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Modeling And Simulation Of Absorption Rate Of Zinc From Polluted Soil By Bushgreen Roots

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Abstract: *The rate of absorption of Zinc by Bushgreen roots was studied. Empirical model was used to model the concentration of Zinc absorbed by Bushgreen roots with time. It was observed that the empirical equation relating the concentration of Zinc in Bushgreen roots with time is a polynomial of second degree with a correlation ratio of R^2= 0.977. The rate of absorption follows second order rate equation. The mass transport coefficient (k) was determined to be 1.30779 x 10^{-4} ug/g-day. The model was validated and the experimental values of concentration of Zinc in Bushgreen roots agree between 92.41 to 99.29 percent with the value predicted by the model developed. The model was also simulated to predict absorbed concentration of Zinc at early stage of root development when the concentration was difficult to measure experimentally. It was observed that the trend of the values predicted was similar to that of the experimental measured values.*

Key Words: *Modelling, Simulation, Absorption, Zinc, Bushgreen roots*

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I. Introduction

The potential adverse impact of heavy metal deposits in the environment has been recognized for a long time. Numerous studies [6, 7, 8, 9] indicates that the main sources contributing to heavy metal pollution in the environment include motor vehicle emissions, industrial emissions and wastewater effluent, urban waste water, pesticides, fertilizer applications and those caused by power plants. The heavy metals are widely spread from point sources to the environment and reached high levels in soils; roadside deposits and those released as particulate in air are taken up by plants through the soil or deposited on leaves.

Vegetables supply trace elements such as Iron, Copper and Zinc which are involved in the functions of several enzymes and are essential for maintaining good health throughout life [4]. Zinc is an essential trace element in human body where it is found in high concentration in red blood cells as an essential part of enzyme carbonic anhydrase, which promotes many reactions relating to carbon dioxide metabolism [4]. A daily intake of zinc is required to maintain a steady state because the human body has no specialized zinc storage system. High concentration of zinc has been reported to cause diarrhoea, depressed immune function impairment of growth and production [1].

Many species of plant has been successful in absorbing contaminants such as lead, cadmium, chromium, arsenic and various radionuclides' from soil. Bushgreen roots have shown ability to absorbed high concentration of some heavy metals including Zinc [3]. This study will model and simulate the rate of adsorption of Zinc from polluted soil by Bushgreen roots.

II. Theory

The models are entirely empirical, it does not attempt to explain the growth processes, but it enables the relation between the concentrations of the heavy metals absorbed with time during the growth period and therefore makes it easy to see any departure from a particular relationship. .

For the absorption mechanism in bushgreen vegetable, the following dynamics was preferred to other candidate functions [2]

Rate of absorption $r_A = \frac{dC_A}{dt} = KC_A^n$ (1)

Where C_A is the concentration of the metal in parts of vegetable at any given time t and K is the mass transport coefficient governing the rate of metal uptake, and n is a constant that signifies the order of rate of absorption.

The above kinetic model is a special case of Fick's law where the mass transfer is governed by the change in concentration in parts of the vegetable with time.

The kinetic model is based on the following assumptions:

- Uptake of metals is considered to take place in the axial (upward) direction.
- The rate is per unit length of transfer from the rhizosphere to the root
- The concentration of the metal ions is uniform along the length of root, stem and leaf

- The absence of any reaction between absorbed ions
- The mechanism of ion transfer is by molecular diffusion

III. Methodology

1.1 Pot Culture Experiment

The method used by [3] was adopted for the pot culture experiment to determine Zinc uptake by roots of Bushgreen vegetable from polluted soils. 3 kg of soil from the polluted area were weighed into five plastic pots; all samples were soaked with distilled water and allowed to stand for three days. 0.3 g of Bushgreen seeds were weighed and planted into each pot and allowed to germinate. After germination the plants were allowed to grow and each pot were irrigated with 250 ml of clean tap water every evening. The pots were kept in a green house away from aerial pollution of heavy metals. Each pot was harvested at a specified time interval of 31, 45, 57, 64 and 71 days respectively. The Bushgreen vegetable samples of each pot were taken to the laboratory for analysis.

