Hyperspectrograms – A new way of description, visualization and interpretation of solid samples' chemical inhomogeneity

The hyperspectral imaging in the near-infrared range (HIS-NIR) is a technique used for fast, non-invasive measurements and characterization of main chemical composition of the sample surface. The measurement leads to multidimensional image acquisition, where each individual image pixel represents single spectrum of a certain region of studied sample. According to the most recent research, the HSI-NIR technique is successfully applied in the analytical chemistry, including examination of a painting's authenticity, searching for marks and traces in the forensic chemistry and identification of a counterfeit medications.

To make full use of an information contained in the complex and multidimensional HSI-NIR data, it requires modern chemometrical and statistical tools. The common initial approach is to reduce multidimensional data to set of spectra that will characterize only certain regions of the image. The choice of the regions is equivalent to the selection of the sample in laboratory and it have a significant impact on further stages of the analysis. It should be mentioned that the knowledge about image sampling, as well as the way of determining the degree of sample's inhomogeneity in the hyperspectral imaging technique, is still incomplete and needs to be improved. In HS imaging, the sample could be defined as the set of spectra, as the region of the image, or whole hyperspectral image. Nevertheless, in the worldwide surveys based on the HSI-NIR technique, the sample generally is described by the individual spectrum or average spectrum of the neighbouring pixels. As a result, part of information about chemical compounds distribution among the sample surface is ignored. Reduction of original variables is related with limitations of computational power of computers and methodological difficulties in application of algorithms that use three-dimensional structured data (as the hyperspectral images). New, promising way of sample description, using hyperspectral imaging technique, and including simultaneously reduced spatial and spectral information, is a hyperspectrogram.

Proposed project concentrate on the conception of an individual sample defined as a set of spectra, which represents certain, specific region of the hyperspectral image. The sample defined that way can be described with hyperspectrogram, a one-dimensional signal constructed by augmenting frequency distribution curves of reduced spectra occurring within that sample. In this way spectral information about studied material is enriched with complementary information about the sample's chemical inhomogeneity. The concept of hyperspectrogram also opens new opportunities for visualization, quantification and interpretation of chemical changes occurring on a studied sample surface.

The aim of the project is to study and to develop the idea of hyperspectrogram which considers the sample's chemical inhomogeneity. Using hyperspectrograms we plan to develop objective measures of chemical inhomogeneity (descriptors), which will be testified on the samples of chosen cereal grains and manufactured tablets. The descriptors and the new methodology of the HSI-NIR sample analysis promises broad functionality which is going far beyond NIR spectral range. The evolved procedure may thereby be used for image sample description in Raman spectroscopy, in mass spectrometry or in X-ray fluorescence spectroscopy. Proposed methodology of a sample description may significantly facilitate resolving various analytical issues such as evaluation of authenticity of the food and drug products, longitudinal monitoring of the studied material and the quality control in the broad sense. The character of the project is interdisciplinary. It matches spectroscopic research with novel chemometrical and statistical methods and image processing methods. Developed approach can be used for comprehensive sample description. That will ensure future efficient samples comparison and allow for development of new, advanced classification and calibration approaches possible to use in the different fields of analytical chemistry.