

# Computer Modelling of the Concentration of Heavy Metals in Artificial Borings

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**Abstract** This study describes the computer modelling of the concentrations of some heavy metals; Fe, Zn, Cd, Cu and Pb in a deep well, undertaken to simulate the subsequent concentrations of the metals with respect to the passage of time. This was with the view of providing further insight to the possibility of bio-accumulation and or bio-degradation of these heavy metals in the wells. With the aid of the Minitab computer software, time-series models (time-dependent) and multi-regression models (pH and temperature-dependent) were developed for each metal using quarterly measurements of concentrations obtained from spectrophotometric analysis of these heavy metals for a period of two years. The obtained models were of the form  $y = a + bt - ct^2$  (time-series or time-dependent) and  $y = a + b[\text{pH}] + c[\text{T}^\circ\text{C}]$ . These models were shown to be reliable from statistical analysis at 95% confidence interval. Finally, by simulating the concentrations of the heavy metals from the respective models, it was found that bio-accumulation was on the increase in Cu and Cd while bio-reduction or bio-degradation was the case with Fe, Zn and Pb. This observation was a clear indication that underground seepage activities were going on, contrary to the believe, especially by rural dwellers, that borehole (deep well) water was very pure and fit for drinking.

**Keywords:** *bio-accumulation, bio-degradation, heavy metals, minitab, time-series model, pollution*

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## 1. Introduction

Most developing nations, chiefly in Africa, have been facing the problem of access to portable drinking water due probably to the short-comings of their respective governments. Drinking water is often collected at springs, extracted from artificial borings in the ground or wells. Building more wells in adequate places is thus a possible way to produce more water, assuming the aquifers can supply an adequate flow [1]. This fact has been so exploited leading to the proliferation of boreholes in major cities and villages without recourse to the contributions of both the environmental and industrial impact on these wells. Even in developed nations like the United States, over half of the population receive their water from private ground water wells. Environmental Protection Agency (EPA) regulations that protect public drinking water systems do not apply to privately owned wells, requiring private owners to be responsible for ensuring that their water is safe from contaminants [2]. Consequently, there may be a continuous consumption of impure or contaminated deep well water under the false notion of consuming portable water or as a result of lack of resources to carry out test and periodic cleaning [3] and [18].

Furthermore, people had over the years believed that the soil and sediment layers deposited above an equifer acted as a natural filter that kept many unnatural pollutants from the surface from infiltrating down to ground water. However, by the 1970s, this erroneous believe was jettisoned upon the realisation that this was not necessarily so. Scientists have also realised that once an aquifer becomes polluted, it may become unusable for decades, and is often impossible to clean up quickly and inexpensively, [4,16]. Several sources of ground water pollution exists [17]. Ground water pollution can be caused by seepage through landfills, failed septic tanks, underground fuel tanks, fertilizers and pesticides, and runoff from urban areas. However, the pollutants of interest in this research study are the heavy metals which come chiefly from the underground rocks and soils.

These may contain arsenic, cadmium, chromium, lead, selenium, copper and nickel, and they remain very common sources of heavy metals occurring naturally in drinking water or wells [5]. These pollutants are non-conservative in nature and their concentrations depend on salinity and pH, which may vary with time and along a river. As a result, the dissolved metal may come out of solution or even redissolve, depending on conditions at that time or channel [6]. It has been reported by [7] that the adverse alteration of water quality presently produces large scale illness and deaths, accounting for approximately

50 million deaths per year worldwide, most of these deaths occurring in Africa and Asia.

Such concerns in recent years, have necessitated the development of computer models that predict the level of pollutants in natural water systems. The main attraction of such models, in contrast with physical models, is their low cost and their ease of adaptability to new situations. Thus the widespread popularity of mathematical modelling techniques, justifies any attempt to develop new models based on novel and rigorous approaches. In other studies by [8,9] and [10,11,12] assumed a constant reaction coefficient with time, whereas in the field, this coefficient may vary according to the changes in pH, salinity, temperature or even other chemical substances and other hydraulic characteristics of the river.

This research was therefore aimed at developing suitable mathematical models using specialised computer softwares such as the Minitab for predicting the levels of such heavy metals in deep wells or boreholes and thereby ascertaining the safety of the water. However, computer-based tools used for predicting such heavy metal concentrations are still used infrequently, even though they can support decision-making by the regulatory authorities, marine environment agencies and industry [13]. Such tools like the Minitab statistical software which offers you an extensive utilization of multivariate analysis, time-series, cross-tabulations, simulations and distributions. Others are; high-resolution graphics, which enables you to produce a comprehensive array of graphs and simple data analysis graphs, to impressive, presentation quality graphs, including 3D graphs.

