Automated algorithm for removing continuous flame spectrum based on sampled linear bases

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Abstract—In this paper, an automated algorithm to estimate and re-move the continuous baseline from measured spectra containing both continuous and discontinuous bands is proposed. The algorithm uses previous information contained in a Continuous Database Spectra (CDBS) to obtain a linear basis, with minimum number of sampled vectors, capable of representing a continuous baseline. The proposed algorithm was tested by using a CDBS of flame spectra where Prin-cipal Components Analysis and Non-negative Matrix Factorization were used to obtain linear bases. Thus, the radical emissions of natural gas, oil and bio-oil flames spectra at different combustion conditions were obtained. In order to validate the performance in the baseline estimation process, the Goodness-of-fit Coefficient and the Root Mean-squared Error quality metrics were evaluated between the estimated and the real spectra in absence of discontinuous emission. The achieved results make the proposed method a key element in the development of automatic monitoring processes strategies involving discontinuous spectral bands.

Keywords—Flame spectra, removing baseline, recovering spec-trum.

I. INTRODUCTION

SEVERAL processes involving spectral emission or ab-sorption bands are evaluated by using these information, allowing a quantitative analysis of the influence of many variables or parameters in the process. Flame spectroscopy is effective in the combustion process characterization, where previous studies have shown that the intensity of several radicals radiated by a flame (discontinuous emissions) in the combustion process provide important information about the air/fuel ratio, the CO pollutant emission or the combustion efficiency [1]. On the other hand, the continuous emission (baseline) of flame provide important information about the flame temperature and soot formation [2]. Thus, for some applications it may be necessary or desirable to separate the discontinuous bands and baseline spectra from a flame measured spectrum in order to extract the aforementioned information.

Typical spectra are classified depending on the energy distribution on *Continuous* and *Discontinuous* spectra [3], [4]. The continuous spectra is characterized because the emit-ted or absorbed energy is distributed in a continuous non-discrete spectrum over a wide region of wavelengths and usually exhibits a maximum (or minimum) intensity over the spectral bands of interest. The discontinuous spectra is characterized because the emitted or absorbed energy is mainly

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concentrated in a narrow band of the spectrum. Usually, a continuous spectrum exhibits low frequency components while the discontinuous emission is characterized by high frequency components [5]. Typical flame spectra in the visible (VIS) band can be seen in Fig. 1, where it is possible to identify several discontinuous emissions, like CH^*, C_2^*, Na^* and K^* radicals at 430 nm, 515.5 nm, 588 nm and 766 nm respectively, added to continuous baseline. The flame discontinuous emissions are attributed to the energy emitted by isolated atoms or molecules, while the continuous flame emission is given mainly by the soot formation (*yellow zone*). It is predominant along the flame, after the reaction zone, and its intensity change locally depending on the flame temperature and emissivity [6], [7], [8]. The formation of the mentioned radicals is predominant in the reaction zone, whereas along the flame the emission of these radicals disappear and the soot radiation becomes predominant [6], [8], [9].

The main goal of this paper is to provide a methodology to separate both the continuous and discontinuous spectral information from a measured flame spectrum. Several methods which essentially are algorithms of signal recovery have been developed with this goal, and have been classified on auto-mated and manual methods [5], [10]. The former methods are automated computed to estimate the continuous baseline from a signal, while the latter require the operator intervention by choosing several baseline points. However, both methods are sensible to signal parameters like noise, being mainly affected
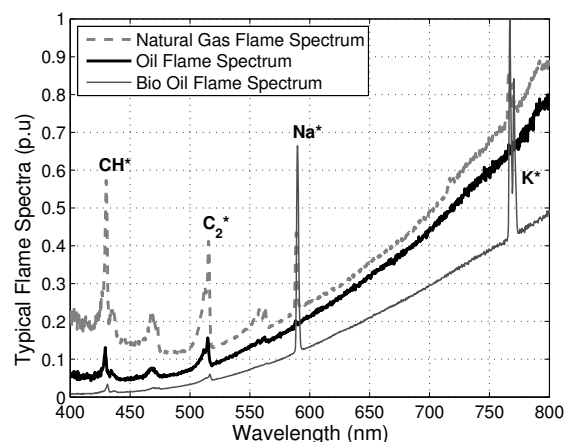

Fig. 1: Typical flame's spectrum (normalized) of natural gas, oil and bio-oil hydrocarbon fuels, where discontinuous emis-sions are added to continuous baseline.

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the automated methods.

