

# Optimizing the Spectral Properties of the Chemical Sensor to Detect Concentrations of Gas Mixtures

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**Abstract:** Monitoring aromatic hydrocarbons is environmentally important because these chemical pollutants are ubiquitous. While waiting for powerful sensors capable of detecting hydrocarbons at extremely low levels, the current study demonstrates how each of the pure gas mixtures can be quickly and accurately identified. A noise removal unit was created for the chemical sensor data and then processed on the basis of the proposed algorithms in order to achieve matching and calibration. This method can be extended to other important aromatic hydrocarbon pollutants.

**Keywords:** fluorescence background, Aromatic hydrocarbons, filter, noise

## 1. Introduction

Aromatic hydrocarbons like naphthalene, (benzene, and toluene) and can cause great human health harm. Thus, prolonged exposure can lead to consequences such as anemia, reproductive dysfunction, damage to the nervous system, as well as some types of cancer. The situation is also aggravated by the fact that the production of gasoline is increasing every year [1].

This requires more efficient and easily accessible methods for monitoring the concentration of these substances in the air, both in various institutions and on city streets. There are many solutions to meet this need, but they have various drawbacks, such as the time to determine the concentration, the cost of production, the need for laboratory conditions to work, low accuracy, or the inability to determine the concentration of several different gases [2; 3].

The development of complex systems for detecting hazardous chemicals through portable sensors has become an urgent necessity because it requires rapid on-site analysis, because advanced detection systems rely on these devices, and thus their response may be with lower partially unclear. Such as, implementing a good sensors requires detecting this response in a target-molecule, and other interfering molecules [4; 5]. Studying the noise signal is an important consideration when studying and implementing sensor systems. There are several types of noise that affect the accuracy of measuring devices and they depend on the working principle of direct absorptiometry. The literature has reported an explanation of source noise, its causes, how it is described, and the types of noise to which the optical detector is exposed [6].

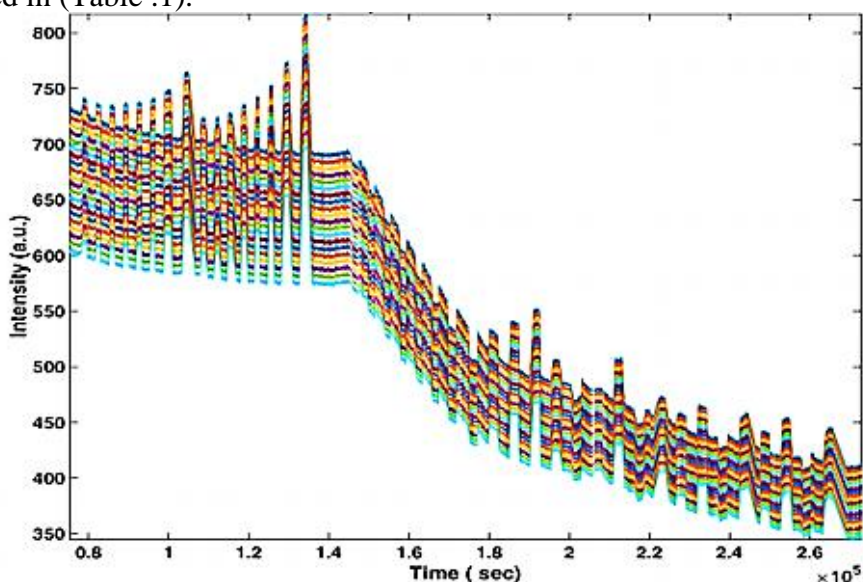
At the same time, in order to solve these problems, new research is constantly being carried out. For example, a method has been developed for determining the concentration of aromatic hydrocarbons based on the use of spectral data from chemical sensing materials.

Numerical methods are applied to the data obtained to determine the concentration of gases, which determines the scientific novelty of this study.