In Minitab, Pareto charts, statistical process control charts, process capability graphs, probability plots, analysis of means, and cause-and-effect (fishbone) diagrams have also been improved. The design of experiment capabilities allows you to generate and analyze full and fractional designs, response surface, and mixture and custom designs, [14]. This soft ware, with an array of the above highlighted capabilities was used to generate the pollution models.

## 2. Methodology

### 2.1. Sampling

Borehole water was sampled in Kassa-Mines area, in Jos, Jos North Local Government Area, Plateau State. The samplings were carried out quarterly from July 2010 to April 2012. Water samples were collected in plastic bottles previously washed, soaked in 10% HNO<sub>3</sub> overnight and rinsed with de-ionized water before use. During sampling, sample bottles were rinsed three times with the sampled water and then filled after a five minutes runoff was allowed from the tap. The samples were labelled and taken to the Department of Chemistry Laboratory, University of Jos for analysis.

### 2.2. Sample Preparation

All reagents used were of analytical grade and distilled water was used for all the preparations. Water samples were filtered using Whatman No. 41 filter paper to remove any suspended particles. 100cm<sup>3</sup> of the filtrate was transferred into a beaker and 5cm<sup>3</sup> concentrated HNO<sub>3</sub> was added. The beaker with the content was placed on a hot plate and evaporated down to about 20cm<sup>3</sup>. The beaker was covered with a watch glass and returned to the hot plate. The heating was continued, and then small portion of HNO<sub>3</sub> was added until the solution appeared light coloured and clear. The beaker wall and glass were washed with distilled water and the sample was filtered to remove any insoluble material. The volume was adjusted to 100cm<sup>3</sup> with distilled water (Radojevic and Bashkin, 1999) [15].

Finally, 100cm<sup>3</sup> of distilled water was transferred in to a beaker and digested as above. This was the blank sample used for blank corrections. Determination of heavy metals (Fe, Zn, Cd, Cu & Pb) in triplicate was made directly on each final solution using the Perkin-Elmer AAnalyst 400 Atomic Absorption Spectroscopy (AAS) as described by (Floyd and Hezekiah, 1997). Triplicate measurements of temperature and pH of water samples were also taken immediately after sampling using the Ertco thermometer model 063FBLSF and the sper pH meter model 840087 respectively. The mean and standard deviations of these measurements were recorded as shown in the various tables below.

**Table 1. Mean Concentration of Heavy metals in Borehole water in Kassa mines Area, Jos North**

Time (Quarterly)	Ph	Temperature (°C)	Mean Concentration of Heavy Metal (mg/l)				
			Fe	Zn	Cd	Cu	Pb
Q1	7.7±0.22	17.21±0.45	4.8±0.13	0.13±0.01	0.5±0.11	0.9±0.03	0.4±0.06
Q2	7.2±0.03	22.19±1.47	5.1±0.06	0.21±0.08	0.54±0.12	1.2±0.14	0.5±0.03
Q3	7.9±0.06	25.84±1.01	47±0.16	2.6±0.11	1.23±0.02	2.19±0.11	0.76±0.04
Q4	8.1±0.12	20.14±0.11	32±0.02	1.4±0.04	0.72±0.01	1.4±0.12	0.58±0.03
Q5	7.6±0.34	18.12±0.24	4.9±0.61	0.12±0.06	0.52±0.01	0.11±0.06	0.38±0.02
Q6	7.4±0.26	23.16±1.55	5.4±0.42	0.26±0.03	0.53±0.06	1.10±0.08	0.53±0.21
Q7	7.4±0.11	27.21±1.16	6.9±0.18	2.96±0.09	1.21±0.16	1.99±0.11	0.73±0.11
Q8	7.8±0.12	23.11±0.66	6.2±1.15	1.48±0.21	0.91±0.13	1.36±0.21	0.64±0.08

