XVI IMEKO World Congress
Measurement - Supports Science - Improves Technology - Protects Environment ... and Provides Employment - Now and in the Future
Vienna, AUSTRIA, 2000, September 25-28

COMPUTER-AIDED ANALYSIS OF MULTICOMPONENT SUBSTANCES USING A MINI-SPECTROPHOTOMETER

A. Miekina, R.Z. Morawski and N. Obarski
Warsaw University of Technology
Warsaw, Poland

Abstract: Spectroscopic methods have been for years widely used in analytical laboratories. However, their application in industrial and environmental practice has been up to now relatively limited because of the high costs of spectrometric instrumentation. This is only recently that the advances of micro- and optoelectronics have made feasible integrated implementation of some spectrometric techniques and the design of low-cost spectrometers for industrial applications. The integration implies a significant reduction of instruments precision – mainly due to miniaturisation. This loss, however, may be partially compensated for by digital signal processing of raw spectrometric data. An algorithmic basis for a low-cost computer-assisted spectrometric system – that can be effectively used for qualitative and quantitative analyses of multicomponent chemical substances – is proposed in this paper.

Keywords: spectroscopy, chemometrics, spectrogram interpretation, chemical analysis

1. INTRODUCTION

Spectroscopy is an analytical technique concerned with measurement characterisation of interactions of radiant energy with matter, including the instruments designed for this purpose, called *spectrometers*, and corresponding means of the interpretation of the interaction both at the fundamental level and for practical analysis. The distribution of radiant energy, absorbed or emitted by a sample of a substance under study (an analyte), is called its *spectrum*. The interpretation of spectra provides fundamental information at atomic and molecular energy levels; at the practical level, comparisons of spectra provide a basis for the determination of qualitative chemical composition and chemical structure, and for quantitative chemical analysis [1].

Various spectroscopic methods are currently used in analytical practice; however, their use in industrial laboratories, except pharmaceutical industry, has been up to now relatively limited because of the high costs of spectrometric instrumentation. This is only recently that the advances of micro- and optoelectronics have made feasible integrated implementation of some spectrometric techniques, and – consequently – their industrial applications, *e.g*. [2 - 7]. The integration implies a significant reduction of costs of corresponding instrumentation, but at the same time a loss of precision and accuracy mainly due to miniaturisation – *cf.* [8 - 10]. This loss, however, may be partially compensated for by digital signal processing of raw spectrometric data. In [11], a set of algorithms, dedicated to low-cost low-resolution integrated spectrometers measuring spectra composed of clearly-cut peaks, was proposed. In this paper, an alternative solution dedicated to a computer-assisted spectrometric system, based on the mini-spectrophotometer *SpectraMatch GT* (manufactured by *CVI Laser Corporation*), is presented.

2. NOTATION AND ASSUMPTIONS

The following notation is used hereinafter in this paper:

l – wavelength; $l \in [l_{\min}, l_{\max}]$;

N – the number of data acquired by the spectrometer;

Δl – the step of wavelength discretisation; $\Delta l = (l_{\max} - l_{\min})/(N-1)$;

l_n – the *n*-th discrete value of wavelength; $l_n = l_{\min} + (n-1)\Delta l$ for $n = 1,...,N$;

$x^{\mathrm{Tr}}(l)$ – the transmittance spectrum of the analyte;

$x^{\mathrm{Ab}}(l)$ – the absorbance spectrum of the analyte; $x^{\mathrm{Ab}}(l) = -\log_{10}\left[x^{\mathrm{Tr}}(l)\right]$;

$\mathbf{c}$ – the vector of concentrations to be determined (measured); $\mathbf{c} = [c_1 \ldots c_J]^T$;

$\hat{\mathbf{c}}$ – an estimate of $\mathbf{c}$.