## 2. Material and methods

### 2.1 sensor

The experiment used a described sensor based on the use of chemically sensitive elements based on FDM1. This makes a sensor materials deposited with a glass-substrate, a fibers optic-probe connected with an LED light source, and a spectrometer used to measure fluorescence spectra[7]. The glass substrate containing the sensing material is located in an airtight cell, to that cleaned air or a mixing of air and vapors of aromatics hydrocarbons in main concentration which supplied. In accordance with the Bouguer-Lambert-Beer law and the principle of superposition, the absorption spectrum of the mixture recorded by the spectrometer is presented as a lined combinations of the spectrum of substances included in the Data obtained from this sensor (Fig.1). According to this, there is specific needful to the target spectrun, are Naphthalene, benzene and toluene (Kinetics of wavelength 460 nm) and different temperatures described in (Table .1).



**Figure 1:** Aromatic compounds received from the sensor

**Table 1** Gas supply parameters

<i>Naphthalene</i>	<i>0.2 <math>\mu\text{g}/\text{min}</math></i>
<i>Benzene</i>	<i>44.0 <math>\mu\text{g}/\text{min}</math></i>
<i>Toluene</i>	<i>10.1 <math>\mu\text{g}/\text{min}</math></i>
<i>Temperatures, <math>^{\circ}\text{C}</math></i>	
<i>Naphthalene</i>	<i>50 <math>^{\circ}\text{C}</math></i>
<i>Benzene</i>	<i>110 <math>^{\circ}\text{C}</math></i>
<i>Toluene</i>	<i>100 <math>^{\circ}\text{C}</math></i>

### 2.2 Spectra retrieval and processing

Spectra is stored and imported in several database's and registered with many tools that have many properties. So, algorithm has been developed to input spectral data and vary

wavelength averages, resolved and inputting of file formats, and then process them with proposed filters, exploiting in this way the high possible resolution.

### 3. Results and discussion

#### 3.1 Obtaining reference spectra

The concentration is specified through the (Bouguer Lambert Beer) law (BLB) in the ultra-violet and visible spectrum of light. The decrease in intensity ( $dI$ ) at wavelength ( $\lambda$ ), that happens when monochromatic lighting  $I(\lambda)$ , penetrates via a sample of thick ( $dz$ ) along the  $z$ -axis including injected particles at a molar concentration ( $c$ ). So intensity is known as:

$$-dI(\lambda) = I(\lambda) \cdot c \cdot k(\lambda) \cdot dz \quad (1)$$

integrate over the path length  $l$ :

$$\int_{I_{ref}(\lambda)}^{I_{sam}(\lambda)} \frac{1}{I(\lambda)} \cdot dz = k(\lambda) \cdot \int_0^l c \cdot dz \quad (2)$$

Where:  $I_{ref}(\lambda)$  represent the initial, or so called reference intensity,  $I_{sam}(\lambda)$  represent the intensity transmitted via the sample, the so called sample intensity, and  $k(\lambda)$  is the proportional factor. Assuming the concentration ( $c$ ) represent the uniform and does not depending on ( $z$ ), this is lead to :

$$\ln \frac{I_{ref}(\lambda)}{I_{sam}(\lambda)} = k(\lambda) \cdot c \cdot l \quad (3)$$

often we can express of the (BLB-law) as :

$$I_{sam}(\lambda) = I_{ref}(\lambda) \cdot 10^{-\epsilon(\lambda) \cdot c \cdot l} \quad (4)$$

Usually, the (BLB-law) is valid for dilution analytic solutions, for strength monochromatic, equivalent, and cohesive radiations in optical homogeneous (iso-tropic) medium. There must be no luminescence or propagation in the observed solution, and the length of the optically path must be strictly defined.

The sensitivity of the measurements can be perfected by increase the path length for materials with less molar absorption co-efficients, as the absorption of light energy in visible and UV-rays is related with several types of electronic transitions [8; 9].

