Modeling of the optical schemes of small-sized spectrometers

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Modeling of the optical schemes of small-sized spectrometers

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Abstract. The main task of this work was the selection of the optimal geometry of the optical system for practical application in a small portable device for water resources analysis. Using the COMSOL Multiphysics software the Czerny–Turner and Paschen–Runge optical schemes were modeled, which differ in the number of used elements and spectral resolution. The obtained simulation results allow concluding that the most suitable scheme for a portable device is the Paschen–Runge optical scheme.

1. Introduction
Fields of application of spectrometric equipment are very extensive today: it is used for the analysis of metals and alloys, measurement of thin films parameters, study of the radiation sources. The new field is its use for carrying out ecological monitoring for the purpose of structure research of aqueous solutions of various compositions [1]. Spectrometer consists of several parts, the most important of which is the optical scheme, the correct selection of which affects the obtained spectral data [2]. As the selection criteria of the appropriate optical scheme can be used the following values: optical resolution, dimensions, number of pixels and optical elements involved.

The main optical schemes used in the small-sized optical spectrometers are the Czerny–Turner and Paschen–Runge schemes, which differ in the number of used elements and spectral resolution [3].

2. Results and discussion
Modeling of optical schemes was performed in COMSOL Multiphysics software to determine the passage of light rays in the system, the correspondence of CCD pixels to the incident rays of each wavelength and spectral resolution of the system. The main task was the selection of the optimal geometry of the optical system for application in a small portable device for water resources analysis.

A number of equations were used for objective modeling and evaluation [4]. First, the numerical aperture $NA$, a parameter characterizing the efficiency of light rays entering into the optical fiber, was determined. This value was calculated using the following equation:

$$NA = n \cdot \sin(\Theta),$$

where $\Theta$ – angle of entry of light into the system; $n$ – refractive index of the propagation medium.

The ray trajectories obtained during the simulation were then used to calculate the resolution of the spectrometer. The number of pixels $P_{num}$ involved is calculated using the next equation:

$$P_{num} = \text{ceil} \left( \frac{N}{2} \cdot \frac{q_s - Q_{\alpha}}{w_p \cdot \cos(\Theta_\alpha)} \right),$$
where \( \text{ceil()} \) – mathematical function that returns the lowest integer number greater than or equal to the value in the brackets; \( N \) – number of pixels of the CCD matrix; \( q_x \) – \( x \)-coordinate of the particles hitting the detector; \( Q_{dx} \) – \( x \)-coordinate of the center of the CCD matrix; \( w_p \) – pixel width; \( \Theta_d \) – angle of inclination of the CCD matrix.

The spectral resolution of the element \( \delta \lambda \) was determined using the expression:

\[
\delta \lambda \approx \frac{\Delta \lambda}{N w_p} \frac{w_i}{N w_p},
\]

where \( \Delta \lambda \) – spectral region of the detector; \( w_i \) – slit width on the CCD matrix.

Modeling was performed in 2D mode, which was a sufficient condition for finding the required parameters of the system. It should also be mentioned that only the rays of the first diffraction order were considered. First modeled optical scheme was a Czerny–Turner scheme of “X” configuration.

There are several different variations of this system that vary in the location of rays, but they are rarely used in the small-sized spectrometers. The configuration of the Czerny–Turner scheme consists of four optical elements: two mirrors, one of which plays the role of a collimator, and the second – a focusing mirror, a flat diffraction grating and a CCD matrix. Optical design of the Czerny–Turner scheme of “X” configuration is shown in figure 1.

![Figure 1. Optical design of the Czerny–Turner scheme of “X” configuration.](image)

The obvious advantages of this scheme include the use of simple optical elements, which are also in an acceptable price range. As the disadvantages should be considered that in some cases, there is a double diffraction, increasing the level of scattered radiation; and also the asymmetry of the entrance slit and the complexity of the alignment due to the presence of a large number of elements.

Optimal angles of inclination of mirrors, detector and grating were calculated for this configuration. An already calculated system with a simplified ray diagram is shown in figure 2.

The separation of the light wave on the CCD matrix is shown in figure 3. The wavelength is specified by a color expression. The rays reflected from the diffraction grating propagate in all directions and fall to different places of the CCD matrix, allowing to reveal the spectral resolution and the optimal arrangement of the CCD matrix relative to the mirrors.

Figure 4 shows the calibration by a wavelength. This parameter is important because it affects the accuracy of determining the spectrum of a source. If the calibration is incorrect, it is impossible to talk about the correctness of the received spectral data.
Figure 2. Modeled optical scheme.

