Comparison processors spectral analysis concentrations for aromatic compounds using the application of mathematical models

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(Communicated by Ehsan Kozegar)

Abstract

Prolonged exposure to gases in enclosed spaces, can cause health problems that may not be easily eliminated, several methods have been developed to determine the concentration of aromatic hydrocarbons. But these methods have certain limitations, which complicate the titration. Regression-based methods can be used using the software and applying numerical methods to the data obtained to determine the concentration of gases. The main idea of this paper: is to keep up with the ideal balance, and limit the deficiency of necessary to obtained from spectroscopic data, and the effect of mutilations presented by different noise decreases and autofluorescence background elimination algorithms was determined from the comparison data. And these changes ratios were in remove background fluorescence (benzene, toluene, xylene), for the (PolyFit) method they were 3% and 5% and 2%, and for the (ModPoly) method they were 1% and 2% and 2%, and for the gas processor method, they were 2% and 5% and 2%, respectively. So, it was noticed it has been noticed here that the proposed method (GasesProcessors) is better in terms of filter performance and autofluorescence background removal compared to other methods.

Keywords: Sensors, Aromatics hydrocarbons (BTX), Fluorescence, Polynomial FIT (Polyfit), GasesProcessors
2020 MSC: 32E30

1 Introduction

As it is known the great damage to public health is caused by mixtures of gases in general, and aromatic hydrocarbons like (BTX) Benzene, Toluene, as well Xylene in particular. Therefore, prolonged exposure to gases in enclosed spaces when the concentrations of these mixtures may be low in the air, even if the concentration of benzene is less than 0.1 mg/m^3 [21].

This can cause health problems that may not be easily eliminated and may become a disease that accompanies us throughout our lives, such as normal or acute anaemia, reproductive weakness, and damage to the nervous system,

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in addition to many types of cancer. Simultaneously, its percentage exceeds the Maximum Permissible Concentration of chemical elements and their compounds in the environment (MPC). Where the ratios of these concentrations to benzene and other aromatic hydrocarbons in most countries the above-mentioned ratio was $0.1 mg/m^3$ [12, 28].

This indicates the aggravation of the situation due to the fact that the production of gasoline increases only every year. Here, it requires finding more efficient and effective ways that can be easily worked on to monitor the concentration of these mixtures in the air, in closed areas in general or in city streets. Indeed, there are many solutions and ways to meet this need, but their advantages differ in addition to having different disadvantages, such as the duration of determining the concentration, the cost of production, the need for laboratory conditions to work, or low accuracy, or the inability to determine the concentration of several different gases at the same time.

Regression-based methods can be used using the software's. Applying numerical methods to the data obtained to determine the concentration of gases, which may help in overcoming these difficulties. Spectral analysis methods are widely used by the software's. However, the methods for solving the problem of fluorescence spectrometry for gases differed, which determines the scientific novelty of this study.

In order to solve these obstacles, I conducted a lot of research. A method has been developed for determining the concentration of aromatic hydrocarbons based on the use of data from chemical sensing materials and obtained hyperspectral data [14, 22, 30].

However, those method has particular determinants, such as the want to use several different chemicals at the same time, which complicates the titration, and makes work not convenient.

So, the intent of the assignment was to determine the better way to save the core components according to the sensor spectroscopy data, and to develop an algorithm to correct the core components of the aromatic hydrocarbon sensor spectra data from distortions that occur during processing.

The use of data obtained from spectroscopic previously improves the concentration calculation of aromatic (BTX) in the air using previously proposed methods [15] and develops a model that allows us to analyze the spectral data of gas fluorescence for determining its concentration, also compare the data we obtained through the use of the methods used and the proposed methods, and the possibility of applying this approach in practice to solve real problems [31].

The fluorescence spectra obtained from this method of Processing, are different from the usual methods, and hopefully will overcome the limitations encountered when using several materials simultaneously, to disband the trouble of determining the concentration of gases based the fluorescence spectra taken by sensors [15].

The scientific novelty of the study was determined, and a new algorithm has been developed and implemented (the method name is ProcessorsGases) which is based on a polynomial method using a mean-pass filter. It was developed and implemented to improve the calibration method in a gas analyzer. In view of the outcomes obtained, it is proven that this method removes the background ratio.