1.2 Preparation of Bushgreen roots samples

The bushgreen root samples were reduced to fine powder in a grinder prior to drying at 60^{o}C in an oven to a constant weight. 0.5 g of the fine powdered Bushgreen roots was weighed into a 250 ml conical flask and digested in 4 ml concentrated perchloric acid ($HClO_4$), 2 ml of concentrated sulphuric acid (H_2SO_4), 25 ml concentrated nitric acid (HNO_3) and 1 ml of hydrogen peroxide (H_2O_2) at 100^{o}C on a hot plate for two hours in a fume cupboard [5]. The resulting solution was made up to 100 ml with distilled deionised water. The samples were analysed using Atomic Absorption Spectrometer (AAS).

IV. Results And Discussion

The variation of Zinc concentration in bushgreen roots with time is shown in Fig. 1. The empirical equation relating the concentration in roots with time is a polynomial of second degree as shown by equation (2) with correlation ratio of R^2 = 0.977

$$C_{Z_{n\ rt}} = 0.005t^2 - 0.013t + 37.79 \qquad (2)$$

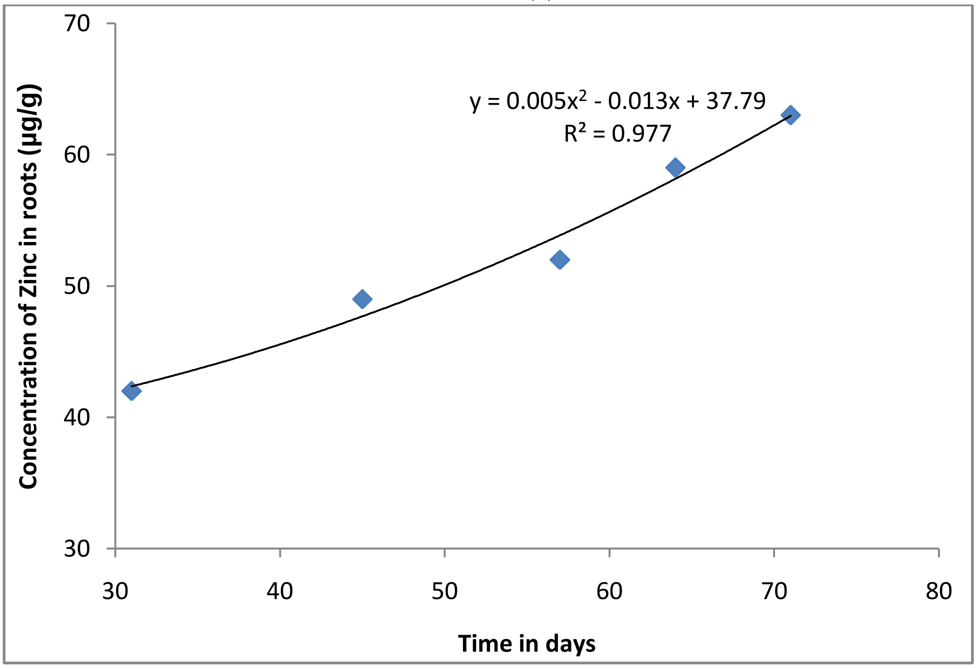

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Figure 1: Variation of zinc concentration in bushgreen roots with time

The rates of Zinc uptake $R_{Z_{n\ rt}} = \frac{dC_{Z_{n\ rt}}}{dt}$ at different times are shown in Table 1.

Table 1: The rate of absorption of zinc in roots at different times

Time in days	Rate ($R_{Z_{n\ rt}}$) in μg/g-day
31	0.297
45	0.437
57	0.557
64	0.627
71	0.697

Applying the absorption kinetics :

$$R_{Z_{n\,rt}} = \frac{dC_{Z_{n\,rt}}}{dt} = K_{Z_{n\,rt}}\ C^{n}_{Z_{n\,rt}} \quad (3)$$

$$\text{In}\ R_{Z_{n\,rt}} = \text{In}\ K_{Z_{n\,rt}} + n\ \text{In}\ C_{Z_{n\,rt}} \quad (4)$$

The plot of In $R_{Z_{n\,rt}}$ against In $Z_{n\,rt}$ gives a linear relationship with slope n and intercept In $K_{Z_{n\,rt}}$.

