

## XRF ANALYSIS - THEORY, EXPERIMENT, AND REGRESSION

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### ABSTRACT

Numerous papers in the past indicate that experimental - regression obtained - alphas may do not have a physical meaning when they contradict theory. This paper will show that the key to the problem is the basic equation applied. If both the theoretical and experimental basic equations are the same then experimental alphas will have the same physical meaning. Actually, experimental alphas based on standards should have more meaning than theoretical alphas. Besides, theoretical alphas are dependent on coefficients that must be determined experimentally. So why use the left hand to reach into the right pocket when a more direct route is available. It has been shown in that for some models the alphas can be expressed as ratios of corresponding regression coefficients. In practice theoretical physicists are frequently forced back to the "drawing board" when their theories cannot be experimentally confirmed. Besides, physicists usually use least squares fitting to link theory with experiment. One is talking here about the linearity in coefficients that have to be determined, and because of that, one can utilize a logarithmic scale or any other mathematical transformation prior to applying multiple linear regression. Theoretically derived computing terms can be very long and/or complicated but often the result is quite simple as in the classic example below:

$$1 - 1/3 + 1/5 - 1/7 + 1/9 - \dots + (-1)^{n-1} * 1/(2n-1) = \pi/4$$

Whenever possible valid shortcuts should be used to simplify the situation so that the purpose served by derived equations is not lost. In all situations an equipment factor should be included in the equation. When the basic equation is properly defined, i.e., is realistic, all the constants can be determined by using multiple linear regression and applying an appropriate set of standards.

### INTRODUCTION

Two types of regressions are described in the literature.<sup>4, 11, 12, 15</sup> The simple one variable, and the more complicated multidimensional regression. Simple regression, of course, can be considered as a particular case of multidimensional regression. One variable regression is often a preprogrammed function in pocket calculators. However, multidimensional regression requires the use of a statistical or spreadsheet program such as Statistica, Quattro Pro, Excel, or Lotus 1-2-3.<sup>24, 25</sup> In a multidimensional approach there is a great deal of freedom in the selection of variables. These variables can be expressed not only in simple terms but also in more

complicated forms such as cross products or other combinations. The analytical problem or system will determine how many variables are required.

It has been shown that by preselecting variables, coordinates for example, and applying multidimensional regression the Lachance - Traill or another matrix correction equation can be derived.<sup>11</sup> This demonstrates that the same mathematical formula can have different origination and be derived differently. Because there is only one algebra, equal equations, no matter how they were derived, can be algebraically and statistically processed and the physical interpretation and computed values should be the same as long as they describe the same physical system.

## **MATHEMATICAL MODELING IN XRF**

The literature contains about twenty models describing XRF matrix correction procedures.<sup>4, 5, 6, 7</sup> Some like the Fundamental Parameters Method assumes that all behaviors of X-rays in a sample are known so the theoretical alphas can be easily computed. At the 1987 Denver X-Ray Conference, Criss and Lachance concurred that the theoretically derived fundamental parameter method formula has the same mathematical form as the Lachance -Traill equation.<sup>1</sup> It means the experimental alpha approach and fundamental parameters essentially merged together. This author has shown that the Lachance-Traill equation can be derived from statistical assumptions which generates the following conclusions:

**if CRISS = LACHANCE and if LACHANCE = STATISTICAL,  
then CRISS = STATISTICAL**

This is an expression of the *transitive* principle of mathematics that: if  $x=y$  and  $y=z$  then  $x=z$ .

This means that theoretically delivered alphas should pass statistical tests based on regression and one cannot say that regression as a multidimensional application is invalid.

## **PAST HISTORY - REGRESSION WITH A "BAD REPUTATION"**

Significant previous literature has indicated that the use of regression is not a valid approach.<sup>4</sup> In a private communication with this author, John Criss concluded that in the past the use of one variable regression was invalid and, therefore, its use obtained a bad reputation. He had no objections to the use of multidimensional regression, however, the details presented in this paper were not yet fully developed at that time.<sup>8</sup>

## **SIMPLE REGRESSION VERSUS MULTIDIMENSIONAL REGRESSION**

The X-ray fluorescence matrix correction phenomenon is a multidimensional process which cannot be described by regression with only one variable. To fully describe the system several variables are required.

To express this mathematically one can write:

$$Y=A_0 + A_1 * X_1 \text{ (one variable case)}$$

$$Y=A_0 + A_1 * X_1 + A_2 * X_2 + A_3 * X_3 + \dots + A_{n-1} * X_{n-1} + A_n * X_n \text{ (multidimensional case)}$$

In a multidimensional approach sets of terms can be grouped such that the 3-dimensional equation of a plane can be derived as described in a previous publication.<sup>13</sup>

## EXAMPLE OF THE CONICAL PROBLEM - MORE GENERAL APPROACH

Application of multidimensional modeling is a very general and can be used to help understand the X-Ray system. The use of geometrical examples to visualize physical phenomena is often a very useful tool to aid in our perception of the processes involved.<sup>2</sup>

The volume of a cone can be written:

$$V = (\pi * r^2 / 3) * H$$

where:

V - volume  
r - base radius  
H - height

For a truncated cone the formula contains additional terms:

$$V = (\pi / 3) * H * (r^2 + r * R + R^2)$$

As is shown, truncation introduced the two additional terms (**2 variables**) and if  $r=1$  then the formula becomes:

$$V = (\pi / 3) * H * (1 + R + R^2)$$

This, **1 + something** expression closely resembles the Lachance-Trail equation.

To accurately compute the volume of a truncated cone all of the terms must be used. The same truth holds for an X-Ray system. To fully describe the matrix correction phenomenon in an X-ray system one has to use sufficient terms to cover the multidimensional aspects of the system.

