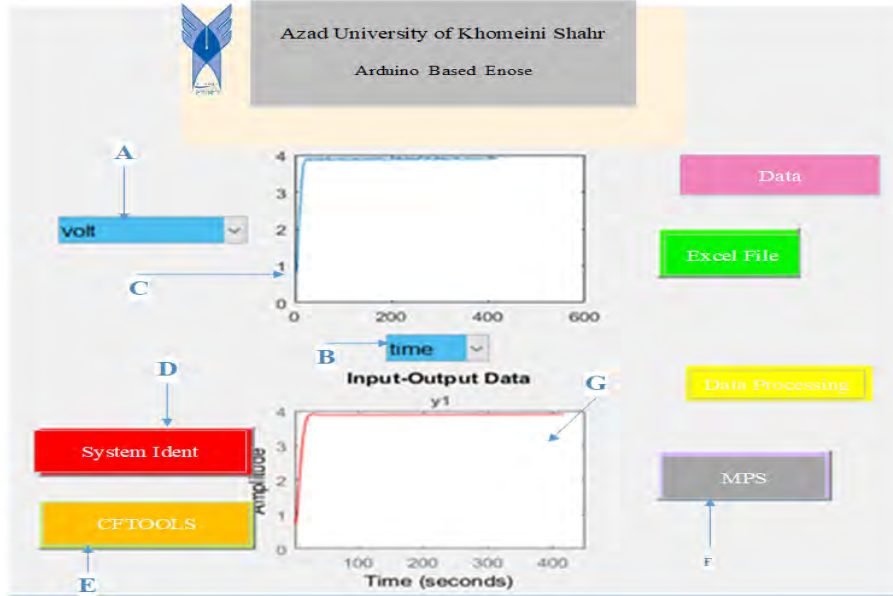


Fig. 3 Overview of the GUI; A: The axis displays the voltage sensor, B: The axis displays the time of biopsy, C: Showing the sensor response, D: System identification, E: The sensor response to binomial view, F: The sensor response using the MPS, G: Drawing out the sensor response using the binomial model MPS.

### 3. A theory for MPS model

As it was mentioned before, the purpose of the study is to present a reducing model depending on ethanol temperature, humidity and gas density for metal-oxide semi-conductive sensors. Therefore, it tries to find a related TGS response with fewer parameters. According to the output signals for different densities, the sensor’s behavior consists of a First Order Pulse Dead Time (FOPDT). In this study, the model is used as an MPS model to reduce the parameters and factors. The proposed MPS model consists of simple and fewer parameters, which leads to the more accurate simulation of the sensor behavior, and finally establishes a better short response. Since the multiple undesirable changing of ethanol from a syringe to the container, PPM calculation is not accurate [24] and ML unit is used to make a modeling calculation, and responses are gathered with ethanol density (C) verified from 0.1ML to 1ML in three steps by varying separately the temperature and humidity. Furthermore, controlling parameters in simultaneous variant temperature and humidity state is difficult, this step has been neglected intentionally. The MPS model based on the 1st order response parameters shown in Equation: 7 with three different parameters ( $K_p, \theta, \tau$ ).

$$H(s) = \frac{K_p e^{-\theta s}}{1 + \tau s} \tag{7}$$

According to Equation: 7,  $H(s)$  is the relation between density’s changes and the sensor response,  $K_p$  is the efficiency of the process,  $\theta$  is a time delay and  $\tau$  is a fixed time. Then the calculation of parameters based on the responses is done (Figure 4). We can use Equation: 8 to calculate the efficiency of the system.

