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Simultaneous Spectrophotometric Determination of Some Polycyclic Aromatic Hydrocarbons Using Salting-Out Assisted Liquid-Liquid Extraction Coupled with Doolittle Multivariate Calibration Algorithm

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Abstract

Simultaneous spectrophotometric determination of some polycyclic aromatic hydrocarbons (PAHs) in wastewater samples after preconcentration by salting-out assisted liquid-liquid extraction was achieved using a doolittle multivariate calibration algorithm (DMCA). The DMCA was applied by lower and upper (LU) triangular matrix decomposition which is efficient, powerful and easily. Results were shown that DMCA has advantages such as, simplicity, rapidness, avoiding matrix inverting and reducing the orders of matrices. The influence of various parameters, such as extraction solvent and volume, type and amount of salt, vortex time and sample pH were studied and optimized. The net analyte signal (NAS) method was used for calculating figures of merit. Linear range (LR) of calibration graphs for naphthalene, anthracene and pyrene were between 0.20 - 2.00, 0.10 - 1.50 and 0.07 -1.00 µg mL^{-1}, respectively. The root mean square errors of prediction (RMSEP) for naphthalene, anthracene and pyrene using DMCA model were 0.0367, 0.0331 and 0.0305, respectively.

Keywords

Polycyclic Aromatic Hydrocarbons; Simultaneous Determination; Spectrophotometry; Doolittle Multivariate Calibration Algorithm; Salting-Out Assisted Liquid-Liquid Extraction.

1. INTRODUCTION

Polycyclic aromatic hydrocarbons (PAHs) are hazardous organic pollutants for their teratogenicity, carcinogenic and mutagenic potential. Hence, monitoring of these compounds in environmental and during industrial process are important [1, 2].

The simultaneous spectrophotometric determination of several active components in a mixture can be a major problem, specifically for components that have become excessively overlapped as a result of similar analytical characteristics [3]. Also, it is not easy to determine these PAHs with conventional methods. Nowadays, rapid spectrophotometric techniques in combination with chemometric methods are used to solve the overlapping spectrum [4, 5]. A review of several literatures showed that a variety of techniques such as gas chromatography- mass spectrometry (GC-MS) [6], high performance liquid chromatography (HPLC) [7, 8] ultra performance liquid chromatography [9] and excitation-emission fluorescence spectroscopy [10] have been reported for the determination of PAHs. Some of these methods possess disadvantages such as being a time-consuming and complicated procedure, use of hazardous organic solvents, as well as produce waste with a high percentage of organic solvents. Spectrophotometric methods are the most popularly used methods due to common availability of instrumentation, wide application range, experimental speed, precision and accuracy of the technique [1, 11].

The salting-outassisted liquid-liquid extraction (SALLE) is a liquid–liquid extraction (LLE) method which used for extraction of polar and nonpolar compounds from aqueous solutions. In this method a suitable amount of salt was added to a mixture of water sample and water–miscible solvent which lead to separate of two phases and transferring of target analytes to organic phase [7, 12-16].

Pre-processing of orthogonal signal correction (OSC) [17, 18] is aimed at eliminating undesired information in the response matrix, to make it mathematically orthogonal to the concentration matrix. The wavelet transform is an excellent mathematical technique, created purposely for the denoising of raw spectral data [19]. In PLS [20-21]

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regression, errors in both the concentrations and analytical signals were considered in the calculation to improve predictive ability. The doolittle multivariate calibration algorithm (DMCA) is a very simple, accurate, efficient, and constant numerical analysis algorithm with an easy computational method. The DMCA can avoid performing matrices inversion, which is often involved in chemometrics such as PCR and PLS methods; decrease the orders of matrixes; accelerate the operation of matrixes; and enhance the efficiency of computation [22-26].

In this work, DMCA in combination with SALLE were used for the simultaneous preconcentration and spectrophotometric determination of some PAHs in aqueous samples.