## FITTING EQUATIONS TO EXPERIMENTAL DATA THE CONICAL PROBLEM - Part II

If one were to make a set of truncated cones from some material their dimensions can be measured and their weight determined with reasonable accuracy. Knowing the mass (m) and the specific gravity of the construction material ( $\rho$ ) the volume of each can be calculated:  $m = \rho * V$ . For a set of cones a system of equations can be written and by using multidimensional regression the regression coefficients can be determined. In this case the following variables ( $X_1, X_2, X_3$ ) should be considered:

$$X_1 = \rho * H * r^2, \quad X_2 = \rho * H * r * R, \quad X_3 = \rho * H * R^2$$

where:

$\rho$  - specific density  
H - height  
r - small base radius  
R - large base radius

The system of equation for nine conical samples can be written as follows:

$$m_1 = A_1 * \rho * H_1 * r_1^2 + A_2 * \rho * H_1 * r_1 * R_1 + A_3 * \rho * H_1 * R_1^2$$

$$m_2 = A_1 * \rho * H_2 * r_2^2 + A_2 * \rho * H_2 * r_2 * R_2 + A_3 * \rho * H_2 * R_2^2$$

$$m_3 = A_1 * \rho * H_3 * r_3^2 + A_2 * \rho * H_3 * r_3 * R_3 + A_3 * \rho * H_3 * R_3^2$$

$$m_4 = A_1 * \rho * H_4 * r_4^2 + A_2 * \rho * H_4 * r_4 * R_4 + A_3 * \rho * H_4 * R_4^2$$

$$m_5 = A_1 * \rho * H_5 * r_5^2 + A_2 * \rho * H_5 * r_5 * R_5 + A_3 * \rho * H_5 * R_5^2$$

$$m_6 = A_1 * \rho * H_6 * r_6^2 + A_2 * \rho * H_6 * r_6 * R_6 + A_3 * \rho * H_6 * R_6^2$$

$$m_7 = A_1 * \rho * H_7 * r_7^2 + A_2 * \rho * H_7 * r_7 * R_7 + A_3 * \rho * H_7 * R_7^2$$

$$m_8 = A_1 * \rho * H_8 * r_8^2 + A_2 * \rho * H_8 * r_8 * R_8 + A_3 * \rho * H_8 * R_8^2$$

$$m_9 = A_1 * \rho * H_9 * r_9^2 + A_2 * \rho * H_9 * r_9 * R_9 + A_3 * \rho * H_9 * R_9^2$$

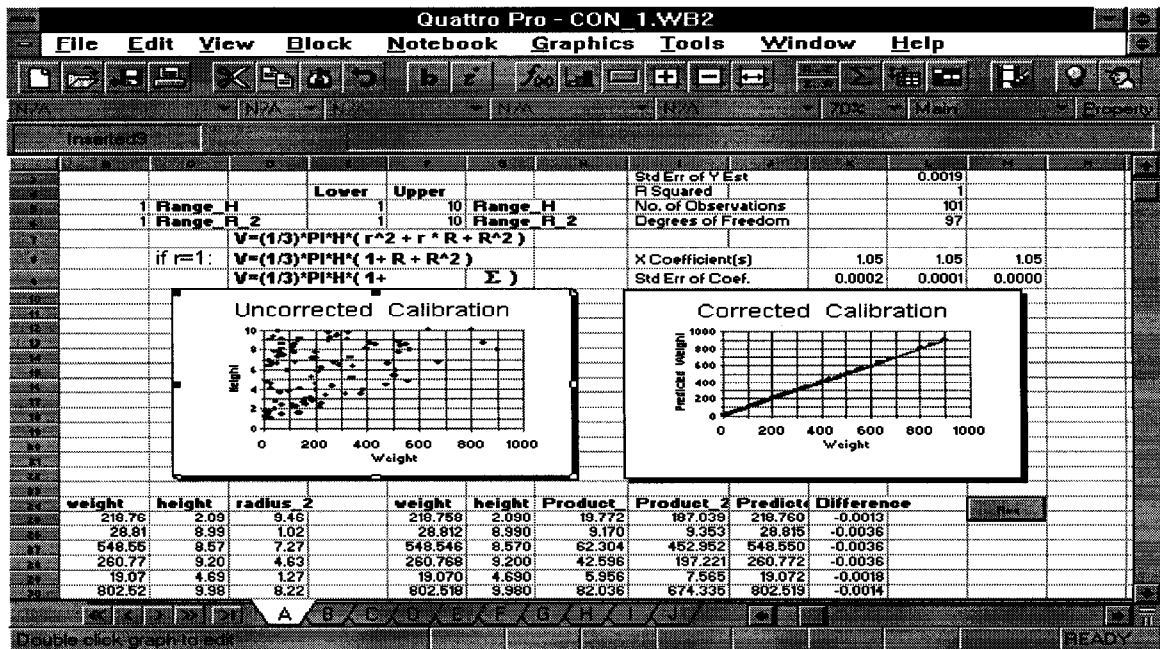


Figure 1. Multiple Linear Regression for the conical problem; Left side presents uncorrected data; Right side presents corrected data. Computations and Graphing done with the help of Quattro Pro V.6 spreadsheet.

Please note the columns with the same regression coefficient in the above equations.

Entering the data in the above format in a spreadsheet in the order of defined regression coefficients as follows:  $A_1, A_2, A_3$  the spreadsheet statistical subroutine will deliver the correlation coefficient and the regression coefficients for the set of equations. If the experiment was carefully conducted we should get the same value of regression coefficient for all 3 terms ( $A_1=A_2=A_3$ ):

$$A_1 = \pi / 3 \quad A_2 = \pi / 3 \quad A_3 = \pi / 3$$

If the value of  $\pi$  was not known one could calculate it using this method. (The theoretical method to determine the value of  $\pi$  is shown in the abstract above.) The values of experimental and theoretical  $\pi$  should be equal. One cannot say here that theoretically obtained  $\pi$  is any better than  $\pi$  experimentally obtained. Granted, one can discuss experimental error, however, the physical meaning of  $\pi$  in both the cases is the same. Multiple Linear Regression for the conical problem is briefly presented in Figure 1. The randomly generated dimensions will simulate a set of truncated cones.

