MODELLING AND SIMULATION ON PARTIAL DEPOSITION OF SELENIUM IN SILTY CLAY PENETRATING PHREATIC BED IN TRANS-AMADI INDUSTRIAL LAYOUT OF PORT HARCOURT

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Abstract

The deposition of selenium in silty clay penetrating phreatic bed has been express in the system, the study were to monitor the deposition of selenium in silty clay at various depths penetrating unconfined depositions, several experts has express the migration process of heavy metal, but this type of mathematical concept has not been applied to monitor the rate of selenium concentration in silty clay. The study has generated the rate of selenium concentration penetrating phreatic deposition, thus expressing decreasing in concentration with respect to change in depths, the decrease in concentration were as a results of impermeable depositions found between three and twelve metres. The generated values were from the simulation produced from the developed model, the study is imperative because the developed model applying this type of mathematical concept has been use to develop model for selenium transport penetrating unconfined bed in the study area. This conceptualized approach is to monitor selenium migrations in soil and water environment.

Keywords: modelling and simulation, selenium, silty clay and phreatic bed.

INTRODUCTION

Generally in soil environment, sorption is the dominating speciation process and thus the largest fraction of heavy metal in a soil is related with the solid phase of that soil. Pollution quandary arises when heavy metals are mobilized into the soil solution and taken up by plants or transported to the surface/ground water. The properties of the soil are thus very important in the attenuation of heavy metals in the environment (Sherene; 2010). The solubility of heavy metals in soil is controlled by reactions with solid phases. Understanding the process governing the migration and plant availability of trace metals in soils is essential for predicting the environmental impact of spreading metal containing wastes on agricultural land. The adverse effect of heavy metals is inseparably related to the soil's ability to absorb and retain sub elements. The pH of the soil solution maintained at neutral to slightly alkaline condition showed low mobility of all heavy metals. To increase the mobility of heavy metals, the pH of the soil solution should be lowered. The solubility of Pb in soil solution was pH dependent, increasing as the pH was adjusted from 6 to 3. At near neutral pH, the activity of Pb2+ showed no clear relationship to pH and a small but significant increase resulting from changing organic matter content. In the near neutral pH range, higher Soil Organic Matter (SOM) increases the Dissolved Organic Matter (DOM), thereby promoting the formation of organo Pb complexes and increasing Pb solubility (Sebastien Sauve; 1998; Friest;2001). Soil Organic Matter is a key for sorbing phase for metals. The dissolution of humic acid at higher pH is responsible for dissolution of Cu and Pb from soil. Organic matter is important for the retention of metals by soil solids, thus decreasing mobility and bioavailability. However because of the complexation of metals by soluble OM, the addition of OM can result in release of metals from solids to the soil solution (Chieshwari, 1999; Thompson el at 1994). The increase in the solubility of the Cu and Pb is related to the dissolution of the HA component of the organic matter. This indicates that solution phase speciation reactions with organic matter dominate the partition of these metals at higher pH. This due to high pH, the [DOM] increases as a result solubility of HA. In general, sorption increases with increasing pH. That is, the lower the pH value the more metal can be found in solution and thus more metal is mobilized. When pH falls is below five, mobility is enhanced as a result of the increased proton concentration (khan and igbaio1991). High solubility of heavy metals in soil solution at alkaline pH was attributed to enhanced formation of organic matter metal complexes after ionization of weak acid groups. Extensive evidence exist that in this pH range most dissolved heavy metals are present as metal soluble organic ligand complexes (khaitak and page 1992). The degree of stabilization

