Diagnostics of harmful impurities in aqueous media using spectroscopic methods and machine learning algorithms

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In the modern era of active development of industry, transport, energy, the pharmaceutical industry, the problem of controlling the environmental situation in megacities is becoming especially relevant. Violation of the qualitative and concentration balance of ions, the presence of drugs in surface, waste and groundwater has a negative impact on both human health and the ecological state of the environment. According to the results of research by the Roshydromet organization, which monitors environmental pollution and the radiation situation in the territory of Moscow and the Moscow Region, in 2020-2021 14 cases of high pollution of water resources were registered. Thus, the control of the ionic composition, as well as the treatment of wastewater from industrial enterprises and urban housing and communal services, is an extremely urgent problem.

Currently, for the diagnosis of aqueous media, mainly chemical contact methods are used, that make it a time-consuming procedure. However, for continuous monitoring of natural waters, remote and express methods are required that allow working and monitoring the situation in real time. The most promising in this regard are spectroscopic methods, which provide remote and rapid operation, as well as a wide range of identification features of the determined components of aqueous media. Due to the complexity of solving the multi-parameter inverse problem of spectroscopy, the identification of many individual components, as well as determination of the concentration of each of them in the presence of others, required the use of machine learning methods (MLM).

In this work, we present the results of using MLM for the obtained Raman scattering, fluorescence, optical absorption, and IR absorption spectra of aqueous solutions of lithium, ammonium, iron (III), nickel, copper, and zinc cations, as well as sulfate and nitrate anions. The concentration ranges varied from 0 to 0.9 M, which correspond to the ranges of observed concentrations in wastewater from non-ferrous metal plants (for example, in spent pickling solutions). The simultaneous use of several spectroscopic methods at once and the use of neural networks ensured a high accuracy in determining the concentrations of these heavy metal ions and sulfate and nitrate anions in aqueous media.

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