Recent Modifications to the Software of a Miniature X-ray Fluorescence Spectrometer for Radiological Glovebox Applications

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The Analytical Development Directorate in the Savannah River National Laboratory develops and maintains capabilities to characterize highly radioactive materials to support the missions of the Savannah River Site and the Department of Energy. Over the last several years a miniature x-ray fluorescence (XRF) spectrometer was installed and operated into an existing radiological glovebox which houses a powder x-ray diffractometer. The instrument has the capability of much larger laboratory-grade Energy Dispersive X-ray Fluorescence Spectrometer, but was easily installed in a glove box. The XRF spectrometer provides fast and rapid semi-quantitative elemental analysis with minimal sample preparation and significantly enhances the analytical capability of the powder x-ray diffractometer by providing chemical composition information which narrows the potential crystal phase matches in the search-match software for the x-ray diffractometer software.

Software to interpret the XRF data was implemented using Microsoft Excel macros. Novel features incorporated into the data analysis program include an adaptive-peak-shape algorithm to enhance, locate and quantify peaks in the XRF spectrum, and improved methods to automatically identify elements from peak data. Recently, the macros were updated with the X-ray Transition Energies from National Institute of Standards and Technology (NIST) and National Physical Laboratory (NPL). The upgraded energy lines were implemented into the second derivative calculation where they made tremendous improvement to the automatic identification feature of the custom software. Another new feature to the software was a search/scan energy lines macro. One can now call up this macro a scan across all the energy lines for a particular sample.

A comparison between the miniature XRF and the Graphite Furnace Atomic Adsorption for low level Hg determination in a radioactive organic extractant will be presented along with the upgraded features of the XRF software.