IMPLEMENTATION OF THE MONTE CARLO - LIBRARY LEAST-SQUARES METHOD TO ENERGY DISPERSIVE X-RAY FLUORESCENCE ANALYSIS

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An integrated Monte Carlo – Library Least-Squares (MCLLS) System has been developed and implemented to model the complete spectral response of energy-dispersive X-ray fluorescence (EDXRF) spectrometers and perform an inverse analysis by an iterated Library Least-Squares method for sample composition when an initial guess is provided. This software is a visualization system developed on the Borland C++ Builder platform and has a user-friendly interface to accomplish all qualitative and quantitative tasks easily . That is to say, the software enables users to run the forward Monte Carlo simulation (if necessary) and complete the sample composition inverse analysis just by click selecting several modes of operation and providing simple inputs. An overview of the software is illustrated in the following.

The software contains three advanced technologies developed by CEAR researchers since 1970; a comprehensive and accurate Monte Carlo forward simulation code – **CEARXRF5**, Differential Operators, and Detector Response Functions.

CEARXRF5, a CEAR proprietary Monte Carlo code for simulating the total and individual library spectral responses of all elements, has been recently upgraded, with several key improvements including: input file format compatibility with MCNP5, a new general geometry package, versatile source definition, variance reduction (tally angle forcing), a new cross section loading method and updated data, while keeping all the capabilities of the previous version.

Differential Operators is a very powerful method for measurement sensitivity study and system optimization. For our EDXRF analyzer system, it becomes an important technique for quantifying the matrix effect in near real time when combined with the MCLLS approach.

Detector Response Functions are needed for many applications involving X-ray spectroscopy. An improved Si (Li) detector response function model over energy ranging from 5 to 60keV and an accurate Germanium detector response have been developed at CEAR and implemented in this integrated system.

Benchmark results on Standard Reference Materials (stainless steel samples from NIST and aluminum alloy samples from Alcoa) are provided for a simple reproducible prototype system using a ^{109}Cd radioisotope source and a Si(Li) detector. The results show excellent agreement between our calculated sample compositions with those of the reference standards and the approach is very fast. The software is easy to use with user-friendly features and the capability to accomplish all related tasks in a visualization environment. It can be a powerful tool for EDXRF analysts.

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