2 Practical Part and Mathematical Model of Signal Registration

To meet the need for devices that determine the concentration of gases, he developed a sensor based on the use of chemically sensitive elements based on dibenzoyl boron difluoride (DBMBF2) [3, 14]. The experiment used a sensor. This sensor includes a sensor material deposited on a glass substrate, a fibre optic probe connected to an LED light source that serves as a fluorescence exciter, and a spectrometer used to measure fluorescence spectra. The glazed substrate with the sensor item is situated in a sealed chamber, inside to which immaculate air or a blend of air with vapors of spectrum (BTX) of a specific concentration is supplied.

After that, an effort to analyze the facts gained from two or more sensitive chemical elements that react differently to changes in gas focus showed the incomplete influence of this process in the described problem [9]. The data obtained from the spectrometer is displayed using the elements of the chemical sensor, the data obtained from one spectrometer (1300 samples, 2048 channels) (horizontal - wavelength, vertical - sample number, in cell - spectrum emission intensity value at the wavelength specified in the row for the sample specified in the column). The experiments took data from five different chemical sensory materials that react with the presence of 3 different gases, namely benzene, toluene, and xylene in different concentrations. The value of their concentration for each moment measured by spectrometers in training is used as an output (for the proposed method-GasesProcessors). The complete data set was divided into training and testing. As test data, 15% of the measurements from the original data set were used, and they were randomly selected.

The datum and store of principal components congruent with the spectral characteristics have been pre-cured using MATLAB (R2013a, MathWorks). Attention was highlighted the characteristic peaks for components BTX. The

spectrum of aromatics hydrocarbons in the scope of heed is shown in Figure 1.
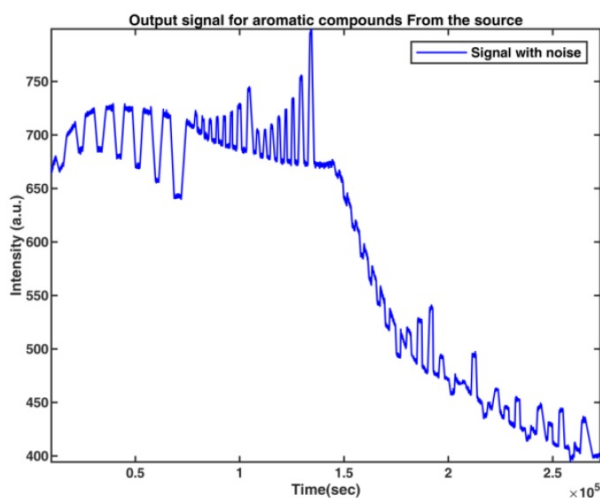

Figure 1: A noisy signal from the output of the sensor spectra $O(\lambda n)$ with given concentrations

2.1 General Scheme of the Algorithm

After we obtain data, "raw BTX" spectra [10], noise is removed in the data processing step to make the spectra more informative, one more non-informative parameter is removed, namely, the autofluorescence background. After successful removal of the background, a "immaculate" spectrum of the sensor is obtained, as shown in the general scheme of the algorithm in Figure 2.
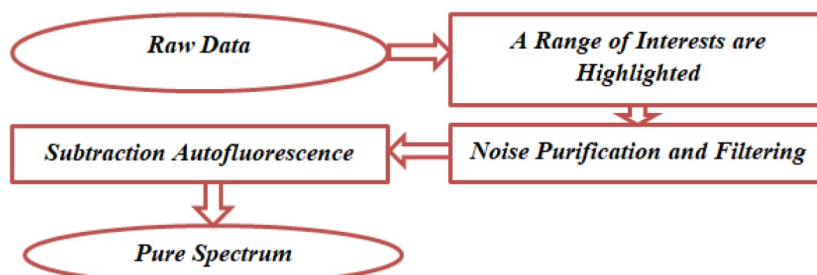

Figure 2: Block diagram of data processing

2.2 Noise Filtering and Autofluorescence Background Removal Algorithms

The noise in scattering indicative is diverse, too used a medium filter to suppress them, we remove noises (mainly impulse ones) using a medium filter [15, 16], as shown in the Spectrum Processing Process in Figure 3.
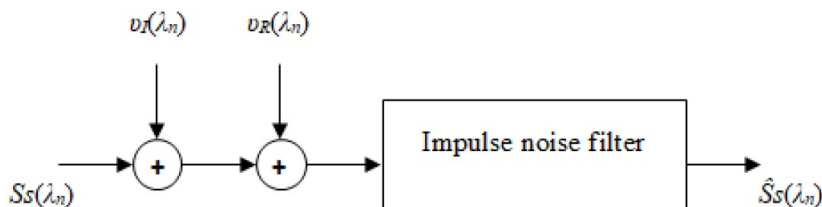