The algorithms for spectrometric data interpretation, described in this paper, are based on the following assumptions:

- the absorbance spectrum of a multicomponent substance equals a linear combination of the absorbance spectra of all its components [12]:
$$x^{\mathrm{Ab}}(l) = c_1 x_1^{\mathrm{Ab}}(l) + \ldots + c_J x_J^{\mathrm{Ab}}(l) \tag{1}$$
where $x_1^{\mathrm{Ab}}(l), \ldots, x_J^{\mathrm{Ab}}(l)$ are normalised absorbance spectra of the components, and $c_1, \ldots, c_J$ are the concentrations of those components;
- the spectrometric data $\left\{\tilde{y}_n^{\mathrm{Tr}} \mid n = 1, \ldots, N\right\}$ may be adequately modelled with the convolution-type equation:
$$\left\{\hat{y}_n^{\mathrm{Tr}}\right\} = \left\{\hat{g}(l) * x^{\mathrm{Tr}}(l)\Big|_{l=l_n} \mid n = 1, \ldots, N\right\} \tag{2}$$
where $\hat{g}(l)$ is an estimate of the apparatus function, determined during calibration of the spectrometer;
- the analyte is composed of $J - \Delta J$ ($\Delta J = 0, 1, \ldots$) components out of J components which may appear in a given application, and whose exact spectra are stored in a reference data library (RD).

3. PROCEDURE FOR INTERPRETATION OF SPECTROMETRIC DATA

The estimation of the concentrations of the components of the analyte, directly from the acquired spectrometric data, is in many practically important cases problematic due to instrumental imperfections of the spectrometer, and to some natural phenomena in the analyte. The imperfections of the spectrometer and some quantum phenomena in the analyte produce blurring in the data representative of the measured spectrum. Both effects may be eliminated or reduced by means of the algorithms of deconvolution [13 - 14]. As a rule, the deconvolution algorithms are designed and assessed using the criteria of the quality of deconvolution, which are not specific of spectrometry; *e.g.* the root-mean-square errors of approximation. Consequently, the estimates of the concentrations, determined on the basis of the results of deconvolution, may turn out to be very poor. On the other hand, the curve-fitting algorithms, used for estimation of concentrations, may be very inefficient if not provided with a good initial guess of the sought-for estimates [15]. Both the algorithms for spectrum reconstruction and the algorithms for estimation of concentrations require some information on the mathematical model of the spectrometric data; this information is acquired during *calibration* of the spectrometer.

Numerical algorithms potentially applicable for calibration of spectrometers, reconstruction of spectra and estimation of concentrations are available in many software libraries [16 - 17], *e.g.* in some MATLAB Toolboxes [18 - 19], including specialised libraries dedicated to processing of spectrometric data, *e.g.* [20]. None of them, however, offers full support for the methodology of spectrometric data interpretation, mainly due to the fact that there is no closed procedures of such interpretation. The demand for such procedures in the domain of spectroscopy is generated by numerous and widespreading applications of spectroscopic methods and techniques in many important areas of science, technology and economy, in particular – in chemical, biochemical and pharmaceutical industries, as well as in environmental monitoring. The procedure described in [11], responding to this demand, is applicable provided the spectra of the components are composed of clearly-cut peaks; it fails if this assumption is not satisfied. A procedure for estimation of concentrations, proposed in this paper (called hereinafter *selection-based procedure*), is free of such limitations. It is based on the least-squares curve fitting, performed in the domain of absorbance, applied to the spectrometric data corrected by means of a deconvolution algorithm. The ill-conditioning effects [21] are overcome by introducing a selection mechanism that involves two actions:

- repetitive curve fitting, under various assumptions concerning the absence of the components from RD in the analyte, and selection of a subset of estimates corresponding to the best fits;
- choosing the estimate corresponding to the maximum number of the absent components.

A more formal description of the selection-based procedure, presented below, contains the symbol J_s that denotes a subset of integers belonging to the set $\{1, \ldots, J\}$ such that the binary representation of the index s is $s_J \ldots s_1$, where:

$$s_j = \begin{cases} 1 & \text{if } j \in \mathrm{J}_s \\ 0 & \text{if } j \notin \mathrm{J}_s \end{cases} \tag{3}$$

The proposed procedure comprises the following steps:

- Compute an estimate of the spectrum using the Tikhonov-regularisation-based algorithm of deconvolution described in [22]:
$$\hat{x}^{\mathrm{Ab}}(l) = \mathrm{TIKH}\left[\left\{\tilde{y}_n^{\mathrm{Tr}}\right\}, \hat{g}(l), \hat{s}_h^2\right] \tag{4}$$
where $\hat{s}_h^2$ is an estimate of the variance s_h^2 of errors in the spectrometric data $\left\{\tilde{y}_n^{\mathrm{Tr}}\right\}$.
- For $s = 2^J - 1, 2^J - 2, 2^J - 3, \ldots$, compute the estimates of concentrations according to the formula:
$$\hat{\mathbf{c}}_s = \arg_{\mathbf{c}} \inf\left\{Q_s(\mathbf{c}) \,\middle|\, \mathbf{c} \in \mathsf{C}\right\} \tag{5}$$
where:
$$Q_s(\mathbf{c}) = \left\| \hat{x}^{\mathrm{Ab}}(l) - \sum_{j \in \mathsf{J}_s} c_j x_j^{\mathrm{Ab}}(l) \right\|_2 \tag{6}$$
- Compute:
$$s_{\min} = \arg_s \inf\left\{Q_s(\hat{\mathbf{c}}_s) \,\middle|\, s = 2^{J-1}, 2^{J-2}, \ldots\right\} \tag{7}$$
- Find a subset $\mathsf{S}_{\min}$ of the values of s that indicate the estimates $\hat{\mathbf{c}}_s$ producing the smallest values of the objective function $Q_s(\hat{\mathbf{c}}_s)$, and such that:
$$\left|Q_s(\hat{\mathbf{c}}_s) - Q_{s_{\min}}(\hat{\mathbf{c}}_{s_{\min}})\right| \le \Delta q \cdot Q_{s_{\min}}(\hat{\mathbf{c}}_{s_{\min}}) \quad \text{for} \quad s \in \mathsf{S}_{\min} \tag{8}$$
where Δq is tolerance margin that should be adjusted to the level of errors in the data $\left\{\tilde{y}_n^{\mathrm{Tr}}\right\}$.
- Choose $\hat{s} \in \mathsf{S}_{\min}$ whose binary representation contains the smallest number of the digits 1.
- Set $\hat{\mathbf{c}} = \hat{\mathbf{c}}_{\hat{s}}$.

The above-described procedure is of heuristic nature, and *does not guarantee* the correct solution, but – according to the computational experience – it is capable to provide such a solution with high probability.

4. METHODOLOGY AND RESULTS OF COMPUTATION

The applicability of the proposed procedure for interpretation of the data from a mini-spectrophotometer *SpectraMatch GT*, whose optical resolution is 5 nm, was studied in the following way:

- A library RD of exact spectra $x_1^{\mathrm{Ab}}(l)$, ..., $x_8^{\mathrm{Ab}}(l)$ of 8 real substances containingTh, U, Zr, Hf, Fe, La, Ho or Ce was compiled – *cf.* Fig. 1.

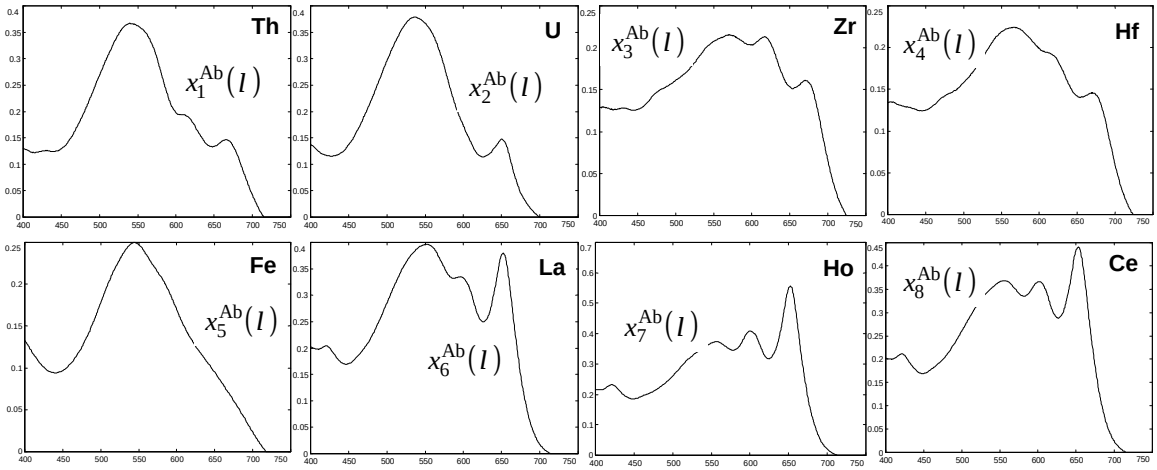

Figure 1. The spectra $x_1^{\mathrm{Ab}}(l)$, ..., $x_8^{\mathrm{Ab}}(l)$ of 8 real substances used for experimentation.

