



Detecting Levels and Innovative Applications for the Detection of Aromatic Compounds Using Multivariate Curve Analysis and Spectroscopy Data

Al-Ibadi Zeyad^{1*}, Muthana Alboedam², Ilya Katanov³, Al-Zubaidi Sura⁴

Abstract

Rapid technological developments and the increasing complexity of matrix work are increasing interest in finding robust technical solutions and fast and assertive data analysis. The data can be filtered to obtain spectral data in more useful spectral bands, the developed algorithms allow quantification of the spectral mixture, and it can be measured with or without titration.

We focused in this study is on samples within the range of wavelengths (459,466,462,464 nm), different strategies are utilized to check Aromatic compounds. These enable us to survey a specific degree of ordinary compounds, much the same as benzene, toluene and xylene, and so on. In this study compares data analysis, received from sensor between A polynomial approximation PolyFit method and Processors Gases method, and compares the results of each, a method with the multivariate curve resolve - alternate least squares (MCR - ALS) regression strategy of analyzing spectral data of information with a different concentration.

Additionally, adequately moor deviations of the anticipated values were accomplished from the genuine values, the standard deviation. And, the amended range was normalized to their region and to some degrees smooth. The autofluorescence establishment was subtracted, for the pure extend investigation, by utilizing logical approaches.

Key Words: Aromatic Compounds, Sensors, Fluorescence, Ultraviolet Spectroscopy, PolyFit, ProcessorsGases, PCA, MCR.

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Introduction

Benzene, toluene, and xylene (BTX) emission are commonplace poisons, benzene emission has pulled in a few environmental concern, since of the carcinogenic nature of benzene. Significant advance within the diminishment of benzene emission has been accomplished.

nevertheless, to achieve further emanation diminishments, the major issue is to find a strategy

which is moderately cheap and basic to function for wide utilize in industry. Photolysis and photocatalysis are two promising procedures that seem to drop into this category.

Application of UV photolysis depends on wavelength. It is categorized as close UV, middle UV and distant UV. The commonplace wavelength for close UV is 350 nm. Close UV light requires a catalyst to be effective.

Corresponding author: Al-Ibadi Zeyad

Address: ^{1*}Faculty of Informatics, Department of Technical Cybernetics, Samara State University, Samara, Russia; ²Faculty of Informatics, Department of Technical Cybernetics, Samara State University, Samara, Russia; ³Faculty of Informatics, Department of Technical Cybernetics, Samara State University, Samara, Russia; ⁴Faculty of Biology, Samara State University, Samara, Russia.

^{1*}E-mail: alibadi2017@yandex.com

²E-mail: mumu_thth@yahoo.com

⁴E-mail: sura.alzubaidi@yandex.com

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Electron transfer constitutes an important chemical process of its expansions in chemistry and biology. The quenching of the fluorescence of particles by electron-withdrawing or electron-donating species is well set up (Fox MA 1988), (Mirzaei A 2018). In a few cases, this quenching is accompanied by a weak and broad emission at wavelengths longer than the quenched fluorescence (Acharyya D 2015), (Sekhar PK 2014).

Dibenzoylmethanato boron difluoride (DBMBF2) shows exceptionally distinctive photoreaction and photophysical designs in alkylbenzenes from those in acetonitrile or dichloromethane as solvents (Safonov AA 2015). And these days we are living within the data age with the quick advancement of computational innovations and advanced facilities. Bigger information sets are delivered by tests and computer recreations. In differentiate to routine logical approaches where basic models are built to fit the information, computerized methods are encouraged to get bits of knowledge into the centre messages carried by the huge volume of information (I. 2002).

Principal component analysis (PCA), as concocted by Karl Pearson in 1901, maybe a method to change over a set of connected factors into uncorrelated ones called foremost components (Azzouz T 2008). Utilizing numerical calculations such as eigenvalue decay of the covariance tensor or single value decomposition (SVD), PCA strategies discover effective applications in numerous areas.

Multivariate Bend Determination Substituting Slightest Squares (MCR-ALS) has been proposed and broadly utilized to resolve different pure reactions and concentrations of the components show in obscure mixtures (Garrido M 2008).

It has been connected to analyse multicomponent chemical frameworks like chemical responses, industrial forms, chromatographic coelution issues, spectroscopic blends, natural checking information (Jaumot J 2005), and it can be connected to numerous other sort of blend examination cases. In MCR-ALS, the measured explanatory signals are expected to take after a generalized bilinear added substance demonstrate (just like the expansion of Beer's law in retention spectroscopy (Bro R 1997)). The commitment of each component to the measured signal depends on its concentration and on its own spectral affectability reaction (pure range).

MCR-ALS can moreover be connected to get quantitative data and it gives physical and chemical

significant arrangements. This is often finished since in MCR-ALS, any sort of limitations can be effectively connected to the looked for arrangements, like non-negativity, unimodality, and trilinearity (De Juan A 2004), (Tauler R 1998).

It is the point of the display article to discover an attainable and effective strategy for benzene degradation, through to create strategies for measuring concentrations in expansion to measuring air quality, for BTX (benzene, toluene and xylene) sensors, after denoise and autofluorescence from gas-based on ultraviolet light, utilizing algorithms MATLAB.