$$K_p = \frac{\Delta Meas}{\Delta Value} \tag{8}$$

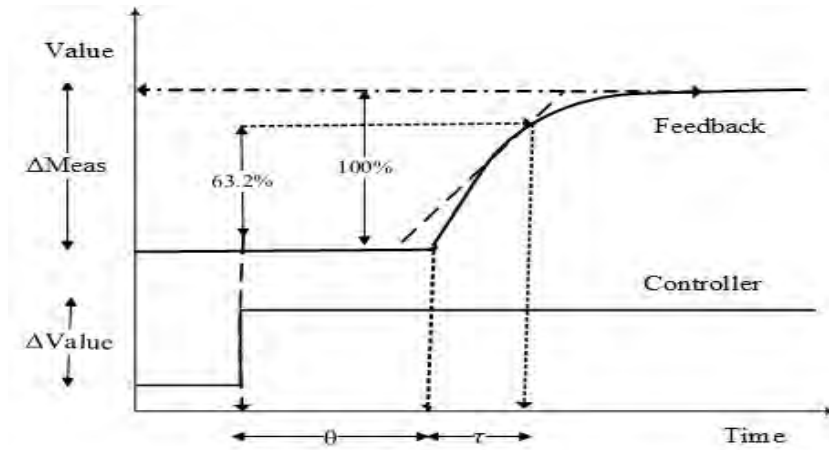


Fig. 4 First Order Response System

With A Dead Time In Accordance With The MPS Model

In this formula  $\Delta\text{Meas}$  means the total change in the amount of feedback and  $\Delta\text{Value}$  shows the total changes in the controller output command. To calculate  $K_p$  by Equation: 9, the maximum amount of output  $V_m$  is related to input density  $C$ , i.e.:

$$K_p = \frac{V_m}{C} \tag{9}$$

By sampling three times, it can be seen that  $K_p$  is not related to temperature and humidity and it is only related to ethanol density  $C$  (in ML). Hence, the relation between density and efficiency could be calculated from Equation: 10;

$$K_p = \frac{3}{C} \tag{10}$$

The time between controller changes to feedback changes is denoted by  $\Theta$  which is called "dead time". To calculate by the drawing method, the initial feedback change points are determined and then the time duration of the controller is increased. In this case, it is proved that this parameter is not related to temperature and humidity. The fixed time  $\tau$  is the time duration when the feedback initialize to change up to 63.2% of the maximum amount of feedback. This parameter is related to density  $C$ , temperature, and humidity. By using the drawing method in the feedback round, a line is drawn at the intensive change of the level point to cut the fixed feedback horizontal slashed line. The initial time of abutted line indicates the system's fixed time. Therefore, a line at the point of 63.2% is drawn horizontally that would cut the vertical line and it could be used to calculate the system's fixed time. To follow up, the E-nose hardware designing, sampling processes, MPS parameters calculation, results and analysis based on R-squared value ( $R^2$ ) determination are introduced.

#### 4. Results and model evaluation:

The model evaluation has been done by using the real sensor output comparison as well as an exponential model.

##### 4.1. Evaluation of the sensor output:

As it was stated before, sampling is conducted by the following three steps.

NO	C(ML)	Kp	$\tau$	$\theta$	R <sup>2</sup>
1	0.1	30.6	28.11	22.39	0.98
2	0.2	15.20	10.9	21.2	0.96
3	0.4	7.9	4.11	8.39	0.97
4	0.5	6.42	2.57	16.43	0.93
5	0.6	5.16	5.25	46.75	0.99
6	0.7	4.32	6.36	6.14	0.95
7	0.8	3.77	36.83	37.17	0.96
8	0.9	3.37	14.77	16.73	0.98
9	1	3.2	41.91	13.09	0.99

Table 1: Response System With Mps Model(The Temperature = 27 ° And Humidity =% 30).

4.1.1. Step 1(Fixed temperature - fixed humidity):

100 samples are collected for this model. The results from 0.1 ML to 1ML amount of ethanol density at temperature 27° C. and %30 humidity in the MPS model are shown in Table I. As it is shown in Table I, the response of bases on MPS model parameters and sensors data has the rate of the R2 relation between the minimum %93, and a maximum of %99.The sample data for the density of 0.6 ML at temperature 27 ° C and %30 humidity is shown in Figure 5.

NO	C(ML)	Kp (27 °)	$\tau$ (27 °)	$\theta$ (27 °)	R <sup>2</sup> (27°)	Kp (40 °)	$\tau$ (40 °)	$\theta$ (40 °)	R <sup>2</sup> (40 °)
1	0.1	32.7	4.54	20.66	0.99	29.9	2.6	7.4	0.99
2	0.2	16.35	5.55	28.65	0.99	15.7	3.76	2.74	0.96
3	0.3	10.83	7.9	10.6	0.98	10.43	3.05	13.45	0.99
4	0.4	8.02	13.66	28.84	0.98	7.22	5.9	31.1	0.97
5	0.5	6.3	10.54	22.46	0.99	5.22	13	65.5	0.96
6	0.6	5.33	14.24	7.26	0.98	5.15	4.97	3.53	0.99
7	0.7	4.67	6.53	17.97	0.97	4.47	6.5	29.5	0.99
8	0.8	4.02	13	20.5	0.98	3.88	4.04	9.46	0.99
9	0.9	3.62	8.82	7.68	0.98	3.42	3.75	7.05	0.91
10	1	3.02	2.91	13.59	0.99	3.11	5.68	33.32	0.97

Table 2: Response System With Mps Model(The Temperature = 27 ° And Humidity =% 30).