- An absorbance spectrum $x^{\mathrm{Ab}}(l)$ of a mixture of 5 substances containing U, Zr, Hf, Fe or La, mixed in a known proportions ($\dot{c}_2 = 1.0\,\%$, $\dot{c}_3 = 1.0\,\%$, $\dot{c}_4 = 1.0\,\%$, $\dot{c}_5 = 1.0\,\%$ $\dot{c}_6 = 1.0\,\%$) was synthesised according to Eq. (1), transformed into the domain of transmittance, convolved with the

estimate of the apparatus function $\hat{g}(l)$ of the mini-spectrophotometer *SpectraMatch GT* (Fig. 2), and disturbed additively according to the formula:

$$\left\{\tilde{y}_n^{\mathrm{Tr}}\right\}=\left\{\hat{y}_n^{\mathrm{Tr}}+h_n \,\middle|\, n=1,...,N\right\} \tag{9}$$

where $\{h_n\}$ is a white sequence of pseudorandom numbers distributed as $\mathrm{N}\left(0; s_h^2\right)$ – *cf.* Fig. 3.

- The data were processed using the procedure described in the previous section for $s_h^2 = 1\cdot10^{-2}, 5\cdot10^{-3}, 1\cdot10^{-3}$; each experiment was repeated $R=20$ times, and the resulting estimates of concentrations were averaged.

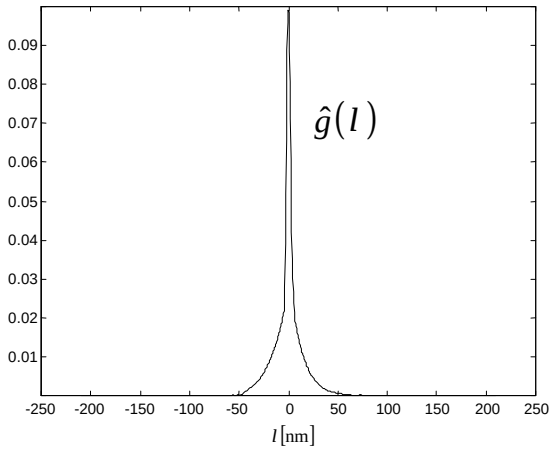

Figure 2. The apparatus function $\hat{g}(l)$ of the mini-spectrophotometer *SpectraMatch GT*.

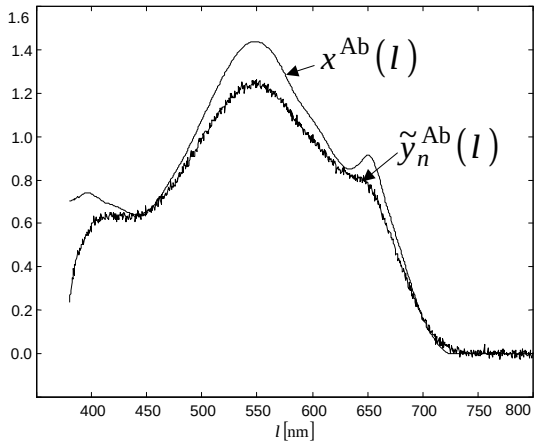

Figure 3. The spectrum of the mixture $x^{\mathrm{Ab}}(l)$ and the data representative of this spectrum $\left\{\tilde{y}_n^{\mathrm{Ab}}\right\}$.

The normalised mean-square error of the estimates of concentrations, was used for characterisation of the measurement uncertainty:

$$\partial_2 = \sqrt{\sum_{j=1}^{8}\left(\hat{c}_j - \dot{c}_j\right)^2 \Big/ \sum_{j=1}^{8}\dot{c}_j^2} \tag{10}$$

The results obtained for various combinations of concentrations were compared with the corresponding result obtained by means of a commonly used method based on direct fitting of the linear combination of the data $\left\{\hat{y}_{j,n}^{\mathrm{Tr}}\right\}$, simulated for all the components in the RD library ($j=1,...,8$), to the raw spectrometric data $\left\{\tilde{y}_n^{\mathrm{Tr}}\right\}$ representative of the analysed mixture.