The Experimental Section

Chemicals Preparation

(Dibenzoylmethanato) boron difluoride was prepared agreeing to the method depicted by Brown and Bladon (Brown NMD 1969). The test checks of multicomponent mix concentrations; they were recorded utilizing a (sensor) comprising of a sensor texture mixed on a glass slide. The complex optical fiber test is related to the back of the chip. The glass slide with the sensor fabric is found in a fixed cell in which clean air or a mixture of air is provided with aromatic hydrocarbon vapours at a certain concentration. 47

The sensor is related with ultraviolet (LED Nichia, $\lambda = 375 \text{ nm}$), and location with the Ocean Optics S2000 fiber spectrometer, and Filtration of identified radiation with Lee Filters 226 LEE U.V. a 200 millisecond beat signal detection scheme and a 185 moment period were utilized.

Material and Titration Methods

All chemicals are of spectroscopic or explanatory review and are utilized without further purification, from the laboratory in the (Samara State University). Combinations of the concentrations, Indicators were Gas supply, for Naphthalene $0.2 \mu\text{g} / \text{min}$, Benzene ($44.0 \mu\text{g} / \text{min}$, Toluene ($10.1 \mu\text{g} / \text{min}$, Xylene ($2.4 \mu\text{g} / \text{min}$, and temperatures at which the Pixie is kept up for Naphthalene (50°C), Benzene (110°C), Toluene (100°C), Xylene (90°C). Air cleanse flow, ml/min 200.

Were introduced into the cell, and direct recording of spectral characteristics, altogether we performed our study for more than 5739 samples. Experimental studies of the samples were performed within 185 seconds from the minute of



testing. A standardized recording of the spectra was carried out. The focus of this study is on samples within the range of wavelengths (459,466,462,464 nm). Here it ought to be noted that it is vital to neglecting values tests taken and all of the estimations at which the concentration of all gasses was zero from the study. The program execution of the method of storing principal components concurring to spectral characteristics information was performed within the MATLAB R2013a mathematical package.

Titration strategies utilized depending on the concentration extend of benzene and toluene and Xylene. When the fragrant hydrocarbon concentration is tall sufficient to be considered as a co-solvent of cyclohexane, when the analytical method of Work (P. 1928), (Hill ZD 1986), (Lipskier JF 1993), was utilized, arrangements of DBMBF2 in cyclohexane and benzene (or toluene) in cyclohexane with a proportion of concentrations $[Aromatic]/[DBMBF2] > 10$, at slightest, were arranged. Expansion of little aliquots of the benzene arrangement in cyclohexane at that point gave modern blends where DBMBF2 and the fragrant hydrocarbon remained solutes over the total extend of concentration of the included compound.

Preprocessing and PCA and MCR Analysis

A monochromatic light event on a sample is characterized by phenomena such as reflection, absorption, or scattering. Scattering of light may be a phenomenon in which an intermediate interaction with a light beam comes about within the rise of electromagnetic radiation of the same composition, or the arrangement of a diverse range in different bearings does not seem like the original (Quintero L 2007).

Within the common case, the scattering process competes with its absorption process. When radiation is absorption, the molecule moves to a less activity electronic state. The return move to the ground state can be either completely lit or went with by light radiation at a lower repeat. This radiation is called radiance (Luminescence). And through numerical models for recording signals, the signal gotten from the sensor can be talked to by a few included logical models that contain the spectrometer signal and the establishment of self-sparkle and clamour (noise of all sorts) (Shreve AP 1992), (Khalaf AIZ 2020).

They don't require alteration of the system and have

no limitations on test sample preparation. Among the important methods, The of the methods of the first and second derivative in the selection of peaks. The manual polynomial approximation estimation, due to its effortlessness and convenience, has gotten to be the foremost prevalent strategy for removing fluorescence foundation in a wide assortment of circumstances. However, a manual polynomial approximation requires user intervention to select areas where the curves coincide with the original data (Khalaf AIZ 2020).

But due to the trouble of choosing a fitting wavelet change edge and the specified level of determination, pattern show can influence the background removal comes about (Quintero L 2007). To get a "pure" spectrum, it is essential to subtract the autofluorescence foundation from the original filtered and smoothed signal. The foundation can be displayed by a polynomial Equation (1).

$$p(x) = p_1x^n + p_2x^{n-1} + \dots + p_nx + p_{n+1} \quad (1)$$

The altered polynomial algorithm is based on a progressive guess, so that the primary polynomial contrasts from polynomial $(i - 1)$ Equation (2).

$$\sigma = |\sigma_{i-1} - \sigma_i/\sigma_i| < \varepsilon, \quad (2) \quad 48$$

where σ_{i-1} is the standard deviation of the $i - 1$ polynomial; σ_i is the standard deviation of the i polynomial, and the standard deviation σ is calculated by the Equation (3).

$$\sigma = \frac{\sqrt{(R(v_1) - \bar{R})^2 + (R(v_2) - \bar{R})^2 + \dots + (R(v_2) - \bar{R})^2 / n}}{n} \quad (3)$$

To play down the distortion of the approximating polynomial, the most crests are decided based on the imbalance the original signal is more prominent than the polynomial and the standard deviation. Presently the "clean" spectrum is gotten by implies of the contrast between the polynomial estimation from the original signal (Cai TT 2001).