## 3. Results and Discussion

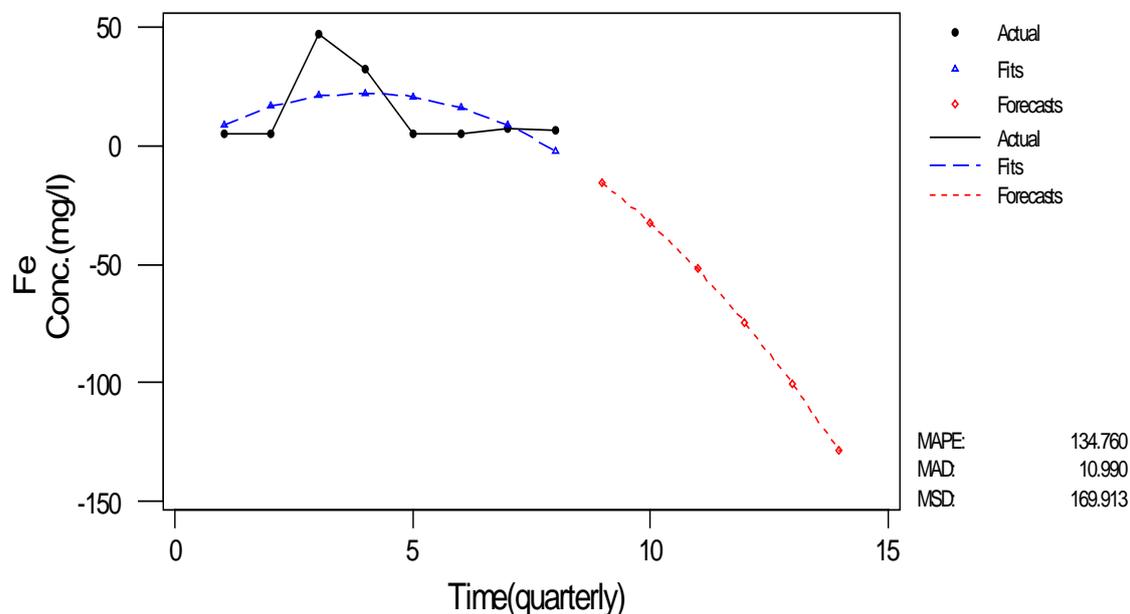
Figure 1 showed the time-series plot for the mean concentration of Fe in the water sample. This model,

quadratic in nature, generally showed a decreasing trend in the concentration of the metal with time. This model, with the aid of the Minitab computer software, was found to be  $Fe(mg/l) = -1.39464 + 11.9530 * t - 1.50417 * t^{**2}$ . Additionally, the pH and temperature dependent model was also found to be;  $Fe(mg/l) = -352 + 42.0 pH + 2.04$

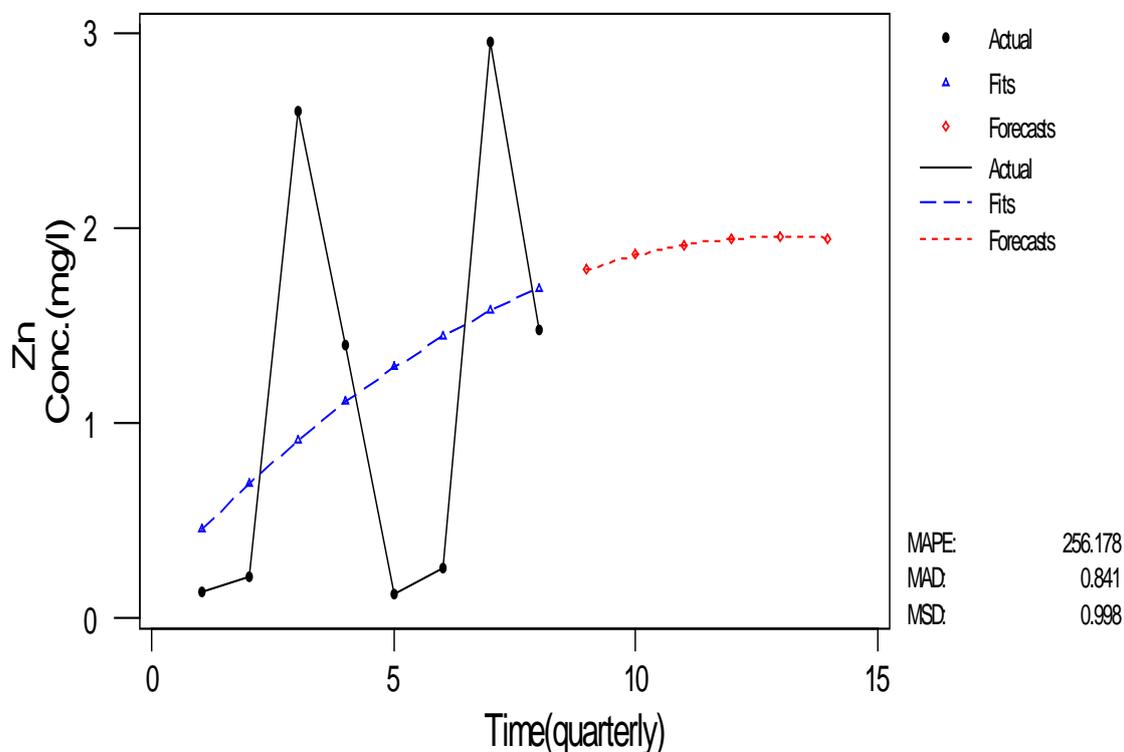
$T$  ( $^{\circ}\text{C}$ ) with the overall coefficient of correlation as 65.4%. This is a measure of the strength of the model at 95% confidence level which to a large extent, is indicative of strong reliance on the model. Thus, the concentration of Fe in the borehole could be forecasted with efflux of time by simple substitution into the time-series model. Alternatively, simple measurement of pH and temperature of the borehole water and substitution into the multi-