Figure 3: Spectrum Processing Process

The software technique turned into the measure for remedying the commitment of fluorescence to the background. They don't need framework adjustment and have no taking sample preparation limitations. Through the numerical process, first and second derivative [20], frequency separating [18], polynomial approximation [4] and wavelet alter

[5] methods are suggested as beneficial methods for foundation evacuation in specific circumstances. The precision of the first and second derivative methods is high in peak extraction. Because of the onerousness of distinguishing tops, losing some of them can make the range overlap with the foundation, resulting in an indigent appraisal of the ultimate [24].

Filtering is based the Fourier modification [18], one of the frequency filtering techniques requires separating the recurrence parts of the sensor range from the removing fluorescence. This technique is one of the most dependable for eliminating fluorescence, however, it relies upon direct human intervention to precisely decide the upper and lower cutoff points of the recurrence scope. Not exclusively is this time-consuming, however, the cutoff points change from one case to another.

The polynomial approximation [7], because of its simplicity and convenience, has turned into the most famous strategy for eliminating the fluorescence foundation for a wide assortment of research working conditions, nonetheless, the manual polynomial estimation requires client intercession to choose regions where the bends match the original data [1].

Albeit programmed polynomial estimate stays away from human mediation, its utilization is restricted because of the great degree of noise. Wavelet transform techniques [5] can likewise be utilized with automated curve fitting, however, because of the trouble of choosing a proper wavelet change edge and required goal level, baseline planning can influence background removal results [25].

2.3 Modified Polynomial Approximation

This is a reduplicate algorithm that found successive approximations until the i-th polynomial differs from the (i-1) polynomial by lower than the amount of ε. It is, as a rule, admissible that the spectra are analogous [19] if they diverge during no more than 5% ($\varepsilon < 0.05$) Quantitatively, the yield condition for their iterative process can be expressed by the following formula (2.1):

$$\sigma = |\sigma_{i-1} - \sigma_i/\sigma_i| < \varepsilon, \tag{2.1}$$

where σ_{i-1}- standard deviation $i-1$ of the polynomial;

σ_i- standard deviation i of the polynomial.

2.4 Proposed Sensor Algorithm (GasesProcessors)

The proposed algorithm is a sensor algorithm, improved in comparison with the previous algorithm in a different way [4].

This method takes inside regard the hubbub disfigurement of the signal and the influence of great sensor peaks on the polynomial approximation. The method is similar to ModPoly, but at the first iteration, an additional procedure is added - the removal of peaks [23].

Peak removal is according to the following norm. To lower the disfigurement of the approximating polynomial, the prime peaks are particular from the inequality $Oo(v) > P1(v) + \sigma1$. The points corresponding to the main peaks are removed from the spectrum and are not taken into account in subsequent steps. Peak removal is needful to ban superfluous outliers in the data [6, 31, 32].