4.1.2. Step 2 (fixed humidity- variant temperature):

For this step, 400 samples are collected. The results from 0.1 ML to 1ML amount of Ethanol’s density at 27° C, 40° C, 50 ° C and 60 ° C at the fixed humidity of %30 in MPS model are shown in Table III and IV. Figure 6 and Figure 7 show the sensor response as compared to the MPS model. According to Table II and Table III, the sensors response is calculated using the MPS model.The level R2 at 27° C, 50 ° C, 60 ° C is between the minimum of 0.96 and the maximum of 0.99. Also at 40 ° C, the level R2 is between the minimum of 0.91 and the maximum of 0.99.

4.1.3. Step 3 (Fixed temperature- variant humidity):

Above 300 samples are collected for this model. Results from %20,%30,%35,%40 and %50 ethanol density at different degrees and variant humidity in the MPS model are shown in Table IV and Table V. As shown in Table V and Table VI, the sensor’s responses in humidity %20 to %50 in concentrations of 0.2 ML to 1ML with the MPS model are obtained. R2 is between the minimum 0.94 and the maximum 0.99. Figure 8 shows the sensor’s response as well as the MPS model for the mentioned step.

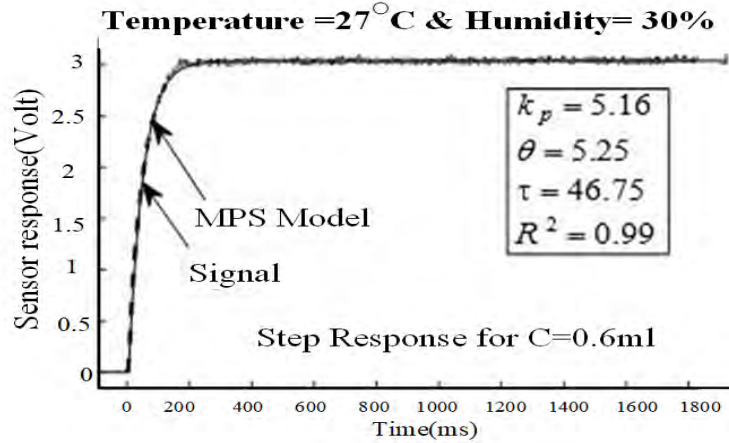


Fig. 5 Comparison of the response of the sensor for C = 0.6ML ethanol at a constant temperature of 27° C and humidity %30 with the MPS model

NO	C(ML)	Kp (50 °)	τ (50 °)	θ (50 °)	R <sup>2</sup> (60°)	Kp (50 °)	τ (60 °)	θ (60 °)	R <sup>2</sup> (60 °)
1	0.1	30.9	4.44	10.06	0.98	30	3.62	10.88	0.99
2	0.2	15.65	2.76	10.04	0.99	14.9	6.64	10.36	0.97
3	0.3	7.13	7.56	50.94	0.97	10.16	5.64	7.16	0.98
4	0.4	7.77	3.9	5.1	0.99	7.7	4.37	7.63	0.98
5	0.5	4.92	3.64	21.86	0.99	6.06	2.56	8.94	0.97
6	0.6	4.58	12.78	43.22	0.96	5	10.54	35.46	0.98
7	0.7	4.47	3.73	3.97	0.99	4.4	1.79	2.81	0.97
8	0.8	3.92	3.76	2.94	0.97	3.86	1.89	5.61	0.98
9	0.9	3.45	4.42	5.48	0.99	3.2	14.86	7.24	0.99
10	1	3.12	4.91	27.29	0.97	3.11	1.87	3.63	0.97

Table 3: Response System With Mps Model(The Temperature = 27 ° And Humidity =% 30).