The PCA strategy is to discover a lower-dimensional space or PCA space (W) that's utilized to convert the information ($X = \{x_1, x_2, \dots, x_N\}$) from a higher-dimensional space (RM) to a lower-dimensional space (Rk), where N speaks to the whole number of tests or perceptions and xi speaks to i th test, design, or perception. All tests have the same measurement ($xi \in RM$). In other words, each test is spoken to by M factors, i.e. each test is spoken to as a point in M -dimensional space (Wold S 1987). And dimensionality decrease is one of the preprocessing steps in numerous machine learning applications and it is utilized to convert the highlights into a lower measurement space. Central Component



Investigation (PCA) technique is one of the foremost popular unsupervised dimensionality lessening procedures. The objective of the PCA is to discover the space, which speaks to the heading of the greatest change of the given information (Shenai PM 2012).

The steps within the PCA calculation is to build an information or include network (X), where each test is spoken to as one column and the number of lines speaks to the measurement, i.e. the number of highlights, of each test. The point by point steps of calculating the lower-dimensional space of the PCA procedure utilizing the covariance Equation (4).

$$\mu = 1/N \sum_{i=1}^N Xi \quad (4)$$

where N represents the total number of samples and xi represents the i th sample. After that subtract the cruel from each a test and compute the covariance framework (co) Equation (5,6).

$$U = \{d1, d2, \dots, dN\} = \sum_{i=1}^N Xi - \mu \quad (5)$$

$$\Sigma = (1/N - 1) U * U^Q \quad (6)$$

the eigenvectors V and eigenvalues of the covariance framework (Σ), eigenvectors agreeing to their comparing eigenvalues, and the eigenvectors that have the biggest eigenvalues $W = \{v1, \dots, vk\}$. The chosen eigenvectors (W) represent to the projection space of PCA. All tests are anticipated on the lower-dimensional space of PCA (W) as takes after, $Y = W^Q U$.

The fundamental thought of MCR is to decompose down the crude spectra matrix D , into the result of two littler matrices C and ST by a bilinear demonstrate model Equation (7).

$$D = C.S^T + E \quad (7)$$

Where D is the information lattice to be rebuilt, ST compares to the cross section of the crude range, this implies ST is the immaculate spectra, C is the related fixation profiles for each one of the sections or concentrations, and E is all that should do with commotion within the shape of a framework or in other words, it is the mistake network (D. J. Jaumot J 2015).

For the most part, in visual spectroscopy, it isn't essential that the concentrated of assimilation of the radiation in each pixel be negative, and as is the case with (physical limitations) it ought to not be negative. When performing the least-squares strategy appeared over, non-negative limitations are utilized on all immaculate spectra. Furthermore, in arrange to induce freed of the compelled constraining and steadiness of the ALS iterative enhancement, until convergence is come (Eilers PH

2005).

Through the utilization of a MATLAB based MCR-ALS tool set (Zhang D 2013), the ST range framework is normalized. Rather than levelling the spectra, there are a few limitations that are utilized to suitably expand the run of arrangements gotten by mass adjust or closure condition in lattice C , this implies and demonstrates that the relative concentrations or amounts of all components on the whole of pixel values create a consistent esteem. The C framework can be rebuilt after the ALS alteration has been completed, the utilize of MCR-ALS application is exceptionally distinctive within the case of analyzing chemical forms that tend to appear ceaseless smooth shapes, from those that we ordinarily get to other spectral concentrations (Feng X 2017).

MCR-ALS application method through its utilize, we are able moreover to analyse multiple groups at the same time into customary charts in one structure, and so, by self-replicating Equation (1).

The gotten information combinations can be assessed after applying the MCR-ALS strategy, the differentiate proportion appeared is assessed utilizing Equation (8), and in the event that no suitable information is accessible the proportion within the irregularity (lock of fit) Equation (9) you'll not be able to evaluate the distinction between the experimental Information Lattice (D) and the information that has been organized and created MCR-ALS (Kumar K 2012).

$$R^2 = 100 \frac{\sqrt{\sum i, jd_{ij}^2 - \sum i, je_{ij}^2 / \sum i, jd_{ij}^2}}{\text{lock of fit} (\%)} \quad (8)$$

$$100 \sqrt{\sum i, je_{ij}^2 / \sum i, jd_{ij}^2} \quad (9)$$

Where: d_{ij} , e_{ij} are a component of the information framework D , the components of the frameworks E , is the related leftover esteem gotten from the distinction between the information network D and the replicated data (CS^T matrix MCR-ALS), (Garrido M 2008).

Study Results

Spectral Properties of the Aromatic Compounds

Ultraviolet-visible spectroscopy is utilized to get the absorbance spectra of a compound in the arrangement or as a solid. What is really being watched spectroscopically is the absorbance of light energy or electromagnetic radiation, which energizes electrons from the ground state to the



primary singlet energized state of the compound or fabric. The UV-vis locale of vitality for the electromagnetic range covers 1.5 - 6.2 eV which relates to a wavelength extend of 800 - 200 nm. The Beer-Lambert Law is the rule behind absorbance spectroscopy.

