Application and Comparison of Spectral Data Filtering for Aromatic Hydrocarbon Concentration Identification by Using an Algorithm

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Abstract: Every year the production of benzene increases, thus as Benzene, Toluene and Xylenes cause significant harmful to human veracity, and the situation is exacerbated by that is the fact, which of exceeding the Maximum Permissible Concentration (MPC) of 0.1 mg/m3. Prolonged exposure to the concentration of benzene, can lead to such consequences as some types of cancer, reproductive shortcomings, harm to the nervous system, as well as pallor. The techniques used to decide focus depend on the utilization of information from substance sensors and mathematical strategies for deciding the convergence of gases. all this method has certain limitations, which leads to the complexity of the calibration. The main from of this study removing all unnecessary noise, and it is necessary to minimize the loss obtained from the spectroscopic data, for improving for working on the exactness of ascertaining the convergence of aromatic hydrocarbons. Has been comparing the data of aromatic compounds obtained, It started from receiving the data, and through the process of filtering the signal using the Median filter, as well as autofluorescence Background Removal and Polynomial Fit(Polyfit), and finally, a method has been used, (GasesProcessors), all that separately for(benzene, toluene, xylene), the classification results are presented in the form of a box with a "whisker These changes were 2.5%, 2%, and 2.8%, for the ratio (before processing to using the Medium filter), respectively, and the changes were 3% for the ratio of the PolyFit method to the Medium filter, and 8%, 9%, and 4%, for the ratio method use(PolyFit) to Medium filter, and 3%,8% and 0% for the ratio of method use(PolyFit) to method use(PolyFit), respectively. It should be noted here that the proposed method (GasesProcessors) is superior in terms of filter performance and autofluorescence background removal compared to previous methods.

1.   Introduction

Air pollution is a severe global problem that directly or indirectly affects all components of the biosphere. The adverse health effects of air pollution are undeniable. Among this extended family of gaseous pollutants, the aromatic hydrocarbons benzene, toluene, and xylene (BTX) have fatal effects on human health in the short, medium, and long term[1].

Despite the high level of effectiveness of monitoring methods commonly used to monitor the concentration of BTX in the air, their need for use in fixed air quality monitoring stations, as well as their bulkiness, complexity, and high cost, are the main disadvantages. Thus, it is not possible to imagine equipment for carrying out large-scale measurements of pollutants in real-time or monitoring human exposure to these substances. However, low-cost, miniaturized, and mobile sensor devices capable of real-time measurement of gaseous pollutants in public spaces, indoors, passenger

compartments and large industrial facilities are needed[2].

Spectroscopy is one of the modern diagnostic methods that allow obtaining data on the elemental and chemical composition, crystal variables, type of defects, their concentration and localisation, and other parameters and properties. The main task of spectroscopic studies is to determine the properties of a substance that cannot be observed directly using radiation spectra. Spectra, in turn, directly depends on both the determined characteristics and external factors, so the use of modern methods of data analysis in spectroscopy is becoming increasingly important.

But the advantages of spectral data make many of the existing filtering methods unable to effectively suppress noise components and at the same time preserve the informative part of the spectrum. And, as a rule, the problem is solved by processing specific spectra, taking into account the experimental conditions, known noise sources and other information[3].

This requires more proficient and effectively available techniques for observing the convergence of such substances in the air, both in different ventures and on city roads.

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There are numerous answers to address this issue, however, they have different hindrances, for example, the span of determination of the concentration, the expense of production, the requirement for research facility conditions for work, low precision, or the powerlessness to decide the concentration of a few distinct gases simultaneously.

Beforehand, he fostered a few techniques, for instance, a strategy was progressed for deciding the fixation regarding sweet-smelling hydrocarbons proportion the utilization of information from chemo sensor materials and hyperspectral information got with their assistance. Mathematical strategies are applied to the got information to decide the grouping of gases [4].

However, this method has specific limits, for example, uses several different chemosensory materials at the same time, which leads to the complexity of the calibration. The main idea of this study is to use spectral facts and work on the exactness of the computation of the concentration of aromatic hydrocarbons in the air utilizing profound learning methods[5,6].

