Methodology of Spectral Diagnostics Automation Using Micro Flow Systems

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Abstract - **This paper presents information about the methodology of spectral diagnostics automation using microflow Lab-Chip device. This methodology, provides spectroscopic analysis in micro flow systems automatically, without human interaction.**

Keywords – **spectrum, spectroscopy analysis, FFT.**

I. INTRODUCTION

Microflow system - is a system, which is based on small Lab-chip device that include microchannel mixers, pumps, etc. and allows to conduct on-chip biochemical diagnostics, usually based on spectroscopic analysis.

This type of microflow systems usually have custom-developed software for spectral analysis, which allows to obtain specific data changes in the intensity of radiation on the wavelength. This is the first step in spectroscopic diagnosis, which is the base for future spectroscopic analysis.

Fig.1 Microflow chip with spectrometer and light source

The list of advantages of such microflow chip includes:

- low consumption of fluids (less reagent costs, less waste and smaller amounts of sample for diagnosis);
- analysis and fast response time through short diffusion distance;
- parallelism;
- better management process through faster response system (eg, thermal control for exothermic chemical reactions);
- compact system;
- chemical, radioactive or biological studies are conducted with a high level of security;
- high reproducibility of data;

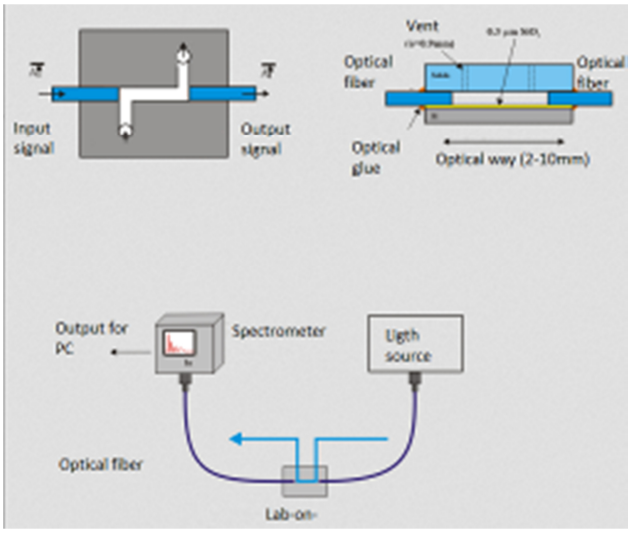

Fig.2. Structure of microflow chip

Microflow chips provides qualitative and quantitative composition of fluids, but their restrictions imposed wavelength light source and spectroscopy.

II. AUTOMATION SPECTROSCOPIC DIAGNOSIS

The data in the spectral analysis contain noise sources, which are all components analysis. Fig. 1 shows a spectrum of 500 mg $FeSO_4$ in diagnostin lab-chip device.

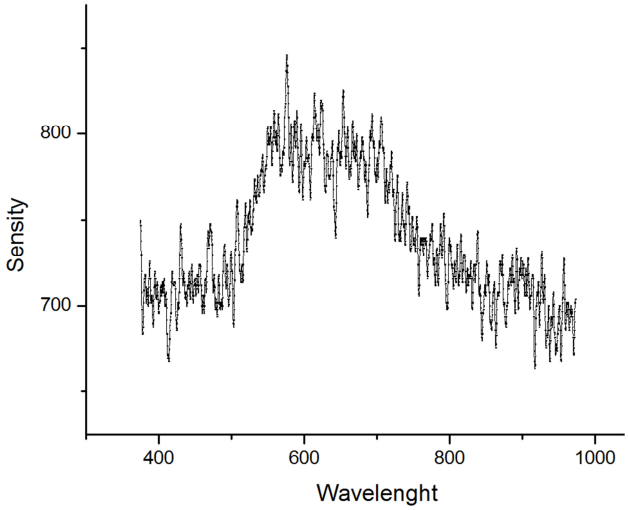

Fig.3 Spectrum of $FeSO_4$

The solution of this problem can be obtained in two ways: by hardware or software filtering. In already designed and existed lab- chip, the hardware filtering may not be available, thus we decided to develop a software variant of spectra filtering method.

Main software filtering methods are based on the arithmetic mean of neighboring pixels and filtering using Fourier and Savitzky–Golay transformations [1]. The best result in noise suppressed saved width and peak value is filtering using Fourier transformation [2].

