

Simulation Methods to Treat Some Factors

Affecting Atomic Absorption measurements

Wafaa.M. Mousa,* Amr.M. Khairat, Shereen.N. Mohamed

Physics Department, Gilr's College,*Faculty of science

Ain Shams University,Cairo, Egypt.

Abstract

Flame atomic absorption spectroscopy (FAAS) is used to quantitatively determine trace metals in the test samples. The purpose of the present study is to treat some of the factors affecting AAS measurements. Some of the factors are under the control of the operator while other factors depend on the used equipment. In the present work equipment was used with low detection limits and high sensitivity but still some factors can't control. Using simulation methods to treat some of these measurements, obtain an estimate of the predicted concentration values for test samples. Two methods of simulation are investigated. The first simulation method is carried out by using line-of-best-fit through the experimental points using Excel programmed and using TREND function to estimate the unknown concentration directly from this calibration function. The second simulation method is based on the approximation programme which is built-in the concept of genetic programming (GP). This is carried out by the introduction of laboratory results of the known concentrations versus the absorption of known elements and finds the best curve of the approximate of each element. The results were rounded up to the laboratory results of most elements with low concentrations, the improvements of the methods were very satisfying and the results reached the imposed limits ($A < 0.05$). Finally, a database was created for all results.

Key words: FAAS, trace element, treat factors, genetic programming, Simulation methods, atomic absorption.

Corresponding author: shereennassef4@gmail.com

1-Introduction

FAAS is used to determine quickly and quantitatively analysis of some metals in the range of a few micrograms per gram or milliliter of tested samples with a good accuracy. Under certain conditions Beer–Lambert law fails to maintain a linear relationship between absorption and concentration.

$$A=\alpha LC$$

$$\text{Or } T = I/ I_0$$

$$A = -(\log I/I_0) = \log \frac{1}{T} \quad \%$$

Where α is the absorption coefficient, L is the path length of the sample which equal 1, T is transmitted beam, I is transmitted intensity, I_0 is the original intensity and C is the concentration of the sample. For optimal measurement results and to comply with the Lambert-Beer Law, the absorbance shall be in the linear range of the instrument.

At very low concentrations, the readings of absorbance can be fluctuating due to the limited resolution of the readout display or because of the signal-to-noise ratio of the light intensity measurement (due to detector noise, photon noise, or light source fluctuation). The suitable range for optimal measurements i.e. the measurement range where the absorbance is directly proportional to the concentration is given as $0.3 < A < 2.5$. Thus, it is recommended to avoid very high absorbance values ($A > 2.5$) as well as very low absorbance values ($A < 0.3$) which may lead to a non-linear behavior of the calibration line. (Mettler,2016).

The present study concentrates on some factors affecting atomic absorption measurements. A sensitive equipment was used with low detection limits to treat some of these factors as follow, the effect of temperature (Boltzmann Equation). By small changes in flame temperatures (~ 10 K) have little effect in atomic absorption but have significant effects in atomic emission spectroscopy. It can be overcome by control Flame temperature for example (nitrous oxide / acetylene instead air / acetylene) (Perkin-Elmer, 2002). A line broadening effect which is a spectral line from any source, or from any absorption or fluorescence cell, will be broadened, the most common broadening effect such as natural broadening, Doppler broadening, Lorentz broadening and self absorption broadening. Chemical interference due to the resonance wavelength may sometimes be dependent on components in the sample solution (Erleben, 2009). This type of interference can be overcome by using higher flame temperature, or by adding releasing agent and/or by adding chelating agent. Ionization interference due to the formation of ions rather than atoms lowers absorption of radiation. Alkali metal ions have lowest ionization energies and are therefore easily ionized in flames. Ionization interference can be overcome by adding ionization suppressors. Physical interferences may arise from differences

between physical properties of samples and standard solutions for calibration curve such as sample viscosity, density, surface tension, It can be overcome by avoiding differences in the amount of sample and standard reaching the flame. It is necessary that the physical properties of both be matched as closely as possible. Spectral interferences due to line overlap is very rare in atomic absorption spectrometry. It can be overcome by either separation of elements or by use of an alternative wavelength. In the present work atomic absorption spectroscopy which has low spectral interference. Background absorption and background correction refers to the relatively small number of atomic absorption lines, the effect can be overcome by one of the following techniques: using Deuterium Lamps for background correction purposes, using an alternating magnetic field (Zeeman-effect) applied at the atomizer (graphite furnace), using solvent extraction to remove the element from the interfering matrix, also repeating the determination at a nearby non absorbing line and subtracting the scatter reading from the signal obtained at the absorbing line. **(García and Báez, 2012).**

