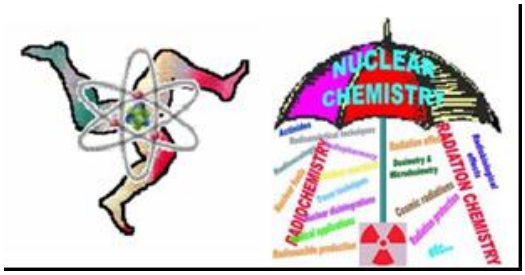

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Processing of UV-Vis spectroscopy data by chemometric tools as a perspective way for online monitoring of SNF reprocessing

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PUREX process of spent nuclear fuel (SNF) reprocessing requires thorough analytical monitoring at every technological stage to minimize economical losses and ecological risks. Spectrophotometric determination of various ions in visible and near UV spectral range is a classical analytical method. It can be successfully employed for determination of various oxidation states of actinides in solutions. However, when several actinides with significantly different concentrations are simultaneously present in the sample, classical spectral analysis of the minor components can become difficult or even impossible without preliminary chemical separation of the elements. UV-Vis spectroscopic analysis in combination with chemometric data processing seems to be promising for express and/or even online determination of various components in SNF reprocessing solutions. The use of modern optical fibers eliminates the limitations of the detector location and all control units of such a spectroscopic system can be placed in the clean zone. Moreover, one can simultaneously apply not only UV-Vis detectors, but also the detectors of IR and other types of radiation.

In this study we attempted to evaluate the potential of UV-Vis spectroscopy in combination with simple chemometric data processing techniques for analysis of the mixture of several elements typical for SNF reprocessing. Spectroscopic measurements were performed with an AvaSpec spectrometer (Avantes B.V., Holland) in the range 184 –1100 nm with 0.53 nm step. The concentrations of both Np and Pu were varied from 0.05 to 1.55 g/L in solutions with constant content of U (50 g/L) and HNO3 (2 mol/L). The experimental spectroscopic data were processed with the Unscrambler 9.7 (CAMO, Norway) software package using PLS1 algorithm.

It was found that the prediction of plutonium content in the model mixtures is possible with rather small relative errors (in 9 of the 10 predicted samples the relative error was lower than 10%). Somewhat worse results were obtained for neptunium (in 8 of the 10 predicted samples RE is lower than 10%). The highest error for prediction of Np concentration was found for the mixture containing rather large concentrations of the elements in question (Np - 300 mg/L, Pu -1300 mg/L, and U50 - g/L). This result can be due to the noisy spectral signal of Np(V) at 980 nm obtained during the measurements that leads to the «noisy» latent variables responsible for Np concentration. However, the mean relative error for 10 test set samples is 4.4 and 7.1 % for plutonium and neptunium, respectively.

The same spectral data were also subjected to the traditional univariate calibration procedure. Absorbance values at 980 nm were used for calibration against neptunium content, signal intensities at 475 nm, for plutonium. Linear fit of the experimental data points yielded regressions with R2 0.98 and 0.95 for plutonium and neptunium, respectively. In spite of the high correlation, predictive ability of these regressions was much poorer than those of PLS models and average relative error of prediction for 10 unknown test samples was 12,7 and 21% for plutonium and neptunium, respectively.

Hence, feasibility of the optical spectroscopy in combination with chemometric data processing was demonstrated for the analysis of the model solutions simulating the PUREX SNF reprocessing. This approach allows fast and simple analysis of plutonium and neptunium in a wide concentration range in the presence of uranium. Further experimental studies are now in progress to improve these results with more complex model solutions as well as by use of more sophisticated chemometric techniques.

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