regression model would estimate the metal concentration at that particular time.

As an example, by the use of the time-series model, the concentration of Fe (22.35mg/l in the year 2011) was evaluated to be -36mg/l by 2015. This would be a case of non detection, implying a complete bio-reduction or bio-degradation of the heavy metal by the year 2015.



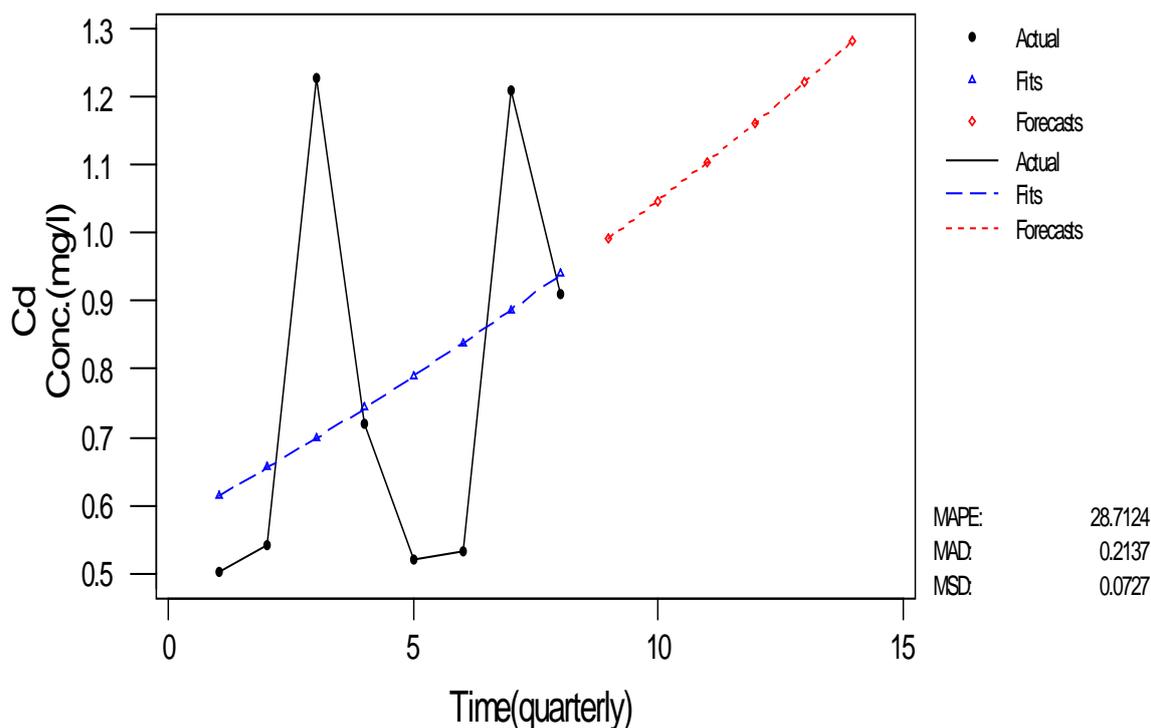
**Figure 1.**  $\text{Fe}(\text{mg/l}) = -1.39464 + 11.9530 * t - 1.50417 * t^2$  (Time-series model),  $\text{Fe}(\text{mg/l}) = -352 + 42.0 \text{ pH} + 2.04 T$  ( $^{\circ}\text{C}$ ) (Multi-regression model),  $R^2 = 65.4\%$