If we could overcome most of these interferences, still some factors cannot be controls which are the reasons for non-linearity (deviations from Beer- Lambert law) of calibration graphs; these effects can be overcome by using simulation methods to treat its measurements. Such as unabsorbed radiation, stray light must be absorbable to the same extent, unequal light path lengths across the light beam, hollow-cathode lamp line width broadening due either to the age of the source or the use of high lamp currents, also disproportionate decomposition of molecular species at high concentration this results in a lower proportion of free atoms being available at higher concentration for a constant atomization temperature, Polychromatic light effect, which occurs if the absorber's absorption coefficient α varies over the wavelength interval of light passing through the sample and varies as a function of wavelength, temperature, solvent, PH, and other chemical conditions. Change in PH as a function of concentration, change in refractive index of the solution at high analytic concentration **(Mettler, 2016).**

2-Materials and Methods

2.1-Instruments

FAAS is used to analysis of samples was performed using thermo elemental atomic spectrometer S4 to determine the concentration of (Fe, Mg, Mn, Ni, Zn and K) sample. The operating conditions for elements measured by this technique were given in table (1). The elements were determined using air-acetylene flame. Table(1) operating conditions for elements measured by FAAS.

Element	Wave length (nm)	Lamp current (mA)	Burner height (mm)	Fuel flow (L/min)	Band pass (nm)
Fe	248.3	15	5.4	0.8	0.2
Mg	285.2	4	7	1	0.5
Mn	279.5	12	7	1	0.2
Ni	232.0	15	4.9	0.8	0.2
K	766.5	8	3.8	1.2	0.5
Zn	213.9	10	4.7	1	0.5

2.2 Sample Preparation

The elements (Fe, Mg, Mn, Ni, Zn and K) were analyzed by FAAS in three types of different samples, sediment samples collected from Suez canal, Egypt at different depths, digested by using HNO₃, H₂SO₄ and HF acids, fertilizers samples (urea, onium phosphate, super phosphate, organic and nitrogen) collected from different Egyptian markets and industries, digested by using HCL or mixture of HCL + HNO₃ and HF acids and plants samples (fruit and vegetable) collected from plants in Cairo, Egypt digested by using HNO₃, H₂SO₄ and HF acids.

2.3 Prepared of Standard Solution

Standard solutions were prepared from stock solution containing 1000 µg/ml, were purchased from Merck for each element. This stock solution was diluted with distilled water once to give different concentrations ranging from 0.25 to 10 ppm of different elements. The standard solutions were freshly prepared.

2.4 Sensitivity

The sensitivity is the concentration of an element in milligrams per liter required to produce a 1% absorption (0.0044 absorbance) signal.

$$\text{Sensitivity (mg/L)} = \frac{\text{Conc. of std. (mg/L)} \times 0.0044}{\text{Measured absorbance}}$$

As long as measurements are made in linear working region, the sensitivity of an element can be determined by reading the absorbance produced by a known concentration of the element and applying the above equation (Jams and Ishwar, 1993).

2.5 Analytical Calibration Curves

The standard solutions were used to construct the calibration curves of the elements. The PH value for the standard solution, the samples and blank were adjusted to the same value. Under the optimal condition, the absorbance was determined for (Fe, Mg, Mn, Ni, Zn and K) then absorbance were plotted against the concentration. Fig.(1) shows an example for the obtain calibration curve for K and Mg. It was observed from fig.1 that the line is curved by increasing the concentration of standard solution.