At present, a lot of, many methods of Chemistry are used to check body fluids and gases that aim to determine a specific procedure that is acceptable during laboratory diagnoses. These chemical methods enable us to quantify a certain level of natural and mineral parts, just like Aromatic compounds (benzene, toluene, xylene), etc. And

determine its deviations from the standard and their concentrations (Lelevic A 2020). Qualitative assessment of the degree of signs that are remembered in the standard chemical examination is conceivable when thinking about other strange properties of gases. Raw spectra were documented and included for comparison of concentrations and contribution of Aromatic compounds.

Through this analysis, we can discover the variance in the formation of Aromatic compounds components. (Figure 1), show the raw spectra of the specific Aromatic compounds for (20 wavelengths).

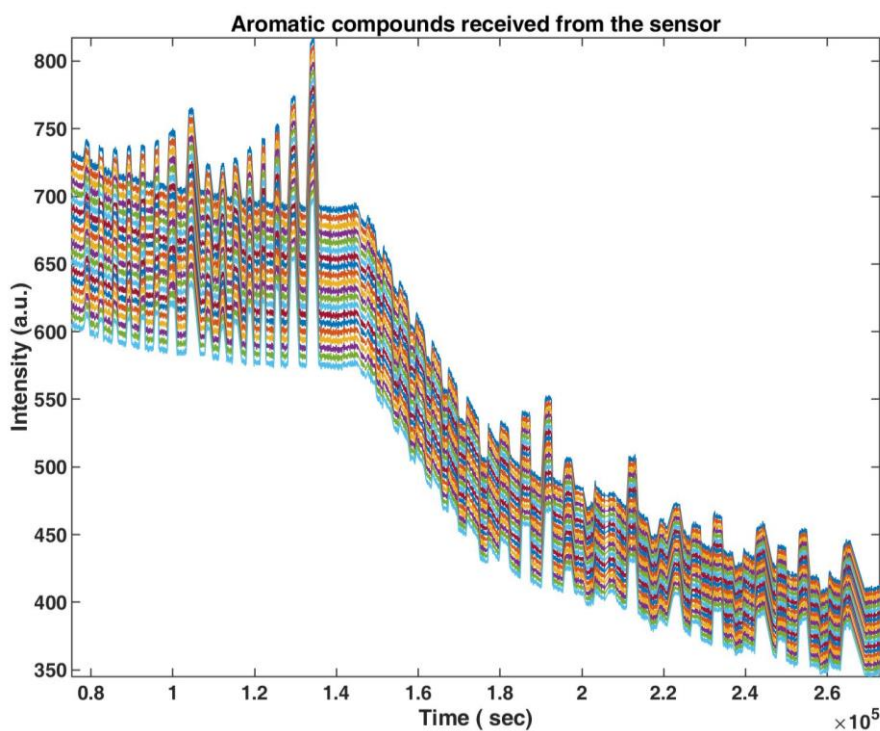


Figure 1. General view of 20 samples within the range of output data from the device

Because the noise filtering nature in signals is diverse, and to remove impulse noise at the preliminary stage, we apply a median filter, and the median filter out to be more efficient than linear filters in cases when the differences in signal values are large compared to the variance of the Gaussian noise, as it gives a lower value of the root mean square error of the output signal in relation to the input, noise-free signal when compared with optimal linear filters (Khalaf AIZ 2020).

The smoothing procedure is carried out using the Savitzky-Golay filter, or Medium filter. The smoothing procedure is carried out using the Savitzky-Golay filter, or medium filter. The Savitzky-

Golay filtering method is better than simple medium because it retains the characteristic features of the spectrum, such as the height and width of the peaks, which are usually smeared with a moving averaging filter. The main advantage of this approach is that it tends to maintain local extrema, which are usually smoothed out by other averaging methods, the formula for Savitzky-Golay filter (Luo J 2005). This study concerned four samples within the range of wavelengths, (Figure 2), Spectrum of Aromatic compounds in the range of interest obtained at four samples within the range of wavelengths (459,466,462,464nm) of output data from the device, it was observed that there was a very large

discrepancy between the signals in (the upper part before smoothing and bottom after smoothing).