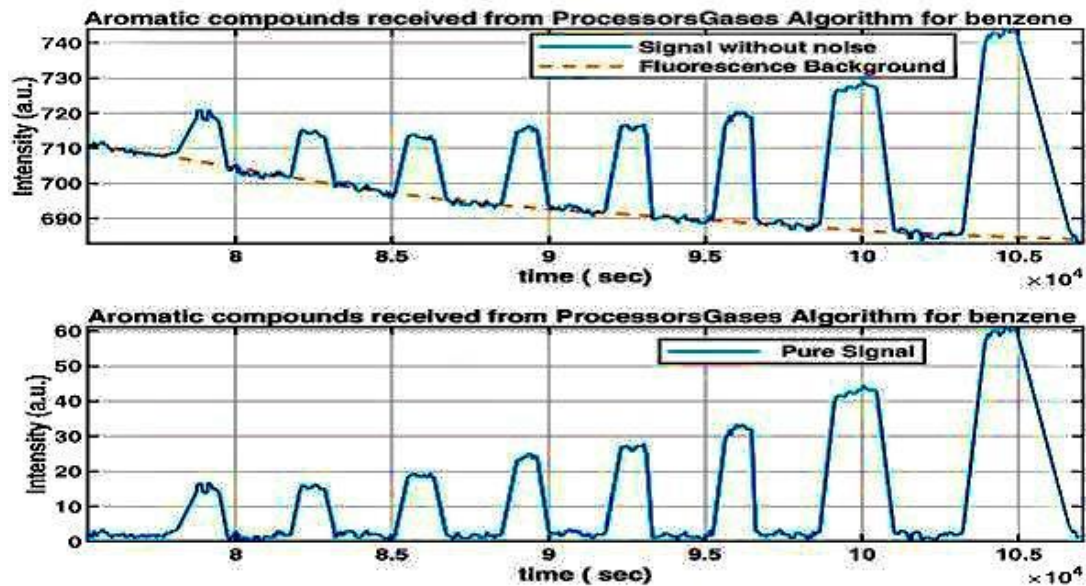
#### 3.2 Mathematical model of spectrum registration

The spectrograph receives a signal from one point, integrating in a natural way both in time and in space coordinates. In summary, the signal from the spectrograph output  $O(\lambda_n)$  can be represented by an additive model consisting of the fluorescence background  $P(\lambda_n)$  (usually a smoothly varying line) and various noises (impulse noise  $vI(\lambda_n)$  and thermal noise  $vR(\lambda_n)$ ) [10-12]. As a result, the mathematical model of the recorded "raw" signal can be written as follows.

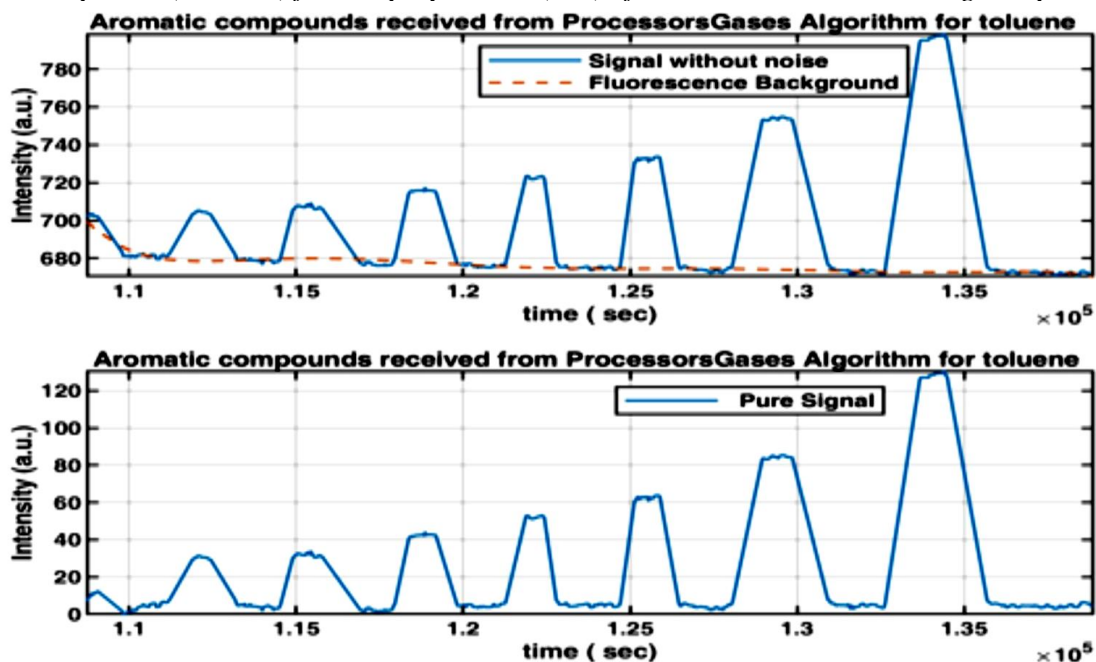
$$O(\lambda_n) = P(\lambda_n) + RS(\lambda_n) + v_f(\lambda_n) + v_R(\lambda_n). \quad (5)$$