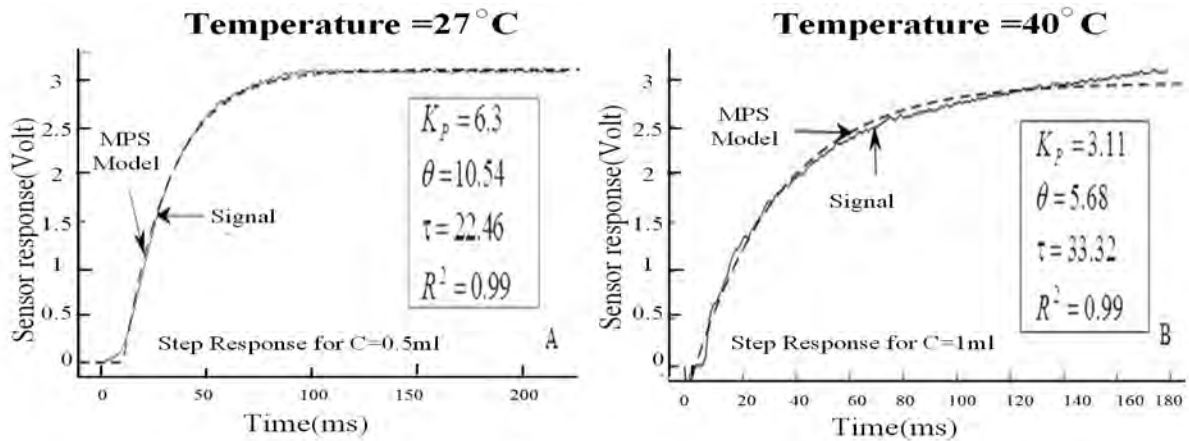


Fig. 6 Comparing The Response Of The Sensor (V) At Different Temperatures With An MPS Model In Every Different Concentration Of Ethanol, A: Temperature =27 ° C, B: Temperature =40° C

4.2. MPS model verification with the exponential model:

One of the models with the least number of parameters is the exponential model with regard to Equation: 5. As the fitted data is based on the exponential model, the least number of parameters is bi-sentence,

NO	C(ML)	Kp %20Hum	$\tau$ %20Hum	$\theta$ %20Hum	R <sup>2</sup> %20Hum	Kp %30Hum	$\tau$ %30Hum	$\theta$ %30Hum	R <sup>2</sup> %30Hum
1	0.2	15.7	4.3	8.2	0.97	15	12.03	6.77	0.98
2	0.4	8.02	5.25	23.7	0.97	7.97	12.88	29.12	0.99
3	0.6	5.28	1	4	0.98	5.08	5.77	5.03	0.98
4	0.8	3.86	1.8	3	0.96	3.76	1.1	5.4	0.99
5	1	3.54	4.75	2.75	0.99	3.37	1.89	5.61	0.94

Table 4: Response System With Mps Model in Humidity %20,%30

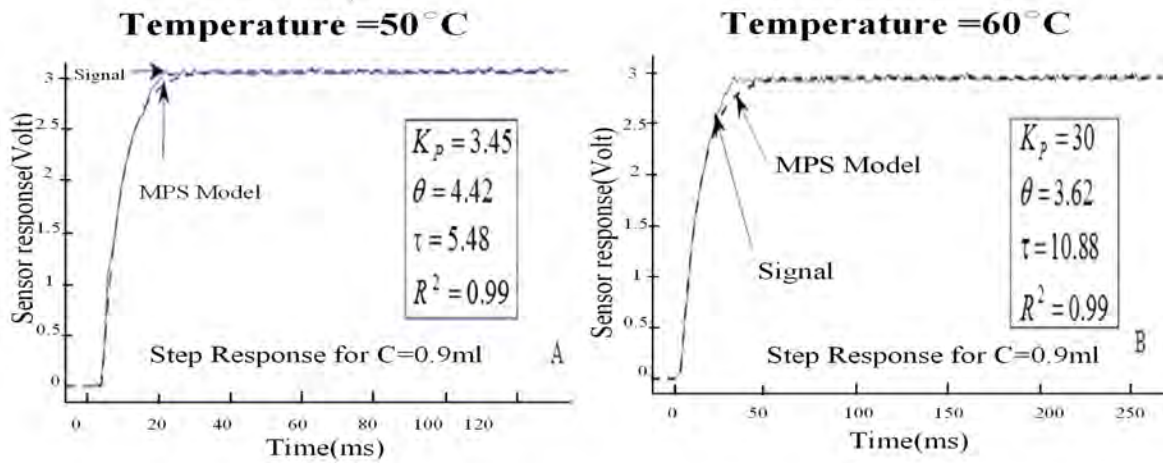


Fig. 7 Comparing The Response Of The Sensor (V) For Every Different Concentration  $\tau$  Of Ethanol At Different Temperatures With MPS Model A: Temperature =50 C, B: Temperature =60 ° C.

