ACCURACY OF THEORETICAL INFLUENCE COEFFICIENT METHODS

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Theoretical (computed) influence coefficient methods are widely used in practice for quantitative XRF, efficient to use, and in most cases sufficiently accurate. A variety of software products exists for their application, based on various mathematical approaches ("models") and schemes for the computation of the coefficients. If used according to the limitations imposed by their authors their results agree usually within a very narrow frame of variation. Nevertheless, errors occur for various reasons and the agreement of results is not necessarily proof of their trueness.

Influence coefficient methods require a careful choice of standards in terms of similarity of their composition with that of the unknown, and of their preparation. The various models, however, differ in their behavior when these requirements are not well met. In general, models with a larger number of coefficients appear to be more robust in this respect than simplistic formulae. The interpretation of influence coefficient methods as a local approximation for the (classical) fundamental parameter approach is obvious from this point of view.

Errors may occur anywhere in the chain of measurement, raw data treatment (determination of net intensities), and numerical computation, but also in the fundamental parameter models (neglected interactions), the numerical values of the parameters, and deficiencies in the numerical computation. As a result the obtained data may be simply inaccurate or show conspicuities such as sums of concentrations different from unity. This paper investigates these errors and their propagation.