The automated algorithm proposed here is based on previous information extracted from a Continuous Database Spectra (CDBS), which allow to obtain a minimum number of real bases to reconstruct any continuous baseline spectrum. Thus, in order to estimate the continuous emission from a real spectrum containing both, continuous and discontinuous radiations, a sampled version of the bases is used. Then, the discontinuous emission is estimated subtracting the continuous estimated baseline to the measured spectrum. The proposed algorithm was tested by using a CDBS of flame spectra, from where Principal Components Analysis (PCA) and Non-negative Matrix Factorization (NNMF) were used to acquire the respective bases. Thus, the radical emissions of natural gas, oil and bio-oil flames spectra at different combustion conditions were obtained. In order to validate the performance in the baseline estimation process, the Goodness-of-fit Coefficient (GFC) and the Root Mean-squared Error (RMSE) quality metrics between the estimated and real spectra in absence of discontinuous emission were evaluated.

This paper is organized as follows. The theory of continuous spectral reconstruction based on sampled bases, and therefore the discontinuous flame spectrum estimation is presented in Section II. Additionally, two quality metrics used to assess the spectral match between a real and a recovered spectrum are presented in this section. In Section III, the experimental validation results of the proposed algorithm are shown. Finally, in the last section, our conclusions are drawn.

II. Theory of continuous spectral reconstruction from sampled bases

It is know that emitted flame spectrum E_e in the VIS band corresponds to the sum of continuous E_c and discontinuous E_d spectral emissions [3], [4], that is:

$$E_e = E_c + E_d \qquad (1)$$

where each term is wavelength dependent.

The idea is to reconstruct the continuous flame radiation E_c from the measured E_e by using previous knowledge about E_c. Then, E_d can be estimated. This *a priori* knowledge is obtained from a CDBS constructed with continuous flame spectral measurements, from which *representative* bases containing much of information from the CDBS are extracted.

The recovering process of continuous spectral emission from E_e is described in the following subsection.

A. Continuous spectrum recovering algorithm

Different methods are based on *a priori* knowledge about the kind of spectra to be represented. For example, PCA, NNMF or independent component analysis (ICA) [11], provide sets of bases which can be linearly combined to represent a given spectrum. The advantage in the use of these methods is that these bases can be extracted from real database.

Thus, a continuous flame spectrum can be linearly expressed as:

$$\hat{E}_{c_{N \times 1}} = B_{N \times n} \cdot c_{n \times 1}, \qquad (2)$$

where B is a matrix containing the *n representative* vectors forming a basis extracted from the CDBS at N wavelengths, and the vector c contains the coefficient of the linear combination. The *hat* symbol over E_c represent the fact that $\hat{E}_c$ is an approximated linear representation using only $n < N$ vectors to represent E_c. The number of chosen vectors obeys to reduce the computational time consumed when the pseudoinverse of the B matrix is needed to be computed [12]. The idea is to define a method which allow to estimate the continuous flame spectrum by calculating the coefficients of the linear combination c from the measure of E_e.

It can be seen from (2) that by computing the pseudoinverse of the matrix B (that is, B^+) then the vector c can be obtained, when a continuous real spectrum E_c^{Re} is represented by the linear model. Thus,

$$c_{n \times 1} = [B]_{n \times N}^+ \cdot E_{c_{N \times 1}}^{Re}. \qquad (3)$$

Assuming that the continuous baseline from a measured real spectrum E_e can be represented by a sampled version of B (that is, B^m) at the same spectral dimension (samples of B with other data vector to zero), therefore, Eq. (3) can be written as follows:

$$c_{n \times 1}^m = [B^m]_{n \times N}^+ \cdot E_{e_{N \times 1}}, \qquad (4)$$

where c^m represents the response of the sampled basis B^m sampling E_e. By assuming that this sampling process is such that continuous samples are observed from E_e in the absence of discontinuous emission, then c^m can be also expressed as follows:

$$c_{n \times 1}^m = [B^m]_{n \times N}^+ \cdot E_{c_{N \times 1}}^{Re}. \qquad (5)$$

Then, pluging E_c^{Re} from (3) in (5), the process transforming the response c^m of the sampled vector basis into the coefficient c, is expressed as follows:

$$c_{n \times 1}^m = [B^m]_{n \times N}^+ \cdot B_{N \times n} \cdot c_{n \times 1}, \qquad (6)$$

$$c_{n \times 1} = \left[[B^m]_{n \times N}^+ \cdot B_{N \times n} \right]^+ \cdot c_{n \times 1}^m. \qquad (7)$$

From the matrix transformation $\left[[B^m]_{n \times N}^+ \cdot B_{N \times n} \right]^+$, the recovered continuous spectrum $\hat{E}_c$ can be calculated by pluging (7) in (2):

$$\hat{E}_{c_{N \times 1}} = B_{N \times n} \cdot \left[[B^m]_{n \times N}^+ \cdot B_{N \times n} \right]^+ \cdot c_{n \times 1}^m, \qquad (8)$$

where the vector c^m is calculated from Eq. (4). Note that the spectral dimension (wavelength resolution) of the continuous recovered spectrum depends on the spectral dimension of the training matrix in the chosen vector basis B.