The specificity of the spectral data obtained from the mathematical model lies in the change in the number of repetitions of spectral readings, depending on the problem being solved, the set of points (from units to tens) used in measurements and calculations. Therefore, the spectral data obtained from the model is a variable length array. Since the nature of noise filtering in signals is varied, we can apply a medium filtration at the preliminary stage for the eliminated of impulse noise. In addition, the median filter is more effective than linear-filters in cases where the varieties in non-signaling amounts are high comparing to the variance of the Gaussian-noise, due to the fact that it gives a less amount of the RMS error of the output signals

comparing to the input signal without noise compared to optimal line filters. Permanent baseline correction is smoothed and performed followed by normalization of the rectified spectrum by their area. The autofluorescence basis is subtracted for pure range analysis using scientific approaches: polynomial evaluation (PolyFit) and gas improvement method for processors. Another algorithm used is polynomial approximation and wavelet shift, which are suggested as useful techniques for background removal in certain situations where it is necessary to separate the frequency components of the spectrum from the background and noise. (Fig .2 and 3). In this study, the following two modifications of the polynomial approximation were also used: ModPoly and I-ModPoly[12-15]. The data obtained from the spectrometer using the chemical sensor elements and the processing using the algorithms are presented in (Table .2).



**Figure 2:** Smoothed spectra with auto-fluorescence background highlighted (top.) and "clean" spectra (bottom.) for the polynomial (7th) of the benzene aromatics signal spectrum.



**Figure 3:** Smoothed spectra with autofluorescence background highlighted (top) and "clean" spectra (bottom) for the polynomial (7th) of the aromatics signal spectrum for toluene

**Table 2.** showing the parameters, models and algorithms used in signal cleaning.

	<i>Time (sec)</i>	Signal pre-processing	Aromatic compounds from the sensor after (wavelength all 460 nm) for benzene			
			the median filter	PolyFit	ModPoly	I-ModPoly
1	7,52E+04	708,950	708,950	715,182	718,829	710,724
2	7,53E+04	709,690	709,690	714,909	718,053	710,712
3	7,53E+04	711,100	710,050	714,632	717,282	710,702
4	7,53E+04	711,240	710,050	714,373	716,572	710,690
5	7,53E+04	708,940	711,100	714,121	715,892	710,670
6	7,54E+04	710,050	710,050	713,875	715,243	710,639
7	7,54E+04	711,610	710,050	713,636	714,622	710,608
943	1,07E+05	685,250	683,340	693,296	687,539	684,011
944	1,07E+05	683,340	683,340	692,654	685,310	683,987
945	1,07E+05	682,810	683,450	691,671	681,861	683,970
946	1,07E+05	681,400	683,450	691,003	679,488	683,956