3 Results

Its primary feature is that it reacts weakly to reading that stands outside pointedly with the background of neighbouring ones, which allows it to be widely used to eliminate anomalous values in data arrays. In addition, as a non-linear filter, the medium filter is more effective than linear filters in cases where the differences in signal values are big compared to the variance of the Gaussian fuss since it gives a smaller rate of the RMS error of the output signal in relation to the input, non-noisy signal at comparison with optimal linear filters [29]. an example of the median filter can be seen in Figure 4, and for order (n=7), in Figure 5. Based on the experiments performed, the 7th-order polynomial gives the best approximation for the spectra, in comparison to (3th,5th,15th) order polynomials approximations. The shown signal smoothed spectra After using the medium filter (with order n=3, n=5, n=15) are in Figure 6.
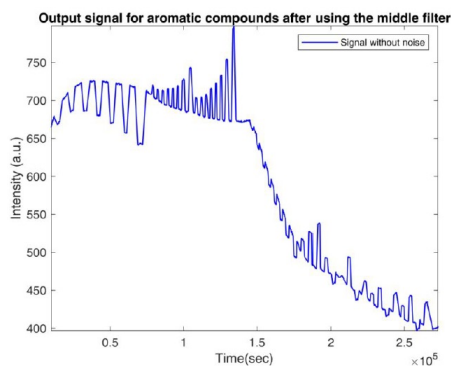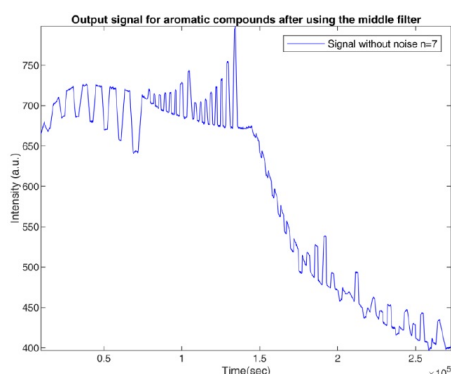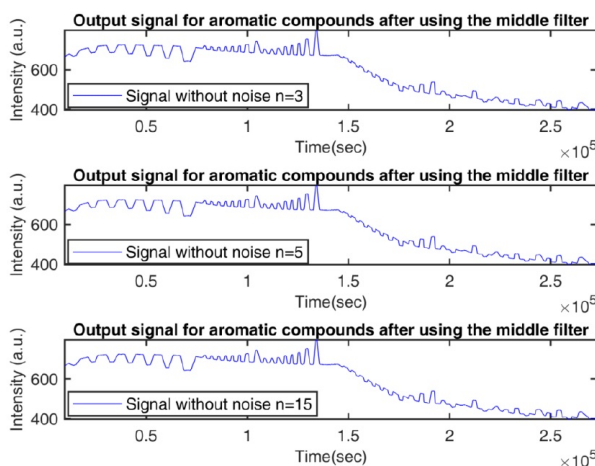
Figure 4: Signal smoothed spectra After using the medium filter

Figure 5: Signal smoothed spectra After using the medium filter (with order n=7)

Medium filtering is implemented as a procedure for local processing of samples in a sliding window, which includes a certain number of signal samples. For each position of the window, the samples selected in it are ranked in ascending or descending order. The average report in its position in the ranked list is called the medium of the considered group of samples. This sample replaces the central sample in the window for the processed signal [2]. The medium filter window is usually set to odd. In the general case, the window can be even, and the medium is set as the arithmetic mean of two average samples [8].

The width of the $(2n + 1)$ medium filter is chosen so that it is able to suppress an n-sample wide pulse [11]. Too large a window can lead to the loss of informative signal components since the filter causes flattening of the peaks. An example of the medium filter can be seen in Figure 6.

Figure 6: Signal smoothed spectra After using the medium filter (with order n=3,n=5,n=15)

In the Polynomial Approximation (Polyfit), and to get a "perfect" spectrum range, the sensors should subtract the autofluorescence background from the pristine filtrated and smoothed signal [13]. The background can be displayed by a polynomial (7), the request for which is picked in view of how to successfully eliminate it and simultaneously limit the expulsion of tops in the sensor signal. In light of the trials played out, the fifth and seventh request polynomials give the best estimation for the spectra of gases [31].

$$p(x) = p_1 x^n + p_2 x^{n-1} + ... + p_n x + p_{n+1} \qquad (3.1)$$

The primary benefit of this procedure is its simplicity and efficiency. It is quicker than different manner and has been widely used in studies of the spectra of gases [26]. The disadvantage of this approximation is its reliance on the spectral zone and on the order of the polynomial [27]. The shown smoothed spectra with a selected autofluorescence background and " immaculate" sensor spectra are in Figure 7, for the method Polynomial Approximation (Polyfit).
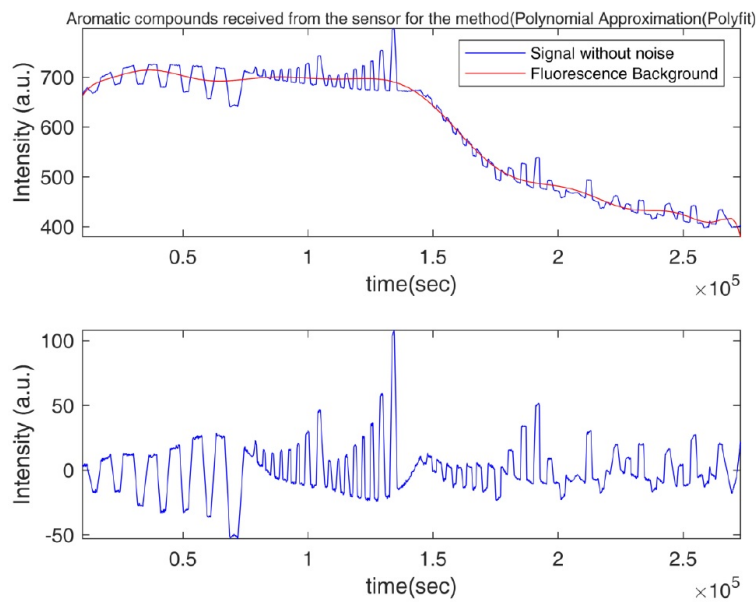