The methodology described above can be understood as follows. The continuous spectral information contained in E_e is extracted by sampling the measured spectrum, and then a matrix transformation $\left[[B^m]_{n \times N}^+ \cdot B_{N \times n} \right]^+$ it is used to transform $c_{n \times 1}^m$ to $c_{n \times 1}$, whereas the spectral dimension of $\hat{E}_{c_{N \times 1}}$ is given by the spectral dimension of $B_{N \times n}$, which appears in (8).

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B. Recovering discontinuous flame emissions

The recovered discontinuous flame's emissions $\hat{E}_d$ can be estimated by replacing the Eq. (8) on Eq. (1):

$$\hat{E}_d = E_e - B_{N \times n} \cdot \left[[B^m]^+_{n \times N} \cdot B_{N \times n}\right]^+ \cdot c^m_{n \times 1}. \quad (9)$$

The proposed algorithm is a general method that can be used when a process provides continuous spectral information and a CDBS can be constructed. Thus, it can be used to recover the discontinuous emission/absorption bands present in the process. As mentioned before, the combustion process monitored by using the flame spectrum is a process which can provide, depending on the spatial measurement zones, continuous spectra (soot formation zone) and both, continuous and discontinuous emission (reaction zone) simultaneously. Therefore, the validation of the proposed method will be carried out by using a flame spectrum database.

C. Metrics for quality evaluation in the spectral reconstruction process

Traditionally, different metrics have been used to assess the performance on the spectral reconstruction process. The RMSE and the GFC are two of such metrics [13], [14]. The RMSE numerically quantify the differences between both, the real and the reconstructed spectrum, while the GFC evaluates the spectral projection of the reconstructed spectrum onto the real spectrum. The RMSE between the real and the reconstructed spectrum is defined as:

$$RMSE = \sqrt{\sum_{j=1}^{N} \left(E_e\left(\lambda_j\right) - \hat{E}_c\left(\lambda_j\right)\right)^2}, \quad (10)$$

where, in this work λ_j is the spectral band in absence of discontinuous emission.

The GFC metric between the real and the reconstructed spectrum is defined as:

$$GFC = \frac{\left|\sum_j E_e\left(\lambda_j\right)\hat{E}_c\left(\lambda_j\right)\right|}{\left[\sum_j \left[E_e\left(\lambda_j\right)\right]^2\right]^{1/2}\left[\sum_j \left[\hat{E}_c\left(\lambda_j\right)\right]^2\right]^{1/2}}. \quad (11)$$

An accurate estimation yields a GFC in [0.995,0.999), while a GFC in [0.999,0.9999) means quite good spectral matches and a GFC larger or equal than 0.9999 means an excellent spectral match [15].

III. EXPERIMENTAL RESULTS

To validate the proposed model, the continuous radiation of natural gas, oil, and bio-oil flame spectra was reconstructed and then subtracted to the measured spectrum, thereby recovering the discontinuous emissions. Five representative spectra (labelled from S1 to S5) containing both, continuous and discontinuous radiation, where measured at different air/fuel conditions, each condition evaluated with the variable lambda(1+e). Different air/fuel conditions were considered because they generate data at different continuous and discontinuous radiation intensities. The variable lambda(1+e) represents
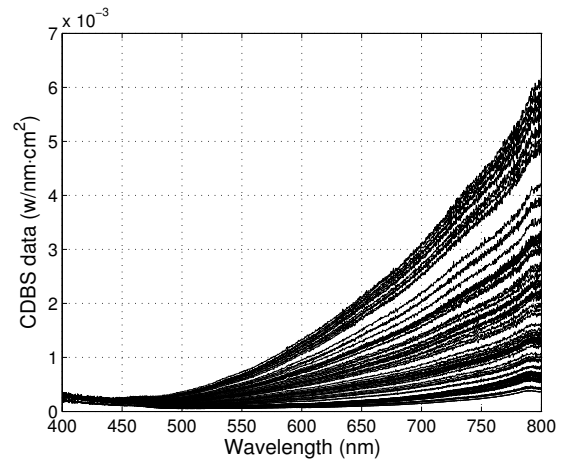