## XRF MATRIX CORRECTIONS BY MULTIDIMENSIONAL REGRESSION

The above process of thinking can be applied to quantitative XRF. It has been shown that starting with multiple linear regression and performing suitable substitutions the Lachance-Trail equation is obtained.<sup>11</sup>

For the sake of clarity this is outlined below:

$$Y = A_0 + A_1 * X_1 + A_2 * X_2 + A_3 * X_3 + \dots + A_{n-1} * X_{n-1} + A_n * X_n$$

Performing the following substitutions:

$$Y = C_k$$

$$X_1 = I_k \quad \text{- intensity}$$

$$X_2 = I_k * C_2 \quad \text{- cross products with "neighboring" elements}$$

$$X_3 = I_k * C_3$$

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$$X_{n-1} = I_k * C_{n-1}$$

$$X_n = I_k * C_n$$

Applying the above substitutions, the following equation is obtained:

$$C_k = A_{k0} + A_{k1} * I_k + A_{k2} * I_k * C_2 + A_{k3} * I_k * C_3 + \dots + A_{kn} * I_k * C_n$$

factoring out  $I_k$ , one gets:

$$C_k = A_{k0} + A_{k1} * I_k \{ 1 + (A_{k2}/A_{k1}) * C_2 + A_{k3}/A_{k1} * C_3 + \dots + (A_{kn}/A_{k1}) * C_n \}$$

Which can be condensed to the Lachance-Trail equation:

$$C_k = A_{k0} + A_{k1} * I_k \left\{ 1 + \sum_{k \neq i} \alpha_{ki} C_i \right\}$$

In the above case the additional term,  $A_{k0}$ , is helpful when using no background subtraction. For those cases with background subtraction  $A_{k0}$  can be forced to zero.

## PHYSICAL AND MATHEMATICAL MEANING OF THESE EQUATIONS

Mathematical correctness and physical meaning are two separate and different criteria which should be distinguished from one another. There are some equations that are mathematically correct, however, they have no physical meaning. On the other hand any equation which has physical meaning is mathematically correct. One simple linear relationship is Ohm's Law which equates the voltage drop across a resistor to the current passing through it. This law is the basis for analog computers and one should realize that if linear problems cannot be modeled on an analog computer then the basic equation describing the phenomenon is not correct.

In the case of Ohm's Law the coefficient of proportionality is called the resistance of a conductor. In a simple case for XRF, one can say that the weight % concentration of an analyte is proportional to its peak height. The coefficient of proportionality for the XRF case contains several components which are very well described by Criss.

Once the equation has been defined and experimental measurements performed one can apply statistical methods to verify the equation. If the equation cannot be tested statistically then it has not been properly defined. Statistical verification of the equation should yield a correlation coefficient approaching 1.0.

In some cases it is difficult to perform experiments without the introduction of instrumental bias. In such situations the equipment contribution should be determined experimentally with the help of standards and included in the formula.

## SET OF XRF STANDARDS DESCRIBED BY SYSTEM OF EQUATIONS

When we have a group of experimental measurements intended to verify a model, we automatically have a system of equations which can be solved by using algebraic and statistical tools. Because few models are 100% correct, least squares techniques should be used in order to take into the account the variation from the ideal. The coefficients of proportionality in the system of equations can be determined and their physical meaning interpreted by applying analog modeling such as used to interpret Ohm's law.

## COLUMNS AND ROWS OF THE MATRIX OF EQUATIONS

Once a system of equations representing the multivariable system is established, appropriate mathematically allowed manipulation of the columns and rows will produce a solution to the system of equation. This manipulation of columns and rows can be programmed to automatically generate a solution for the system of equations.<sup>17, 18</sup> These mathematical manipulations can produce a situation where a determinant becomes zero. To avoid this condition that confuses computers and generates error messages, one can add randomly generated small value numbers

such as 0.00015, 0.00023 to the measured values producing a random low noise level. This low noise level will circumvent a zero determinant situation.

## **SYSTEM OF EQUATIONS TESTED BY STATISTICAL METHODS**

A piece of paper is very patient and one can write down any system of equations one can imagine, however, these equations could contradict each other, or one or more may be inappropriate to the group.

When working with standards, their behavior in the sense of matrix problems is described by an equation like the Lachance-Trail. The system of equations is obtained from standards (one standard - one equation, 2 standards - 2 equations, n standards - n equations) and these equations must fulfill certain criteria which act to bind them together. Statistical mathematics solves this problem using testing algorithms.<sup>18</sup> Multiple linear regression correlates one variable with n observations (variables). Correlation coefficients for multiple linear regression are well defined and can be automatically determined from data in a spreadsheet format using a program such as Quattro Pro.

## **THE +/- SIGN IN FRONT OF THE REGRESSION COEFFICIENTS IS DETERMINED BY THE SYSTEM OF EQUATIONS (STANDARDS)**

Please note that the signs in front of the regression coefficients belong to the group of standards and can be algebraically determined like anything else in algebra. For example, we know that a straight line can intersect a parabola at two points  $X_1, X_2$  that can be computed automatically and the signs are part of the computed results.

This author is fully aware of the two physical phenomena of absorption and enhancement which take place in a given sample. However, in order to describe these phenomena one has to use differential equations and one should realize that such processes also take place in a sample simultaneously. Manipulation of the sign in front of a regression coefficient is algebraically forbidden and doesn't have any sense. Association of "+" with **enhancement** and "-" with **absorption** simplifies and distorts the system. The system of equations based on a system of standards will automatically take care of the signs.