Signal pre-filtering as a way of identifying and separating overlapping peaks using numerical differentiation of measurements is important because it allows a denoised signal to be obtained. This stage can be considered as a preliminary procedure preceding the main stages of processing.

An intermediate filter was used to smooth the original signal. The basic working principle of spectrum processing is to remove the autofluorescence component from the original signal obtained from portable sensors using a polynomial curve fitting (PolyFit) function based on the previously proposed polynomial fitting method. (GasesProcessors) using Matlab software environment[7].

Thus, the aim of the study is to improve a model that would allow us to successfully analyze the spectral data of the fluorescence of gases and determine their concentration, and obtain information about the applicability of this approach in practice to solve real problems.

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. Based on results obtained, it is proven that this method removes the background ratio.

2. The Practical and Mathematical

To assist with addressing the requirement for gas focus, a few sensors have been created, and a sensor in light of the utilization of fluorescent chemosensitive components in view of the fluorophore dibenzoylmethane boron difluoride (DBMBF2) has also been developed at the Center for Photochemistry of the Russian Academy of Sciences [4].

This sensor incorporates a sensor material kept on a layer of glass, a fiber optic test associated with a LED light source that fills in as a fluorescence exciter and a spectrometer used to gauge fluorescence spectra. The glass substrate utilizing the sensor material is situated In a fixed compartment, into which clean air or a blend of air with fumes of (BTX), of a given concentricity is given. During the analysis, the phone was provided with fumes fixations displayed in Figures 1, 2, and 3, separately, as well as sets of their mixtures.

It was treat this data as reference data, and apply to that data our proposed method to remove noise and shine from the reference signal in order to obtain a pure signal and thus we will obtain new concentrations. We compare the data we obtained, before and after filtering the data through the use of the Medium filter , through the method (PolyFit- Polynomial curve fitting) and ending with the use of the gas processing method (GasesProcessors), and we compare between what was obtained from new data for each independent element of data Aromatic compounds (BTX), and reference data[7,8].
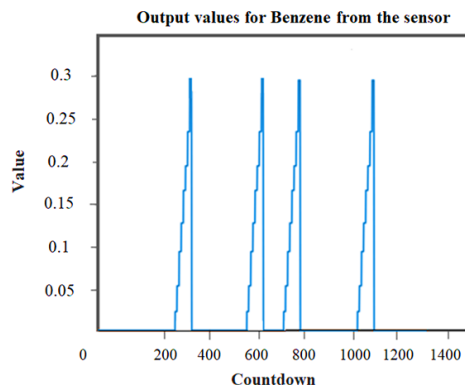

Fig. 1: Normalized data of benzene concentration versus time, Y-axis - normalized values of gas concentration,X-axis - time step (step size 185 seconds)

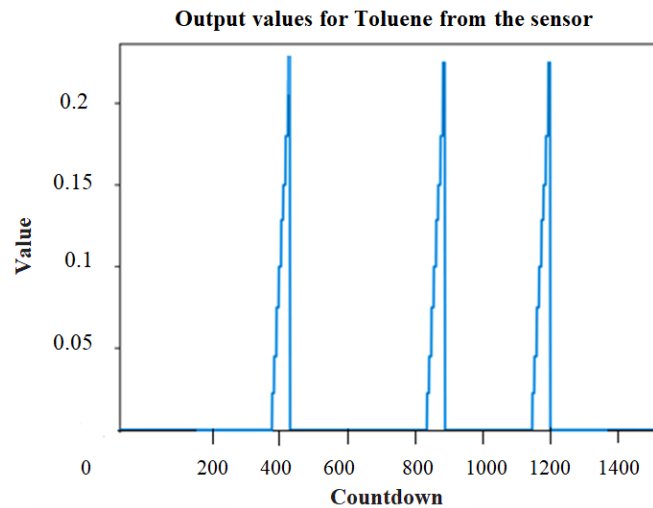**Output values for Toluene from the sensor**

