

## ON THE USE OF MONTE CARLO BASED METHODS TO EDXRF QUALITATIVE ANALYSIS

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The CEARXRF GUI-Based MCLLS analysis approach can accurately calculate elemental weight fractions by fitting the measured characteristic X-ray spectrum (excited by a Gamma-ray or X-ray source) with the computer generated elemental libraries. The elemental stratified sampling variance reduction technique has been implemented and verified in the CEARXRF5 code. Results from an improved EDXRF Analyzer indicate significant improvement in the statistics of the elemental libraries of elements with low concentrations. The stratified sampling technique enables each component in the measured sample to have equal opportunity to be sampled with adjusted weights and essentially all elemental libraries in the sample will have the same statistical precision. This is very important since some elements of interest may have very low concentrations - such as traceable lead (Pb) in plastic toys. The analog sampling scheme cannot generate satisfactory results for these low concentration elements due to the low probability of their sampling.

This MCLLS approach consists of three major parts as follows: (1) an improved EDXRF Analyzer that utilizes a Cd-109 chemical source to excite the individual elements in a sample together with an X-ray detector and a multi-channel analyzer to simultaneously collect the fluorescence radiation spectra emitted by the sample; (2) a Monte Carlo Simulation code (CEARXRF5) that generates the incident photon spectra on the detector surface for all required elemental libraries with predetermined guesses of elemental weight fractions for the sample of interest [These computed library spectra are convolved with detector response functions (DRFs), which take Gaussian energy broadening and other detector features into account and are then regressed with an experimental spectrum to yield a better estimate of each elemental weight fraction]. Iterations may be needed to obtain the desired results if the initial guesses are not close enough to the actual values. The differential operators (DOs) that are incorporated in the CEARXRF5 code can be used to accelerate the iterative procedure; and (3) a visualization software package (MCLLSPro) that first uses qualitative analysis to predetermine the elements present and obtain an initial guess of their concentration in the sample. Results show that the elemental library stratified sampling scheme improve the overall accuracy of the MCLLS approach compared to the analog sampling method.