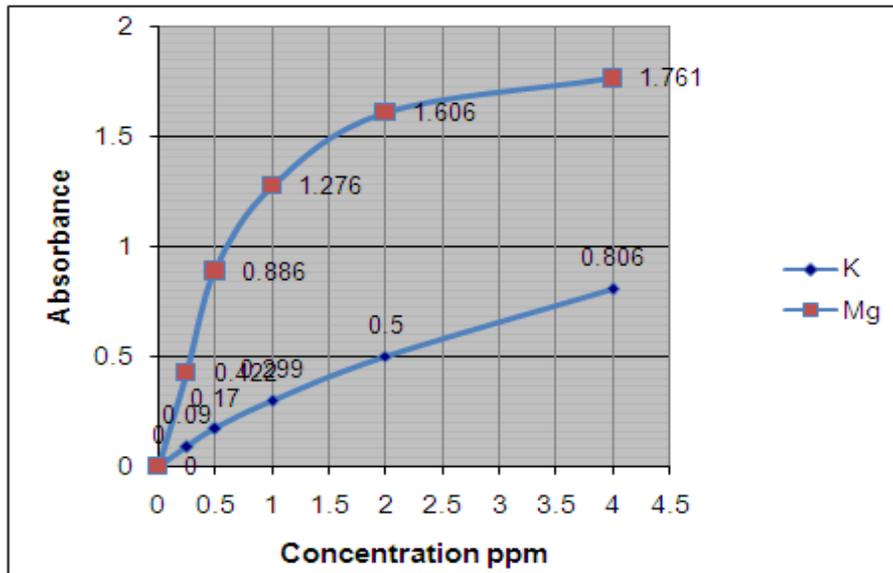


Fig.(1) Calibration Curve for Ka and Mg

The calibration data are judged to be satisfactory the calibration equation (i.e., the gradient and the intercept) can be used to estimate the concentration of the analyte in test samples, the prediction interval gives an estimate of the uncertainty associated with predicted values of x(concentration) and is illustrated in Fig.(2). (Lehtonen and Sihvonen, 2006)

The standard deviation (standard error), describes the dispersion of the measurements around the mean value. The standard deviation of the individual measurement describes also the precision of the measurements Standard deviation(S) of the absorbance were calculated as:

$$s(r) = \sqrt{\frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n - 1}}$$

Where y_i is measured values of y for a given value of x_i , \hat{y}_i is the predicted value by the equation of calibration line for a given value of x_i and n = the number of measurements.

The relative standard deviation (RSD) (Barwick ,2003).

$$(\%)RSD = \frac{\text{st.dev}}{\text{mean}} \times 100\%$$

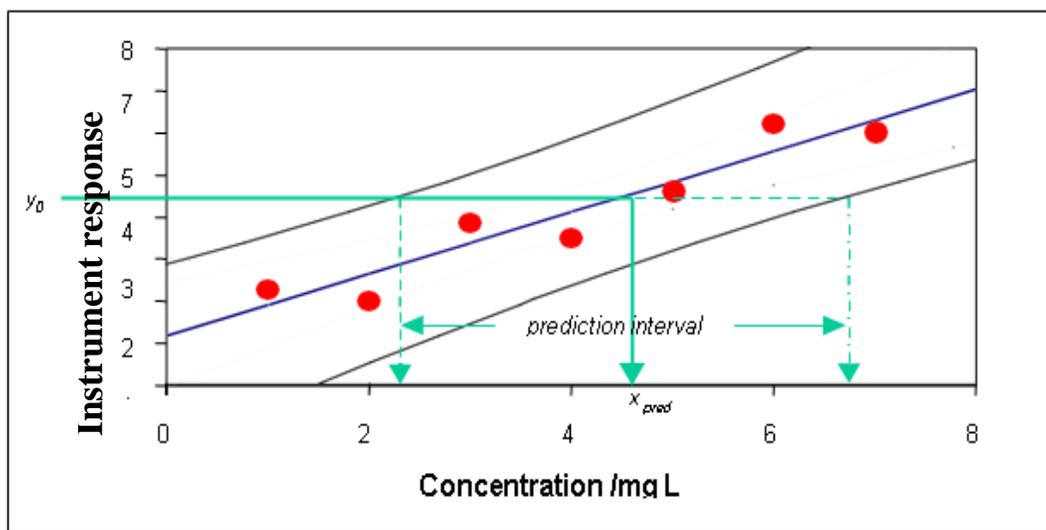


Fig.(2) the prediction interval for x and y

A residual is the difference between an observed y value, and the y value calculated using the equation of the fitted line. The residuals give an indication of how well the line fits the data.

3-Results and Discussion

A set of six standards were prepared then the absorbance for each standard sample is measured. The experimental result shows that the samples have absorbance greater than the working curve for K and Mg for an example.

In this case, the calculated concentration of sample will not be accurate by using the line equation obtained from the Beer's Law plot and can't be calculate for any dilutions carried out, (according to the matrix effect),which taken from the AAS user guide (Mettler,2016). So by using some experimental results for three type of samples such as sediment samples collected from Suez canal (Fahmy, 2006), different fertilizers consumed in Egypt (Mousa et al., 2014) and plants sample. Under the same optimal condition, the sample solutions were nebulized and the absorbance was determined. Concentration in ppm of K and Mg elements for fertilizers sample, plants sample and sediment Sample with different simulation methods are tabled in table (2).

Table (2): Concentration in($\mu\text{g/ml}$) ppm of K and Mg elements for fertilizers sample, plants sample and sediment Sample .