1.1 THEORY

1.1.1. Calibration

The calibration set $C_{15\times3}$ was designed. The absorbance matrix $A_{15\times111}$ was obtained from the spectral data of 15 calibration samples. According to Lambert-Beer law:

$$C_{15\times3}B_{3\times111} = A_{15\times111} \tag{1}$$

Thus

$$C^{T}_{3\times15}C_{15\times3}B_{3\times111} = C^{T}_{3\times15}A_{15\times111} \tag{2}$$

The process of triangle decomposition of matrix, is

$$C^{T}_{3\times15}C_{15\times3} = LU \tag{3}$$

Solving the following equation

$$LY = C^{T}_{3\times15}A_{15\times111} \tag{4}$$

Y is turn out; with another equation

$$UB = Y \tag{5}$$

The absorption coefficient matrix B is obtained.

1.1.2. Prediction

By estimating the coefficient matrix B gotten previously and the spectra data $A_{6\times111}$ of the real samples, the matrix $C_{6\times3}$ of the concentrations of real samples is obtained. The absorbance matrix $A_{6\times111}$ of 6 real samples was obtained from the spectra data of the samples. The multivariate calibration techniques are based on, Lambert-Beer Law, that is A=bc.

$$C_{6\times3}B_{3\times111} = A_{6\times111} \tag{6}$$

So

$$C_{6\times3}B_{3\times111}B^{T}_{111\times3} = A_{6\times111}B^{T}_{111\times3} \tag{7}$$

The process of triangle decomposition of matrix is

$$B_{3\times11}B^{T}_{111\times3} = MN \tag{8}$$

Solving the following equation

$$YN = A_{6\times111}B^{T}_{111\times3} \tag{9}$$

We get Y; by solving equation

$$CM = Y \tag{10}$$

The concentration matrix $C_{6\times3}$ of real samples could be gained.

2. EXPERIMENTAL

2.1. Reagents and Chemicals

Acetonitrile, tetrahydrofuran (THF), ethanol, acetone, isopropanol, ammonium sulfate, sodium chloride, sodium carbonate, were purchased from Merck Chemical (Darmstadt, Germany). All solutions were prepared with deionized water (Milli-Q system, Millipore, USA). Naphthalene, anthracene and pyrene were obtained from Sigma-Aldrich (USA). The universal buffer solution was prepared according to reported procedure [27].

2.2. Instrumentation and Software

A Perkin Elmer Lambda 25 (Perkin Elmer, USA) spectrophotometer equipped with a 350 µL quartz microcell was employed for all experimental. The Centurion Scientific centrifuge (model EBA 200 Hettich) was used for centrifuging. A vortex mixer (50 Hz) from Scientific Industries, CSLVORTEX (England) was used. All evaluations for this work were carried out in MATLAB (Version 7.8.0 (R2009), Mathwork Inc.) on a personal computer. The programs for DMCA and NAS calculations were written in MATLAB Version 7.8.0 (R2009a) and run on a VAIO Personal Computer (4GB RAM) equipped with the Windows 8 operating system. PLS, OSC, and Wavelet orthogonal signal correction (WOSC) estimates were obtained using the PLS-Toolbox version 4.0 from Eigenvector Research Inc.

2.3. Sample Preparation

Standard stock solutions of naphthalene, anthracene and pyrene were prepared by dissolving each analyte in methanol with concentration of 100 µg mL^{-1}. Working standard solutions at different concentrations were freshly prepared by mixing the appropriate volumes of the stock solutions and diluting with deionized water. Wastewater samples were collected from Shazand Petrochemical Corporation. Samples were filtered using a 0.45 µm membrane filters prior to extraction.

2.4. SALLE Procedure

In this study, 4.0 mL of aqueous sample containing PAHs was transferred into a test tube with conical bottom. 1.0 mL of acetonitrile as extraction solvent and 1.0 g of $(NH_4)_2SO_4$ were added, and the mixture was vortexed using a vortex mixer at 3000 rpm for 3.0 min. The cloudy mixture was centrifuged for 2.0 min at 4000 rpm. Finally, 300 µL of the organic phase was withdrawn and transferred into a 350 µL spectrophotometric cell. Absorbance data were taken in the range of 200-400 nm against acetonitrile as blank. The spectra were analyzed by the DMCA method for simultaneous determination of PAHs.