Figure 7: Smoothed spectra with a selected autofluorescence background (upper) and " immaculate" sensor spectra (bottom) for a 7th-order polynomial for the method(Polynomial Approximation (Polyfit).

Presently more about this mode (Modified Polynomial Approximation), everything begins with a solitary polynomial estimate $P1_{(v)}$ as per equation (3.1), utilizing the "crude" sensor signal $Oo_{(v)}$, where v is the shift of the sensor range, estimated in (cm^{-1}) or (nm) or time (seconds) [15]. Then the root-mean-square deviation σ is determined by the recipe (3.2).

$$\sigma = \sqrt{(R(v_1) - \bar{R})^2 + (R(v_2) - \bar{R})^2 + ... + (R(v_n) - \bar{R})^2/n} \qquad (3.2)$$

where $R_{(v)} = O_{(v)} - P_{(v)}$ is the contrast between the polynomial estimate and the first sign, and $\bar{R}$ is the typical worth of these distinctions.

In the event that there are focuses in the ongoing range that surpass the related polynomial guess, considering the RMS, then, at that point, they are supplanted by polynomial focuses with a mean square blunder, in this manner considering clamour impacts and staying away from fake pinnacles, in any case, the range focuses stay unaltered [31].

The autofluorescence background will be the polynomial gained at the last iteration. An "immaculate" sensor spectrum is gained by moulting this polynomial approximation from the original signal [17]. The shown smoothed spectra with a selected autofluorescence background and "immaculate" sensor spectra are in Figure 8, for the method Modified Polynomial Approximation.

What's more, we'll get the autofluorescence background from (GasesProcessorse algorithm), as in the past case, which will be the polynomial acquired at the last emphasis. A "immaculate" sensor range is gotten by subtracting this polynomial estimation at the first sign, where in light of progressive approximations and the (i-th) polynomial varies from the polynomial (i-1) [16].
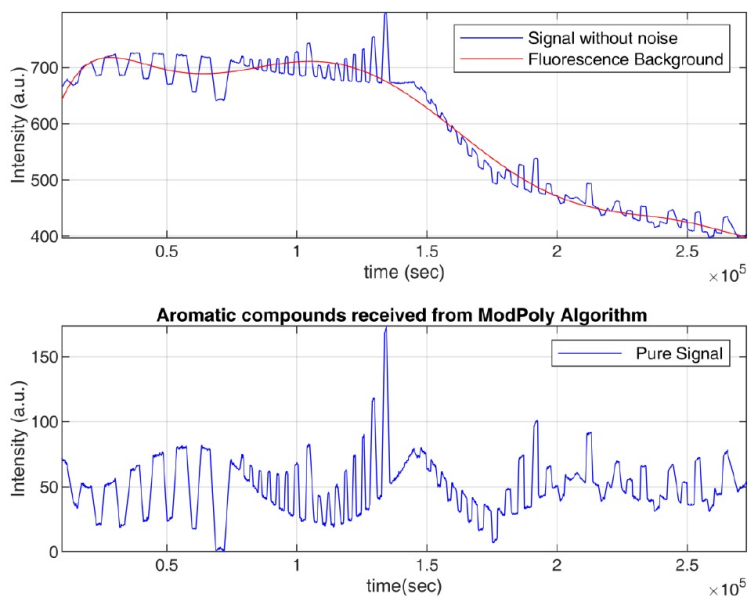
Figure 8: Smoothed spectra with a selected autofluorescence background (upper) and "immaculate" sensor spectra (bottom) for a 7th-order polynomial for the method(Modified Polynomial Approximation).