NO	C(ML)	Kp %40Hum	$\tau$ %40Hum	$\theta$ %40Hum	R <sup>2</sup> %40Hum	Kp %50Hum	$\tau$ %50Hum	$\theta$ %50Hum	R <sup>2</sup> %50Hum
1	0.2	15.1	6.35	22.15	0.98	14.06	8.7	31.3	0.99
2	0.4	7.55	9.19	10.31	0.97	7.5	5.28	46.22	0.97
3	0.6	5.26	7.66	8.34	0.94	5.06	3.52	5.98	0.98
4	0.8	3.95	14.18	20.32	0.99	3.8	12.92	40.08	0.95
5	1	3.48	7.58	39.52	0.99	3.53	13.75	23.25	0.99

Table 5: RESPONSE SYSTEM WITH MPS MODEL IN HUMIDITY % 20, % 30

which is used to reevaluate the MPS model as in Equation: 7. Although both models (the two-term multi-exponential and MPS) in Laplace domain have the same function, the MPS model has a simple and fewer number of coefficients  $K_p, \theta$  and  $\tau$ , with respect to multi-exponential model's coefficients of  $G_1, \tau_1, G_2,$  and  $\tau_2$ . Moreover, with respect to the effect of the processing time in optimization, having the least number of coefficients can significantly reduce the processing time and provide a faster estimation of sensor's responses[5]. The comparison between the MPS as well as bi-sentence exponential models is shown in %30 humidity, in Table VII and Table VIII. According to the Tables VIII and IX, the results of few parameters are close to the sensor response by R<sup>2</sup>, while in the numerous parameters situation, bi-sentence exponential model is closer to the true response. Figure 9 and 10 show the sample data belonging to Table VII and Table VIII. Based on Figure 9 and Figure 10 and the related tables and according to the results, both models have a common point with regards to Laplace transform, but the MPS model is simpler and has fewer parameters, which is significantly beneficial in reducing the processing steps and is closer to a real response.



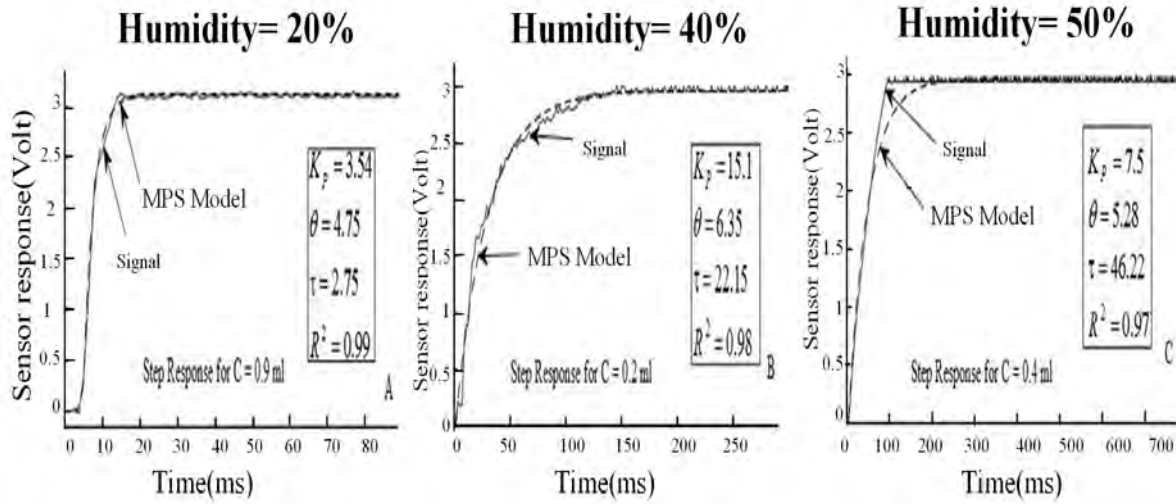


Fig. 8 Comparing The Sensor Response For The Constant Humidity At %20,%40 and %50 Concentration With Calculated MPS Model Coefficients