3. RESULT AND DISCUSSION

In this study, the effect of various parameters on the extraction efficiency of the SALLE procedure of analytes were studied and optimized. The absorption spectra of naphthalene, anthracene, pyrene, and their mixture are shown in (Figure 1). The Figure shows spectra of these analytes were overlapped. To resolve this problem, a useful and satisfactory technique such as the DMCA regression which presents versatility results is used. Thereafter, at optimal experimental conditions, DMCA was used as a useful chemometric method in the analysis of overlapping spectra and simultaneous spectrophotometric determination of several PAHs mixtures.

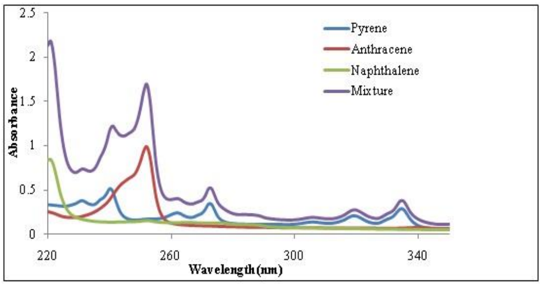

Fig. 1. The absorption spectrum of 0.2 µg mL^{-1} of pyrene, 0.2 µg mL^{-1} of Anthracene, 0.2 µg mL^{-1}naphthalene and 0.21 µg mL^{-1} of pyrene, 0.3 µg mL^{-1} of Anthracene and 0.48 µg mL^{-1} naphthalene in a mixture after SALLE procedure.

3.1. Optimization of Extraction Conditions

3.1.1 Selection of the Organic Solvent

In most sample preparation methods, the selection of a suitable extracting solvent is a key step. The organic solvent must be very polar, miscible in aqueous phase and induce phase separation upon addition of suitable inorganic salts [28]. This inference is wrong and applies only to the Salting-out assisted liquid–liquid extraction procedure. Various water-miscible organic solvents, such as acetonitrile, tetrahydrofuran (THF), isopropanol, ethanol, acetone, and their binary mixture, were tested as the extracting solvent (Figure 2). Using acetone and ethanol two phase system was not obtained. Under the similar conditions, the results showed that acetonitrile exhibited the highest extraction recoveries when compared with the other solvents. Thus, acetonitrile was chosen as extracting solvent.

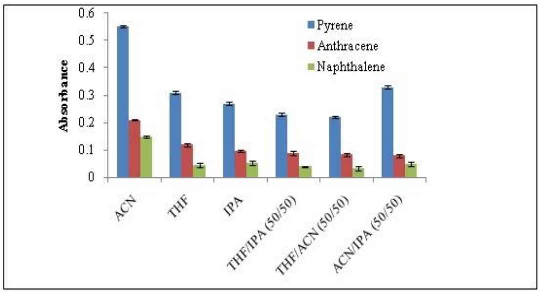

Fig. 2. Effect of water-miscible organic solvent on the extraction efficiency. Extraction conditions: extraction solvent volume, 1.0 mL; salt amount, 1.0 g; vortex time, 3 min; IPA, isopropanol; ACN, acetonitrile; and THF, tetrahydrofuran.

3.1.2. Effect of Acetonitrile Volume

The effect of acetonitrile volume on extraction was considered in the range of 0.8-2.0 mL (Figure 3). As can be seen, the highest extraction efficiency was obtained at 1.0 mL volume of acetonitrile. At higher volumes of acetonitrile due to analyte dilution absorbance values were decreased.

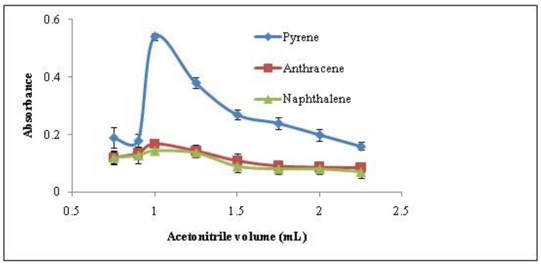

Fig. 3. Effect of acetonitrile volume on the extraction efficiency. Extraction conditions: extraction solvent, acetonitrile; salt amount, 1.0 g and vortex time, 3 min.