## **XRF THEORY VERSUS XRF EXPERIMENTS**

For any theory to be valid it must be verified experimentally. If experimental data contradicts the theory the theory must be modified. The growth of physics is an example of the cooperation between theoretical and experimental physicists. One group has pushed to create more accurate theoretical models while the other one had to develop better experimental tools to verify theoretical models. The experimental physicists act like a quality control department checking the reliability of the products of theoretical physicists.

Saying that the experimentally determined alphas do not have any physical meaning contradicts the above point of view. This attitude is counterproductive because theory needs experimentation and experimentation needs theory. There can be no difference in the meaning - physical or otherwise - between theoretical and experimental alphas since the equations are the same. Both methods should deliver the same values with an accuracy of  $\pm$  the standard deviation.

With reference to Ohm's law, one can imagine that the resistance of a conductor can be predicted theoretically and if model is adequate the value should be easily obtained from an experiment within the uncertainty of the measurements.

## **FITTING EQUATIONS TO EXPERIMENTAL DATA**

Good experimental data needs a theory that will describe the model, such as XRF matrix corrections. The goal of most researchers is to continuously refine the equations that describe their experimentals. Fitting equations to data is a natural process in theory development. We are justified bending theory to fit experimental data, however, the converse is prohibited. Theoretical derivations are invalid if they cannot be verified experimentally.

## **SPREADSHEET ENVIRONMENT FOR MULTIDIMENSIONAL REGRESSION**

It has been shown that an electronic spreadsheet is a practical and efficient environment for data storage. A good spreadsheet will have a set of statistical tools, including multiple linear regression built in. Additionally, with the help of good graphics one can present the data visually as is illustrated in Figures 2 & 3. Processes can be simplified by using macros which can automate large segments of the calculations. Since most modern high-end spreadsheets are similar, this approach for XRF matrix corrections is largely vendor independent. In addition to manuals supplied with each product, there is substantial third party instructional materials available for all the major spreadsheets.<sup>24-38</sup>

## **APPLYING MULTIPLE LINEAR REGRESSION TO THE AVAILABLE INDEPENDENT THEORETICAL WORK PUBLISHED IN THE PAST**

It should be mentioned here that in our Laboratory the commonly used k-alpha ratio X-Ray intensity coding is not used. Instead, the normalized intensity coding is used and alphas for such a system will differ from the classic alphas. It has been suggested that the method presented in this paper should be checked against something that is well known and accepted and for this reason Rousseau's work seems to fulfill this criterion.

The initial steps for the classic Lachance-Traill approach are a little different from our methodology, however, it was possible to reprogram our spreadsheet for the classic Lachance-Traill data processing.

First, the original Lachance-Traill formula -  $C_i = R_i (1 + \sum_{j \neq i} \alpha_{ij} * C_j)$  - is rewritten as:

$$C_i - R_i = \sum_{j \neq i} \alpha_{ij} * (R_i * C_j)$$

This way the right side is in the form of Multiple Linear Regression to which the computing power of a spreadsheet can be easily applied.

Table 1 illustrates the side by side comparison of experimental and theoretical alphas. There are some very close alpha values and there are also differences which should be expected. The following tables (Table 2, Table 3, and Table 4) illustrate how close computed values are to the true concentrations; computed values using the theoretical and experimental alphas are presented.



