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Chemometric Approach to Modeling the Extraction Method Parameters for Toxic and Strategic Elements from Fly Ash Samples

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The modern development of industry brings with it an increasing energy demand. In Serbia, a significant portion of electricity is generated by burning coal in thermal power plants, which results in the production of large amounts of industrial waste: fly ash, bottom ash, and slag. These waste materials can contain both toxic and strategically important elements. By determining the quantity of toxic elements present, proper handling of this hazardous waste can be ensured. Additionally, extracting strategic elements from waste materials could offer an ecological alternative to mining.

In this study, a comparison of two digestion methods was conducted: HNO_3/HCl/HF and HNO_3/H_2SO_4 with V_2O_5. Additionally, modeling of microwave digestion parameters was performed, including temperature, time, catalyst, and type of mineral acids. The investigations were carried out on seven different fly ash samples.

The obtained results were processed using advanced techniques of multivariate chemometric analysis: artificial neural networks (ANN), cluster analysis (CA) and principal component analysis (PCA). The results indicated that lower temperatures and the method HNO_3/H_2SO_4 with V_2O_5 are more suitable for volatile toxic and some strategic elements, whereas higher temperatures and the method HNO_3/HCl/HF are more suitable for other elements, including most of the strategic elements.

Keywords: Fly ash, Strategic Elements, Artificial Neural Networks, Cluster Analysis, Principal Component Analysis

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