**Figure 2.**  $\text{Zn}(\text{mg/l}) = 0.191429 + 0.270595 * t - 1.04E-02 * t^2$ ,  $\text{Zn}(\text{mg/l}) = -19.3 + 1.83 \text{ pH} + 0.293 T$  ( $^{\circ}\text{C}$ ), ( $R^2 = 85.1\%$ )

Figure 2, also a quadratic model, showed that the general trend in the concentration of Zn in the water was also decreasing with time. The time-series model was found to be  $\text{Zn}(\text{mg/l}) = 0.191429 + 0.270595 * t - 1.04E-$

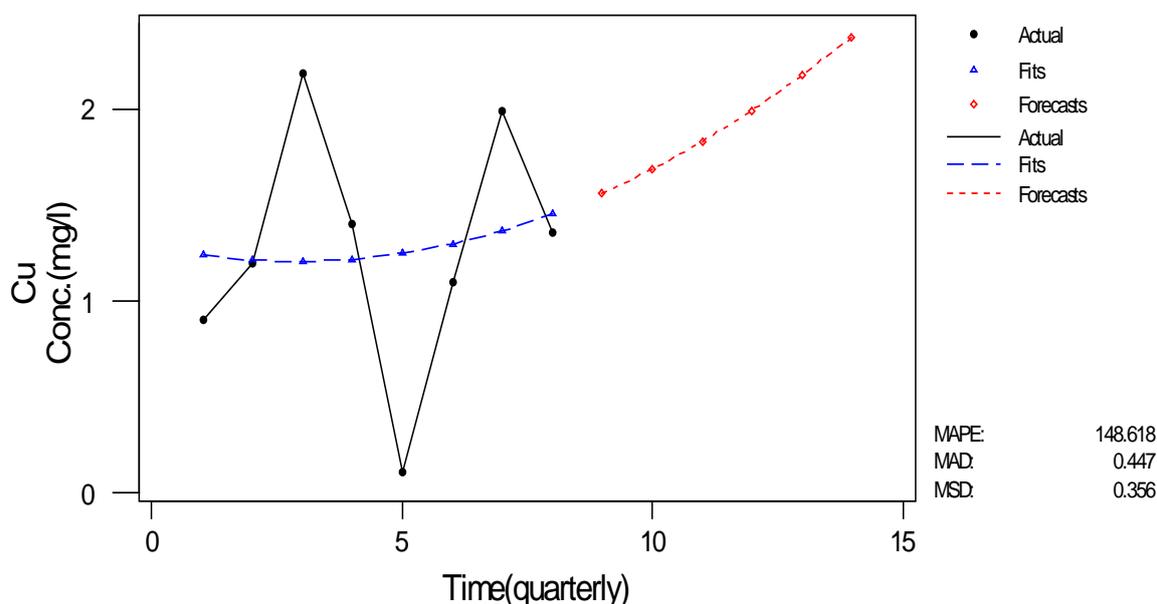
$02 * t^2$  while that of the multi-regression for this metal was  $\text{Zn}(\text{mg/l}) = -19.3 + 1.83 \text{ pH} + 0.293 T$  ( $^{\circ}\text{C}$ ). The strength of this model was however higher than that for Fe as it was found to be 85.1% at 95% confidence level.



**Figure 3.**  $Cd(mg/l) = 0.5725 + 3.92E-02*t + 8.33E-04*t^{**2}$ ,  $Cd(mg/l) = -4.46 + 0.453 pH + 0.0803 T(^{\circ}C)$ ,  $R^2 = 85.7\%$

In Figure 3 however, the concentration of Cd was seen to be increasing steadily with time and its time-series and multi-regression models were developed as  $Cd(mg/l) = 0.5725 + 3.92E-02*t + 8.33E-04*t^{**2}$  and  $Cd(mg/l) = -4.46 + 0.453 pH + 0.0803 T(^{\circ}C)$  respectively. The strength of this model was 85.7% which was also indicative of a very strong reliance. Modelling the concentration of Cu on the

other hand, was 82% error-free and the general trend also showed that the concentration was increasing steadily with time as could be seen in Figure 4 below; and its developed models were found to be  $Yt = 1.28339 - 5.41E-02*t + 9.46E-03*t^{**2}$  and  $Cu(mg/l) = -8.24 + 0.765 pH + 0.166 T(^{\circ}C)$  respectively. The reliability on the models was also very high.