The intermediate results of computation, obtained for $s_h^2 = 5\cdot10^{-3}$, are shown in Table 1. The grey fields correspond to $s \in \mathrm{S}_{\min}$ defined for $\Delta q = 1\%$. Since the binary representation of $s = 62\,|_{10}$, *i.e.* $00111110\,|_2$, contains the smallest number of the digits 1 among the binary representations of $s \in \mathrm{S}_{\min}$, the final result of estimation is $\hat{\mathbf{c}}_{62}$.The final results of study are summarised in Table 2.

5. CONCLUSION

The results of numerical experiments described in this paper have demonstrated some essential advantages of the procedure for spectrometric data interpretation, proposed by the authors, in comparison to the currently used procedures for estimation of concentrations based on the least-squares curve fitting in the domain of raw spectrometric data. When applied to the data acquired by means of the low-resolution mini-spectrophotometer *SpectraMatch GT*, the proposed selection-based procedure provides much more reliable estimates of concentrations: they are subject to 2-20 times less mean-square errors. If compared to sophisticated statistical methods of estimation, such as Bayesian procedure developed in [23], the selection-based procedure requires much less statistical *a priori* information on the concentrations, and less computing time. It seems to be, therefore, an attractive software tool for computer-aided applications of low-resolution mini-spectrometers in industrial or environmental monitoring.

Table 1. The intermediate results of computation, obtained for $s_h^2 = 5 \cdot 10^{-3}$ ($J' = J - \Delta J$ is the number of the digits 1 in the binary representation of s, *i.e.* the number of components present in the mixture). The grey fields correspond to $s \in \mathsf{S}_{\min}$ for $\Delta q = 1\%$.

s	J'	$Q_s(\hat{\mathbf{c}}_s)$	∂_2	s	J'	$Q_s(\hat{\mathbf{c}}_s)$	∂_2	s	J'	$Q_s(\hat{\mathbf{c}}_s)$	∂_2	s	J'	$Q_s(\hat{\mathbf{c}}_s)$	∂_2	s	J'	$Q_s(\hat{\mathbf{c}}_s)$	∂_2
255	8	0.36	0.59	221	6	0.63	0.76	182	5	0.38	0.58	127	7	0.37	0.52	87	5	0.40	0.54
254	7	0.36	0.50	220	5	0.88	1.42	181	5	0.59	0.56	126	6	0.37	0.39	86	4	0.41	0.55
253	7	0.59	0.72	219	6	0.37	0.73	180	4	0.72	1.11	125	6	0.59	0.66	85	4	0.63	0.63
252	6	0.72	1.07	218	5	0.38	0.67	179	5	0.84	0.87	124	5	0.72	1.09	83	4	0.84	0.93
251	7	0.37	0.78	217	5	0.64	0.65	178	4	0.92	1.24	123	6	0.38	0.71	79	5	0.48	0.92
250	6	0.37	0.73	216	4	0.89	1.42	177	4	0.85	0.88	122	5	0.38	0.69	78	4	0.49	1.11
249	6	0.61	0.63	215	6	0.39	0.64	175	6	0.43	0.91	121	5	0.61	0.52	77	4	0.88	0.91
248	5	0.75	1.01	214	5	0.40	0.57	174	5	0.44	0.94	120	4	0.75	1.01	75	4	0.48	0.90
247	7	0.38	0.72	213	5	0.63	0.72	173	5	0.75	0.75	119	6	0.38	0.67	71	4	0.61	0.63
246	6	0.38	0.67	212	4	0.88	1.51	172	4	2.31	1.19	118	5	0.38	0.58	63	6	0.37	0.41
245	6	0.59	0.66	211	5	0.84	0.87	171	5	0.44	0.92	117	5	0.59	0.56	62	5	0.37	0.03
244	5	0.72	1.09	210	4	0.92	1.24	170	4	0.44	0.95	116	4	0.72	1.11	61	5	0.59	0.56
243	6	0.84	0.89	209	4	0.84	0.83	169	4	0.75	0.68	115	5	0.84	0.95	60	4	0.72	1.11
242	5	0.92	1.20	207	6	0.45	0.95	167	5	0.53	0.71	114	4	1.01	1.54	59	5	0.39	0.73
241	5	0.84	0.87	206	5	0.46	0.99	166	4	0.55	0.85	113	4	0.84	0.93	58	4	0.39	0.65
240	4	0.99	1.45	205	5	0.88	0.93	165	4	0.80	0.69	111	6	0.43	0.91	57	4	0.61	0.30
239	7	0.43	0.92	204	4	3.06	2.30	163	4	1.13	0.90	110	5	0.44	0.94	55	5	0.38	0.58
238	6	0.44	0.95	203	5	0.45	0.94	159	6	0.37	0.50	109	5	0.75	0.75	54	4	0.38	0.41
237	6	0.75	0.80	202	4	0.46	0.99	158	5	0.37	0.31	108	4	2.31	1.19	53	4	0.59	0.39
236	5	2.31	1.15	201	4	0.88	0.91	157	5	0.70	0.69	107	5	0.44	0.92	51	4	0.97	0.84
235	6	0.44	0.93	199	5	0.59	0.74	156	4	0.88	1.48	106	4	0.44	0.95	47	5	0.43	0.89
234	5	0.44	0.96	198	4	0.61	0.92	155	5	0.38	0.68	105	4	0.75	0.68	46	4	0.44	0.92
233	5	0.75	0.75	197	4	0.93	0.97	154	4	0.38	0.57	103	5	0.53	0.71	45	4	0.75	0.68
232	4	2.31	1.19	195	4	1.13	0.90	153	4	0.71	0.48	102	4	0.55	0.85	43	4	0.44	0.90
231	6	0.53	0.77	191	7	0.37	0.50	151	5	0.40	0.58	101	4	0.80	0.69	39	4	0.53	0.62
230	5	0.55	0.88	190	6	0.37	0.35	150	4	0.40	0.41	99	4	1.16	0.92	31	5	1.04	0.90
229	5	0.80	0.77	189	6	0.59	0.66	149	4	0.70	0.59	95	6	0.37	0.45	30	4	1.04	0.87
228	4	2.65	1.08	188	5	0.72	1.09	147	4	0.84	0.83	94	5	0.38	0.38	29	4	1.37	0.88
227	5	1.13	0.92	187	6	0.38	0.74	143	5	0.45	0.94	93	5	0.63	0.70	27	4	1.05	1.65
226	4	1.65	0.99	186	5	0.38	0.68	142	4	0.46	0.99	92	4	0.89	1.61	23	4	1.06	1.24
225	4	1.14	0.87	185	5	0.61	0.52	141	4	0.92	0.83	91	5	0.38	0.64	15	4	1.04	1.00
223	7	0.37	0.58	184	4	0.75	1.01	139	4	0.45	0.93	90	4	0.39	0.66	…			
222	6	0.37	0.48	183	6	0.38	0.67	135	4	0.59	0.66	89	4	0.64	0.52	…			