3.1.3. Effects of Salt Type and its Amount

In SALLE, the solubility of hydrophilic compounds and organic solvent in the aqueous phase decreased on addition of salt and consequently, increased the transfer of analytes into the organic phase. In order to obtain phase separation and highest extraction recoveries, different salts, including sodium chloride, ammonium sulfate, and sodium carbonate were evaluated. The results showed that the extraction recovery with ammonium sulfate was higher than other salts. Afterwards, the effect of ammonium sulfate concentration on the extraction recoveries was tested by adding various amounts of this salt in the range of 0.75-2.00 g to the aqueous sample solution. (Figure 4) shows the extraction efficiency of the three analytes were improved as the amount of salt increased from 0.75-1.00 g and remained constant upon addition of higher amounts of salt. Thus, 1.00 g of ammonium sulfate was selected as the optimal concentration throughout the study.

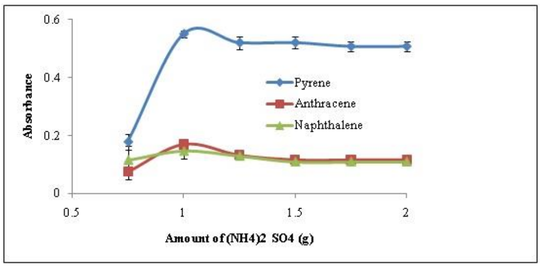

Fig. 4. Effect of salt amount on the extraction efficiency. Extraction conditions: extraction solvent; acetonitrile; extraction solvent volume, 1.0 mL; vortex time, 3 min.

3.1.4. Effect of Sample pH

The effect of sample pH on the extraction recoveries was evaluated in the range of 2.0-11.0. The results obtained clearly show that the extracted analytes were constant in the studied pH range. Therefore, no pH adjustment was performed for subsequent experiments.

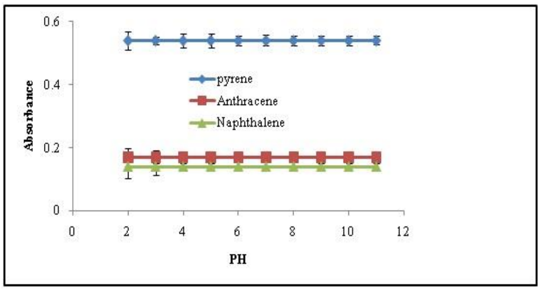

Fig. 5. Effect of PH on the extraction of PAHs of interest. Extraction conditions: extraction solvent; acetonitrile; extraction solvent volume, 1.0 mL; vortex time, 3 min.

3.1.5. Effect of Vortex Agitation Time

Agitation of the sample mixture due to which increase the contact surface between the extracting solvent and analytes plays a major role in SALLE. Also, agitation leads to the dissolution the added salt which results in salting-out phenomenon. Therefore, a vortex time was investigated in the range of 1–5 min, and efficiency extraction recoveries were obtained at a vortex time of 3 min. (Figure 6) indicates 3 min is the optimal vortex time.

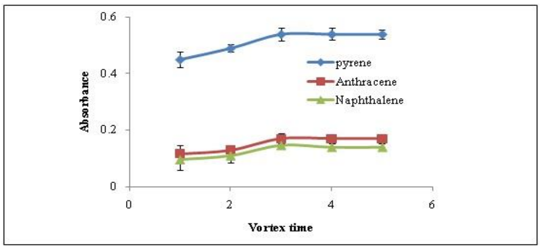

Fig. 6. Effect of vortex time on the extraction of PAHs of interest. Extraction conditions: extraction solvent, acetonitrile; extraction solvent volume, 1.0 mL; salt concentration, 1.0 g.

3.1.6. Effect of Centrifugation Time

Centrifuge time and rates are very necessary to preconcentrate trace amounts of PAHs with high efficiency in a short time. Thus, under optimal reagent conditions obtained, the effect of the centrifuge time and rate were studied in rage of 1–5.0 min and 2000–5000 rpm, respectively. The results showed that centrifugation for approximately 2.0 min at approximately 4000 rpm was selected as optimum as complete separation occurred within this time.

3.2. Individual Calibration

Individual calibration curves were constructed with several points as absorbance versus naphthalene, anthracene and pyrene concentrations. The linear regression equations for naphthalene in the concentration range of 0.2- 2.0 µg mL^{-1}, anthracene in the concentration range of 0.1-1.5 µg mL^{-1} and pyrene in the concentration range of 0.07-1.0 µg mL^{-1} were A= 0.571C + 0.03, A= 2.26C + 0.09 and A= 3.12C + 0.025, respectively. The limit of detection values for naphthalene, anthracene and pyrene were 0.017, 0.016 and 0.014 µg mL^{-1} respectively. These values were calculated using the net analyte signal (NAS) method [30].