achieved by compost appears to be very important in determining potential mobility of heavy metals. Carillo et al., (2000 reported that, Cd can move readily in sandy loam soils, but OM in the surface layer will act as a sink for Cd and will reduce the rate of movement. Destructions of heavy metals between soil and solute is the key for evaluating the environment impact of the metals. For Cu, in particular OM both solid and dissolved can affect its mobility substantially. (Temming hoff et al., 1997). Naidu and Harter (1998) reported that, the role of organic acids in Cd mobilization is especially important since modern agriculture increasingly involves minimum tillage practices that recycle plant residues. Complexations of metals by organic ligands play an important role in controlling metal solubility. The amount of metals adsorbed decreases with increasing ionic strength for minerals with permanent surface charge density (Boekhold et al., 1993). Casagrande, (2001) reported that regardless of pH, Zn adsorption was always superior for the most diluted $CaCl_2$, solution utilized. This shows that the reaction took place on the negative surface of colloids. For these surfaces, the reduction of ionic strength makes the surface electric potential more negative, and thus ion adsorption is greater. The soil texture plays an important role in mobility of metals in soil. Texture reflects the particle size distribution of the soil and thus the content of fine particles like oxides and clay. These compounds are important adsorption media for heavy metals in soils. The clay soil retains high amount of metals when compared to sandy soil. Jeanne and Roy (1991) concluded that the fine textured soils contain higher amounts of Pb (3889 mg kg-1) and coarse textured soil contains (530 mg kg-1) lower amount of Pb. (Michael et al 1994) reported that the metal content of top and middle layer of soil was comparatively higher than bottom layer of soil. Jeyabaskaran and Sree Ramulu, (1996) concluded that the content of DTPA- extractable metals in light textured soils were low in soils irrigated with sewage water for the past 50 years. Alesi et al. (1980) reported that the soil texture and structure as evaluated by bulk density i.e. the solution flux. This plays a part in diffusion of metal ions into and out of soil aggregates in such a way that movement of elements through soil may be predicated with greater accuracy by having some knowledge of flow velocities. Karathanasis (1999) reported that colloids with high surface charge and soils with greater macro porosity contributed more Pb mobility and transport. When the temperature raises the metal activity in the soil solution as well as that the plant roots may be more active and has faster absorption rates. Furthermore, the absorption rate of the roots may be increased as a result of higher evapo transpiration from the plant. Yu Ling et al., (1998) concluded that considerable enrichment of heavy metals in the sub-micron range occurs during evaporization of heavy metals in the high temperature environment and the subsequent condensation in lower temperature regions of the systems. Duration and temperature increased the percentage of Pb that was bound to the carbonates decreased with a concomitant increase of residual Pb. Sheaffer et al., (1980) reported that, higher soil temperature enhances the degradation soil organic matter, thereby releasing organic acids, which increase the mobility of heavy metals in soils. Thereby the availability is increased.

Governing equation

$$\Delta\tau^1 \frac{d^2c}{dx^2} - V_x \frac{dc}{dx} + \phi_t \frac{dc}{dx} = 0$$

$$\text{......................} \qquad (1)$$

$$\Delta\tau^1 \frac{d^2c}{dx^2} - (V_x - \phi_t)\frac{dc}{dx} = 0$$

$$\text{......................} \qquad (2)$$

Let $C = \sum_{n=0}^{\infty} a_n x^n$

$$C^1 = \sum_{n=1}^{\infty} n a_n x^{n-1}$$

$$C^{11} = \sum_{n=2}^{\infty} n(n-1) a_n x^{n-2}$$

$$\Delta\tau^1 \sum_{n=2}^{\infty} (n-1) a_n x^{n-2} - (V_x - \phi_t)\sum_{n=1}^{\infty} n a_n x^{n-1} = 0 \text{ ......}(3)$$

Replace n in the 1st term by $n+2$ and in the 2nd term by $n+1$, so that we have;

$$\Delta\tau^1 \sum_{n=2}^{\infty} n(n+2)(n+1) a_{n+2} x^n - (V_x + \phi_t)\sum_{n=0}^{\infty} (n+1) a_{n+1} x^n = 0$$

$$\text{..............} \qquad (4)$$

i.e. $\Delta\tau^1 (n+2)(n+1) a_{n+2} = (V_x - \phi_t)(n-1) a_{n+1}$

$$\text{......................} \qquad (5)$$

$$a_{n+2} = \frac{(V_x - \phi_t)(n+1) a_{n+1}}{\Delta\tau^1 (n+2)(n+1)}$$

$$\text{......................} \qquad (6)$$

$$a_{n+2} = \frac{(V_x - \phi_t) a_{n+1}}{\Delta\tau^1 (n+2)}$$

$$\text{......................} \qquad (7)$$

for $n = 0$, $a_2 = \frac{(V_x - \phi_t) a_1}{2\Delta\tau^1}$

$$\text{......................} \qquad (8)$$

for $n = 1$, $a_3 = \frac{(V_x - \phi_t) a_2}{3\Delta\tau^1} = \frac{(V_x - \phi_t)^2 a_1}{2\Delta\tau^1 \bullet 3\Delta\tau^1}$