Exper.	0.009630	0.011024	0.011962	<b><u>-0.006936</u></b>	<b><u>-0.052056</u></b>	0.045750	0.054874	0.074995	0.125754	0.095225	0.156291
<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	0.004156	0.005602	0.009714	0.014406	0.0199873	0.041254	0.050568	0.073334	0.124176	0.142788	0.162920
Exper.	0.048038	0.002719	0.007064	0.052546	0.074753	0.035463	0.034620	0.058502	0.032212	0.032933	0.108821
<b>Mg</b>	<b>Na</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	0.092356	0.002134	0.005252	0.008718	0.012634	0.027396	0.03702	0.048957	0.080222	0.092663	0.106127
Exper.	0.060198	0.080141	0.000816	0.005525	0.019670	0.022068	0.024534	0.036379	0.051343	0.039635	0.067578
<b>Al</b>	<b>Na</b>	<b>Mg</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	0.060378	0.081373	0.000923	0.003298	0.005986	0.016305	0.020770	0.031565	0.052632	0.061274	0.070631
Exper.	0.039017	0.053718	0.071584	0.002784	0.004541	0.011337	0.015111	0.025837	0.042468	0.052892	0.046704
<b>Si</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	0.039697	0.054623	0.072029	0.001411	0.003750	0.012156	0.015575	0.023497	0.034965	0.041106	0.047757
Exper.	0.026092	0.034982	0.054282	0.060547	<b><u>-0.117154</u></b>	0.010057	0.003930	<b><u>-0.033879</u></b>	0.055631	0.039050	0.038104
<b>P</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	0.025410	0.036121	0.048547	0.061061	<b><u>-0.001495</u></b>	0.004195	0.006681	0.012617	0.022061	0.026486	0.031283
Exper.	0.015685	0.020827	0.032514	0.041005	0.107627	<b><u>-0.010529</u></b>	<b><u>-0.002505</u></b>	0.005923	0.112038	0.048201	0.021537
<b>S</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	0.015517	0.023283	0.032250	0.041355	0.052168	0.001159	0.003055	0.007525	0.013319	0.016527	0.020008
Exper.	<b><u>-0.000280</u></b>	0.002940	0.006649	0.010334	0.011419	0.024376	<b><u>-0.002673</u></b>	<b><u>-0.002041</u></b>	0.001578	0.001820	0.001969
<b>K</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	0.000035	0.003137	0.006673	0.010341	0.014622	0.018997	<b><u>-0.002418</u></b>	<b><u>-0.000474</u></b>	<b><u>-0.000563</u></b>	0.000710	0.002096
Exper.	<b><u>-0.002120</u></b>	0.000044	0.002433	0.005343	0.011687	0.011174	0.023408	<b><u>-0.003051</u></b>	<b><u>-0.002377</u></b>	<b><u>-0.001776</u></b>	<b><u>-0.000768</u></b>
<b>Ca</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	<b><u>-0.002431</u></b>	<b><u>-0.000089</u></b>	0.002570	0.005345	0.008567	0.01883	0.024227	<b><u>-0.001110</u></b>	<b><u>-0.002785</u></b>	<b><u>-0.001833</u></b>	<b><u>-0.000794</u></b>
Exper.	<b><u>-0.005637</u></b>	<b><u>-0.004197</u></b>	<b><u>-0.002540</u></b>	<b><u>-0.000915</u></b>	0.001603	0.003700	0.010013	0.013211	<b><u>-0.005184</u></b>	<b><u>-0.004543</u></b>	<b><u>-0.004575</u></b>
<b>Ti</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Cr</b>	<b>Mn</b>	<b>Fe</b>
Theory	<b><u>-0.005539</u></b>	<b><u>-0.004144</u></b>	<b><u>-0.002567</u></b>	<b><u>-0.000906</u></b>	0.001008	0.003002	0.010388	0.01309	<b><u>-0.005713</u></b>	<b><u>-0.005144</u></b>	<b><u>-0.004524</u></b>
Exper.	<b><u>-0.004308</u></b>	<b><u>-0.003147</u></b>	<b><u>-0.001770</u></b>	0.000397	0.000208	0.001857	0.014060	0.016895	0.024228	<b><u>-0.001784</u></b>	<b><u>-0.006317</u></b>
<b>Cr</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Mn</b>	<b>Fe</b>
Theory	<b><u>-0.004898</u></b>	<b><u>-0.003292</u></b>	<b><u>-0.001487</u></b>	0.000434	0.002629	0.004943	0.013471	0.016652	0.023913	<b><u>-0.001520</u></b>	<b><u>-0.004695</u></b>
Exper.	<b><u>-0.005657</u></b>	<b><u>-0.004098</u></b>	<b><u>-0.002299</u></b>	<b><u>-0.000852</u></b>	0.001627	<b><u>-0.000733</u></b>	0.010041	0.013534	0.019188	0.004675	<b><u>-0.000556</u></b>
<b>Mn</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Fe</b>
Theory	<b><u>-0.005522</u></b>	<b><u>-0.004107</u></b>	<b><u>-0.002522</u></b>	<b><u>-0.000826</u></b>	0.001103	0.003149	0.010672	0.013494	0.019920	<b><u>-0.001084</u></b>	<b><u>-0.001559</u></b>
Exper.	<b><u>-0.006075</u></b>	<b><u>-0.004866</u></b>	<b><u>-0.002986</u></b>	<b><u>-0.001859</u></b>	<b><u>-0.000981</u></b>	<b><u>-0.001515</u></b>	0.007847	0.010897	0.015962	0.029651	0.003018
<b>Fe</b>	<b>Na</b>	<b>Mg</b>	<b>Al</b>	<b>Si</b>	<b>P</b>	<b>S</b>	<b>K</b>	<b>Ca</b>	<b>Ti</b>	<b>Cr</b>	<b>Mn</b>
Theory	<b><u>-0.005996</u></b>	<b><u>-0.004745</u></b>	<b><u>-0.003349</u></b>	<b><u>-0.001850</u></b>	<b><u>-0.000151</u></b>	0.001659	0.008298	0.0010801	0.016489	0.023140	<b><u>-0.001048</u></b>

Table 1. Empirical and theoretical influence coefficients. Expanded Table based on Rousseau's publication.<sup>9</sup>

Please note that the negative coefficients are printed in bold, underlined italic font.