Fertilizers Sample no.	Measurement by AAS	
	K	Mg
F1	44.1	0.6544
F2	2.33	3.20941
F3	6.8	4
F4	52.02	2.073
F5	0.23	0.991
F6	0.390	2.85
F7	0.2	0.016
F8	0.4	3.604
Plants Sample no.	K	Mg
1	11.06	1.796
2	15.01	6.275
3	15.8	5.0457
4	11.12	0.8769
5	13.25	2.3954
6	10.999	2.551
sediment Sample no.	Measurement by	Measurement by
	Flame photometry	UV-VIS
	K	Mg
1	10.036	1612.95
2	10.864	1497.35
3	9.683	1656.55
4	10.174	2500
5	10.547	1504.55
6	9.6	942.55
7	11.572	1719.8
8	10.864	1656.1
9	10.817	1534.25
10	11.386	1690.5

3.1 Estimating the uncertainty in predicted concentrations by Using MS EXCEL Programme to fit curves

Using MS Excel programme to enter and graph the data, linear regression simply calculates the values for m and b that minimize the sum of the squared residuals. For this reason, this type of regression is often referred to as, “least squares regression” (Barwick, 2003).

Fig.(3), shows the analytical curves for K with Linear fit as an example. The fit-equation is $y=mx+b$, the predicted concentrations by the fit-equation is $x=(y-b)/m$ or using TREND function to estimate the unknown concentration directly from this calibration function. Where x is concentration(C), y is absorbance (A) and (m,b)are constant .

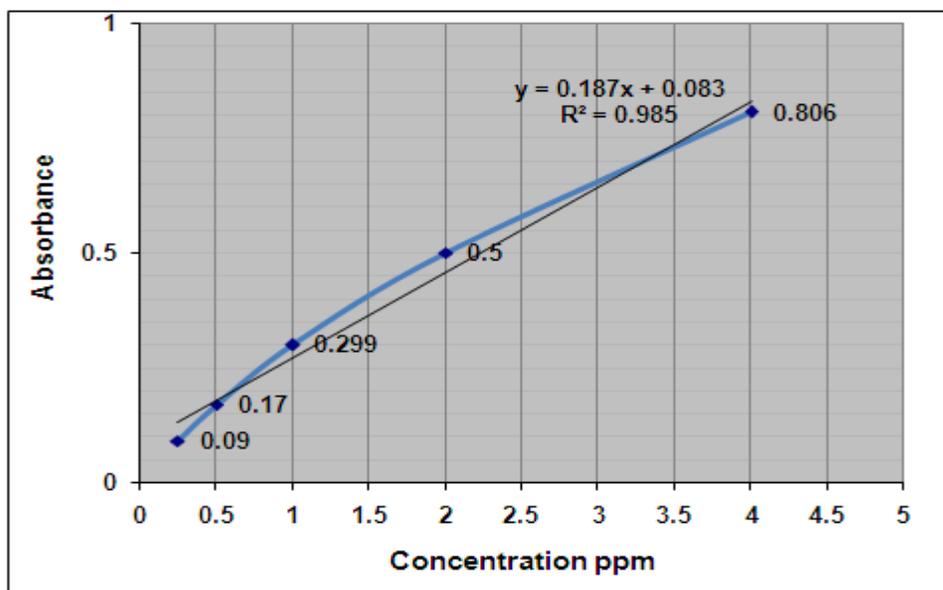


Fig.(3)analytical curves for K with linear fit

The correlation coefficient, (r^2) is a measure of the strength of the degree of correlation between the y and x values. From fig.(3) $r^2 = 0.985$, this gives an idea of the error that is caused by the slight residual non-linearity of the calibration curve (Emeritus and O’haver,2008). The residual plots for the improved method of the K as an example are shown in fig.(4).

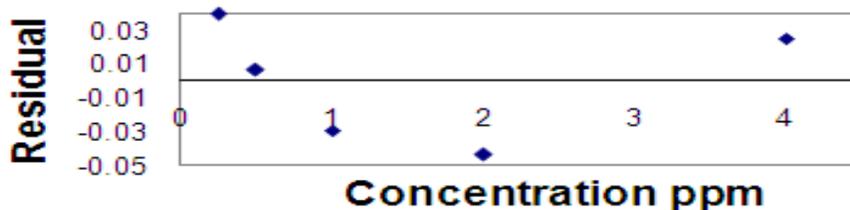


Fig.(4) The residual plots for K with linear fit

Second method to improve r2 by using quadratic fit, Fig.(5) shows the analytical curves for K with quadratic fit as an example. The equation is $y = a*x^2 + b*x + c$, estimate the predicted concentrations by the fit-equation of calibration line, namely

$$x = \frac{-b + \sqrt{b^2 - 4*a*(c-y)}}{2*a}$$

Where x is concentration(C), y is absorbance (A) and (a,b,c) are constant .