	<i>Time (sec)</i>	Signal pre-processing	Aromatic compounds from the sensor after (wavelength all 460 nm) for toluene			
			the median filter	PolyFit	ModPoly	I-ModPoly
1	1.09E+05	703.020	701.830	694.600	696.435	699.490
2	1.09E+05	703.610	701.950	694.523	696.619	698.961
3	1.09E+05	700.990	702.590	694.407	696.869	698.443
4	1.09E+05	704.560	703.020	694.289	697.093	698.101
5	1.09E+05	704.110	703.020	694.211	697.218	697.598
6	1.09E+05	701.950	703.540	694.092	697.385	697.250
7	1.09E+05	702.590	702.590	694.012	697.477	696.785
700	1.38E+05	673.510	672.600	676.494	661.614	672.866
701	1.38E+05	672.600	672.240	676.204	661.233	672.849
702	1.38E+05	672.220	672.240	675.771	660.682	672.805
703	1.38E+05	672.240	672.240	675.339	660.169	672.787
704	1.38E+05	670.540	672.220	675.052	659.852	672.753

	Time (sec)	Signal pre-processing	Aromatic compounds from the sensor after (wavelength all 460 nm) for Naphthalene			
			the median filter	Poly Fit	ModPoly	I-ModPoly
1	9.29E+04	708.95	665.81	658.562	668.047	668.099
2	9.29E+04	709.69	665.81	658.898	668.156	668.162
3	9.29E+04	711.1	665.81	659.229	668.263	668.225
4	9.29E+04	711.24	665.82	659.558	668.368	668.288
5	9.29E+04	708.94	665.81	659.883	668.472	668.351
6	9.29E+04	710.05	665.81	660.206	668.573	668.415
7	9.29E+04	711.61	665.81	660.5259	668.672	668.478
1529	7.58E+04	754.62	713.94	691.429	696.548	703.978
1530	7.58E+04	753.78	713.94	692.081	698.083	704.815
1531	7.58E+04	755.39	713.94	692.717	699.585	705.658
1532	7.58E+04	673.12	712.5	693.360	701.112	706.509
1533	7.58E+04	676.63	712.5	694.011	702.662	707.401

### 3.3 Noise structure of sensor spectra

For obtaining the concentrations of gas mixtures (naphthalene benzene coloring) noise and background autofluorescence must be reduced. The noise structure was determined using the equation below for estimating noise as a role of signal-strength.

$$\hat{N}_s(i) = b_l \times I(i) \quad (6)$$

where for each point  $i$  of the signal, the estimate of the standard deviation of the noise  $\hat{N}_s$  ( $i$  is obtained by multiplying the corresponding intensity of the noise-reduced signal  $I(i)$  by  $b_l$ , i.e., the average value of the coefficients  $b_l$  of the obtained regression models. The noise structure can be applied to the simulated spectrum  $P$  to obtain the corresponding final spectrum  $S$  using the following equation:

$$S(i) = P(i) + P(i) \times \hat{N}_s(i) \times r(i) \quad (7)$$

where for each point  $i$  of the signal  $\hat{N}_s(i)$  is the noise estimated according to equation 7, based on the intensity of the pure spectrum  $P(i)$  and  $r(i)$

Combinations of concentrations of naphthalene, benzene and toluene are introduced, shown in (Fig.4,5 and 6), respectively, and combinations of their mixtures before and after treatment.

