# Comparison of Four Elemental Mass Balance Methods for Clay Mineral Quantification[1]

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**Abstract:** The quantification of the relative mineralogical composition of clay mixtures by powder X-ray diffraction or chemical mass balance methods has been severely hampered by a lack of representative standards. The recent development of elemental mass balance models that do not require standards for all minerals in the mixture may help circumvent this problem. These methods, which are based on the numerical optimization of systems of non-linear equations using the Marquardt algorithm, show promise for mineral quantification. The objective of this study is to make a preliminary assessment of the accuracy of these methods and to compare them to linear models that require standards for all mineral phases. Methods 1 and 2 are based on weighted average solutions to simultaneous linear equations solved for single samples with known standards. Solutions were achieved by a matrix decomposition algorithm and the Marquardt algorithm, respectively. Methods 3 and 4 are based on a set of simultaneous non-linear equations with reduced non-linearity solved by least squares optimization based on the Marquardt algorithm for multiple samples. Illite and halloysite compositions were fixed in Method 3, only the halloysite composition was fixed in Method 4. All models yielded relative weight fractions of the three mineral components; additionally, Methods 3 and 4 yielded compositions of smectite, and smectite and illite, respectively. Ten clay mixtures with varying proportions of the <0.2 μm size fraction of three different reference clays (Wyoming bentonite, Fithian illite, and New Bedford halloysite) were prepared gravimetrically and analyzed by inductively coupled plasma-atomic emission spectroscopy. Accuracy of the four methods was evaluated by comparing the known mineralogical compositions of the mixtures with those predicted by the models. Relative errors of 5 and 10% (randomly +/−) were imposed on the elemental composition of the smectite standard to simulate errors due to lack of good standards. Not surprisingly, the accuracy of Methods 1 and 2 decreased rapidly with increasing error. Because Methods 3 and 4 optimized for the smectite composition and only used it for an initial guess, they were unaffected by the level of introduced error. They accurately quantified the mineralogical compositions of the mixtures and the elemental compositions of smectite, and smectite and illite, respectively.

**Key Words:** Elemental mass balance • Marquardt algorithm • Non-linear models • Numerical optimization • Quantification

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