Figure 3. Propagation of light rays in the Czerny–Turner scheme.

Figure 4. Calibration of the wavelength.

Figure 5. Dependence of the spectral resolution on the wavelength.
Figure 5 shows the dependence of spectral resolution on the wavelength. From the presented trajectory of the wave propagation and the graph it can be seen that the spectral resolution decreases with increasing wavelength.

Optimal results were obtained with the following parameters of the optical system: \( \theta_g = 28.76^\circ; \theta_c = 11^\circ; \theta_i = 77^\circ; \theta_d = 6.76^\circ \). Focusing and collimating mirrors radiuses are 130 and 100 mm. Calculations were carried out for a CCD matrix with 3648 pixels with 8 \( \mu \)m widths.

Further, modeling of the Paschen–Runge optical scheme was carried out. The feature of this configuration is that all optical elements are located on the Rowland circle. Also concave diffraction grating, performing simultaneously the functions of collimator and focusing mirrors, is used, which allows to get rid of the two mirrors, significantly simplifying the scheme. Also, the minimum number of mirrors increases the sensitivity of the device in the short-wave region of the spectrum. The optical scheme is shown in figure 6.

![Optical design of the Paschen–Runge scheme.](image)

The advantages of this scheme include a smaller number of optical elements than in the Czerny–Turner scheme, as well as the presence of constant dispersion in the spectral range. The disadvantage is the presence of the Rowland circle, which leads to the impossibility of ensuring perfect focus. A simplified optical diagram showing the angles used is presented in figure 7.

![Modeled optical scheme.](image)

The separation of the wave on the CCD matrix is shown in figure 8. The obtained ray decomposition to the spectrum one more time proves the possibility of using a concave diffraction grating as an available alternative to the system “collimator–diffraction grating–focusing mirror”.

Figure 9 presents the calibration of the wavelength for the Paschen–Runge optical scheme. It should be noted that in this case more pixels are involved and a larger wavelength range is obtained, which favorably affects the reception of spectrums.
Figure 8. Distribution of rays in the Paschen–Runge scheme.

Figure 10 shows the dependence of spectral resolution on the wavelength. As can be seen this spectral resolution is significantly different from the Czerny–Turner scheme, since it has a pronounced maximum, indicating that the CCD matrix is placed on the Rowland circle only by its ends, the rest is inside the circle. The value of the spectral resolution of this scheme significantly exceeds the Czerny–Turner scheme.

Optimal results were obtained with the following parameters of the optical system: $\theta_g = 2^\circ$; $\theta_d = 136.36^\circ$. Concave grating radius is 125 mm. Calculations were carried out for a CCD matrix with 3648 pixels with 8 μm widths.

Using the graphs shown above the question of choosing the preferred optical scheme can be discussed. It should be noted that the main selection criterion is the number of optical elements. The Czerny–Turner scheme contains 4 elements: two concave mirrors, a flat diffraction grating and a CCD matrix. The Paschen–Runge contains only two: a concave diffraction grating and a CCD matrix. From this it can be concluded that it is preferable to use the Paschen–Runge scheme for small-sized devices for environmental monitoring of aqueous solutions. Of course, this reduces the cost of the device, but there is a problem in its adjustment. However, through a simple search of parameters in the analysis environment COMSOL Multiphysics it is possible to obtain an optimal distance, the coordinates of the elements and angles.

By analyzing the presented calculation it can be judged that for the realization of optical scheme the following dimensions will be required: system length should be $15 \pm 1$ cm and width – 8 cm. These system parameters are optimal and sufficient for implementing in a portable device.

The next parameter for comparison is the parameter of the wavelength calibration, i. e. the numbers of pixels corresponding to the different wavelengths of the incident light. From the comparison of figures 4 and 9 it can be concluded that the calibration is identical for both cases. The obtained distribution of rays confirms the minimal difficulties in the calibration of a chosen optical system.
An important parameter of the used optical schemes is the spectral resolution or the ability to distinguish in the resulting spectrum lines corresponding to two close frequencies. From figures 5 and 10 it can be seen that the best spectral resolution has the Paschen–Runge optical scheme.

3. Conclusion
The result of this work is the modeling of two optical schemes, which are currently most often used in small-sized spectrometers. The obtained simulation results allow concluding that the most suitable scheme for a portable device is the Paschen–Runge optical scheme, since only a concave diffraction grating and CCD matrix are required for optimal operation, and also it has a higher spectral resolution compared to the Czerny–Turner optical scheme.

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