Fig. 2: Continuous samples spectra used to construct the CDBS.

the air-to-fuel ratio of the actual combustion condition over the corresponding stoichiometric air-to-fuel ratio, and is defined as:

$$\text{lambda(1+e)} = \frac{\text{(air/fuel)}_{\text{actual}}}{\text{(air/fuel)}_{\text{stoichiometric}}}, \quad (12)$$

that is, when lambda(1+e) is close to one the process is near to the stoichiometric condition exhibiting at this point, a stronger continuous spectral emission than when lambda(1+e) values are longer.

In order to generate the vector basis of B, and consequently of B^m, a CDBS of 97 continuous flame spectra was constructed from a flame's spectral database taken in our laboratories since 2005 for different kinds of fuels flames. Spectra were measured along the flame in absence of discontinuous emissions. Both, the data of the CDBS and the testing spectra (S1-S5) were measured using a USB2000 spectrometer (previously calibrated with a HL2000 calibration lamp, Ocean Optics Inc.) in the 400.2-800.31 nm spectral band using N=1145 wavelength channels. Sample spectra of the CDBS are depicted in Fig. 2.

Two different methods were computed to extract orthogonal bases from the CDBS: PCA and NNMF. Due to PCA defines a space with vectors pointing in the direction of maximum variance and orthogonal between them, then the variance of the Principal Components (PCs) extracted from the CDBS was calculated and the results are depicted (in log scale) in Fig. 3. From this figure, it can be concluded that the first three PC's contain the maximum energy representing the CDBS. Therefore, the first three PCs ($n = 3$) where chosen to construct the matrix B and B^m. These PCs are shown in Fig. 4. Additionally, the first three NNMF vectors were used and then, the results in the continuous recovering process were evaluated and compared by using the same number of vector basis. The first three vector basis extracted by means of NNMF are shown in Fig. 5.

In order to define the optimum sampled version of B allowing an accurate reconstruction of E_c, an exhaustive search was made by changing the Period of Sampling (PoS) (in nm) of B from 1 to 1145 channels. The optimum PoS for each

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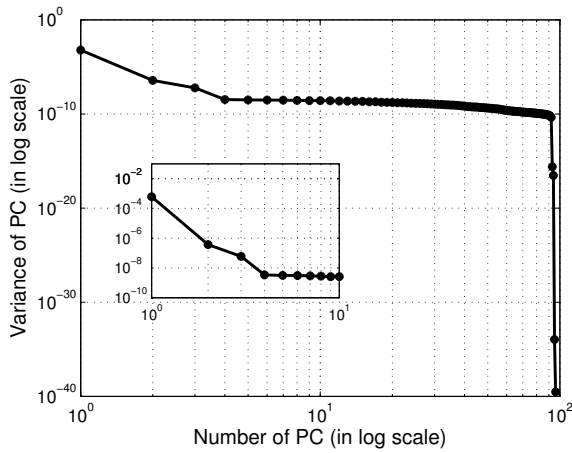fuel spectra was evaluated by calculating the average GFC

Fig. 3: Variance of the principal components extracted from CDBS.
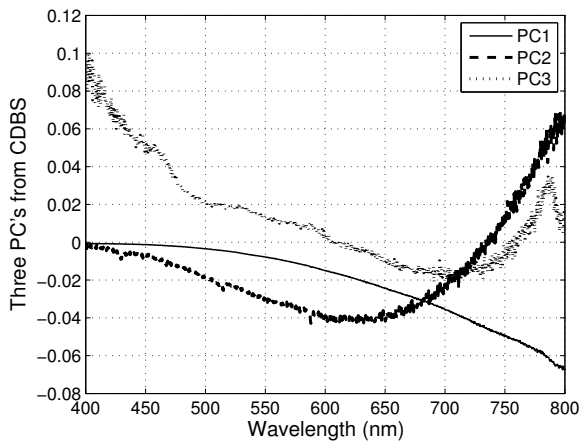

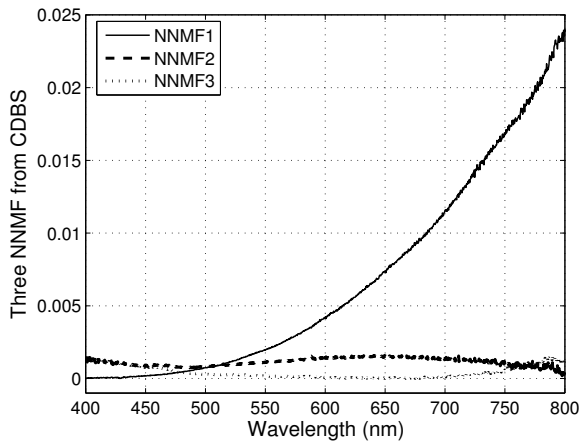Fig. 4: First three principal components extracted from a flame CDBS.