In this case, filtering based on the Fourier transformation includes new feature, which describes coefficients (amplitude and phase) by the decomposition of the input functions on the basic elements - harmonic vibrations with different frequencies.

Thus, filtering based on Fourier transformation involves the use of direct conversion, filter and reverse transformation. Filter formula is written below:

$$F_{cutoff} = \frac{1}{n\Delta t}, \quad (1)$$

where - number of points, which indicates the user and - the distance between two adjacent data points. The function is used for cutting high frequency components, which is a parabola with a value of 1 at zero frequency and 0 at higher cutoff frequency.

The experiments with the definition of the optimal window width permitted to establish the optimal number of points - 35 points (Figure 2)

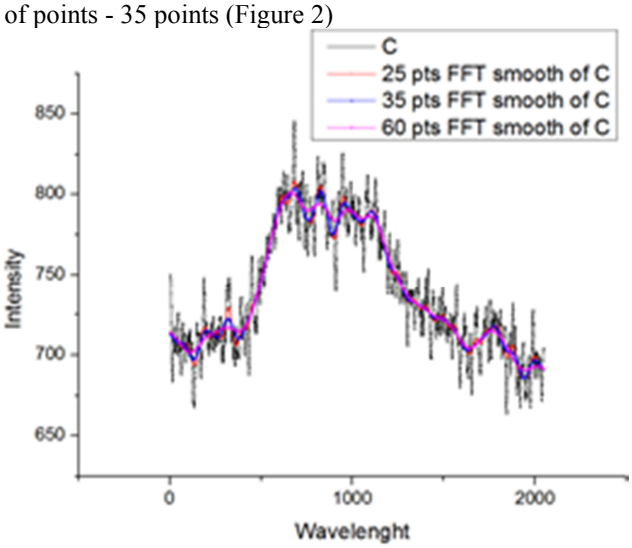

Fig.4 Filter $FeSO_4$ spectrum using Fourier transform

Another component of the data-processing is to bring data into a single representation for the classification problem. For analyzing, the data of spectroscopic diagnostic neural network was selected. The neural network has a certain number of input neurons for different number of neurons. Thus, it is necessary to model a new neural network, which required to conduct many experiments with one fluid for different types of spectrometers. Therefore, it is appropriate to bring the use of data in a single view.

As mentioned above, the next step is to bring spectrum after filtration to single volume settings. There are two cases: the increase and decrease data. To reduce the amount of data, we have developed an algorithm that determines the deviation neighboring points. From the set of values one excludes value with minimum deviation. The number of such exceptions is equal to the difference of volume data. To increase the amount necessary to reverse operation - defining deviations neighboring points, choose the required number of minimum deviation and then duplicate values.

Thus, we have spectral analysis data that used for classification. Using neural network output, we get the probability ratio of liquid to a class of liquids.

The process accompanied by a large number of data and information, as it is appropriate database design, needs to develop tools for its specific processing.

The last stage is the output of a diagnosis. Attainment of the objectives at each stage of diagnosis, will automate the process in spectroscopic diagnostic microflow systems. Fig. 3 shows the general scheme of automation of methods of spectral diagnostics.

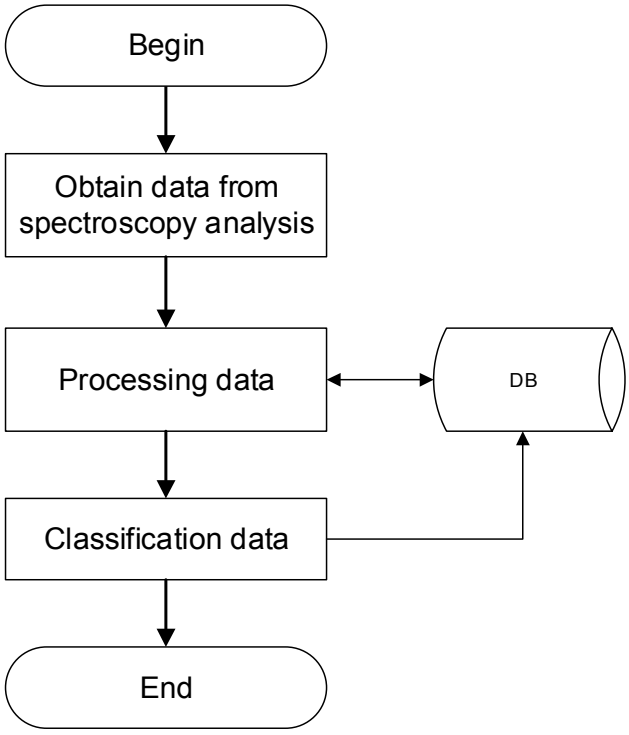

Figure 5. General scheme of spectral diagnostics automation techniques

Holding spectroscopic analysis using portable diagnostic systems requires a sequence of steps:

- If the analysis is to improve data for the study, the analysis carried out with solutions of lower salt concentration to more. This will reduce the impact analysis prior to the next.
- Before starting, work necessary to calibrate the instrument.
- Before the spectral analysis of each channel, solution rinsed with distilled water. This procedure is necessary to clean up remnants of previous solutions, thus reducing the impact on the current preliminary solutions. Number of repetitions of this step depends on the concentration and viscosity of the solution. An indication of the effective channel washed proximity-received spectrum to the spectrum of distilled water. You can also use designed system if the system

detects that this solution is distilled water, and then you can do the following experiment.

- At The analysis necessary to feed was completely filled with a solution.
- Following the analysis for this solution must repeat the preceding paragraph of this several times and then calculate the average. This will reduce the influence of random noise.
- After a series of experiments it is necessary to re-channel wash with distilled water and dry it. This step is necessary to prevent contamination of the canal.

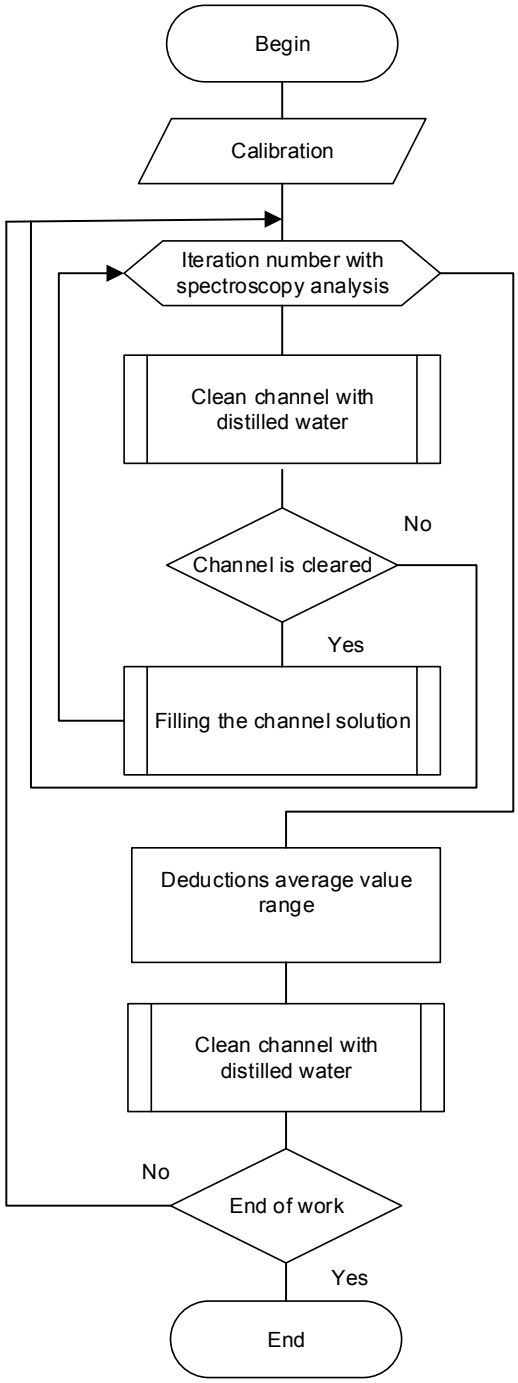

Figure 6. Methodology of spectral analysis.

III. CONCLUSION

The methods of spectroscopic diagnostic automation using microflow system have the following advantages, namely:

- Provide software filtering of the noise spectrum, which may replace the hardware implementation;
- Provide data normalization, which can be used with different types of spectrometers;
- Spectroscopic analysis can be performed autonomously, without user intervention.

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