$$\text{......................} \qquad (9)$$

for

$$n = 2; a_4 = \frac{(V_x - \phi_t)a_3}{\Delta\tau^1} = \frac{(V_x - \phi_t)}{4\Delta\tau^1} \bullet \frac{(V_x - \phi_t)a_1}{3\Delta\tau^1 \bullet 2\Delta\tau^1} = \frac{(V_x - \phi_t)^3 a_1}{4\Delta\tau^1 \bullet 3\Delta\tau^1} \quad \ldots$$

$$\ldots\ldots\ldots\ldots \quad (10)$$

for $\quad n = 3; a_5 = \frac{(V_x - \phi_t)}{5\Delta\tau^1} = \frac{(\phi - V_t)^4 a_1}{5\Delta\tau^1 \bullet 4\Delta\tau^1 \bullet 3\Delta\tau^1 \bullet 2\Delta\tau^1}$

$$\ldots\ldots\ldots \quad (11)$$

for n; $a_n - \dfrac{(V_x - \phi_t)^{n-1} a_1}{\Delta\tau^{1^{n-1}} n!}$

$$\ldots\ldots\ldots\ldots \quad (12)$$

$$C(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 + \ldots\ldots a_n x_n$$

$$\ldots\ldots\ldots \quad (13)$$

$$= a_0 + a_1 x + \frac{(V_x - \phi_t)a_1 x^2}{2!\Delta\tau^1} + \frac{(V_x - \phi_t)a_1 x^3}{3!\Delta\tau^2} + \frac{(V_x - \phi_t)x^4}{4!\Delta\tau^3} + \frac{(V_x - \phi_t)^5}{5!\Delta\tau^4}$$

$$\ldots\ldots\ldots\ldots \quad (14)$$

$$C(x) = a_0 + a_1 \left[x + \frac{(V_x - \phi_t)x^2}{2!\Delta\tau^1} + \frac{(V_x - \phi_t)^2 x^3}{3!\Delta\tau^2} + \frac{(V_x - \phi_t)^3 x^4}{4!\Delta\tau^3} + \frac{(V_x - \phi_t)x^5}{5!\Delta\tau^4} + \ldots \right]$$

$$\ldots\ldots\ldots\ldots \quad (15)$$

$$C(x) = a_0 + a_1 \ell^{\frac{(V_x - \phi_t)}{\Delta\tau^1} x}$$

$$\ldots\ldots\ldots\ldots \quad (16)$$

MATERIALS AND METHOD

Standard laboratory experiment where performed to monitor selenium concentration at different formation, the soil deposition of the strata were collected in sequences base on the structural deposition at different locations, this samples collected at different location generate variation at different depth producing different migration of Selenium concentration through [ASS] at different strata, the experimental result are applied to be compared with theoretical values to determine the validation of the model.

RESULT AND DISCUSSION

Results and discussion are presented in tables 1 to 8 including Figures 1 to 6, representation of conynebacterium concentration.

The study expresses the physical process observation on the deposition of selenium in the strata, the figures from one to two shows selenium are experiencing higher

Table 1: Predictive Values of conynebacterium Concentration at Different Depth

Depth [M]	Selenium Concentration
3	1.03E+00
6	7.00E-01
9	3.60E-01
12	1.60E-01
15	7.20E-02
18	3.00E-02
21	2.00E-02
24	1.50E-02
27	4.60E-03
30	3.52E-03
33	2.67E-04
36	1.00E-04
37	3.74E-05
39	4.63E-05