Fig. 5: First three vectors from NNMF extracted from a flame CDBS.

metric at each PoS between the original and the recovered spectra in absence of discontinuous radiations, considering the S1 to S5 samples. The results of the GFC metric for each PoS defining B^m, by using PCA and NNMF are depicted in Figs. 6 and 7, respectively, for natural gas, oil, and bio-oil fuels spectra. Additionally, Table I summarizes the PoS where the maximum average GFC occurs, and the associated sampling wavelengths. From these results, it can be seen that in order to reconstruct the continuous radiation from a natural gas spectra, 10 wavelengths of sampling should be considered, 11 wavelengths of sampling are needed for oil continuous emission and 6 wavelengths of sampling are needed in PCA while 4 are needed in NNMF to reconstruct the continuous spectra radiation from bio-oil spectra. An important observation can be highlighted from Figs. 6(a), (b), and (c): with a PoS of N/2, that is, with only 2 wavelengths of sampling between 400 nm and 800 nm, an important decrease in the GFC value occurs, which however starts to increase exhibiting an accurate value at a PoS of 928 (associated to the wavelength of 729.09 nm). This means that with only two wavelengths of sampling (420.2 nm and 729.09 nm) an accurate continuous spectral recovery can be achieved.
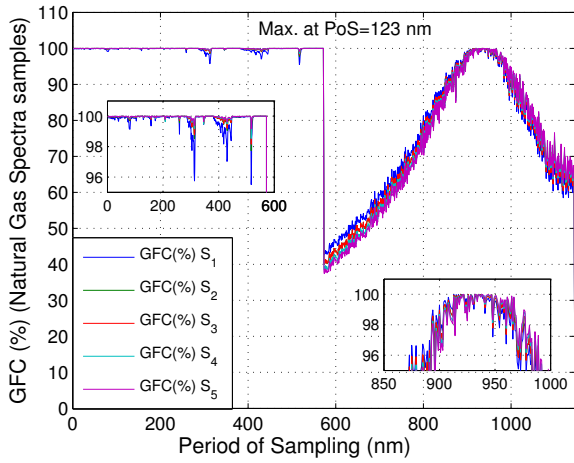
TABLE I: Optimum PoS and their associated sampling wavelengths used to construct the matrix B^m for an accurate continuous radiation recovery

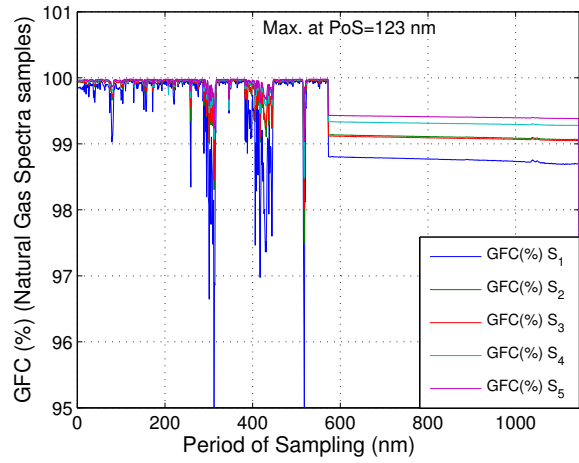| Fuel		Opt. PoS	Max. Avg. GFC	Wavelengths
Gas	PCA	123	99.9938	400.2–445.6–490.8–535.3–579.2–
	NNMF	123	99.9931	622.4–664.9–706.6–747.7–788.0
Oil	PCA	114	99.9940	400.2–442.3–484.2–525.6–566.4–
	NNMF	114	99.9936	606.6–646.3–685.3–723.8–761.5–798.7
Bio-oil	PCA	222	99.9849	400.2–482.0–562.1–640.0–715.7–789
	NNMF	372	99.9845	400.2–536.4–666.9–790.9