		Na	Mg	Al	Si	P	S	K	Ca	Ti	Cr	Mn	Fe	Total	Abs. Deltas
G_1	True Conc.	0.10	4.00	10.00	60.00	0.10	1.00	1.00	10.00	2.50	0.90	0.40	10.00	100.00	0.00
	Th_alphas	0.08	4.02	10.01	60.37	0.12	1.01	1.01	10.07	2.51	0.92	0.39	10.00	100.51	0.51
	Exp_alphas	0.09	4.25	10.07	60.16	0.11	1.01	1.01	10.00	2.50	0.90	0.40	10.05	100.55	0.55
G_2	True Conc.	5.00	1.00	15.00	60.00	0.10	0.10	5.00	5.00	3.00	0.70	0.10	5.00	100.00	0.00
	Th_alphas	4.68	0.99	14.67	59.55	0.12	0.08	5.00	5.02	3.01	0.71	0.10	5.04	98.97	1.03
	Exp_alphas	5.00	0.98	15.05	60.09	0.12	0.08	5.00	4.99	3.00	0.70	0.10	5.05	100.15	0.15
G_3	True Conc.	10.00	0.50	20.00	65.00	0.50	0.50	0.50	0.50	0.50	0.50	0.50	1.00	100.00	0.00
	Th_alphas	9.14	0.50	19.52	63.59	0.49	0.49	0.50	0.51	0.51	0.51	0.50	1.02	97.28	2.72
	Exp_alphas	9.99	0.45	19.98	64.93	0.51	0.51	0.49	0.50	0.50	0.50	0.50	1.02	99.88	0.12
G_4	True Conc.	0.50	0.10	5.00	80.00	0.10	0.10	1.00	2.00	1.00	0.10	0.10	10.00	100.00	0.00
	Th_alphas	0.52	0.11	5.19	80.32	0.13	0.09	1.00	2.01	1.00	0.10	0.10	9.98	100.55	0.55
	Exp_alphas	0.54	0.12	5.13	79.32	0.13	0.09	0.99	2.01	1.00	0.10	0.10	10.00	99.52	0.48
G_5	True Conc.	2.00	25.00	0.10	60.00	0.50	0.10	3.00	3.00	0.50	0.30	0.50	5.00	100.00	0.00
	Th_alphas	1.88	24.83	0.11	59.96	0.52	0.08	3.01	3.01	0.50	0.30	0.50	5.03	99.73	0.27
	Exp_alphas	2.02	25.43	0.11	59.70	0.52	0.08	3.00	3.01	0.50	0.30	0.50	5.01	100.20	0.20
G_6	True Conc.	1.00	50.00	1.00	40.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	100.00	0.00
	Th_alphas	0.91	48.31	1.00	39.26	1.01	0.98	0.99	1.01	1.01	1.01	1.01	1.03	97.53	2.47
	Exp_alphas	1.01	49.88	1.02	39.94	1.00	1.00	0.99	1.02	1.00	1.00	1.00	1.01	99.88	0.12
G_7	True Conc.	2.00	1.00	0.10	35.00	0.30	0.10	0.10	40.00	0.30	0.10	1.00	20.00	100.00	0.00
	Th_alphas	1.97	1.04	0.11	36.21	0.30	0.09	0.11	40.17	0.30	0.10	0.99	19.87	101.26	1.26
	Exp_alphas	1.99	1.05	0.11	35.87	0.29	0.09	0.10	39.99	0.31	0.09	1.00	19.98	100.87	0.87
G_8	True Conc.	0.50	2.00	15.00	75.00	1.00	0.10	1.30	2.00	0.50	0.50	0.10	2.00	100.00	0.00
	Th_alphas	0.46	2.04	15.00	75.07	0.97	0.09	1.31	2.01	0.50	0.51	0.10	2.02	100.08	0.08
	Exp_alphas	0.51	2.22	14.99	74.84	0.98	0.10	1.31	2.01	0.50	0.50	0.10	2.03	100.08	0.07
G_9	True Conc.	2.00	20.00	30.00	40.00	0.10	1.00	0.10	0.50	5.00	0.20	0.50	0.60	100.00	0.00
	Th_alphas	1.79	19.17	29.22	39.40	0.11	0.99	0.10	0.50	5.04	0.20	0.50	0.62	97.64	2.36
	Exp_alphas	2.02	20.19	29.97	40.24	0.11	1.00	0.10	0.50	5.00	0.19	0.50	0.61	100.44	0.44
G_10	True Conc.	2.00	30.00	0.10	0.10	0.20	0.10	0.50	50.00	0.80	0.20	1.00	15.00	100.00	0.00
	Th_alphas	1.96	30.46	0.12	0.13	0.21	0.11	0.51	49.85	0.80	0.20	0.98	14.91	100.24	0.24
	Exp_alphas	2.04	30.29	0.12	0.13	0.20	0.10	0.51	50.00	0.80	0.20	1.00	15.00	100.38	0.38
G_11	True Conc.	0.50	20.00	0.50	50.00	0.10	0.50	0.90	0.50	4.00	1.00	2.00	20.00	100.00	0.00
	Th_alphas	0.50	20.13	0.53	50.30	0.11	0.49	0.90	0.51	4.00	1.03	1.96	19.81	100.27	0.27
	Exp_alphas	0.50	20.41	0.52	50.30	0.11	0.50	0.89	0.51	4.00	1.00	2.00	19.99	100.73	0.73
G_12	True Conc.	0.40	0.40	1.00	95.00	1.70	0.30	0.20	0.20	0.20	0.10	0.10	0.40	100.00	0.00
	Th_alphas	0.40	0.46	1.11	95.74	1.74	0.31	0.20	0.20	0.20	0.11	0.10	0.40	100.97	0.97
	Exp_alphas	0.43	0.53	1.11	95.01	1.70	0.31	0.20	0.20	0.20	0.10	0.10	0.40	100.30	0.29

Table 2. True concentration, computed concentrations with theoretical alphas, and computed concentrations with empirical alphas for standards G1-G12. Expanded Table based on Rousseau's publication.<sup>9</sup>

