D6 Monte Carlo Uncertainty Analysis for the Measurement of Forensic Glass Using Neutron Activation Analysis and Laser Ablation-Inductively Coupled Plasma/Mass Spectrometry (LA-ICP/MS)

Nicholas Sharp, PhD, National Institute of Standards and Technology, Gaithersburg, MD 20899; Ruthmara Corzo, PhD, Gaithersburg, MD 20899-8371; Jamie L. Weaver, PhD, National Institute of Standards and Technology, Gaithersburg, MD 20876; Blaza Toman, PhD, National Institute of Standards and Technology, Gaithersburg, MD 20899; Maria Martinez, PhD, National Institute of Standards and Technology, Gaithersburg, MD 20899; Eric B. Steel, National Institute of Standards and Technology, Gaithersburg, MD 20899-8371; Jose R. Almirall, PhD, Florida International University, Miami, FL 33199*

Learning Overview: The goal of this presentation is to highlight the importance of proper handling of uncertainty analyses for LA-ICP/MS and to show the steps being taken to develop the procedures for certifying a new glass Standard Reference Material (SRM) for the forensics community.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by empowering analysts and technicians to understand their instrument's and technique's uncertainties and enable them to confirm whether their procedures are adequately incorporating uncertainty propagations.

The ubiquity of glass makes it a commonly encountered type of forensic trace evidence. Elemental analysis using sensitive analytical techniques, such as LA-ICP/MS, is routinely used to compare the chemical composition of glass specimens submitted in casework. The forensic community uses several National Institute of Standards and Technology (NIST) Standard Reference Materials (SRM 1831, SRM 610, SRM 612, and SRM 614) and international glass reference materials (Float Glass Standard 1 [FGS1] and FGS2) for quality control and external calibration. However, the community currently relies on consensus or reference (i.e., not certified) concentration values for all elements in the FGS glasses and some elements, particularly the trace elements, in the NIST SRMs. Additionally, many of the certified element concentration values in the NIST SRM certificates were determined over 20 years ago. Finally, several glass reference materials are currently low in stock and will need to be replaced within the next decade. To address these gaps, the elements in the NIST SRMs and three newly designed float glass reference materials produced by Corning®, Inc. (in collaboration with Florida International University) will be evaluated with modern methodology. Neutron Activation Analysis (NAA) and LA-ICP/MS will be used to obtain statistically robust concentration values at the bulk and micro sampling scale, respectively.

To estimate the uncertainty in NAA and LA-ICP/MS measurements, a rigorous Monte Carlo-based method has been developed. The Monte Carlo uncertainty analysis method complements and expands upon the Guide to Expression of Uncertainty in Measurement (GUM) method. The Monte Carlo method accounts for all correlations introduced through common input variables (e.g., standards) and for the dark uncertainty between measurements. An R script that conducts the Monte Carlo uncertainty calculations for NAA has been developed. The uncertainty budget analysis of NAA revealed that an improvement in uncertainties could be achieved by reducing correlations in the standards (a four-fold improvement in uncertainties) and by increasing the number of wafers analyzed. An R script that combines data reduction of the raw LA-ICP/MS signal, quantitation using single-point external calibration, and a Monte Carlo uncertainty analysis has been written for LA-ICP/MS measurements. The uncertainty budget analysis will aid in evaluating LA-ICP/MS as a potential analytical tool for the certification of major, minor, and trace elements in glass at NIST. Additionally, the uncertainty budget analysis will aid in determining a practical number of fragments and replicate measurements per fragment for the certification of elements in the three new float glass reference materials for the forensic science community. The results for the Monte Carlo uncertainty budget analysis of NAA and LA-ICP/MS will be presented.

Glass, Trace Elements, Glass Standard

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*Presenting Author