Fig. 2: Normalized data of toluene concentration versus time, Y-axis - normalized values of gas concentration, X-axis - time step (step size 185 seconds)
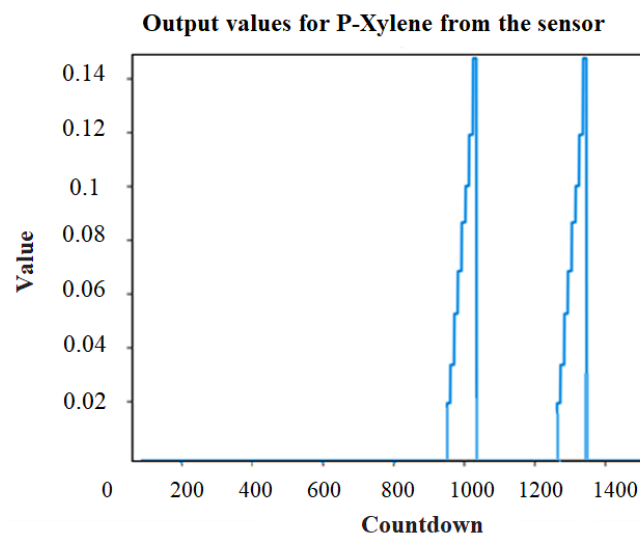
Output values for P-Xylene from the sensor

Fig.3: Normalized data on p-xylene concentration versus time, Y-axis - normalized gas concentrations, X-axis - time step (step size 185 seconds)

2.1 General Properties and Signal Registration Model

Light interacting with matter can give vastly different data about the condition of matter and at a fast. Optical sensors can be established on different optical standards (retention, reflection, iridescence, fluorescence), covering different districts of the range (UV...etc.) and allowing to evaluate of light power as well as other related properties like a lifetime, refractive index, dispersing and diffraction...etc.[9,10]. Despite different advantages, optical sensors in like manner have burdens:

Surrounding light can slow down their performance, long haul steadiness is restricted because of marker leaching or photobleaching selectivity can be low, and mass transfer of the analyte from the sample to the pointer stage is essential to get an analytical sign [11]. So utilized in a great many applications, for example,

clinical diagnostics, there is a developing interest in optical sensors[12-13].

The spectrum signal directed by the sensor $O(\lambda n)$ can be represented by some additional a model comprising the sensor signal $Ss(\lambda n)$, the autofluorescence background $P(\lambda n)$ (normally a easily changing line) [14], and noise (impulse noise $vI(\lambda n)$ furthermore, thermal clamour$vR(\lambda n)$). The bookmark from the directed by of the sensor is in accordance with formula (1), and all three components are shown in (Figures,1,2,3).

$$O(\lambda n) = P(\lambda n) + Ss(\lambda n) + vI(\lambda n) + vR(\lambda n)$$
(1)

Our goal is to propose a method for processing fluorescence spectra obtained from this installation, the method is based on the filtering of the signal from the noise and subtracting the received autofluorescence due to the use of the sample for obtaining a clean signal.

3. Results

3.1 Input data (material and method)

The signal spectra of an optical chemical sensor, obtained using a data recording device, are an array of readings (1300 samples, 2048 channels) (horizontally - wavelength, vertically - sample number, in the cell - the value of the intensity of the spectrum radiation at a certain in the wavelength row for the sample specified in the column) [15]. Data is recorded for wavelengths in such a range that not only autofluorescence is present, but as well as phenomena that forerun it. Figure 4 general view of the output data from the instrument (BTX spectrum), shows the spread of the deviations from the(ref.)signal worth, (Preceding to handling) for each BTX spectrum individually, interquartile range (IQR: the distance between the upper and lower quartiles, respectively (20-35-50), the classification results are presented in the form of a box with a "whisker".
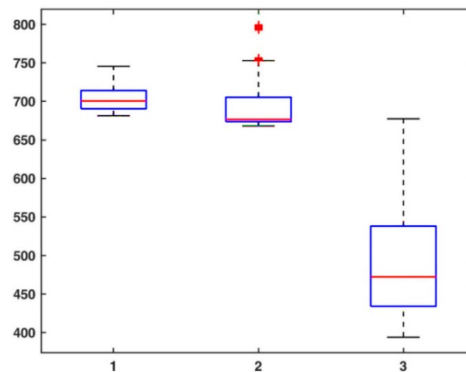

Fig. 4: (Prior to handling and utilizing a medium filter) for each part of (the BTX spectrum)severally

3.2. Noise Filtering

At the next stage, a range of interest is identified in these spectra. The clipped spectra are still heavily noisy, so noise is removed during the data processing step to make the spectra more informative.