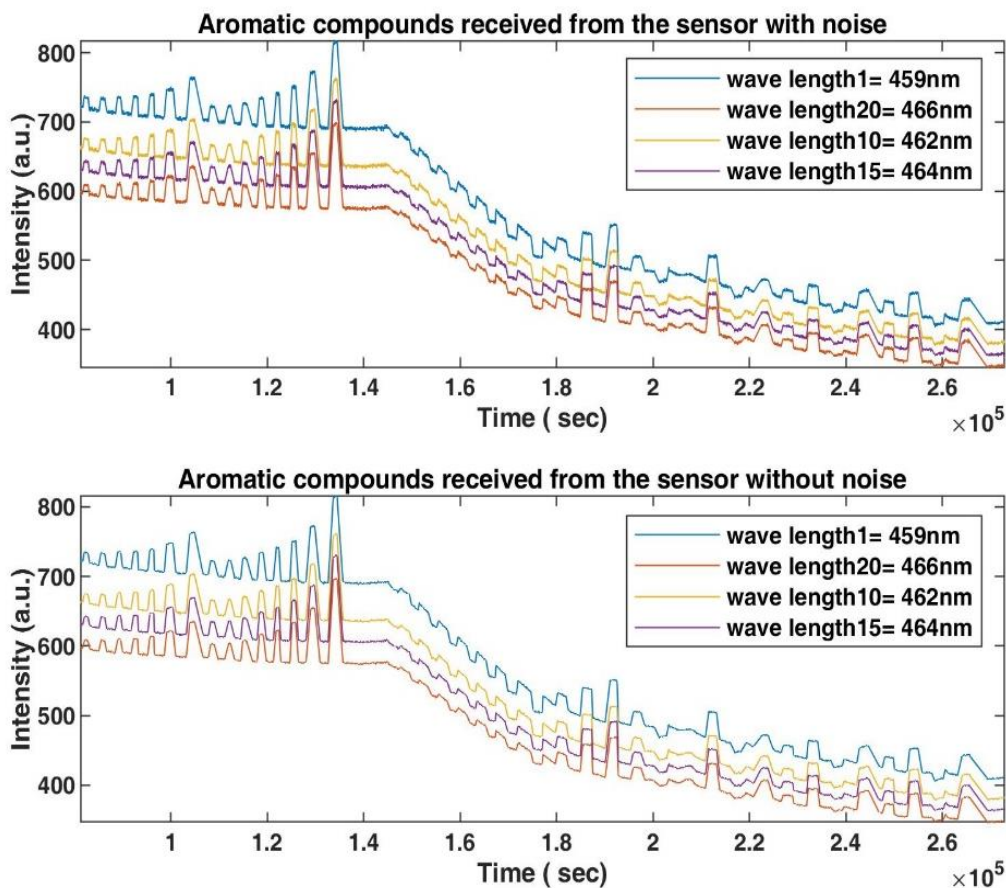


Figure 2. Four samples within the range of wavelengths (459,466,462,464nm) some samples of output data from the device.

Background removal is one of the most difficult tasks for a qualitative analysis of experimental results. A variety of techniques encompass either instrumental or software approaches to remove background fluorescence signals, software methods have become the standard for correcting the contribution of fluorescence to the background (Cai TT 2001).

It is necessary to subtract the autofluorescence background from the original filtered and smoothed signal. The background can be modelled by polynomial, the order of which is selected on the basis of effectively removing it and at the same time minimizing the removal of signal peaks (Pijanka JK 2013). To obtain a “pure” spectrum, we used the method (PolyFit) and the proposed developed

method (ProcessorsGases), and we worked on studying and applying them to the components of Aromatic compounds. (Figure 3), Spectrum of Aromatic compounds in the range of interest obtained at four samples within the range of wavelengths was pre-treated and the pure signal obtained through the use of the method PolyFit, in (Figure 4), Spectrum of Aromatic compounds in the range of interest obtained at four samples within the range of wavelengths was pre-treated and the pure signal obtained through the use of the method ProcessorsGases (Khalaf AIZ 2020).

The pure signal obtained through the use of the two methods, a very large variance was observed in the gasoline portion and also toluene and less variation in the xylene region.



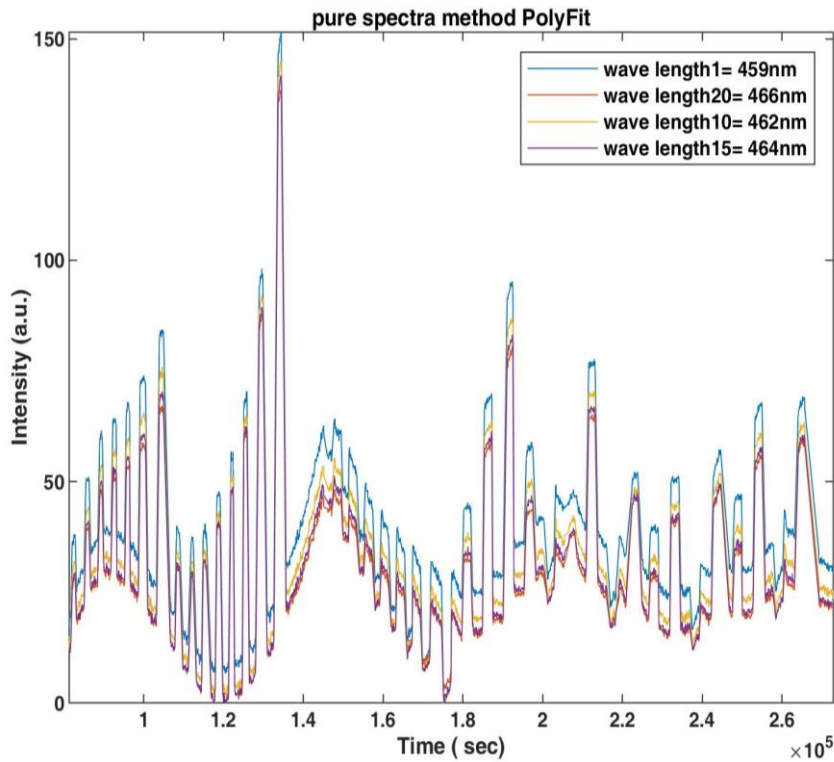


Figure 3. View of 4 samples within the range "pure spectra" received using from PolyFit for the signal spectrum aromatic compounds