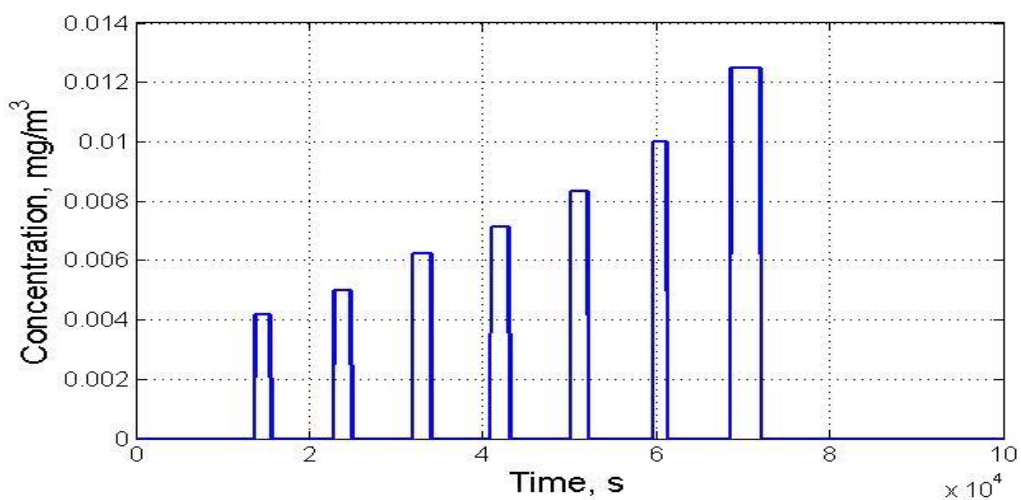
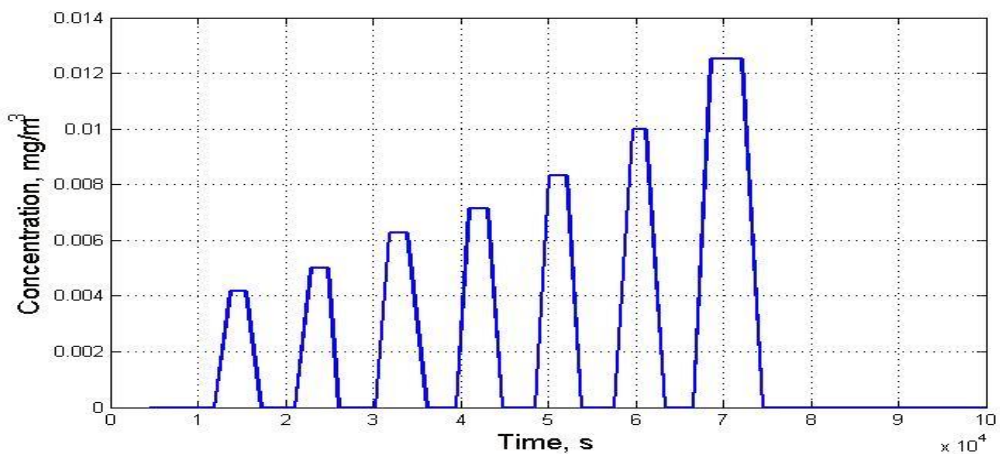
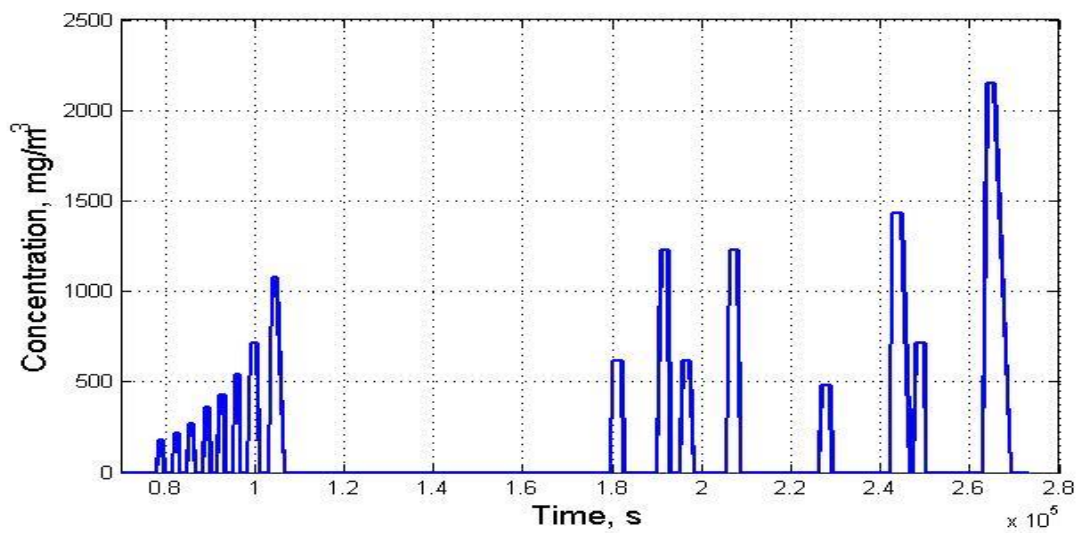
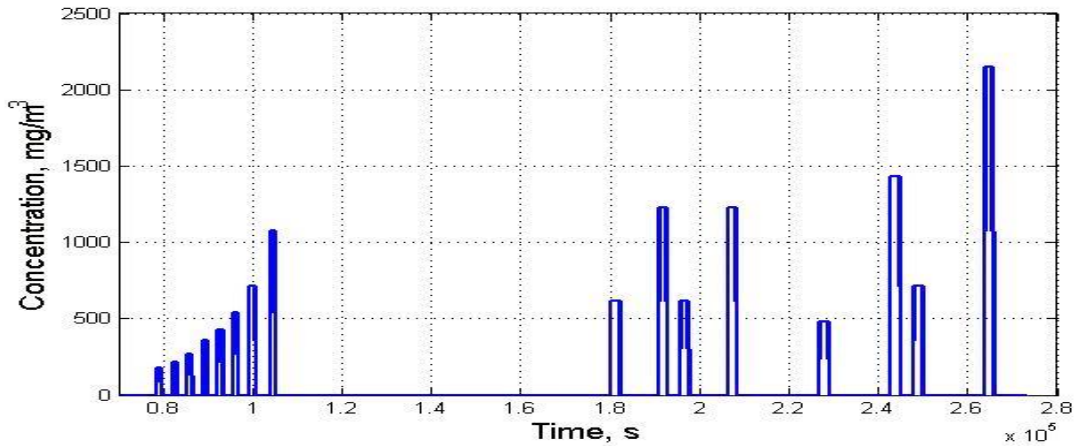