The nature of noise in scattering the signals are varied. To remove pulsation noise at the introductory stage, use apply a filter Medium. Its main trait is that it reacts weakened to readings that stand out pointedly against the background of adjoining ones, which allows it to be widely used to eliminate irregular values in data arrays.

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 are ranked in ascending or descending order. The average report in its position in the ranked list is the Medium of the considered group of samples. This sample replaces the central sample in the window for the processed signal[16]. 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 average of twain samples average [17].

The indicative signal from Medium filter $(y\_k)$of a moving of width$(2n + 1)$ for the current sample k is consists of the time chain input $(..., x\_(k - 1), x\_k, x\_(k + 1), ...)$ as described in formula (2):

$$y\_k = Me(x\_(k - n), x\_(k - n + 1), ..., x\_(k - 1), x\_k, x\_(k + 1,) ..., x\_(k + n - 1), x\_(k + n)) \quad (2)$$

where $(x\_1, ..., x\_m, ..., x\_(2n + 1)) = x\_(n + 1)$

x_m - variation series elements, i.e. arranged in ascending order of x_m values

$$x\_1 = min (x\_1, x\_2, ..., x\_(2n + 1)) \le x\_1 \le x\_2 ... \le x\_(2n + 1) = max (x\_1, x\_2, ..., x\_(2n + 1))$$

The width of the (2n+1) Medium filter is chosen so that it is able to suppress an n-sample wide pulse[18]. 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 operation of the Medium filter can be seen in Figure 5 showing the spread of deviations from the reference value (Medium filter) for each section of BTX spectrum, interquartile range (IQR): the distance between the upper and lower quartiles, respectively (15-35-65), the classification results are presented in the form of a box with a "whisker".
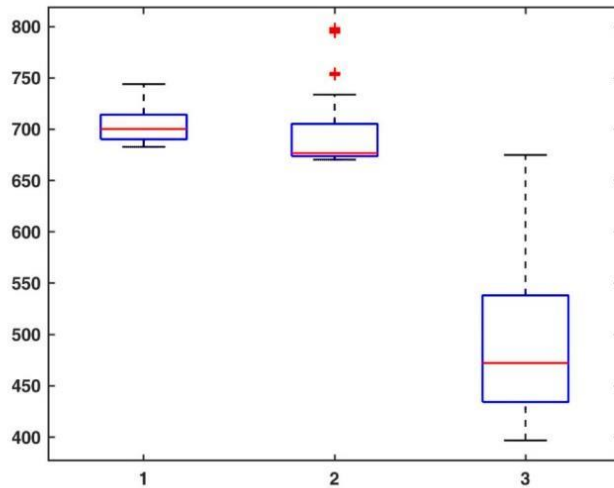
Fig. 5: (filter the median) for each part of BTX spectrum (solo 1,2,3)

3.3. Autofluorescence Background Removal and Polynomial Fit (Polyfit)

Unfortunately, the spectra of BTX sensors from chemical samples are accompanied by internal fluorescence, which can be several orders of magnitude stronger than the weak signal of the sensors [19]. Therefore, removal background is one of the most difficult errands for a qualitative analysis of empirical results.

Finally, to obtain a "clean" sensor spectrum, it is necessary to subtract the autofluorescence background from the original filtered and smoothed signal[20].

The polynomial approximation [21], due to its simplicity and convenience, has become the most popular method for removing the fluorescence background for a wide variety of situations.

The background can be modelled is accordance with formula a polynomial (3), the order of which is chosen accordingly on how to effectively remove it and at the same time minimize the removal of peaks in the spectrum. Based on the experiments performed, the 5th and 7th order polynomials give the best approximation for the spectra of gases,

$$p(x) = p\_1\, x\verb|^|n + p\_2\, x\verb|^|(n-1) + \cdots + p\_n\, x + p\_(n+1) \qquad (3)$$

The main advantage of this method is its simplicity and efficiency. It is faster than other methods and has been widely used in studies of the spectra of gases[22]. The disadvantage of this approximation is its dependence on the spectral range and on the order of the polynomial[23].