concentration between the organic soil deposition due to low permeability that has cause an accumulation to the point where change in depths influences are very high in those depositions, these rate of concentration were observed to reduce in phreatic bed due to this natural purification process, these are based on the structure and the rate of migration between the organic deposition were accumulation were observed. While three and four produced similar results, but its level of concentration varies, it decreases with change in depth base on the structural variation of the strata influencing the deposition of permeability in the formation. Slight change in these deposition were observed to pressure the migration process of the contaminant in the study area, therefore the concentration experienced decreasing rate compared to figure one and two, five and six maintained there degradation process as the rate of accumulation and impermeable formation were observed to reduced their transport process finally reducing the rate of concentration in phreatic bed. Seven and eight experienced more decrease in concentration, the rate of migration were inhibited by impermeable deposition that could not allowed rapid migration to the phreatic bed, the deposited unconfined bed were experienced lower concentration compared to other figures, the study express this results through simulation from the developed model, the theoretical values were compared with experimental results, both parameters generated best fits validating the model for the study. The environmental problems with heavy metals are that they as elements are undestroyable and the most of them have toxic effects on living organisms when exceeding a certain concentration. Furthermore, some heavy metals are being subjected to bioaccumulation and may pose a risk to human health when transferred to the food chain. Soils, whether in urban or agricultural areas represent a major sink for metals released into the environment from a wide variety of anthropogenic sources (Sherene 2010, Niragu, 1991).

Table 2: Predicted and Measured of selenium Concentration Different Depth

Depth [M]	Predictive Selenium Conc.	Measured Values
3	1.03E+00	1.08
6	7.00E-01	0.84
9	3.60E-01	0.42
12	1.60E-01	1.90E-01
15	7.20E-02	8.20E-02
18	3.00E-02	6.00E-02
21	2.00E-02	5.00E-02
24	1.50E-02	1.20E-02
27	4.60E-03	3.22E-03
30	3.52E-03	2.54E-03
33	2.67E-04	2.32E-04
36	1.00E-04	4.00E-05
37	3.74E-05	3.23E-05
39	4.63E-05	4.42E-05

Table 3: Predictive Values of Selenium Concentration at Different Depth

Depth [M]	Selenium Concentration
3	9.10E-01
6	5.50E-01
9	2.50E-01
12	1.04E-01
15	3.80E-02
18	1.46E-02
21	5.20E-03
24	1.83E-03
27	2.08E-03
30	2.12E-04
33	7.12E-05
36	2.37E-05
37	7.85E-06
39	2.56E-06

Table 4: Predicted and Measured of selenium Concentration Different Depth

Depth [M]	Predictive Selenium Conc.	Measured Values
3	9.10E-01	8.80E-01
6	5.50E-01	4.40E-01
9	2.50E-01	2.21E-01
12	1.04E-01	1.01E-01
15	3.80E-02	3.55E-02
18	1.46E-02	1.26E-02
21	5.20E-03	5.00E-03
24	1.83E-03	1.67E-03
27	2.08E-03	2.07E-03
30	2.12E-04	2.04E-04
33	7.12E-05	6.89E-05
36	2.37E-05	2.11E-05
37	7.85E-06	7.66E-06
39	2.56E-06	2.44E-06

Table 5: Predictive Values of Selenium Concentration at Different Depth

Depth [M]	Selenium Concentration
3	8.30E-01
6	4.60E-01
9	1.80E-01
12	6.70E-02
15	2.30E-02
18	1.43E-02
21	2.44E-03
24	7.66E-04
27	2.36E-03
30	7.19E-05
33	2.17E-05
36	6.49E-06
37	1.92E-06
39	5.69E-07

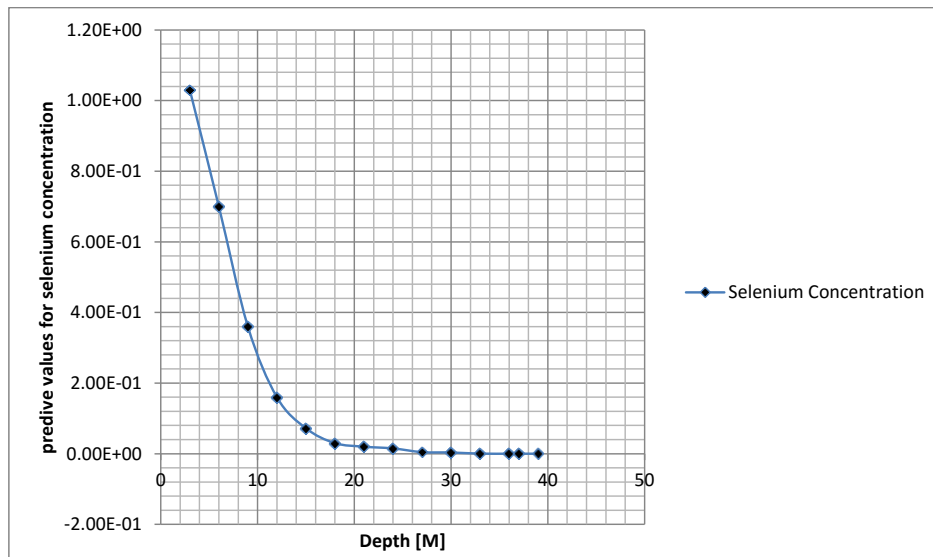**Table 6:** Predicted and Measured of selenium Concentration Different Depth