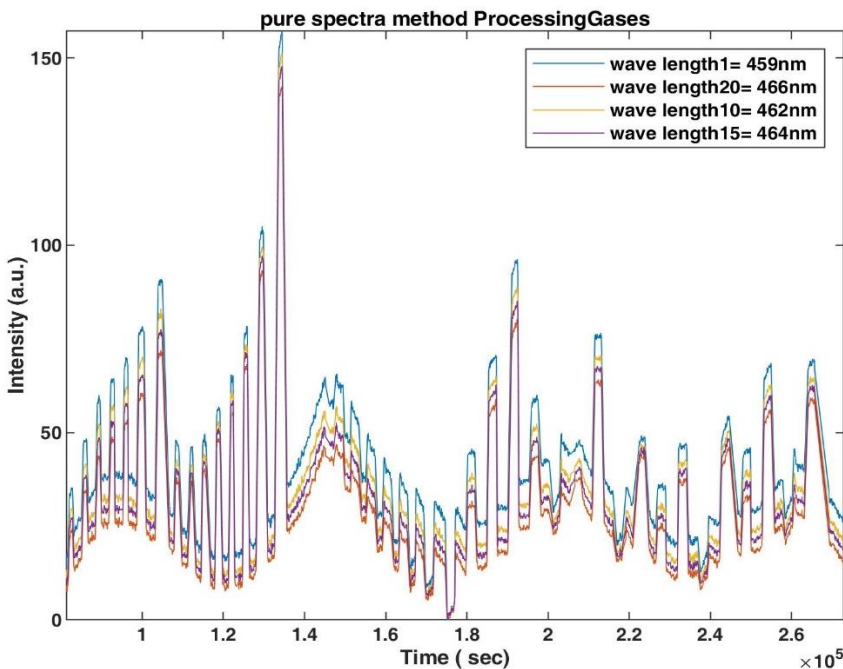


Figure 4. View of 4 samples within the range "pure spectra" received using from processing Gases for the signal spectrum aromatic compounds

Comparing and Analyzing the Spectral Properties of Aromatic Compounds in Gases Using (MCR-ALS)

Through use, method the MCR regression to analyse information spectral data at different

concentrations and compare it with previous methods notable differences were observed between all cases. In addition to a remarkable merging of the wavelengths chosen in this study.



The primary features of in Aromatic compounds (Luo J 2005). We also obtained the concentrations lines are shown in spectral locales and around. (Aromatic compounds) for the spectra that were (Figure 5), illustrates the processors conducted on used. spectra of Aromatic compounds by MCR methods

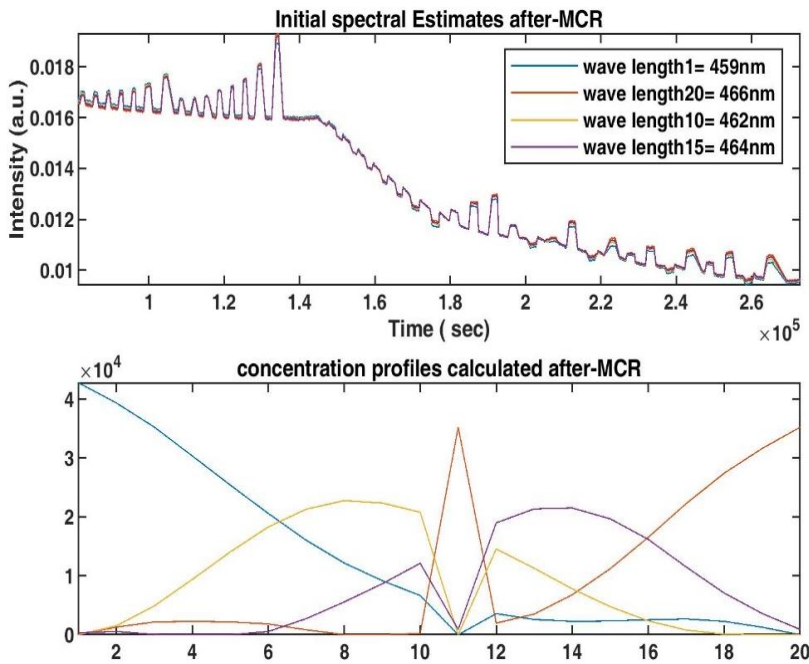


Figure 5. Smoothed spectra with a highlighted autofluorescence background (top) and "Concentrations" spectra (bottom) received using from MCR 53 for the signal spectrum aromatic compounds

In addition, we obtained pure spectra and the (Figure 6), illustrates pure spectra received of concentrations different from the previous, while Aromatic compounds by MCR methods (Feng X preserving the general structure of the gas mixture 2017).