Considering that in all cases the average GFC calculated using PCs was closer to 100% than NNMF, then PCs vectors were used to extract the continuous radiation of the testing samples S1 to S5. By using the optimum empirically found PoS with allows an accurate continuous spectral reconstruction from a measured spectrum, the matrix B^m has been constructed by each fuel. Then, the Eq. (9) has been used estimate the discontinuous emission. These results are depicted in Figs. 8 to 10. In addition, Table II lists the GFC and the RMSE metrics between the original and recovered continuous radiation, calculated by using PCA and NNMF, for each testing sample (S1 to S5) and for each fuel.
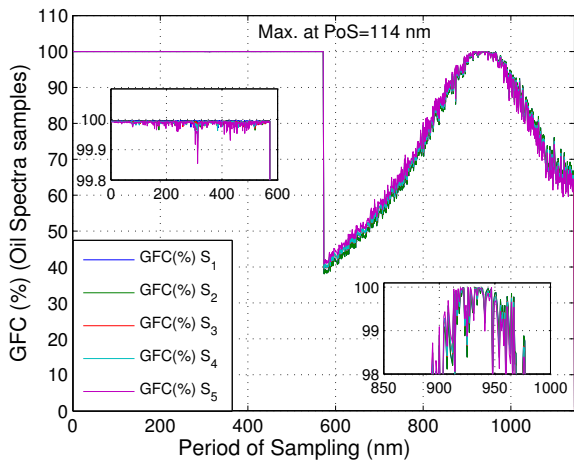
IV. CONCLUSION