Depth [M]	Predictive Selenium Conc.	Measured Values
3	8.30E-01	8.80E-01
6	4.60E-01	4.40E-01
9	1.80E-01	2.21E-01
12	6.70E-02	1.01E-01
15	2.30E-02	3.55E-02
18	1.43E-02	1.26E-02
21	2.44E-03	5.00E-03
24	7.66E-04	1.67E-03
27	2.36E-03	2.07E-03
30	7.19E-05	2.04E-04
33	2.17E-05	6.89E-05
36	6.49E-06	2.11E-05
37	1.92E-06	7.66E-06
39	5.69E-07	2.44E-06

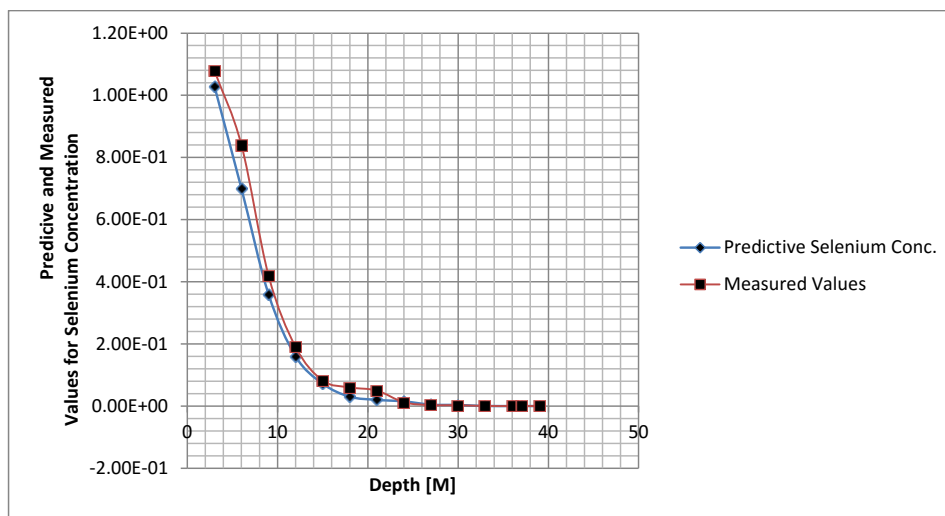**Table 7:** Predictive Values of Selenium Concentration at Different Depth

Time Per Day	Selenium Concentration
10	8.30E-01
20	4.60E-01
30	1.80E-01
40	6.70E-02
50	2.30E-02
60	1.43E-02
70	2.44E-03
80	7.66E-04
90	2.36E-03
100	7.19E-05
110	2.17E-05
120	6.49E-06
130	1.92E-06
140	5.69E-07

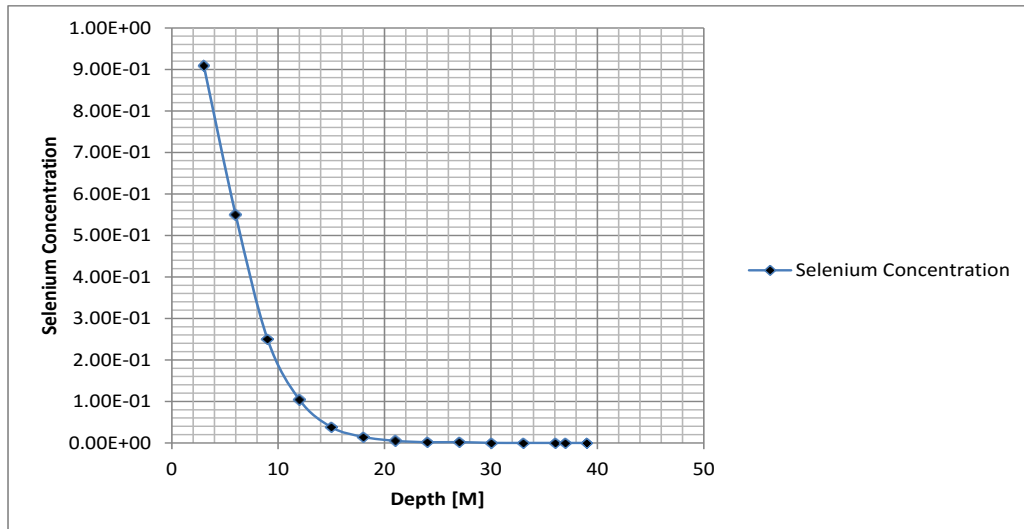**Table 8:** Predicted and Measured of selenium Concentration Different Depth