**Figure 4.**  $Cu(mg/l) = 1.28339 - 5.41E-02*t + 9.46E-03*t^{**2}$ ,  $Cu(mg/l) = -8.24 + 0.765 pH + 0.166 T(^{\circ}C)$ , ( $R^2 = 81.8\%$ )

The general trend with the modelling of the concentration of Pb as seen in Figure 5 above, showed that the concentration was initially increasing and then decreased as time continued to increase. Both models were expressed as;  $Yt = 0.446786 + 3.17E-02*t - 9.52E-$

$04*t^{**2}$  and  $Pb(mg/l) = -1.80 + 0.195 pH + 0.0396 T(^{\circ}C)$  in that order. Furthermore, these models were found to be the most error-free as the strength was 98.5%, therefore, most reliable.

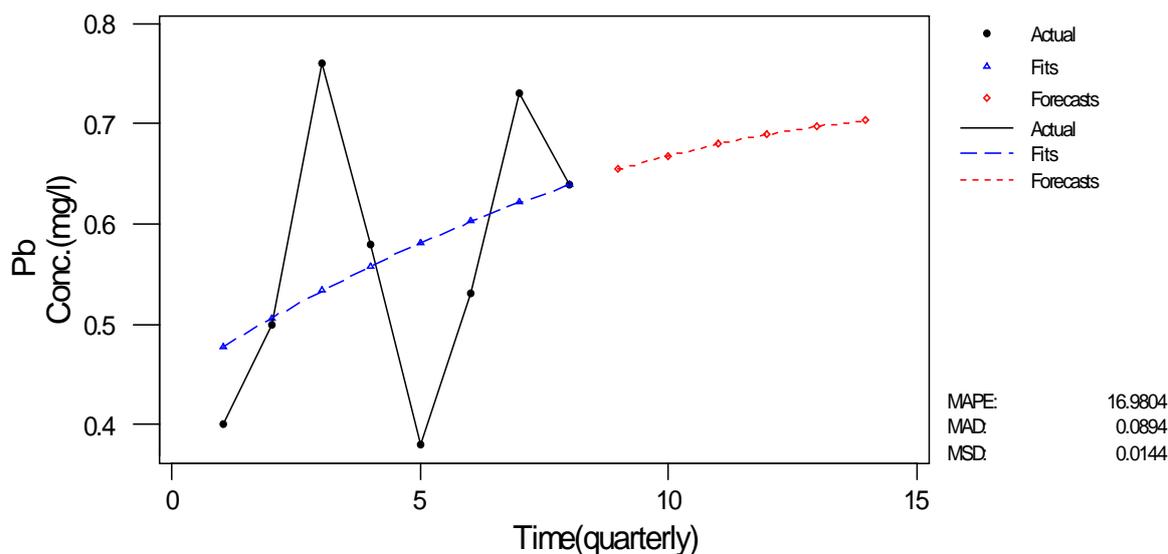


Figure 5.  $Pb(mg/l) = 0.446786 + 3.17E-02 * t - 9.52E-04 * t^{**2}$ ,  $Pb(mg/l) = -1.80 + 0.195 pH + 0.0396 T(^{\circ}C)$

## 4. Conclusion

The concentrations of these heavy metals; Fe, Cu, Cd, Zn and Pb in Kassa-mines deep well were computer-modelled with the view of ascertaining whether pollution activities were still possible even at several metres beneath the ground.

The results showed that there was biodegradation in the concentrations of Fe, Zn and Pb, while there was bio-accumulation in the concentrations of Cd and Cu. The order of increase was found to be  $Cu > Cd > Pb > Zn > Fe$ . This implies that pollution activities were not only possible, but were very much going on either as decrease or increase which may invariably lead to metal accumulation or reduction. This is due probably to seepage into and out of the boring and possibly too from leaching from underground rocks. With the foregoing, it is suggested that the casing for such deep wells or boreholes be checked for any crack or breakage as this may also be the likely channel for the seepage.

Furthermore, this findings portends danger to residents of Kassa Mines area who drink from this deep well because of the danger of accumulating these heavy metals particularly Cd with time. Additionally, it could be seen that the growing believe that borehole water was very pure may not be true.

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