An automated algorithm to estimate and remove the continuous baseline from measured flame spectra containing both, continuous and discontinuous bands, has been proposed. The algorithm is based on a real CDBS from where a minimum number of vector basis which allow a linear representation of a continuous spectrum are extracted. These vector bases and a sampled version of them are used to separate the continuous
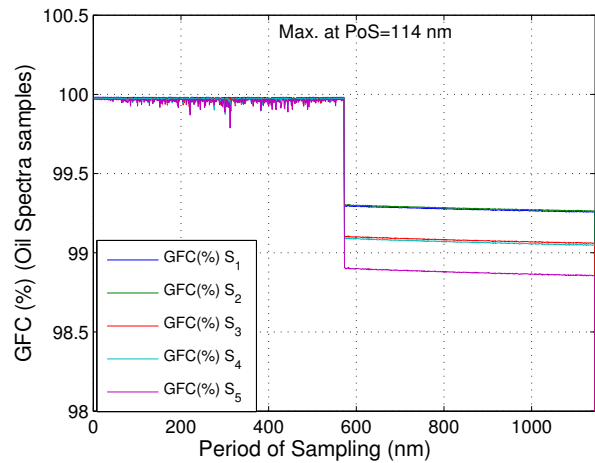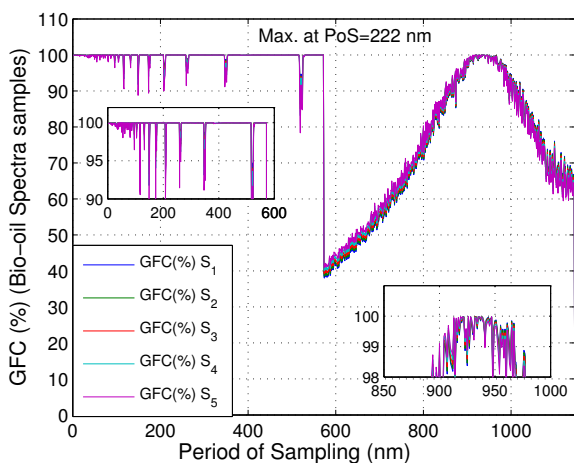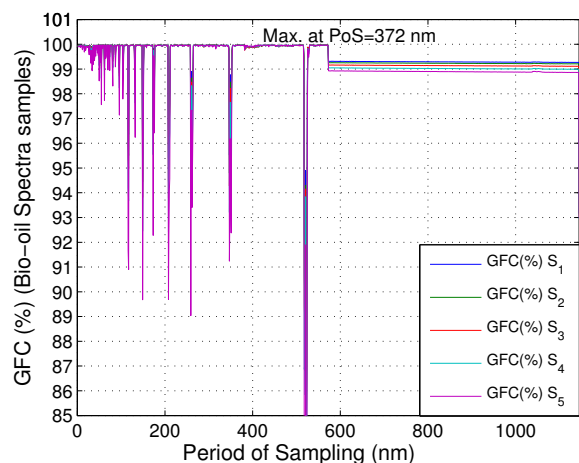
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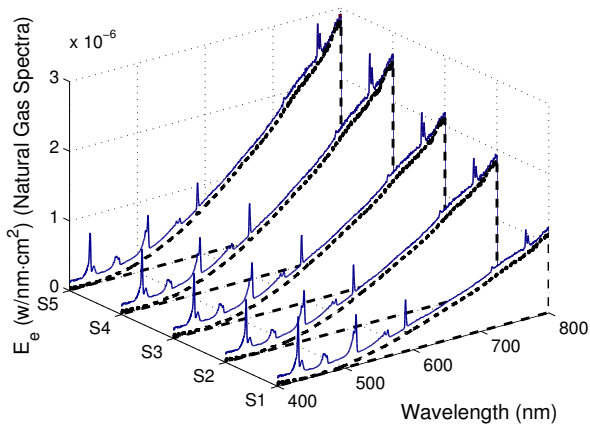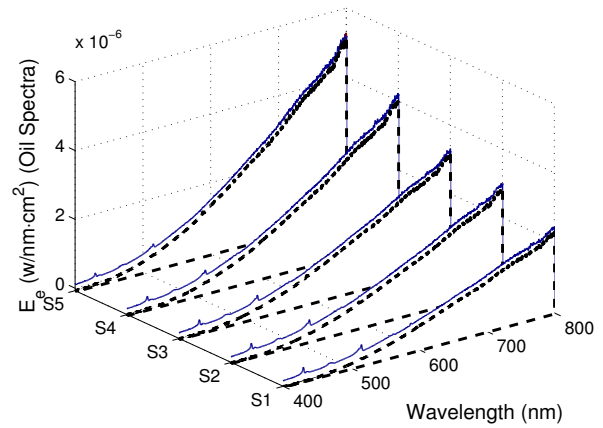International Journal of Mechanical and Mechatronics Engineering
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Fig. 6: GFC values as a function of the period of sampling PoS of vector basis computed with PCA for: (a) natural gas flame samples; (b) oil flame samples; and (c) bio-oil flame samples.
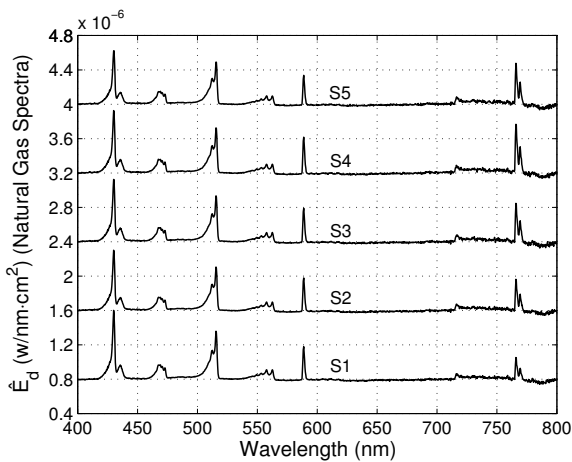
Fig. 7: GFC values as a function of the period of sampling PoS of vector basis computed with NNMF for: (a) natural gas flame samples; (b) oil flame samples; and (c) bio-oil flame samples.
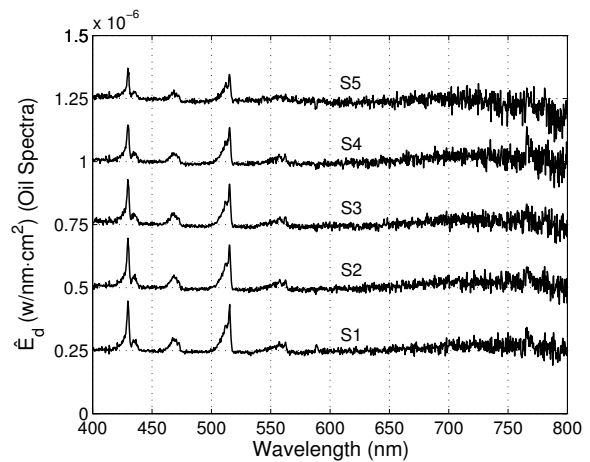
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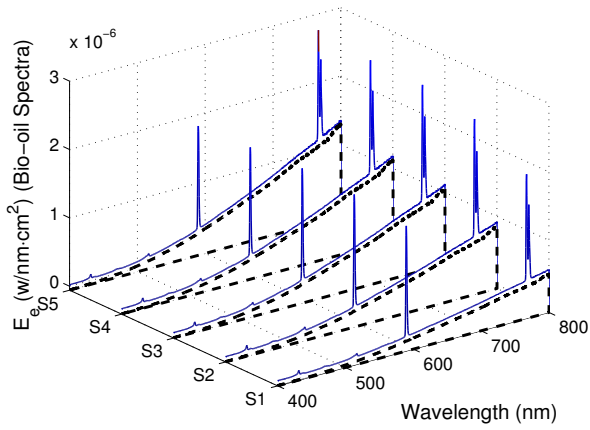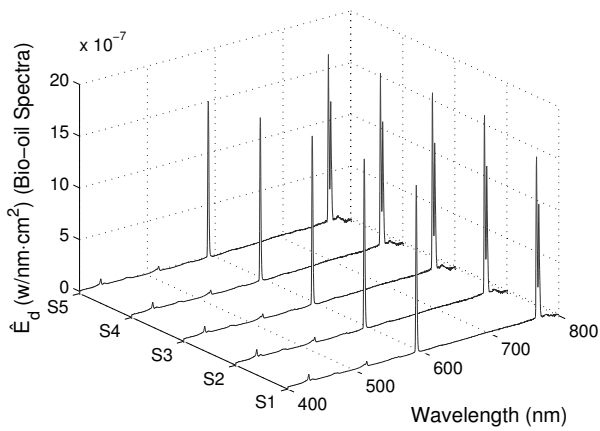
Fig. 8: (a) The original flame spectra (solid lines) and the recovered continuous spectra (dashed lines) of the natural gas flames for different air/fuel conditions. (b) The recovered discontinuous spectra of the natural gas flames with an offset of 0.8 $\mu w/nm \cdot cm^2$ between spectra.