3.3. Multivariate Calibration

The present similarity spectra of the three PAHs could be resolved using DMCA. To have a satisfactory model, 15 mixtures were designed as the calibration set. The model calibration was verified with six synthetic mixtures containing naphthalene, anthracene and pyrene. Thereafter, chemometric models such as wavelet orthogonal signal correction partial least squares (WOSC-PLS) and DMCA were estimated, using the correlation for the training set concentration and its current data. All calibration and validation of synthetic mixtures were constructed in accordance with the SALLE procedure previously mentioned. The spectral zone between 200 and 400 nm with scan rate of 450 nm min^{-1} was measured against acetonitrile as blank. The absorbance data spectral region between 240 and 340 nm was chosen for the analysis, because this is the region with the maximum spectral information about the mixed PAHs of interest.

3.3.1. WOSC-PLS Method

To ensure the predictive ability of the calibration model, raw spectral data are often denoised prior to construction of the model. In this study, two pre-processing approaches orthogonal signal correction (OSC) and wavelet (WT), combined for building the chemometric calibration were chosen due to pre-processing of the raw spectral data with WOSC correction being more of the unnecessary spectral data than that filtered with OSC or WT alone. A couple of WT with OSC was employed in this study, which it is very effective in improving the predictive ability of the PLS model in comparison to other methods used. In this research, various wavelet functions (Coiflet 1, 2, ..., 5, Daubechies 4, 5, 6, and Symmlet 3, 4, 5,...8) as well as decomposition levels (L=1-6) were investigated. To estimate and find the optimum values selection of the mentioned parameters, the root mean square error of prediction (RMSEP) and relative standard error of prediction (RSEP) can be applied. Therefore, optimal value parameters were selected in this method as Symmlet3, L=1, and number of PLS factors=4.

3.4.2. Determination of Naphthalene, Anthracene and Pyrene in Synthetic Mixtures

The predictive ability and verification of DMCA method was determined using 6 three-component PAHs mixtures interest. The results obtained from simultaneous determination of naphthalene, anthracene and pyrene after SALLE by DMCA method are shown in (Table 1).

3.5. Evaluation of the Performance of the Test Methods

The predictive power of DMCA and WOSC-PLS methods were investigated using a set of synthetic mixture samples. To verify the predictive ability of these models, the RMSEP and RSEP can be used (Table 5).

$$RMSEP = \sqrt{\frac{\sum_{1}^{n}\left(y_{pred} - y_{obs}\right)^2}{n}} \qquad (11)$$

$$RSEP(\%) = 100 \times \sqrt{\frac{\sum_{i=1}^{n}\left(y_{pred} - y_{obs}\right)^2}{\sum\left(y_{obs}\right)^2}} \qquad (12)$$

Where y_{pred} is the predicted concentration, y_{obs} observed value of the sample, and n is the number of samples in the validation set. The values RMSEP were minimized when optimum value of latent variables (LVs) is 4 for WOSC-PLS; thus, 4 was chosen as the optimum number of LVs for the training set of the WOSC-PLS method. (Table 2) shows the RMSEP and RSEP for the two methods. The displayed differences were not statistically significant and DMCA and WOSC-PLS are observed to efficiency almost similar results. The square of the correlation coefficient (R^2) which is a sign of the efficiency of fit of all the data to a direct line [31, 32], were estimated and also contained in Table 2. The values of R^2 are similar for DMCA and WOSC-PLS models.

Table 1. Added and found results of synthetic PAHs mixtures interest (µg mL^{-1}).

