

Advances in Chemistry. Part I: Noise, Calibration, and Educational Advances in Analytical Chemistry. Part II: Safety Oversight in Chemical Journals.

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Part I

The accuracy and precision of the results of any chemical analysis depends on the calibration graph and its associated systematic and random errors. Least squares regression generally treats all data with equal weights. A weighted least-squares fit is an improvement but requires knowledge of the imprecision in each point of the calibration graph. The imprecision is not easy to estimate with high confidence because of the large number of replicates needed.

The imprecision depends on the types of magnitudes of the sources of noise. We have characterized the noise sources in ICP-OES and UV/Vis and developed a model that effectively predicts the standard deviation of emission and absorption as a function of concentration.

Once a model is fit to the data, calibration designs were studied. These designs ranged from one to three decades in order to optimize precision over the calibration graph for ultraviolet-visible spectrochemical analyses. Different calibration strategies, composed of different concentrations and number of replicates, have been evaluated determine the calibration design that will minimize imprecision as measured by the average relative concentration error integrated over the entire calibration graph.

A laboratory experiment utilizing potentiometric titrations was prepared to connect electrochemistry, stoichiometry, equilibria and reinforce acid-base titrations. Students were to perform a potentiometric titration to determine the initial analyte concentration and reactant concentrations at varying points in the titration in order to determine the solubility product constant of a solid species.

Part II

Advances in chemistry are highly dependent on the procedures published in peer-reviewed journals. Some chemistry journals require authors to address safety considerations in their manuscripts but others do not. In this study, we examined 726 chemistry journals from 28 publishers to determine if they require the author to mention safety precautions. Journals supply information for authors that generally mention safety in two places. In the guidelines for authors, which are widely read by prospective contributors, 8% mention safety. Most journals have ethics guidelines of which 59% mention safety.

In order to determine the effectiveness of safety policies 100 articles from each of six journals that published research that involved extensive syntheses were selected. The results of the search indicated that the target compounds were mentioned 107 times but only one mention carried any safety precaution.

An outcome of the paper, *Review and Analysis of Safety Policies in Chemical Journals*, is the implementation of new safety policies in chemical journals by the American Chemical Society. The ACS now requires unexpected, new, and/or significant hazards or risks of the published work to be detailed.