Model	C(ML)	0.2	0.4	0.6	0.8
Multi Exponential Model	$\tau_2$	-0.06	-0.01	-0.12	-0.26
	G2	-4.38	-7.1	-4.36	-3.98
	$\tau_1$	-0.003	-0.003	-0.014	0.012
	G1	3.13	6.82	2.99	2.95
	R <sup>2</sup>	0.90	0.99	0.93	0.98
MPS Model	$\tau$	6.77	29.12	5.03	5.40
	$\theta$	12.03	12.88	5.77	1.1
	Kp	15.00	7.97	5.08	3.76
	R <sup>2</sup>	0.98	0.99	0.98	0.99

Table 6: Comparing Binomial System Response With Various Concentration Of Ethanol Per View And Mps Models In Constant humidity %30

Model	C(ML)	0.2	0.4	0.6	0.8
Multi Exponential Model	$\tau_2$	-0.08	-0.11	-0.1	-0.12
	G2	-3.77	-4.07	-3.54	-3.66
	$\tau_1$	-0.04	-0.02	0.01	0.01
	G1	2.98	3.02	2.92	2.98
	R <sup>2</sup>	0.98	0.97	0.97	0.98
MPS Model	$\tau$	10.88	7.16	8.94	7.24
	$\theta$	3.62	5.64	2.56	14.86
	Kp	30	10.16	6.06	3.2
	R <sup>2</sup>	0.99	0.98	0.97	0.99

Table 7: Comparing Binomial System Response With Various Concentration Of Ethanol Per View And MPS Models In Constant Temperature 60 ° C

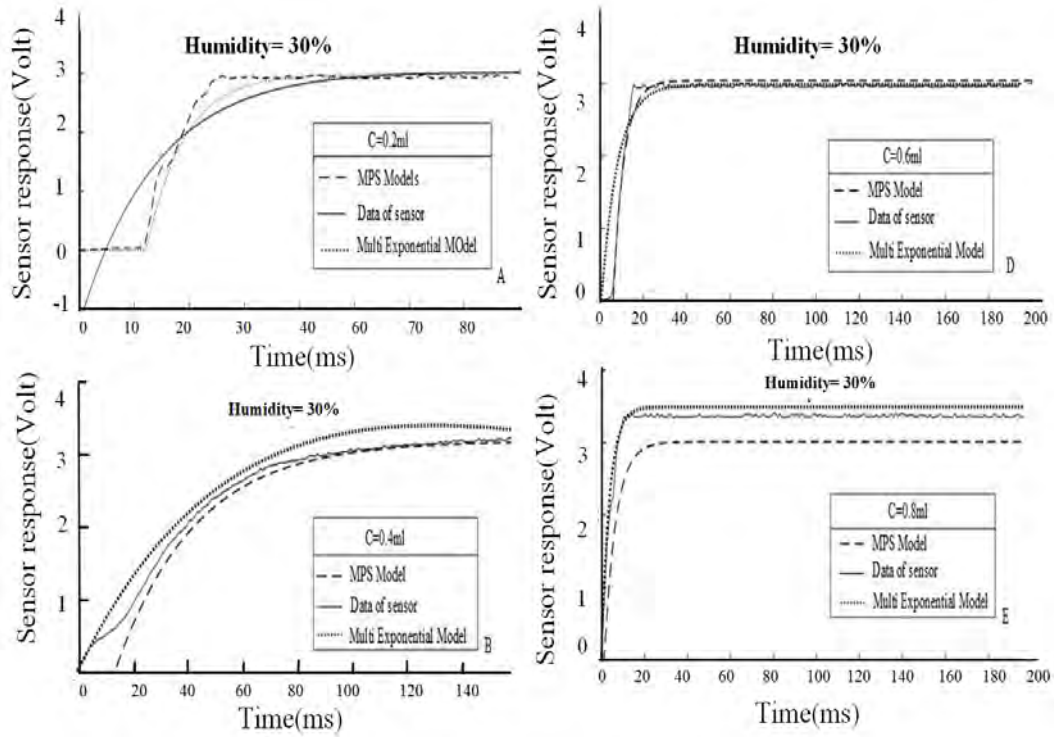


Fig. 9

Comparing the sensor response with different concentrations using the Multi Exponential Model and MPS models in the constant humidity of 30(percentage), A: C=0.2ML, B: C=0.4ML, D: C=0.6ML, E: C=0.8ML