Naphthalene			Anthracene			Pyrene		
Added	Found	Recovery (%)	Added	Found	Recovery (%)	Added	Found	Recovery (%)
0.30	0.32	106.6	0.20	0.23	115.0	0.12	0.13	108.3
0.56	0.53	94.6	0.40	0.37	92.5	0.26	0.25	96.1
0.83	0.83	100.0	0.60	0.58	96.7	0.40	0.40	100.0
1.00	1.04	104.0	0.74	0.76	102.7	0.50	0.51	102.0
1.20	1.24	103.3	0.87	0.84	96.5	0.60	0.58	96.6
2.00	1.97	98.5	1.50	1.50	100.0	1.00	1.02	102.0

Table 2. Statistical parameters obtained by applying the two data treatment methods to the synthetic mixtures.

Methods	WOSC-PLS			DMCA		
	Naphthalene	Anthracene	Pyrene	Naphthalene	Anthracene	Pyrene
NLVs[a]	4	4	4	-	-	-
RMSEP	0.030	0.024	0.013	0.037	0.033	0.030
RSEP (%)	2.7	2.9	2.4	3.3	4.0	5.5
R^2	.997	.996	.998	.997	.994	.994

[a] Number of latent variables.

Table 3. Analytical figures of merit obtained by the NAS method.

Component	Selectivity	Sensitivity	LOD (µg mL^{-1})	LOQ (µg mL^{-1})
Naphthalene	0.077	0.182	0.017	0.055
Anthracene	0.038	0.189	0.016	0.053
Pyrene	0.158	0.056	0.014	0.048

Table 4. Accuracy data for naphthalene, anthracene and pyrene spiked in a wastewater sample.

Compound	Added (µg mL^{-1})	Found (µg mL^{-1})	Recovery (%)	RSD (%) (n=4)
Naphthalene	0.0	N.D[a]	-	-
	0.60	0.62	103.33	7.23
	0.95	0.93	97.90	6.81
	1.32	1.29	97.72	4.72
Anthracene	0.0	N.D	-	-
	0.35	0.34	97.14	5.51
	0.85	0.87	102.35	5.15
	0.93	0.90	96.77	4.94
Pyrene	0.0	N.D	-	-
	0.27	0.28	103.70	5.43
	0.70	0.71	101.42	3.71
	0.82	0.84	102.44	3.47

[a]Not Detected.

Table 5. Comparison of analytical parameters of the proposed SALLE method with some of the methods reported in literature.

Method	Analyte	Instrument	LR (µg mL^{-1})	LOD (µg mL^{-1})	RSD (%)	Recovery (%)	Refs.
DLLE[a] -EDR	Naphthalene	UV/Vis	0.25 - 2.0	0.05	1.1	74.00 - 87.83	1
	Anthracene		0.10 - 0.75	0.01	0.8	102.55 - 104.00	
	Pyrene		-	-	-	-	
SPME[b]	Naphthalene	GC/MS	0.00001 - 0.01	0.000003	< 20	-	33
	Anthracene		0.00001 - 0.03	0.00002	< 20	-	
	Pyrene		0.00001 – 0.01	0.000001	< 20	-	
SAALLME[c]	Naphthalene	HPLC/UV	0.025 – 1.00	0.00834	< 6.6	95.2 – 98.8	7
	Anthracene		0.001 - 0.50	0.00022	< 7.2	92.0 – 96.8	
	Pyrene		-	-	-	-	
SALLE[d] - DMCA	Naphthalene	UV/Vis	0.20 – 2.0	0.017	4.3	97.72 - 103.33	Proposed method
	Anthracene		0.10 – 1.5	0.016	3.9	96.77 – 102.35	
	Pyrene		0.07 – 1.0	0.014	3.1	101.42 – 103.70	

[a] Dispersive liquid–liquid extraction - Extended derivative ratio. [b] Solid-phase microextraction. [c] Salt-and air- assisted liquid-liquid microextraction. [d] Salting-out assisted liquid-liquid extraction - Doolittle multivariate calibration algorithm.

3.5. Analytical Characteristics of the Method

Quantitative specifications of the developed method were achieved under the optimum conditions. Calculation of the NAS, allows the calculation of several figures of merit (selectivity, sensitivity, limit of detection (LOD), limit of quantification (LOQ), useful for method comparison and to describe the quality of the proposed multivariate calibration (Table 3). A linear range (LR) of calibration graphs were determined for naphthalene, anthracene and pyrene, between 0.20 - 2.0, 0.10 - 1.50 and 0.07 - 1.00 µg mL^{-1}, respectively. The limit of detection values of 0.017, .016 and 0.014 µg mL^{-1} were calculated according to the NAS method. The enrichment factors of the chosen PAHs, computed as the ratio of the slope pre-concentration samples to those obtained without pre-concentration, were 25.70 for naphthalene, 34.80 for anthracene and 38.10 for pyrene. The repeatability of the methods was investigated using three repeat measurements of a 0.4 µg mL^{-1} PAHs were 4.30, 3.90 and 3.10 % for naphthalene, anthracene and pyrene, respectively.