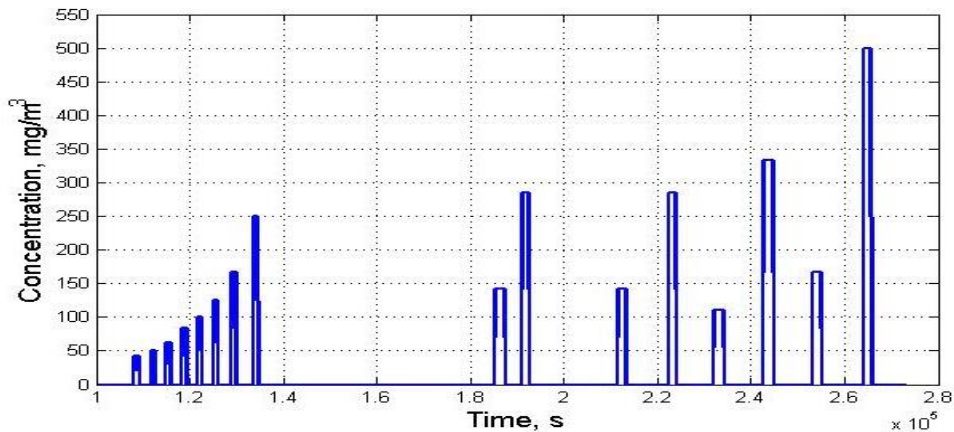
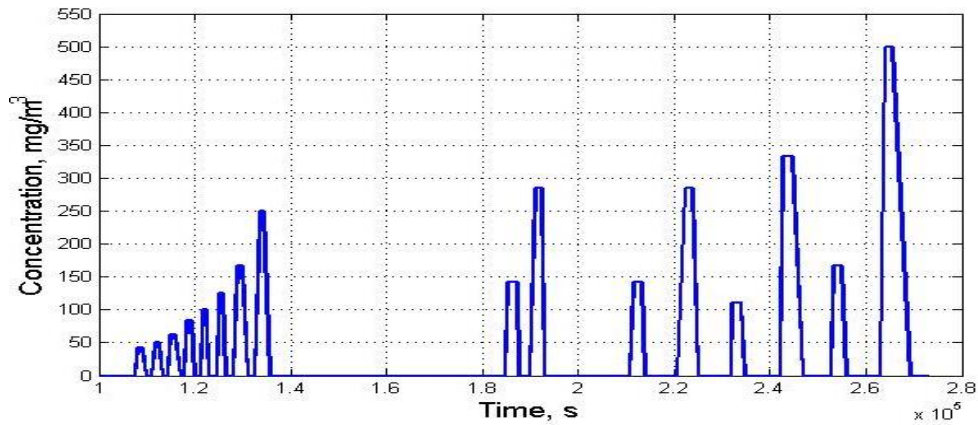
Figure 4: Output values before and after treatment (naphthalene)