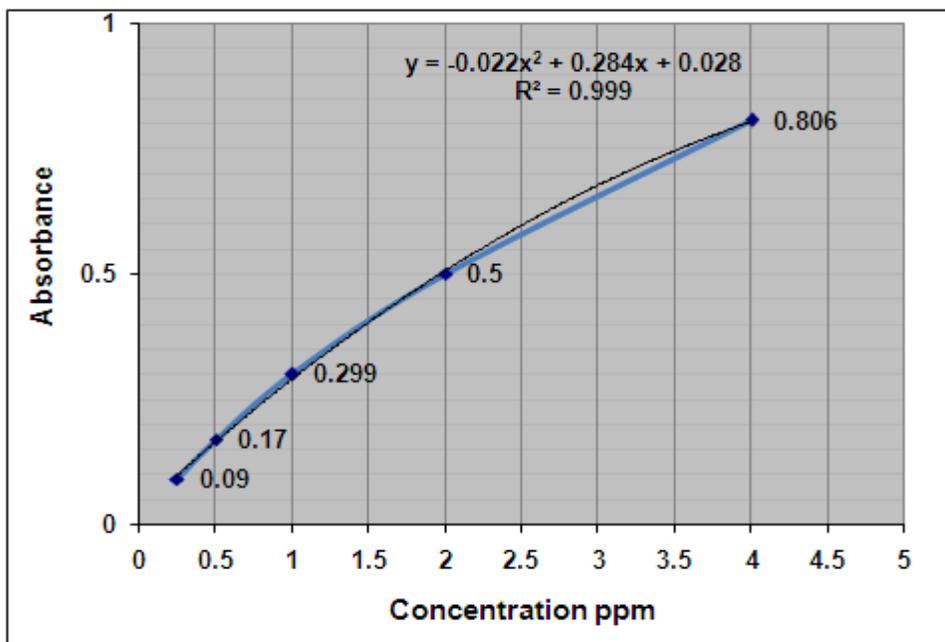


Fig.(5) analytical curves for K with quadratic fit

From fig.(5), $r^2 = 0.999$ which approximates the perfect value 1 and improvement of fitting methods, The unknown concentrations (con.), unknown absorbance (abs.) results for Excel programme are tabled in table (3).

3.2 Estimating of Concentration by Using Approximation programmed built-in with genetic programming (GP) concept

Recently, different modeling methods, based on soft computing systems, include the application of Artificial Intelligence (AI) Techniques. Those Evolution Algorithms have a physical powerful existence in the physics (Cohen et al., 2003). Due to the nonlinear relationship between the interaction parameters and the output, the behavior of the interactions often becomes complicated. To understand the interactions of multipart data analysis are needed and (AI) techniques are vital (Teodorescu and Sherwood, 2008). Those techniques are

becoming useful as alternate approaches to conventional ones. In this sense, AI techniques, such as Genetic Programming (GP), and Gene Expression Programming (GEP), can be used as alternative tools for the simulation of these interactions (Ferreira et al., 2006).

The GP is a Global Optimization algorithm and an Automatic Programming technique that had been applied in Physics. It is a recently developed Evolutionary Computation (EC) method for function discovery and data analysis (Schmidt and Lipson, 2009). GP is established on the assumption of Darwin's theory of evolution in nature. GP uses population of individuals, selects them according to fitness, and produces genetic variation using one or more genetic operators (Koza, 1992). The motivation of using a GP approach is its learning algorithm that learns the relationships between variables in sets of data and then builds models to explain these relationships (mathematically dependence) (Whiteson and Whiteson, 2009).

Approximation programmed built-in with genetic programming (GP) concept to calculate the unknown concentration from equation, which different for each element. Fig.(6) Shows the GP result for K as an example, from fig.(6) the equation of GP for K as an example is ($y=x/(x+2)$), where x: concentration of any element, y: absorbance of any element. The unknown concentrations (con.GP), unknown absorbance (abs.GP) results for GP programme are tabled in table (3).