		Na	Mg	Al	Si	P	S	K	Ca	Ti	Cr	Mn	Fe	Total	Abs. Deltas
G_13	True Conc.	4.00	25.00	10.00	40.00	0.10	0.40	4.00	0.10	0.20	0.20	1.00	15.00	100.00	0.00
	Th_alphas	3.87	24.94	10.09	40.16	0.11	0.40	4.02	0.11	0.20	0.21	0.99	14.93	100.03	0.03
	Exp_alphas	3.98	24.60	9.96	39.87	0.11	0.39	4.00	0.11	0.20	0.20	1.00	14.95	99.38	0.62
G_14	True Conc.	0.10	2.00	1.00	50.00	1.00	0.10	0.10	45.00	0.10	0.20	0.10	0.30	100.00	0.00
	Th_alphas	0.08	1.94	0.96	50.03	1.03	0.10	0.10	44.91	0.11	0.19	0.09	0.31	99.85	0.15
	Exp_alphas	0.08	2.06	1.04	49.74	1.00	0.09	0.10	45.00	0.11	0.20	0.09	0.31	99.81	0.19
G_15	True Conc.	5.00	10.00	5.00	70.00	2.00	0.10	0.30	0.50	3.00	1.00	0.10	3.00	100.00	0.00
	Th_alphas	4.71	10.13	5.15	70.29	2.04	0.09	0.31	0.50	3.00	1.01	0.10	3.03	100.36	0.36
	Exp_alphas	5.00	10.17	5.14	70.04	2.00	0.09	0.31	0.50	3.00	1.00	0.10	3.03	100.39	0.38
G_16	True Conc.	7.00	5.00	25.00	45.00	0.10	0.10	5.00	8.00	0.20	0.10	0.50	4.00	100.00	0.00
	Th_alphas	6.44	4.90	24.27	44.61	0.11	0.12	4.99	8.01	0.21	0.10	0.51	4.06	98.33	1.67
	Exp_alphas	7.00	4.67	24.90	45.24	0.11	0.12	5.00	8.00	0.20	0.10	0.50	4.06	99.91	0.09
G_17	True Conc.	3.00	15.00	10.00	65.00	0.40	1.00	1.50	0.50	0.10	1.00	0.50	2.00	100.00	0.00
	Th_alphas	2.81	14.98	10.20	65.22	0.37	0.99	1.51	0.51	0.10	1.01	0.50	2.02	100.22	0.22
	Exp_alphas	3.00	15.17	10.17	64.87	0.37	1.00	1.51	0.51	0.10	1.00	0.50	2.03	100.22	0.22
G_18	True Conc.	0.50	5.00	20.00	50.00	0.20	2.00	0.10	9.00	1.00	0.10	0.10	12.00	100.00	0.00
	Th_alphas	0.46	5.02	19.85	50.33	0.23	2.03	0.10	9.04	1.00	0.10	0.10	11.99	100.25	0.25
	Exp_alphas	0.47	5.44	19.98	50.14	0.22	2.00	0.10	9.00	1.00	0.10	0.10	11.99	100.54	0.54
G_19	True Conc.	1.00	20.00	0.10	50.00	0.10	0.10	0.10	25.00	2.00	0.10	0.50	1.00	100.00	0.00
	Th_alphas	0.90	19.08	0.10	49.74	0.10	0.11	0.11	24.99	2.00	0.10	0.50	1.02	98.75	1.25
	Exp_alphas	0.99	19.67	0.10	50.38	0.10	0.11	0.11	24.99	2.00	0.10	0.50	1.01	100.05	0.05
G_20	True Conc.	1.50	0.50	15.00	70.00	1.50	0.20	7.50	0.80	0.50	1.00	1.00	0.50	100.00	0.00
	Th_alphas	1.38	0.50	14.64	69.18	1.46	0.18	7.46	0.80	0.50	1.00	1.00	0.50	98.60	1.40
	Exp_alphas	1.49	0.54	14.93	70.31	1.50	0.19	7.50	0.80	0.50	1.00	1.00	0.51	100.25	0.25
G_21	True Conc.	0.20	0.20	18.20	65.00	0.20	0.20	15.00	0.20	0.20	0.20	0.20	0.20	100.00	0.00
	Th_alphas	0.17	0.19	17.16	63.29	0.17	0.21	14.79	0.19	0.20	0.21	0.20	0.20	96.98	3.02
	Exp_alphas	0.19	0.21	18.23	64.91	0.18	0.21	15.00	0.19	0.20	0.21	0.20	0.20	99.94	0.06
G_22	True Conc.	4.00	12.00	10.00	70.00	0.30	0.10	0.10	0.10	0.40	0.50	2.00	0.50	100.00	0.00
	Th_alphas	3.74	12.08	10.27	70.36	0.32	0.09	0.09	0.10	0.40	0.50	1.99	0.50	100.44	0.44
	Exp_alphas	4.01	13.16	10.05	70.27	0.32	0.09	0.09	0.10	0.40	0.50	2.00	0.51	101.49	1.49
G_23	True Conc.	0.10	1.00	1.00	70.00	0.10	0.10	0.10	25.00	0.10	0.10	2.00	0.40	100.00	0.00
	Th_alphas	0.10	1.01	0.99	68.91	0.11	0.12	0.10	24.91	0.10	0.10	2.00	0.40	98.85	1.15
	Exp_alphas	0.11	1.03	1.01	69.46	0.11	0.12	0.10	25.01	0.10	0.10	2.00	0.40	99.55	0.45
G_24	True Conc.	2.00	10.00	5.00	5.00	2.00	1.00	2.00	50.00	1.00	1.00	1.00	20.00	100.00	0.00
	Th_alphas	1.99	10.23	5.19	5.42	2.09	1.04	2.04	50.04	1.00	1.02	0.99	19.86	100.91	0.91
	Exp_alphas	2.00	10.42	5.32	5.34	2.00	1.00	2.00	50.00	1.00	1.00	1.00	20.00	101.08	1.08

Table 3. True concentration, computed concentrations with theoretical alphas, and computed concentrations with empirical alphas for standards G13-G24. Expanded Table based on Rousseau's publication.<sup>9</sup>