Fig. 9: (a) The original flame spectra (solid lines) and the recovered continuous spectra (dashed lines) of the oil flames for different air/fuel conditions. (b) The recovered discontinuous spectra of the oil flames with an offset of 0.25 $\mu w/nm \cdot cm^2$ between spectra.

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Fig. 10: (a) The original flame spectra (solid lines) and the recovered continuous spectra (dashed lines) of the bio-oil flames for different air/fuel conditions. (b) The recovered discontinuous spectra of the bio-oil flames.

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TABLE II: GFC and RMSE metrics calculated between the original and recovered continuous radiation in absence of discontinuous emission.

Fuel	Testing Sample	lambda (1+e)	GFC (%)		RMSE (10^{-5})	
			PCA	NNMF	PCA	NNMF
Gas	S1	1.37	99.9883	99.9872	0.4208	0.5115
	S2	1.29	99.9939	99.9931	0.4309	0.5413
	S3	1.26	99.9943	99.9936	0.4233	0.5378
	S4	1.23	99.9957	99.9952	0.2924	0.4049
	S5	1.11	99.9966	99.9965	0.3414	0.4485
Oil	S1	1.18	99.9920	99.9914	0.6000	0.5880
	S2	1.15	99.9937	99.9933	0.7260	0.7220
	S3	1.12	99.9941	99.9935	0.4200	0.4170
	S4	1.08	99.9945	99.9944	0.4800	0.4850
	S5	1.02	99.9957	99.9956	1.2080	1.2090
Bio-oil	S1	1.65	99.9835	99.9831	0.1118	0.1329
	S2	1.56	99.9846	99.9841	0.1629	0.2769
	S3	1.39	99.9848	99.9844	0.2039	0.2940
	S4	1.20	99.9858	99.9854	0.2350	0.3134
	S5	1.14	99.9858	99.9855	0.2225	0.2773

emission from a real flame spectrum containing continuous and discontinuous spectral information.

The algorithm has been tested by using flame spectra of natural gas, oil, and bio-oil fuels, at different air/fuel conditions. In order to determine the optimum PoS of the vector basis for an accurate recovering process, the GFC between the measured and the recovered spectrum has been calculated in absence of discontinuous emission. The calculated GFC has demonstrated the feasibility of the proposed algorithm to recover the continuous emission from a measured spectrum, by using three orthogonal vector basis computed by PCA and NNMF. A minimum GFC of 0.999835 achieved by using vectors basis from PCA and a GFC of 0.999831 achieved by using vector basis from NNMF mean that a quite good spectral match has been achieved. Moreover, the discontinuous emission has been obtained by subtracting the continuous recovered spectrum to the measured sample.

The algorithm proposed can be extended to other processes which provide continuous spectral information to construct a CDBS, and then to extract the discontinuous emission/absorption bands, being a key element in the development of advanced control strategies for processes monitoring.

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