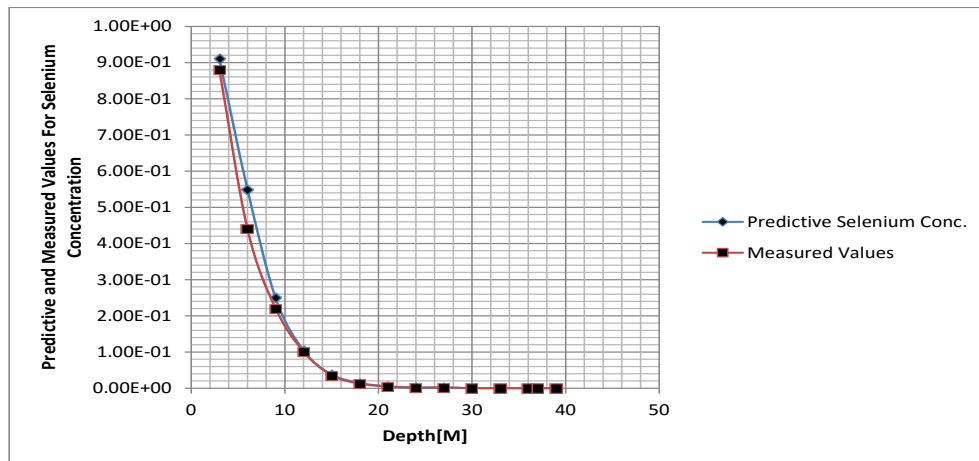| Time Per Day	Predictive Selenium Conc.	Measured Values
10	8.30E-01	8.80E-01
20	4.60E-01	4.40E-01
30	1.80E-01	2.21E-01
40	6.70E-02	1.01E-01
50	2.30E-02	3.55E-02
60	1.43E-02	1.26E-02
70	2.44E-03	5.00E-03
80	7.66E-04	1.67E-03
90	2.36E-03	2.07E-03
100	7.19E-05	2.04E-04
110	2.17E-05	6.89E-05
120	6.49E-06	2.11E-05
130	1.92E-06	7.66E-06
140	5.69E-07	2.44E-06

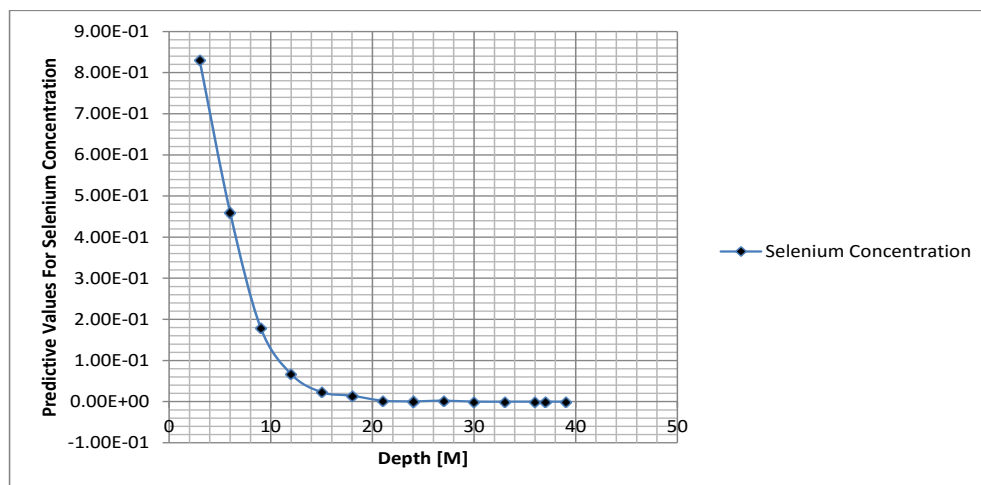**Figure 1:** Predictive Values of Selenium Concentration at Different Depth