		Na	Mg	Al	Si	P	S	K	Ca	Ti	Cr	Mn	Fe	Total	Abs. Deltas
G_25	True Conc.	0.20	2.00	15.00	60.00	0.20	0.50	0.40	20.00	0.10	1.00	0.10	0.50	100.00	0.00
	Th_alphas	0.18	1.93	14.26	59.13	0.22	0.49	0.40	19.92	0.10	1.00	0.09	0.51	98.23	1.77
	Exp_alphas	0.19	2.05	14.92	60.29	0.23	0.49	0.41	19.99	0.10	1.00	0.09	0.51	100.27	0.27
G_26	True Conc.	8.00	1.00	10.00	70.00	0.50	0.10	2.00	0.40	2.50	0.50	0.50	4.50	100.00	0.00
	Th_alphas	7.62	1.03	10.10	69.92	0.50	0.09	2.01	0.40	2.51	0.50	0.50	4.53	99.71	0.29
	Exp_alphas	8.03	0.97	10.15	70.02	0.49	0.09	2.00	0.40	2.50	0.50	0.50	4.54	100.19	0.19
G_27	True Conc.	1.00	1.00	15.00	50.00	1.00	0.10	1.00	5.00	5.00	0.80	0.10	20.00	100.00	0.00
	Th_alphas	0.95	1.01	14.93	50.28	1.01	0.08	1.02	5.05	5.01	0.83	0.10	19.88	100.15	0.15
	Exp_alphas	0.97	1.05	14.88	50.25	1.00	0.08	1.01	5.01	5.00	0.80	0.10	19.98	100.14	0.14
G_28	True Conc.	3.00	2.00	20.00	70.00	0.40	1.00	0.50	0.50	0.40	0.10	0.10	2.00	100.00	0.00
	Th_alphas	2.79	2.02	19.82	69.56	0.39	0.98	0.49	0.50	0.40	0.10	0.10	2.02	99.17	0.83
	Exp_alphas	3.02	2.13	19.98	69.76	0.39	0.99	0.49	0.50	0.40	0.10	0.10	2.02	99.89	0.11
G_29	True Conc.	0.10	30.00	20.00	45.00	0.10	0.10	0.10	2.00	0.10	1.00	0.50	1.00	100.00	0.00
	Th_alphas	0.09	29.10	19.82	44.47	0.12	0.08	0.10	2.01	0.10	1.01	0.50	1.02	98.42	1.58
	Exp_alphas	0.10	29.63	19.96	44.87	0.12	0.09	0.10	2.01	0.10	1.00	0.50	1.03	99.51	0.49
G_30	True Conc.	0.50	30.00	1.00	65.00	0.30	0.10	0.10	0.20	0.20	2.00	0.10	0.50	100.00	0.00
	Th_alphas	0.47	29.71	1.03	64.69	0.31	0.09	0.11	0.20	0.20	2.00	0.10	0.50	99.41	0.59
	Exp_alphas	0.54	30.11	1.02	64.76	0.31	0.09	0.11	0.20	0.20	2.00	0.10	0.51	99.95	0.05
G_31	True Conc.	0.50	2.50	5.00	60.00	0.10	0.20	0.30	15.00	1.00	0.30	0.10	15.00	100.00	0.00
	Th_alphas	0.50	2.53	5.03	60.34	0.11	0.20	0.30	15.06	1.00	0.30	0.10	14.94	100.41	0.41
	Exp_alphas	0.51	2.64	5.05	59.77	0.11	0.20	0.30	15.02	1.00	0.30	0.10	14.99	99.98	0.02
G_32	True Conc.	1.00	6.00	1.00	75.00	0.20	0.10	0.70	10.00	4.00	0.20	1.00	0.80	100.00	0.00
	Th_alphas	0.92	6.02	1.02	74.27	0.18	0.09	0.71	10.02	4.00	0.20	1.00	0.81	99.24	0.76
	Exp_alphas	0.99	6.29	1.04	74.68	0.17	0.09	0.71	10.00	4.00	0.20	1.00	0.81	99.97	0.03
G_33	True Conc.	0.50	40.00	1.00	40.00	0.50	0.20	0.30	3.00	0.20	0.30	2.00	12.00	100.00	0.00
	Th_alphas	0.48	39.68	1.02	40.05	0.49	0.20	0.30	3.02	0.20	0.31	1.97	11.98	99.70	0.30
	Exp_alphas	0.50	39.61	1.00	39.99	0.49	0.20	0.30	3.03	0.20	0.30	2.00	12.02	99.64	0.36
G_34	True Conc.	5.00	20.00	0.10	65.00	0.40	0.30	0.20	5.00	3.00	0.40	0.50	0.10	100.00	0.00
	Th_alphas	4.51	19.50	0.09	63.94	0.41	0.30	0.21	5.01	3.02	0.40	0.52	0.11	98.02	1.98
	Exp_alphas	4.97	19.19	0.10	64.94	0.40	0.30	0.21	5.02	3.00	0.40	0.50	0.10	99.13	0.87
G_35	True Conc.	0.20	20.00	0.50	35.00	0.10	0.10	1.00	30.00	1.00	0.10	2.00	10.00	100.00	0.00
	Th_alphas	0.20	19.73	0.50	35.97	0.09	0.10	1.01	30.12	1.00	0.10	1.99	9.99	100.80	0.80
	Exp_alphas	0.21	19.76	0.50	35.94	0.09	0.09	1.00	30.00	1.00	0.10	2.00	10.04	100.74	0.74
G_36	True Conc.	3.00	0.50	10.00	60.00	0.20	0.10	0.50	5.00	0.10	0.50	0.10	20.00	100.00	0.00
	Th_alphas	2.93	0.51	10.12	60.15	0.18	0.09	0.5	5.03	0.1	0.51	0.09	19.84	100.05	0.05
	Exp_alphas	2.98	0.52	9.99	59.64	0.18	0.09	0.50	5.03	0.10	0.50	0.10	19.97	99.60	0.40

Table 4. True concentration, computed concentrations with theoretical alphas, and computed concentrations with empirical alphas for standards G25-G36. Expanded Table based on Rousseau's publication.<sup>9</sup>

## FINAL CONCLUSIONS

It has been shown that both a theoretical and experimental approach should deliver the same results if the same equation is used in both cases. In the simple case of Ohm's law this is easily demonstrated with rudimentary measurements of current with varying resistances and applied voltage. Calculated values using the statement of the law should be identical to those measured values within the uncertainty of the measurements. This same principle, when expanded to the more complicated case of matrix corrections for XFR systems, also stands. Just as resistance, voltage and current have physical meaning in electrical measurements as well as in the statement of the Ohm's law equation, alphas calculated by regression analysis have just as much physical meaning as those calculated theoretically.

## ACKNOWLEDGMENTS

Thanks are due to Gerald R. Lachance for his friendly consultations and for the selection of theoretical material to be analyzed in order to check the performance of the method described in this paper.

The author would like to acknowledge the support of Robert F. Craig, Manager of the OSRAM SYLVANIA Technical Assistance Laboratory during development of this project and thanks to Dr. Dennis B. Shinn, Manager of the OSRAM SYLVANIA Technical Services Laboratory for critical remarks as well as for reviewing the manuscript.

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