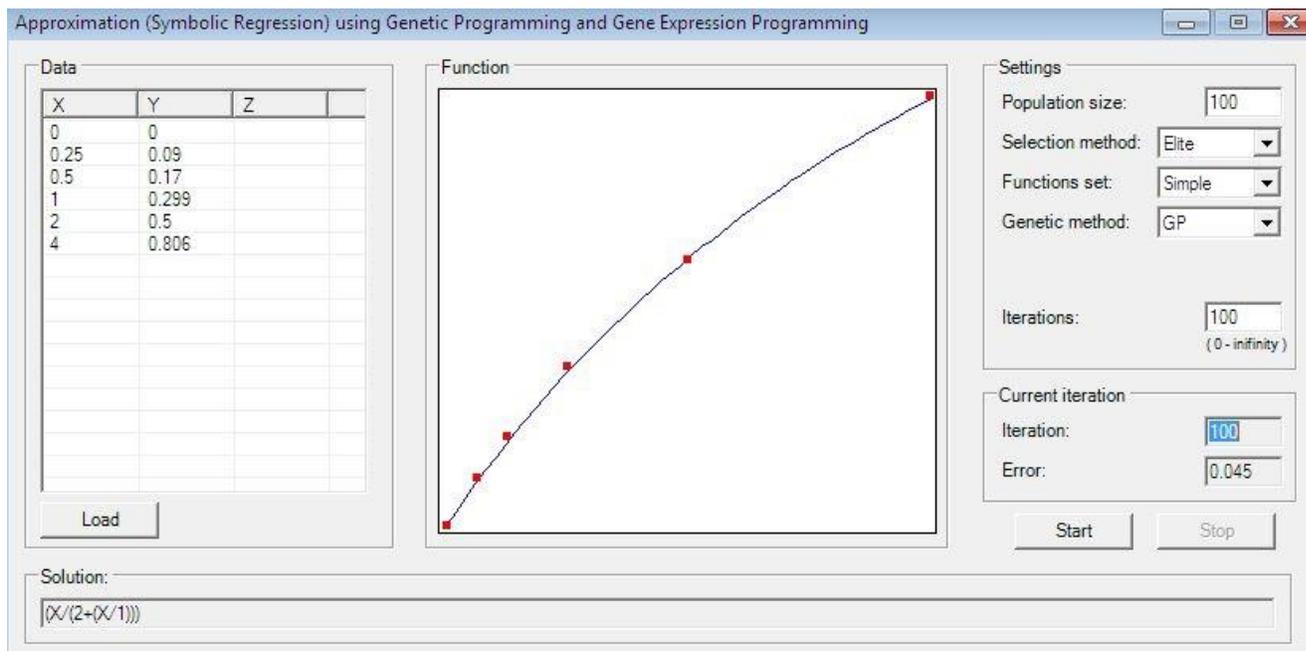


Fig.(6) shows the GP result for K

3.3 Comparison of results between different simulation methods

The concentration in ($\mu\text{g/ml}$) ppm, absorbance results for standard elements for three measurements with different simulation methods are tabled in table (3).

Table (3): The concentration in ($\mu\text{g/ml}$) ppm, absorbance results for standard elements for three measurements with different simulation methods.

Con. of standard (x)	Fe					Mn				
	Con.(x) by (fitting)	Con.(x) by (GP)	Abs.(y) by (AAS)	Abs.(y) by (fitting)	Abs.(y) by (GP)	Con.(x) by (fitting)	Con.(x) by (GP)	Abs.(y) by (AAS)	Abs.(y) by (fitting)	Abs.(y) by (GP)
0.25	0.22	0.12	0.005	0.0062	0.01	0.26	0.27	0.064	0.063	0.08
0.5	0.44	0.36	0.015	0.017	0.020	0.52	0.47	0.106	0.103	0.15
0.625	0.72	0.672	0.028	0.023	0.026	—	—	—	—	—
1	1.04	1.008	0.042	0.040	0.041	1.091	0.91	0.198	0.18	0.3
1.25	1.38	1.392	0.058	0.051	0.052	1.27	0.73	0.227	0.22	0.36
1.75	1.97	2.04	0.085	0.074	0.072	—	—	—	—	—
2	2.13	2.184	0.091	0.086	0.083	2.15	2.33	0.369	0.34	0.54
2.5	2.71	2.856	0.119	0.10	0.10	2.50	1.49	0.427	0.42	0.65
3.5	3.52	3.744	0.156	0.154	0.145	—	—	—	—	—
4	4.00	4.2	0.175	0.177	0.16	4.05	4.14	0.676	0.66	0.92
5	5.00	5.28	0.22	0.22	0.20	—	—	—	—	—
7	6.44	6.84	0.285	0.31	0.29	—	—	—	—	—
8	—	—	—	—	—	6.51	5.09	1.085	1.30	1.41
10	9.11	9.72	0.405	0.45	0.41	6.97	5.57	1.148	1.63	1.57
Con. of standard (x)	K					Mg				
	Con.(x) by (fitting)	Con.(x) by (GP)	Abs.(y) by (AAS)	Abs.(y) by (fitting)	Abs.(y) by (GP)	Con.(x) by (fitting)	Con.(x) by (GP)	Abs.(y) by (AAS)	Abs.(y) by (fitting)	Abs.(y) by (GP)
0.25	0.15	0.24	0.09	0.12	0.11	0.29	0.24	0.422	0.790	0.33
0.5	0.48	0.49	0.17	0.17	0.2	0.67	0.50	0.886	0.867	0.6
0.625	—	—	—	—	—	—	—	—	—	—
1	1.16	0.85	0.299	0.27	0.33	1.75	1.12	1.276	1.021	1
1.25	—	—	—	—	—	—	—	—	—	—
1.75	—	—	—	—	—	—	—	—	—	—