Table 2. The summary of the final results of study, obtained for the selection-based procedure for estimation of concentrations (PROPOSED PROCEDURE) and for the least-squares curve fitting in the domain of raw spectrometric data (REFERENCE PROCEDURE); all estimates in %.

s_h^2	PROCEDURE	$\hat{c}_1$	$\hat{c}_2$	$\hat{c}_3$	$\hat{c}_4$	$\hat{c}_5$	$\hat{c}_6$	$\hat{c}_7$	$\hat{c}_8$	∂_2
$1 \cdot 10^{-2}$	PROPOSED	0.00	1.08	1.42	0.53	0.97	1.02	0.00	0.00	0.22
	REFERENCE	0.00	1.26	1.72	0.47	0.83	0.00	0.51	0.00	0.52
$5 \cdot 10^{-3}$	PROPOSED	0.00	1.00	0.98	1.04	0.93	1.01	0.00	0.00	0.03
	REFERENCE	0.00	1.24	1.92	0.24	0.90	0.00	0.50	0.00	0.59
$1 \cdot 10^{-3}$	PROPOSED	0.00	1.01	1.06	0.95	0.97	1.00	0.00	0.00	0.03
	REFERENCE	0.00	1.23	2.11	0.00	0.98	0.00	0.50	0.00	0.66

ACKNOWLEDGEMENT

This research work was supported by the State Committee for Scientific Research, Poland (grants # 8 T10C 025 11 and # 8 T10C 040 17)

REFERENCES

[1] Parker S. (Ed.): *McGraw-Hill Encyclopedia of Chemistry,* McGraw-Hill, 1983.

