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Les Ebdon and Michael Foulkes

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Optimization in trace atomic spectroscopy

By Les Ebdon and Michael Foulkes

Plymouth Analytical Chemistry Research Unit, Department of Environmental Sciences, Polytechnic South West, Drake Circus, Plymouth PL4 8AA, U.K.

Optimization of analytical instrumentation enables realization of potential and the valid comparisons of techniques, hence the interest in rigorous, mathematically based, optimization procedures. One of the most effective procedures is variable step-size simplex. Using a simple algorithm, sets of initial operating parameters can be tested and instrumental response evaluated. The worst response is rejected and a new set evaluated, thus in a logical manner the optimal conditions are identified. Particular benefits are speed, computer compatibility, relative freedom from false optima and the irrelevance of prior assumptions or knowledge about response surfaces.

The development of inductively coupled plasma atomic emission spectrometry (ICPAES) was controversial as the interdependent operating variables made optimization difficult. Simplex-based procedures have therefore been extensively used to optimize ICPAES for signal-to-background ratios, multielement determinations and to minimize interferences from easily ionized elements. In the analysis of solids by nebulizing suspensions of powders into plasmas (slurry atomization), the aim is to achieve calibration using aqueous standards. Simplex procedures have been used to achieve equivalent analyte response from slurries and aqueous solutions. The compatibility of simplex algorithms with computers offers the potential for microprocessor-controlled optimization of analytical instruments. Work in this area has been pioneered at Plymouth for ICP spectrometry.

Optimization of direct current plasma AES is also facile. Examples of successful optimizations include for signal-to-background ratio; for slurry atomization; and hydride generation. The latter may include the optimization of the chemistry of the hydride generation parameters along with the instrumental parameters, this is particularly valuable for lead.

Inductively coupled plasma mass spectrometry (ICPMS) is a new technique which offers excellent detection limits but uses complex instrumentation. Simplex optimization is being used to develop methodology and instrumentation, e.g. a recent comparison of low-flow and conventional torches for ICPMS showed the latter offered superior sensitivity and freedom from polyatomic interferences.

Optimization offers a powerful tool to enhance trace analysis.