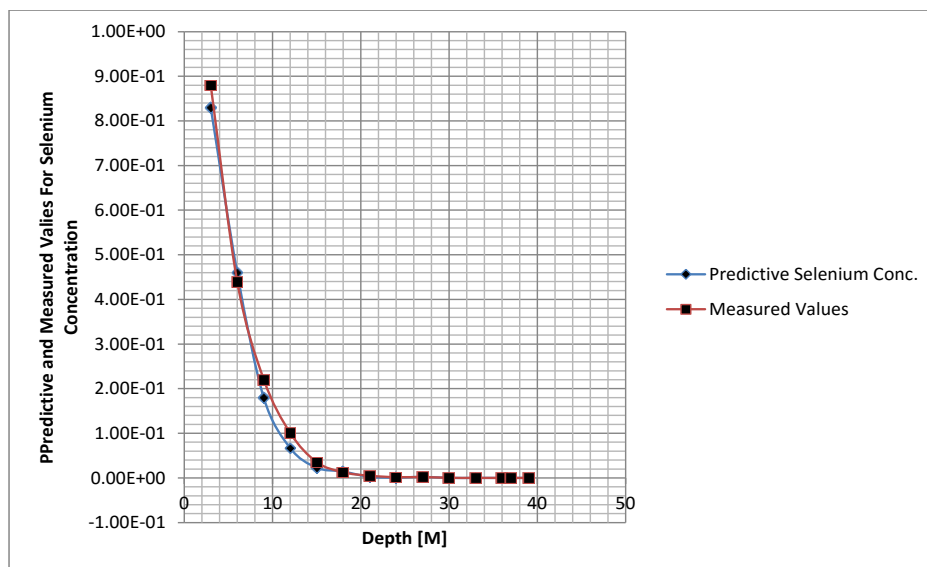**Figure 2:** Predicted and Measured of selenium Concentration Different Depth

Figure 3: Predictive Values of Selenium Concentration at Different Depth

Figure 4: Predicted and Measured of selenium Concentration Different Depth

Figure 5: Predictive Values of Selenium Concentration at Different Depth

Figure 6: Predicted and Measured of selenium Concentration Different Depth

CONCLUSION

The behaviour of heavy metal in soil has been expressed by several experts in different dimensions, the transport of selenium were monitor applying this approach to generate there rate of concentration in various strata to penetrating Phreatic bed]. Several researchers has apply several concept to express the deposition of heavy metal in soil and water environment, the migration process in soil varies due to the influences from geological histories and other deposited minerals that may inhibit the migration process. The behaviour of the metal depend on the depositions of formation characteristics in the study environment, the study applied this approach and discovered there rate of concentration in silty clay. Several factors in heavy metals are found to influence the deposition of heavy metal [selenium] in the study area, environmental conditions are observed to be one the process of heavy metal migration into soil and water environment. Once in soil, some of these metals would be persistent because of their fairly immobile nature. Other metals however would be more mobile therefore the potential of transfer either through soil profile down to ground water aquifer or via plant - root uptake (bio available) is likely. In most soil environment sorption is the dominating speciation process and thus the largest portion of heavy metal in a soil is connected with the solid phase of that soil. Pollution difficulties arise when heavy metals are mobilized into the soil solution and taken up by plants or transported to the surface/ground water. The properties of the soil are thus very imperative in the attenuation of heavy metals in the environment. The solubility of heavy metals in soil is restricted by reactions with solid phases. Once sewage sludge is applied to soil, the heavy metal species experience numerous possible fates including Adsorption/desorption reactions. The soil texture plays an significant role in mobility of metals in soil. Texture reflects the particle size distribution of the soil and thus the content of fine particles like oxides and clay. These compounds are important adsorption media for heavy metals in soils. The developed model were simulated to predict there rate depositions in silty clay penetrating Phreatic bed. There rate of concentration are express through the simulation values.

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