**Figure 5:** Output values before and after treatment (benzene)



**Figure 6:** Output values before and after treatment (toluene)

Under the presumption of linearly relation between the concentrations of a special pure chemicals, and the intensity of the identical spectrum bands, duplicating units of the concentrations' spectrum by the identicate concentration levels in any gas mixture gives not realistic outcomes. Indeed, by this process, the spectral background of the individual-focus is forced for changing as to the identicate focus ratio , so the correct waveform not served. For this reasons, an algorithm raised on a sigmoidal weighted function (SWF) was evaluated to doubly the spectrum attributed to the real sample with respective concentration, But preserving the (framework intensity, and shape) , and thus just worked in the real absorption-bands. Given the sensor spectra  $S$ , composed of (1 ip) data point, the identicate spectra ( $R$ ), gained by



multiplying the (cc 1 ppb.) concentration value, weighted by SWF, for each  $i$  point by the equation:

$$R(i) = \left[ 1 + \frac{1}{1 + e^{-a \left( \frac{s(i) - s_{\Delta N}}{s_{\Delta u} - s_{\Delta Q} - m \right)}}} \times (c - 1) \right] \times S(i) \quad (8)$$

The (SMIN.), and (SMAX.) are the minimal and maximal signal intensity rates ( $S$ ), as arranged ( $a$ , and  $m$ ) are alterable parameters that utilized to determine the (SWF) shape. With this function, the fewest rates of signal intensity ( $S$ ) are multiplied by 1, while the highest rates are linear multiplied by the suitable concentration value ( $c$ ). The mean density amountes are multiply by a factor from  $(1 - c)$ , which is depend on the amounts of the parameters ( $a$ , and  $m$ ). Particularly, ( $m$ ) concernds to the percent of the signal strength that the douplcation factor is  $(c+1)/2$ , and  $a$  determines the slope of the sigmoid function[16-18]. In order to model a spectrum data set fitted for taking in to numerous the complex variables in the forming of gas mixtures in realized conditions, the methods of the algorithms used were used in parallel to obtain the corresponding signal[19; 20].

#### 4. Conclusions:

For the modeling of suitable spectral-data set to take in to account the series variation in the gas composition mixtures in actual conditions, the methods of algorithms used in parallel were used to obtain the corresponding signal. In this paper, four aromatic gases were taken into account: naphthalene, benzene and toluene. To do this, it is necessary to create a matrix for calculating the concentrations for the formation of mixtures. The starting aim is to obtain the spectra of gas mixtures from the chemical sensor, which must be exactly operated to obtain features of equaled size, maximum range, accuracy, etc. Once noise and background fluorescence affected differently the individual spectra, the credible concentration, in several contents were calculated via means of an appropriate concentration matrix. Thus a combination of congregation spectrum of the potential admixtures of the several study species constructed, to form the required data-base.

According to this procedure, the optimum selection of spectrum points will be determined, to achieve the extreme efficient extracted of the required information. The better outcomes will be gained by resolve a knowledge processes which permits the system to obtain new media spectrum and probably reject fewer informative spectra, relying on the measures used regarding noise, potential driftage, etc., and the specific environment that you are operating. This method can be extended to other important contaminants of aromatic hydrocarbons.

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