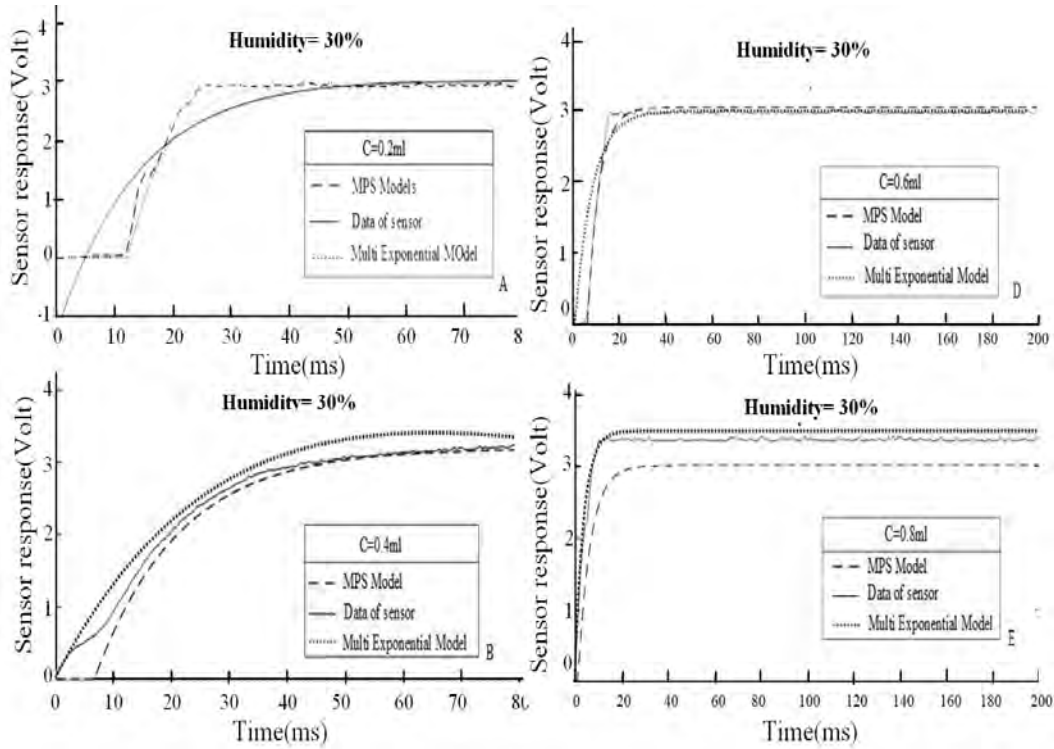


Fig. 10

Comparing the sensor response with different concentrations using the Multi Exponential Model and MPS models in constant temperature 60C, A: C=0.1ML, B: C=0.3ML, D: C=0.5ML, E: C=0.9ML.

Finally, the weak and strong points of each model are shown in Table IX.

Model	Strengths Format of model	Weakness
Multi Exponential Model	-Covers three zones sensors response	-Complex relations for parameters of sensors responses - In some cases is not close to the sensor's response
MPS Model	-Simpler relations for parameters - Fewer factors - More accurately simulation of the response - Creation of better transient time	Could be different based on the type of sensor

Table 8: ADVANTAGES AND DISADVANTAGES OF THE MPS MODEL AND MULTI EXPONENTIAL MODEL.

#### 4.3. CONCLUSION

Because of very small dimensions, reasonable price, short response, and long-lasting functions, metal-oxide semi-conductors are common to be used and they have transient and steady state conditions. The proposed models consist of complex parameters and using them in simulation software is complicated. The purpose of this paper is to find a new helpful model based on fewer parameters and mathematical equations. The most popular model is the bi-sentence exponential model which covers three zones of response, but it has complex relations with many parameters and it is not sometimes simultaneous with the sensor's response. Suggested MPS model has simpler and fewer parameters with closer short responses. 800 data collections are analyzed in three categories: fixed-temperature-fixed humidity in which data has the rate of the R2 relation is between the minimum %93, and the maximum of %99, variable temperature fixed humidity in which the level R2 at 27 C, 50 C, and 60 C is between the minimum of 0.96 and the maximum of 0.99. Also at 40 C, the level R2 is between the minimum of 0.91 and the maximum of 0.99, fixed-temperature-variant humidity in which R2 is between the minimum 0.94 and the maximum 0.99. Results convincingly show that this model could be verified with different sensors. over than vast research area of e nose [25] this work could be applied for further applications like mobile olfaction [26].

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