3.6. Applications

This newly proposed method has been applied in the simultaneous pre-concentration and determination of naphthalene, anthracene, and pyrene after SALLE procedure, under the optimal conditions in the different wastewater samples. The validity of the DMCA method was determined by analysis of the samples spiked with a known concentration of PAHs interest. The satisfactory results are shown in (Table 4). The obtained recovery of the proposed methods shows the ability to predict concentration of PAHs interest in the wastewater samples of matrixes.

3.7. Comparison of the Proposed Method with other Methods

Comparison of the figures of merit of the DMCA method with some of the previously reported methods for the determination of target analytes is shown in (Table 5). The proposed method in comparison with other approaches is simple, cheap, powerful, produces better results, non-polluting, possesses much simpler calibration models, highly sensitive, and similar repeatability. These results show that the DMCA method is successful at the simultaneous spectrophotometric determination of overlapping peaks.

4. CONCLUSION

In this research, an accurate, simple, useful and satisfactory method was applied for simultaneous spectrophotometric determination of these compounds in wastewater samples. The simultaneous spectrophotometric determination of naphthalene, anthracene, and pyrene is extremely challenging and complex due to spectral interferences observed in the absorption spectra of these components. The results show satisfactory and reliability of the SALLE method as a sample preparation method in combination with DMCA approach. As well as, DMCA may be of useful for the extension of automatic calibration processes, as the choice of the optimum number of factors is not necessary. Future research on the DMCA should focus on improving this approach in relation with pre-processing techniques.

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اندازه‌گیری همزمان اسپکتروفتومتری هیدروکربن‌های آرماتیک چندحلقه‌ی با استفاده از پیش‌تغلیظ استخراج مایع-مایع کمک‌شده با نمک‌زنی جفت شده با الگوریتم چند متغیره دولیتل

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چکیده

اندازه‌گیری همزمان اسپکتروفتومتری چند هیدروکربن آروماتیک چند حلقه‌ی در نمونه‌های آبی بعد از پیش‌تغلیظ استخراج مایع-مایع کمک‌شده با نمک‌زنی با استفاده از الگوریتم چند متغیره دولیتل بدست آورده شده‌است. الگوریتم چند متغیره دولیتل از تجزیه ماتریس بالا و پایین مثلثی استفاده می‌کند که روشی آسان و نیرومند است. نتایج نشان می‌دهد که الگوریتم چند متغیره دولیتل دارای مزایای مانند سادگی، سرعت، اجتناب از معکوس نمودن ماتریس و کاهش مرتبه ماتریس می‌باشد. تأثیر پارامترهای مختلفی نظیر حلال استخراج و حجم، نوع و مقدار نمک، زمان ورتکس و pH نمونه مورد بررسی و بهینه سازی شد. برای محاسبه ارقام شایستگی از روش سیگنال خالص آنالیت استفاده شده است. محدوده خطی برای منحنی کالیبراسیون به ترتیب برای نفتالن، آنتراسن و پیرن بین ۲,۰۰–۰,۲۰، ۱,۵۰–۰,۱۰ و ۱,۰۰–۰,۰۷ میلی‌گرم بر لیتر تعیین گردید. میانگین مربعات خطای پیشگویی برای نفتالن، آنتراسن و پیرن با استفاده از مدل الگوریتم چند متغیره دولیتل به ترتیب ۰,۰۳۶۷، ۰,۰۳۰۱ و ۰,۰۳۰۵ بدست آمد.

واژه‌های کلیدی

هیدروکربن های آرماتیک چند حلقه ی؛ اندازه گیری همزمان اسپکتروفتومتری؛ الگوریتم چند متغیره دولیتل؛ استخراج مایع-مایع کمک شده با نمک زنی جفت‌شده.