2	2.21	2	0.5	0.45	0.5	2.54	2.20	1.606	1.32	1.5
2.5	—	—	—	—	—	—	—	—	—	—
3.5	—	—	—	—	—	—	—	—	—	—
4	3.83	4.30	0.806	0.83	0.66	2.92	3.32	1.761	1.94	2
5	—	—	—	—	—	—	—	—	—	—
7	—	—	—	—	—	—	—	—	—	—
8	4.37	20.22	0.91	1.57	0.8	3.19	3.32	1.873	3.17	2.4
10	—	—	—	—	—	—	—	—	—	—
Con. of standard (x)	Zn					Ni				
	Con.(x) by (fitting)	Con.(x) by (GP)	Abs.(y) by (AAS)	Abs.(y) by (fitting)	Abs.(y) by (GP)	Con.(x) by (fitting)	Con.(x) by (GP)	Abs.(y) by (AAS)	Abs.(y) by (fitting)	Abs.(y) by (GP)
0.25	0.12	0.29	0.055	0.074	0.047	0.162	0.25	0.02	0.025	0.02
0.5	0.41	0.52	0.095	0.10	0.090	0.482	0.47	0.038	0.039	0.04
0.625	—	—	—	—	—	—	—	—	—	—
1	1.13	1.18	0.192	0.175	0.166	1.10	0.91	0.073	0.067	0.08
1.25	—	—	—	—	—	—	—	—	—	—
1.75	—	—	—	—	—	—	—	—	—	—
2	2.24	2.62	0.344	0.30	0.28	2.04	1.27	0.126	0.123	0.16
2.5	—	—	—	—	—	—	—	—	—	—
3.5	—	—	—	—	—	—	—	—	—	—
4	3.83	4.26	0.56	0.57	0.44	3.95	4.21	0.233	0.235	0.32
5	4.33	8.47	0.629	0.71	0.5	—	—	—	—	—
7	—	—	—	—	—	—	—	—	—	—
8	5.21	14.92	0.749	1.11	0.61	—	—	—	—	—
10	5.56	19.63	0.797	1.38	0.66	—	—	—	—	—

Con. : Concentration of any element.

Abs. : Absorption of substance

Concentration in ppm of K and Mg elements for fertilizers sample, plants sample and sediment Sample with different simulation methods ,measurement by AAS techniques for all elements while measurement by flame photometry for K in sediment sample and UV-VIS spectrophotometer for Mg in sediment sample ,are tabled in table(4).

Table (4): Concentration in ppm of K and Mg elements for fertilizers sample, plants sample and sediment Sample with different simulation methods.