[2] Niemelä P., Hietala E., Tornberg J.: "Application of FTIR Spectrometry to the On-line Measurement of Organic Substances in Papermaking Process Water", *Proc. XIV IMEKO World Congress (Tampere, Finland, June 1-6, 1997)*, CD-ROM IWC97.HTM, IMEKO & Finish Society of Automation, 1997.
[3] Grant B.: "Photonics Pays Dividends in Process Control - Manufacturers Turn to Spectroscopy to Cut Losses in Large-volume Applications", *Photonics Spectra*, March 1998, pp. 130-132.
[4] Mendosa R. A.: "Raman Spectrometers 'Fingerprint' Gemstones", *Photonics Spectra*, March 1997, p. 136.
[5] Pelletier M. J., Kowalchyk W. K.: "Raman Spectroscopy Keeps Industry under Control", *Photonics Spectra*, October 1997, pp. 112-118.
[6] Tatterson K. G.: "Raman Spectroscopy Could Simplify Pollution Monitoring", *Photonics Spectra*, October 1997, pp. 48-49.
[7] Rauf M., Lori W., Phelan V.: "Testing the Purity of Olive Oil", *Int. Laboratory News*, April 1998, p. 21B.
[8] *MMS1 - Monolithic Miniature Spectrometer*, Product Information, Carl Zeiss OEM - Sensorik/Prozeßanalytik, 1997
[9] *SpectraMatch - User's Manual*, CVI Laser Corp., 1996.
[10] *Spectronic® 20 Genesys™ Spectrophotometer*, Technical Data, Spectronic Instruments, 1997.
[11] Miekina A., Morawski R. Z.: "An Alternative Approach to Interpretation of Spectrometric Data", *Proc. Int. Conf. MEASUREMENT '99 (Smolenice, Slovakia, April 26-29, 1999)*, str. 185-188.
[12] Robinson J. W.: *Undergraduate Instrumental Analysis*, Marcel Dekker, 1995.
[13] Jansson P. A. (Ed.): *Deconvolution of Images and Spectra,* Academic Press, 1997.
[14] Morawski R. Z., Szczecinski L., Barwicz A.: "Deconvolution Algorithms for Instrumental Applications - A Comparative Study", *J. Chemometrics,* 1995, Vol. 9, pp. 3-20.
[15] Gilbert A.: "The Resolution of Bands in Spectroscopy" In: *Analytical Applications of Spectroscopy II* (ed. by Davies A. M. C., and Creaser C. S.), Royal Soc. Chem., Cambridge (UK), 1991, pp. 275-285.
[16] Brown S. D., Bear Jr. R. S., Blank T. B.: "Chemometrics", *Anal. Chem.*, Vol. 64, No. 12, 1992, pp. 22R-49R,
[17] Brown S. D., Sum S. T., Despagne F.: "Chemometrics", *Anal. Chem*. Vol. 68, No. 12, 1995, pp. 21R-61R.
[18] Kramer R.: *Chemometrics Tolbox for Use with MATLAB - User's Guide*, MathWorks Inc., 1993
[19] Krauss T. P., Shure L., Little J. N.: *Signal Processing Tolbox for Use with MATLAB - User's Guide*, MathWorks Inc., 1994
[20] *Grams/32 - User's Guide,* Galctic Industries Corp. 1996.
[21] Morawski R. Z.: "Unified Approach to Measurand Reconstruction". *IEEE Trans. Instrum. & Meas.,* Vol. 43, No 2, April 1994, pp. 226-231.
[22] Morawski R. Z., Ben Slima M., Milewski M., Barwicz A.: "Application of a Digital Signal Processor for Correction of Spectrophotometric Measurements", *IEEE Trans. Instrum. & Meas*., June 1993, Vol. 43, No. 3, pp. 778÷782.
[23] Niedzinski C., Morawski R. Z.: "Bayesian Approach to Spectrophotometric Analysis of Multicomponent Substances", *IEEE Trans. Instrum. & Meas.*, Vol. 49, No. 2, April 2000 (in print).

AUTHOR: Andrzej MIEKINA and Roman Z. MORAWSKI, Warsaw University of Technology, Faculty of Electronics and Information Technology, Institute of Radioelectronics, ul. Nowowiejska 15/19, 00-665 Warsaw, Poland
Phone: (+48 22) 660-7721, Fax: (+48 22) 825-5248, E-mail: R.Morawski@ire.pw.edu.pl and
Norbert OBARSKI, Warsaw University of Technology, Faculty of Chemistry, ul. Noakowskiego 3 - 00-664 Warsaw, Poland