Dependency Model for Visible Aquaphotomics

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Introduction: The main idea of this research is the extension of the aquaphotomics method to the visible range of the spectrum. The motivation is that devices for measuring spectra in the visible range are cheaper and more common.

Already known as the fact that visible changes occur when altering the spectral pattern of water. The spectrum of light reflected from the water surface is different from the spectrum of incident light. Analysis of the concentration of microparticles, chemical elements and detection of bacteria in water by the changes in the molecular water system represented in the form as a water spectral pattern was success in NIR range [1]. And it is obvious extension is in visible range. Because, each element or compound has a specific "fingerprint" pattern in the absorption of electromagnetic radiation. Even in the visible spectrum, it is presented a fingerprinting section. Thus, the absorption in the visible spectrum is giving unique information about the presented elements or compounds in water.

The results presented in this work prove the existence of a correlation between some parameters of water and its spectral characteristics.

Experiments and Methods: The experiment for data collection consisted of two types of measurements: experimental and control. The first was to measure the spectral characteristics of water samples. For these purposes, a spectrophotometer was used, which measures the spectrum in the range from 380 to 730 nm and with step in 10 nm. This precision is not enough for identification of the compound or element from the white absorption spectrum – the patterns differ by much smaller step. Therefore, to increase the harvested information, for each water sample were measured spectra of 18 different color etalons. Reflected spectra from these etalons were measured through the glass square cuvette with water sample in a closed box to avoid the influence of external light [2].

Control measurements were carried out parallel to the experimental for each sample. They included measurements of such parameters: pH, electrical conductivity (EC) and temperature. During the experiment, the parameters varied in such ranges: pH from 2.56 to 10.5; EC from almost 0 to 6.51; temperature from 2 to 50.5 °C.

For the experiments, distilled water (as a zero etalon), pipe water, and water from the aquaponic system were used. Samples were prepared for different types of water, where only one parameter was changed, while the changes of remaining parameters were close to 0. To minimize the error created by the user or device for the same pH, EC, T values, 3 repetitions were performed.

The obtained data were divided into two sets – readings of parameters (pH, EC, temperature) and the results of reading spectra. For each color etalon, the spectrophotometer provides 36 values for different wavelengths. Having 18 etalons for each water sample, 36*18 = 648 values were obtained. And about 100 combinations with different values of parameters for each type of water. Total, the data consists of about 190 000 values.

All data were used for multivariate analysis to confirm the existence of a relationship between the values of the parameters and the spectrum in the visible range. To create and train the model, partial least-squares (PLS) regression method [3] was used: $Y = X * B,$ where Y is matrix of parameters (pH, EC, T), X is matrix of spectra measurements, and B is matrix of regression coefficients.

Results: As a result, a model was created that should predict the values of parameters based on the spectral characteristics of water samples.

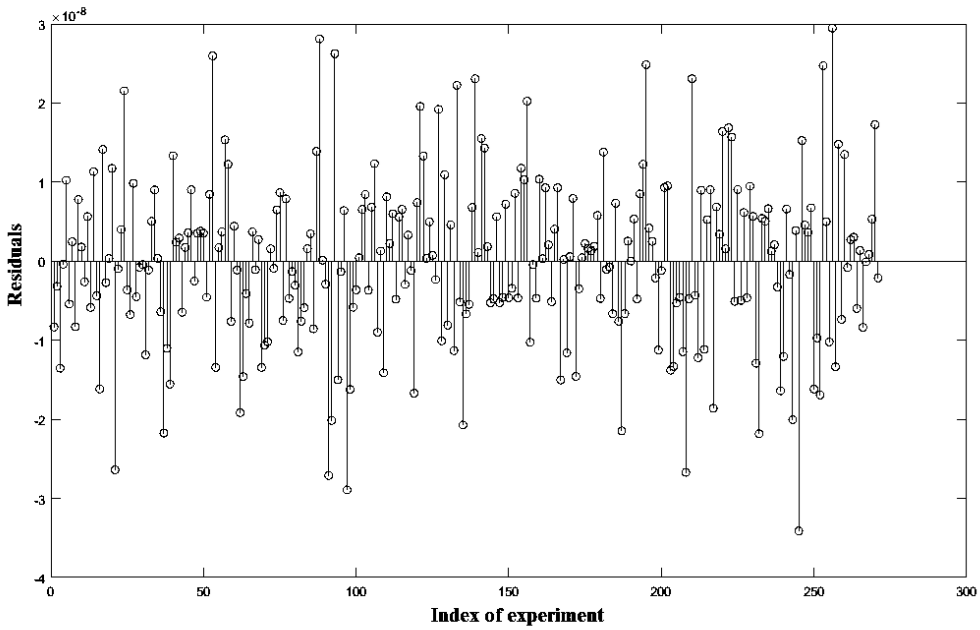

Fig. 1. The results of model running

Figure 1 shows the residuals of the results predicted by the regression model from the real. As can be seen, the deviation is very small and does not exceed the value $4 * 10^{-8}$.

Conclusion and Discussion: At this stage, was created a model with excellent training results. This prove the existence of the dependence of the spectral characteristics of water on tested parameters. To expand this research to a full-fledged method, it is necessary to create the system capable to predict the values of parameters based on spectral measurements. For this purpose, the statistical data obtained during the experiments will be used for more in-depth analysis.

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