by AAs technique	fertilizers sample	No.	Measurement by AAS		Estimating by TREND Function		Estimating by Approximation programmed	
			K	Mg	K	Mg	K	Mg
		1	44.1	0.6544	43.20	0.660	27.36	0.364
		2	2.33	3.209	2.322	2.75	1.415	2.77
		3	6.8	4	6.78	3.317	4.195	4.57
		4	52.02	2.073	51.58	1.95	32.11	1.43
		5	0.23	0.991	0.22	1.072	0.1105	0.62
		6	0.39	2.85	0.39	2.49	0.212	2.24
	7	0.2	0.016	1.816	0.0075	1.1	0.042	
	8	0.4	3.64	0.412	3.036	0.225	3.52	
	Plants Sample		K	Mg	K	Mg	K	Mg
		1	11.06	1.79	6.499	2.43	8.38	2.16
		2	15.01	6.275	8.00	3.11	5.34	3.17
		3	15.8	5.045	8.30	3.04	5.04	3.04
		4	11.12	0.876	6.52	1.58	8.28	1.34
		5	13.25	2.39	7.33	2.68	6.24	2.48
6	10.99	2.551	6.47	2.72	8.47	2.54		
by two different technique	sediment sample	No.	Measurement by Flame photometry	Measurement by UV-VIS	Estimating by TREND Function		Estimating by Approximation programmed	
			K	Mg	K	Mg	K	Mg
		1	10.62	403.6	12.2480	402.8637	11.0892	528.7664
		2	11.5	807.2	13.1280	805.7297	11.8675	1057.509
		3	10.25	2522.5	11.8780	2517.910	10.7620	3304.669
		4	10.5	2018	12.1280	2014.327	10.9831	2643.740
		5	12.75	1816.2	14.3780	1812.894	12.9731	2379.368
		6	11	2018	12.6280	2014.327	11.4253	2643.740
		7	12.25	908.1	13.8780	906.4462	12.5309	1189.695
		8	11.5	1311.7	13.1280	1309.312	11.8675	1718.439
	9	11.5	1210.8	13.1280	1208.595	11.8675	1586.253	
10	12	1614.4	13.6280	1611.461	12.3098	2114.996		

4-Conclusion

- Flame atomic absorption spectrometry (FAAS) was used to determine the concentration of some elements with a good accuracy and sensitivity.
- Once for optimal measurement results and to comply with the Lambert- Beer's Law, unknown concentration of solutions can be measured using the calibration curve. If Beer's Law is deviation, two different simulation methods are used to treat and determine the unknown concentration of samples. These methods which are used GP (a global optimization algorithm), fit linear equation and TREND function.
- The measured standard solutions of elements by AAS technique are a good agreement with the two different simulation methods with each other at low concentration, The improvements of the methods were very satisfying and the results reached the imposed limits ($A < 0.05$).
- In spite of the low concentration of elements was varied between (0.25 and 4 ppm) is a good agreement with GP method and AAS technique, but not agree in high concentration.
- At high concentration of some standard elements above (4 ppm) the K and Mg for direct or by dilutions the measurements are not accurate according to some factors affecting on AAS technique, sensitivity of these elements and for this reason the simulation method must be used.
- The results by fitting method for K, Mg as an example on high concentration are a good agreement with the results by two different techniques (Flame photometry and UV-VIS spectrophotometry) which avoid the factors affecting on the measurements, this show the validity of fitting method on AAS at high concentration.
- The residual standard deviation is used as an estimate of the uncertainty in predicted concentration values, rather than carrying out the full standard error of prediction calculation.

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الملخص العربي

أ.م.د./ عمرو محمد محمود خيرت
أستاذ مساعد الفيزياء النظرية
بكلية العلوم جامعه عين شمس

أ.م.د./ وفاء محمود موسى
أستاذ مساعد فيزياء الاطياف
بكلية البنات للأداب والعلوم والتربية
جامعه عين شمس

يستخدم طيفي الامتصاص الذري للتحديد الكمي للمعادن في العينات المختبرة. و هناك بعض العوامل التي تؤثر على قياسات الامتصاص الذري والتي يتم التحكم فيها عن طريق المشغل ، كما يوجد عوامل أخرى تعتمد على الجهاز المستخدم في التعيين. في هذا البحث تم استخدام جهاز ذو حساسية عالية لتعيين وتحديد دقيق للتركيزات المنخفضة ، ولكن لا تزال بعض العوامل التي لا يمكن السيطرة عليها. باستخدام طرق المحاكاة لعلاج بعض هذه القياسات وتعيين التركيزات العالية للعناصر الغير معروفة للعينات المستخدمة الطريقة الاولى للمحاكاة باستخدام برنامج اكسيل وتحديد افضل خط يمر بالنقاط العملية واستخدام دالة تريند لحساب التركيز غير المعروف مباشرة من هذه الدالة. طريقة المحاكاة الثانية باستخدام برنامج مبنى على مفهوم البرمجة الجينية عن طريق ادخال النتائج العملية للتركيزات المعلومة مقابل الامتصاص لعناصر معروفة وإيجاد افضل منحني تقريبي لكل عنصر. ومن خلال استخدام تلك الطرق للمحاكاة وجدت النتائج مقربة للنتائج العملية لمعظم العناصر ذات التركيزات المنخفضة ، كما وجد استخدام الطريقة الاولى للمحاكاة جيدا مع التركيزات العالية ، واخيرا تم إنشاء قاعدة بيانات لكل النتائج .