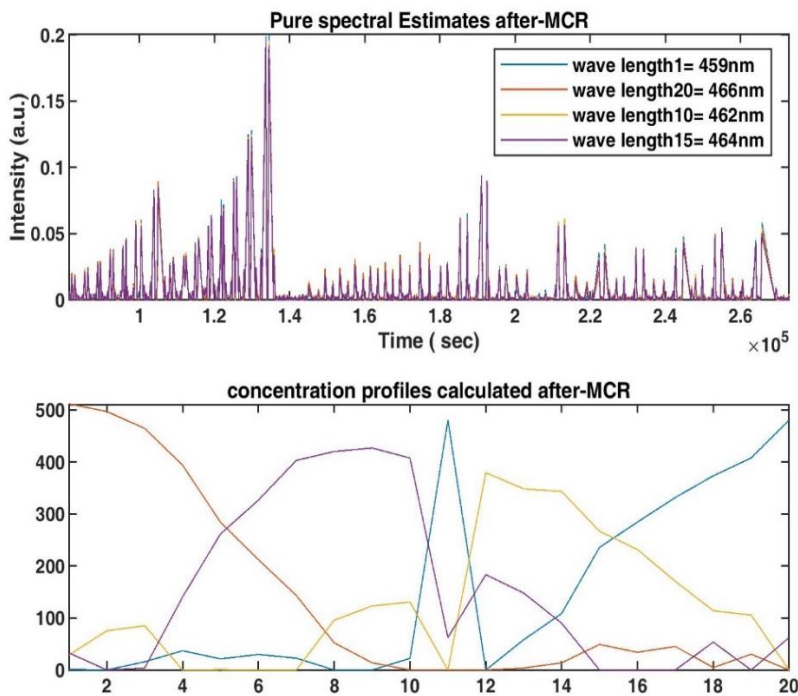


Figure 6. Pure spectra (top) and "Concentrations" spectra (bottom) received using from MCR for the signal spectrum aromatic compounds



Discussion and Conclusion

Aromatic compounds spectra showed a simple affinity for wavelengths (459,466,462,464 nm) the minor variations in intensities and positions of clear Sensors tops.

The best part the most might of the technique for pathologies recognition caused by gases of Aromatic compounds it is Sensor scattering spectra and became a good alternative from available discovery systems of various other conditions utilizing research Centre strategies for gases in general, and Aromatic compounds in particular (D. J. Jaumot J 2015).

With respect to the estimation of the concentrations, particularly the (benzene, toluene and xylene), the spectroscopy, and (Multivariate Curve Resolution) (MCR) analysis, in spectra of Aromatic compounds specimens were recorded using a Sensor. It was found that there were obvious spectral differences at specific (PolyFit, processing Gases, MCR) positions etc. in the groups (Khalaf AIZ 2020).

Results obtained for components: 4 after application of PCA, Initial spectral Estimates after -MCR, to the data matrix maximum of iterations, reached lack of fit (%) at optimum = 0.023854 (PCA) 0.023856(exp) Percent of variance explained (R2) at optimum 100 times are at optimum in iteration 50 results.

And was results for pure spectral Estimates after -MCR, obtained for components: 4 after application of PCA, to the data matrix maximum of iterations reached lack of fit (%) at optimum = 3.9809(PCA) 4.075(exp) Percent of variance explained (R2) at optimum 100 times are at optimum in iteration 15 results.

For this particular purpose, the method employed can be helpful in expediting the determination associated with the difference between tops. After that, it will be easier to research by examining the concentrations of Aromatic compounds in addition to determining their need or perhaps capacity treatment in common.

In another meaning, the proposed relatively simple analysis allows, discriminating between Sensors spectra and absorption cross-sections of molecule in Hitran, by means of the original spectra info. The employment of a low-cost and portable Sensors spectrometer would make the technique available for other applications.

Some of the gases of aromatic compounds are sometimes considered unrealistic, other gases can be used for research purposes for non-invasive

diagnostics, for which they cause various malignant diseases. In the future, this approach may become the basis for screening and diagnostics that will expand the properties of various elements, improving unexplained observable groups.

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References

- Fox MA, Chanon M. (Eds.). *Photoinduced electron transfer*. Elsevier Science Limited 1988.
- Mirzaei A, Kim JH, Kim HW, Kim SS. Resistive-based gas sensors for detection of benzene, toluene and xylene (BTX) gases: a review. *Journal of Materials Chemistry C* 2018; 6(16): 4342-4370.
- Acharyya D, Bhattacharyya P. An efficient BTX sensor based on ZnO nanoflowers grown by CBD method. *Solid-State Electronics* 2015; 106: 18-26.
- Sekhar PK, Subramaniam K. Detection of harmful benzene, toluene, ethylbenzene, xylenes (BTEX) vapors using electrochemical gas sensors. *ECS Electrochemistry Letters* 2014; 3(2): B1-B4.
- Safonov AA, Bagaturyants AA, Sazhnikov VA. Fluorescence spectra of (dibenzoylmethanato) boron difluoride exciplexes with aromatic hydrocarbons: a theoretical study. *The Journal of Physical Chemistry A* 2015; 119(29): 8182-8187.
- Jolliffe I. *Principal Component Analysis*. 2Nd Ed. New York, NY: Springer-Verlag 2002.
- Azzouz T, Tauler R. Application of multivariate curve resolution alternating least squares (MCR-ALS) to the quantitative analysis of pharmaceutical and agricultural samples. *Talanta*, 2008; 74(5): 1201-1210.
- Garrido M, Rius FX, Larrechi MS. Multivariate curve resolution-alternating least squares (MCR-ALS) applied to spectroscopic data from monitoring chemical reactions processes. *Analytical and bioanalytical chemistry* 2008; 390(8): 2059-2066.
- Jaumot J, Gargallo R, De Juan A, Tauler R. A graphical user-friendly interface for MCR-ALS: a new tool for multivariate curve resolution in MATLAB. *Chemometrics and intelligent laboratory systems* 2005; 76(1): 101-110.
- Bro R, De Jong S. A fast non-negativity-constrained least squares algorithm. *Journal of Chemometrics: A Journal of the Chemometrics Society* 1997; 11(5): 393-401.
- De Juan A, Navea S, Diewok J, Tauler R. Local rank exploratory analysis of evolving rank-deficient systems. *Chemometrics and intelligent laboratory systems* 2004; 70(1): 11-21.
- Tauler R, Marqués I, Casassas E. Multivariate curve resolution applied to three-way trilinear data: Study of a spectrofluorimetric acid-base titration of salicylic acid at three excitation wavelengths. *Journal of Chemometrics: A Journal of the Chemometrics Society* 1998; 12(1): 55-75.