• In Figure 6 the deviations from the reference are dispersed esteem Polynomial FIT, for either part of BTX spectrum independently, interquartile range (IQR): the distance between the upper and lower quartiles, respectively (18-36-12), the classification results are presented in the form of a box with a "whisker"[7].
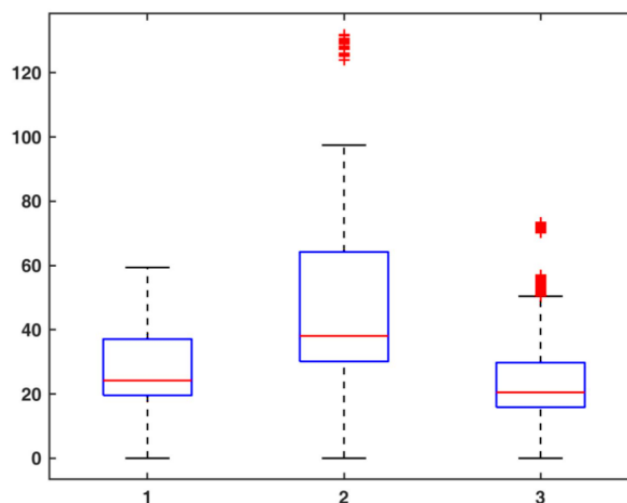

Fig. 6: (PolyFit) for each of BTX spectrum, independently

3.4. Method (*GasesProcessors*) for the components of aromatic compounds separately

And by using the proposed and improved algorithm Figure 7, compared to previous algorithms [24], it is (iteration) based on successive classification to the (I-th) polynomial varies from the polynomial (I-1) [25]. Assuming there are focuses in the ongoing range that surpass the relating polynomial guess given the standard deviation, then they are supplanted by polynomial focuses with standard mistake, accordingly considering noise effects and keeping away from artificial peaks, in any case, the range scores stay unaltered [26].

This style takes into account signal noise distortion and the effect of pure. The first and another iterations in add supplemental parts from peak removal nevertheless to prevent unnecessary outliers, in information for large peak on the polynomial (BTX spectrum)[27]. At the second and ensuing cycles, we carry out a similar system until the condition(7-th) is fulfilled. The polynomial

acquired at the last cycle will be considered as the autofluorescence foundation. The unadulterated range is gotten by molt this polynomial estimate from the authentic spectrum signal[28].

It is usually accepted that the spectra are similar [7] if they differ by no more than 5% ($\varepsilon < 0.05$) Quantitatively, the yield condition for their iterative process can be expressed by the following formula (4):

$$\sigma = |\sigma_{i-1} - \sigma_i / \sigma_i| < \varepsilon, \qquad (4)$$

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

Peak removal is organized according to the next fundamental. To minimize the disfigurement of the approximating polynomial, the main peaks are determined from the disproportion $Oo(v) > P1(v) + \sigma1$ .The points comparing to the principal peaks are eliminated from the spectrum and are not made into account in ensuing strides. Peak elimination is important to forestall superfluous outliers in the reference[29].
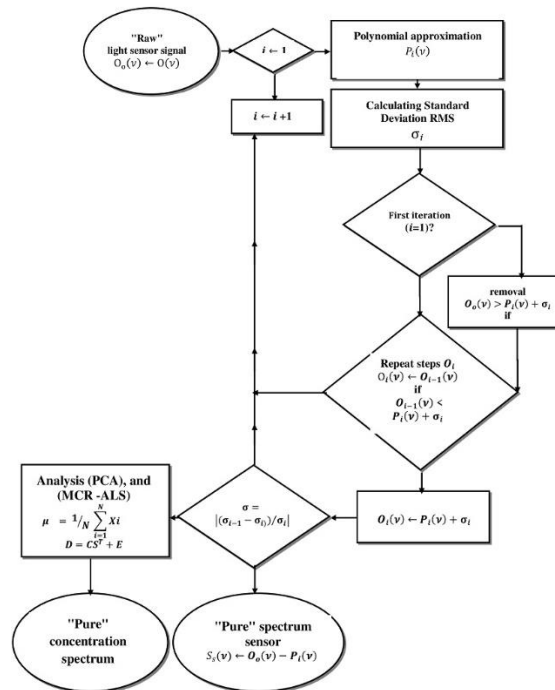

Fig. 7: Algorithm diagram for gas processing method

The autofluorescence background will be the polynomial obtained at the last iteration. A "pure" sensor spectrum is obtained by deducting this polynomial approximation from the authentic signal[30], and an example of the operation of the algorithm (GasesProcessors) is shown in Figure 8.