This process considers signal commotion contortion and the impact of pure, big aromatic (BTX) peaks on the polynomial estimation, Still, the first and second cycles add additional stanzas from peak removal, et cetera to forestall pointless exceptions in the data [15].

At the second and later emphases, we carry out a similar strategy until the condition (3.2) is fulfilled. The polynomial got and the latter emphasis ought to be considered as the autofluorescence background. The pure range is gotten by molt this polynomial estimation at the first sign [18], the shown buffed spectra with a selected autofluorescence background and "immaculate" sensor spectra are in Figure 9, for the method of the algorithm (GasesProcessorse).
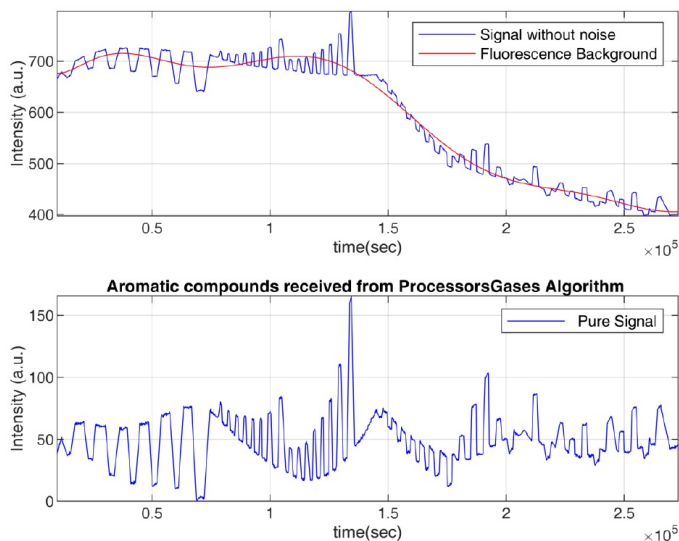
Figure 9: Smooth spectra together with a selected autofluorescence background (upper) and "immaculate" sensor spectra (bottom) for a 7th-order polynomial for the method algorithm (GasesProcessorse).

In addition, measurements from 1 to 15 as well as from (1181 to 3001) were excluded from the sample to reduce the number of zero concentrations in the sample for more even distribution.

And due to the huge amount of data, only a few of them were mentioned (due to the impossibility of including a large database in this study).

Tables 1, 2, and 3 contain pre-and post-treatment sensor data for benzene, toluene, and xylenes aromatics. Each column represents a specific action, the amplitudes of these peaks after filtering by the medium filter were also calculated and the amplitudes of the peaks after the removal of background fluorescence by the PolyFit and ModPoly algorithms and the developed method (gas processors) are shown.

Table 4 shows data on BTX aromatics before and after processing using the above methods.

Table 1: Aromatic compounds from the sensor after (wavelength all 460nm) for Benzene

	Time (sec)	Signal before processing	Using the medium filter	Polynomial approximation (PolyFit)	Method use (ModPoly)	Using method (under development Gas processors)
1	7.52×10^4	708.950	708.950	715.182	718.829	710.769
2	7.53×10^4	709.690	709.690	714.909	718.053	710.744
3	7.53×10^4	711.100	710.050	714.632	717.282	710.719
4	7.53×10^4	711.240	710.050	714.373	716.572	710.694
5	7.53×10^4	708.940	711.100	714.121	715.892	710.670

Table 2: Aromatic compounds from the sensor after (wavelength all 460nm) for Toluene

	Time (sec)	Signal before processing	Using the medium filter	Polynomial approximation (PolyFit)	Method use (ModPoly)	Using method (under development Gas processors)
1	1.09×10^5	703.020	701.830	694.600	696.435	699.496
2	1.09×10^5	703.610	701.950	694.523	696.619	698.969
3	1.09×10^5	700.990	702.590	694.407	696.869	698.451
4	1.09×10^5	704.560	703.020	694.289	697.093	698.112
5	1.09×10^5	704.110	703.020	694.211	697.218	697.610

Table 3: Aromatic compounds from the sensor after (wavelength all 460nm) for Xylene