- Brown NMD, Bladon P. Spectroscopy and structure of (1, 3-diketonato) boron difluorides and related compounds. *Journal of the Chemical Society A: Inorganic, Physical, Theoretical* 1969; 526-532.
- Job P. Formation and stability of inorganic complexes in solution. *Ann. Chim.*, 1928; 9(113).
- Hill ZD, MacCarthy P. Novel approach to Job's method: An undergraduate experiment. *Journal of Chemical Education* 1986; 63(2): 162-167.
- Lipskier JF, Tran-Thi TH. Supramolecular assemblies of porphyrins and phthalocyanines bearing oppositely charged substituents. First evidence of heterotrimer formation. *Inorganic Chemistry* 1993; 32(5): 722-731.
- Quintero L, Hunt S, Diem M. Denoising of raman spectroscopy signals. *In Poster presented at the 2007 R2C Multi Spectral Discrimination Methods Conference* 2007.
- Shreve AP, Cherepy NJ, Mathies RA. Effective rejection of fluorescence interference in Raman spectroscopy using a shifted excitation difference technique. *Applied spectroscopy* 1992; 46(4): 707-711.
- Khalaf AIZ, Alboedam M, Abidalhussein HJ, Hassan AZS. The role of blood proteins and nucleic acids in the detection of multiple Myeloma based on Raman spectroscopy. *EurAsian Journal of BioSciences* 2020; 14(1): 1955-1963.
- Khalaf AIZ, Alboedam M, Jwad Abidalhussein H, Hassan AZS. Detecting levels amino acids for proteins of different for patients with myeloma and comparing them using a portable Raman spectrometer. *EurAsian Journal of BioSciences* 2020; 14(1): 2029-2036.
- Cai TT, Zhang D, Ben-Amotz D. Enhanced chemical classification of Raman images using multiresolution wavelet transformation. *Applied spectroscopy* 2001; 55(9): 1124-1130.
- Wold S, Esbensen K, Geladi P. Principal component analysis. *Chemometrics and intelligent laboratory systems* 1987; 2(1-3): 37-52.
- Shenai PM, Xu Z, Zhao Y. Applications of principal component analysis (PCA) in materials science. *Principal component analysis-engineering applications* 2012: 25-40.
- Jaumot J, De Juan A, Tauler R. MCR-ALS GUI 2.0: New features and applications. *Chemometrics and Intelligent Laboratory Systems* 2015; 140: 1-12.
- Eilers PH, Boelens HF. Baseline correction with asymmetric least squares smoothing. *Leiden University Medical Centre Report* 2005; 1(1): 5.
- Zhang D, Wang P, Slipchenko MN, Ben-Amotz D, Weiner AM, Cheng JX. Quantitative vibrational imaging by hyperspectral stimulated Raman scattering microscopy and multivariate curve resolution analysis. *Analytical chemistry* 2013; 85(1): 98-106.
- Feng X, Moy AJ, Nguyen HT, Zhang J, Fox MC, Sebastian KR, Tunnell JW. Raman active components of skin cancer. *Biomedical optics express* 2017; 8(6): 2835-2850.
- Kumar K, Mishra AK. Application of 'multivariate curve resolution alternating least square (MCR-ALS)' analysis to extract pure component synchronous fluorescence spectra at various wavelength offsets from total synchronous fluorescence spectroscopy (TSFS) data set of dilute aqueous solutions of fluorophores. *Chemometrics and Intelligent Laboratory Systems* 2012; 116: 78-86.
- Lelevic A, Souchon V, Moreaud M, Lorentz C, Geantet C. Gas chromatography vacuum ultraviolet spectroscopy: A review. *Journal of separation science* 2020; 43(1): 150-173.
- Luo J, Ying K, He P, Bai J. Properties of Savitzky-Golay digital differentiators. *Digital Signal Processing* 2005; 15(2): 122-136.
- Pijanka JK, Stone N, Rutter AV, Forsyth N, Sockalingum GD, Yang Y, Sulé-Suso J. Identification of different subsets of lung cells using Raman microspectroscopy and whole cell nucleus isolation. *Analyst* 2013; 138(17): 5052-5058.
- Pandarakalam JP. The physiology of incarnation process; lessons from pre-birth experiences and reincarnation-type case. *NeuroQuantology* 2019; 17(5): 22-34.
- Meijer DKF, Hans G. Life and consciousness are guided by a semi-harmonic EM background field. *NeuroQuantology* 2019; 17(4): 37-44.