A very big contradiction was seen between the benzene spectrum signal that had been preprocessed, showing the

spread to misrepresent the reference rate(GasesProcessors) of each part for compounds BTX spectrum, interquartile range (IQR):the distance between the upper and lower quartiles, respectively (13-22-12), the classification results are presented in the form of a box with a "whisker"[7].
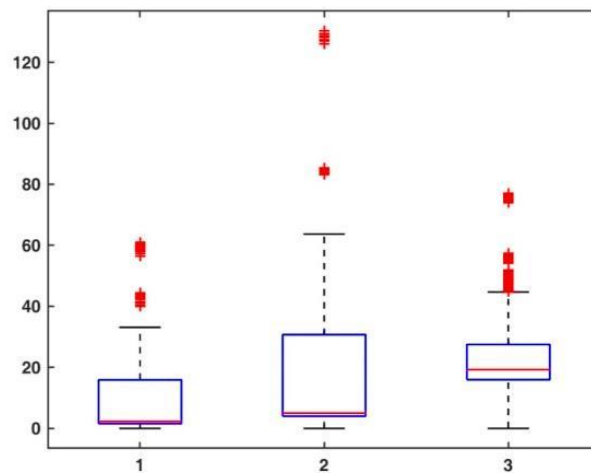
Fig. 8: (*GasesProcessors*) for each portion of BTX spectrum(1=B, 2=T, 3=X) severally.

Comparing the results obtained by us from the methods used in Figures 4-5-6-8), the difference is noted in values, for each portion of BTX spectrum, where the changes in deviations from the reference value in percent were as follows:

These changes were 2.5%, 2%, and 2.8%, for the ratio (before processing to using the Medium filter), respectively, and the changes were 3% for the ratio of the PolyFit method to the Medium filter , and 8%, 9%, and 4%, for the ratio method use(PolyFit) to Medium filter , and 3%,8% and 0% for the ratio of method use(PolyFit) to method use(PolyFit), respectively. Comparing the results obtained, it was found that this method(GasesProcessors Method) removes the largest percentage of the background.

4. Discussion and Conclusion

The motivation behind this labour is to determine the best technique for safeguarding major parts from scattering spectroscopy data. Different strategies were investigated to remove different distortions according to the original signal control model. Been investigated to eliminate various distortions in accordance with the original signal control model. Such as registration noise and background autofluorescence, for example, recording noisiness and the background autofluorescence. The fundamental task was to keep up with the ideal equilibrium: to limit the deficiency of vital data and simultaneously eliminate all superfluous noise.

Information for spectrometer data from the dissipating sensor is placed into the program Matlab. Crude spectra signals are handled (at the first Medium filter, after that method PolyFit, and finally GasesProcessors developed method) which results in "pure" spectra. Then, the subsequent data are compared and the information previously extracted. In light of the extracted data, the effect of distortions presented by different algorithms for

clamor lowering and background elimination from *autofluorescence* was specified.

Scatterplots (whiskers) are plotted for absolute distortions introduced in the main during pre-processing (noise reduction and autofluorescence removal steps). Assuming there are focuses in the ongoing range that surpass the related polynomial estimate, taking into consideration the criterion aberration, then they are supplanted by means of polynomial focuses with RMS blunder, in this manner considering commotion impacts and keeping away from artificial peaks, in any case, the range focuses stay unaltered. In the second and ensuing cycles, until the condition is met (Condition 4). The polynomial acquired at the last cycle will be considered as the autofluorescence background. A "spotless" range is gotten by means of deducting this polynomial estimation from the authentic indicative[7,8].

That the proposed method (GasesProcessors Method) is slightly better than the previous methods for removing fluorescence background. Comparing the results obtained, it was found that this method removes the largest percentage of the background.

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