	Time (sec)	Signal before processing	Using the medium filter	Polynomial approximation (PolyFit)	Method use (ModPoly)	Using method (under development Gas processors)
1	1.39×10^5	672.77	670.800	666.017	669.516	666.537
2	1.39×10^5	671.06	670.800	666.182	669.599	666.688
3	1.39×10^5	671.92	671.060	666.346	669.681	666.788
4	1.39×10^5	670.8	671.060	666.454	669.736	666.936
5	1.39×10^5	669.51	670.800	666.614	669.816	667.083

Table 4: Aromatic compounds from the sensor after (wavelength all 460nm) for Xylene

	Aromatic compounds from the sensor after (wavelength all 460nm) for Benzene			Aromatic compounds from the sensor after (wavelength all 460nm) for Toluene			Aromatic compounds from the sensor after (wavelength all 460nm) for Xylene		
	Polynomial approximation (PolyFit)	Method use (ModPoly)	Using method (under development Gas processors)	Polynomial approximation (PolyFit)	Method use (ModPoly)	Using method (under development Gas processors)	Polynomial approximation (PolyFit)	Method use (ModPoly)	Using method (under development Gas processors)
1	21.890	0.033	13.556	21.890	21.890	21.890	28.094	22.018	23.461
2	22.163	0.798	14.342	22.163	22.163	22.163	28.469	21.867	23.378
3	23.180	1.183	15.853	23.180	23.180	23.180	28.305	22.027	23.836
4	23.799	1.208	16.563	23.799	23.799	23.799	28.457	21.878	23.781
5	24.051	2.282	17.603	24.051	24.051	24.051	28.297	21.471	23.701

4 Discussion and Conclusion

Base objective was into preserve the optimal poise: to minimize the wastage of substantial input and simultaneously remove all unnecessary noise, and the effect of distortions introduced by various hubbub dilution and autofluorescence background elimination algorithms was determined from the comparison data.

It has been noticed here that the proposed method (gas scrubbing) is better in terms of filter performance and autofluorescence background removal compared to other methods.

Influence of various methods of processing the spectra on the fundamental components, which were taken as the characteristic peaks of aromatic hydrocarbons, that respond to changes in concentrations at a wavelength of 460 nm.

The medium filter has a minimal error diffusion compared to other filters, subsequently it is easier to right this diffusion, and inter alia the autofluorescence elimination process, the Gas Processor process has the teeny error diffusion, compared to the most common processes (PolyFit, ModPoly).

If thither are points in the existing spectrum such exceed the conformable polynomial approximation taking into account the RMS. Afterwards, are changed by means of points of the polynomial by the root signify squareness fault, hubbub effects are taken into account and artificial peaks are avoided. The autofluorescence background will be considered the polynomial obtained at the last iteration, "Pure" spectrum, aromatic hydrocarbons are obtained by deducting this polynomial approximation from the authentic signal [31, 32].

"Pure" spectrum (benzene, toluene, xylene), respectively, these changes were 3% for the ratio of the PolyFit method to the medium filter, and 1% for the ratio of the use of the method(ModPoly) to the method (polynomial approximation, (PolyFit)), and 8% for the ratio of method usage (GasesProcessors) to method usage (ModPoly), and 9% for the ratio of method usage (GasesProcessors) to signal before processing. And these changes were 4% for the ratio of the PolyFit method to the medium filter, 1% for the ratio of method use (ModPoly) to the method (polynomial approximation (PolyFit)), and 2% for the ratio of method use (GasesProcessors) to method use (ModPoly), and 2% for the ratio of method usage (GasesProcessors) to signal before processing.

And these changes were 3% for the ratio of method PolyFit to medium filter, 2% for the ratio of method use (ModPoly) to the method (polynomial approximation (PolyFit)), and 2% for the ratio of method use (GasesProcessors) to method use (ModPoly), and 1% for the ratio of method usage (GasesProcessors) to signal before processing.

Background fluorescence (benzene, toluene, xylene), for the PolyFit method they were 3% and 5% and 2%, and for the ModPoly method they were 1% and 2% and 2%, and for the gas processor method, they were 2% and 5% and 2%, respectively.

For this purpose, the mode used may be useful in speeding up the determination associated with the difference between the peaks will then be easier to investigate the concentricity of compounds (BTX)in addition to determining their requirement or perhaps general processing.

Acknowledgments

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