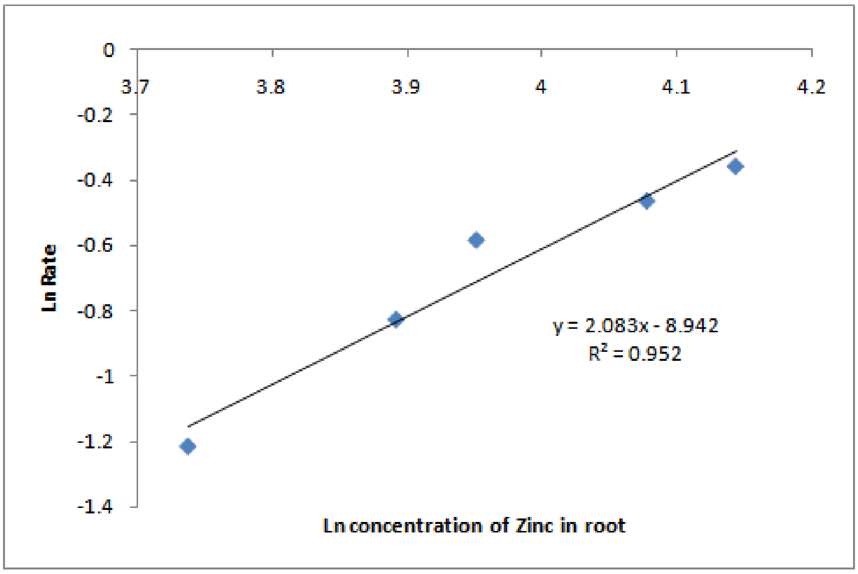

Figure 2: Rate of absorption of zinc with concentration in the roots of bushgreen

From the Fig. 2, slope, n = 2.083 and intercept, In $K_{Z_{n\,rt}}$ = -8.942.
Therefore,

$$K_{Z_{n\,rt}} = e^{-8.942} = 1.30779 \times 10^{-4}\ \left(\frac{\mu g}{gday}\right) \quad (5)$$

From the empirical model, the rate of absorption is of second order since n = 2 and therefore the absorption model is given by

$$R_{Z_{n\,rt}} = \frac{dC_{Z_{n\,rt}}}{dt} = K_{Z_{n\,rt}}\ C^{2}_{Z_{n\,rt}} \quad (6)$$

Integrating equation (6) give the solution

$$C_{Z_{n\,rt}} = \frac{C_{Z_{n\,rt\,o}}}{1 - K_{Z_{n\,rt}}\, tC_{Z_{n\,rt\,o}}} \quad (7)$$

Substituting $C_{Z_{nrt}}$ into equation (6) gives the zinc absorption model of bushgreen root

$$R_{Z_{n\,rt}} = K_{Z_{n\,rt}}\ C^{2}_{Z_{n\,rt}} = K_{Z_{n\,rt}}\ \left(\frac{C_{Z_{n\,rt\,o}}}{1 - K_{Z_{n\,rt}}\, tC_{Z_{n\,rt\,o}}}\right)^2 \quad (8)$$

Therefore,

$$R_{Z_{n\,rt}} = 1.30779 \times 10^{-4}\ \left(\frac{C_{Z_{n\,rt\,o}}}{1 - 1.30779 \times 10^{-4}\, tC_{Z_{n\,rt\,o}}}\right)^2 \quad (9)$$

Equation (9) is the model for the rate of absorption of zinc by roots of bushgreen plant grown on a polluted soil. The experimental values of concentrations of Zinc in bushgreen roots agree well with the values predicted by the model between 92.29 to 99.29 % as shown in Table 2. The Zinc absorption model shows better predictions than the copper absorption model reported by [3].

Table 2: Comparison between the experimental and model Predicted Zn concentration

Time (days)	**Rate** (μg/g-day}	**Conc. (experimental)** (μg/g)	**Conc. (model prediction)(μg/g)**	**% Agreement between model & experimental values**
31	0.297	42	44.63	93.74
45	0.437	49	49.35	99.29
57	0.557	52	52.61	98.83
64	0.627	59	55.27	93.69
71	0.697	63	58.22	92.41

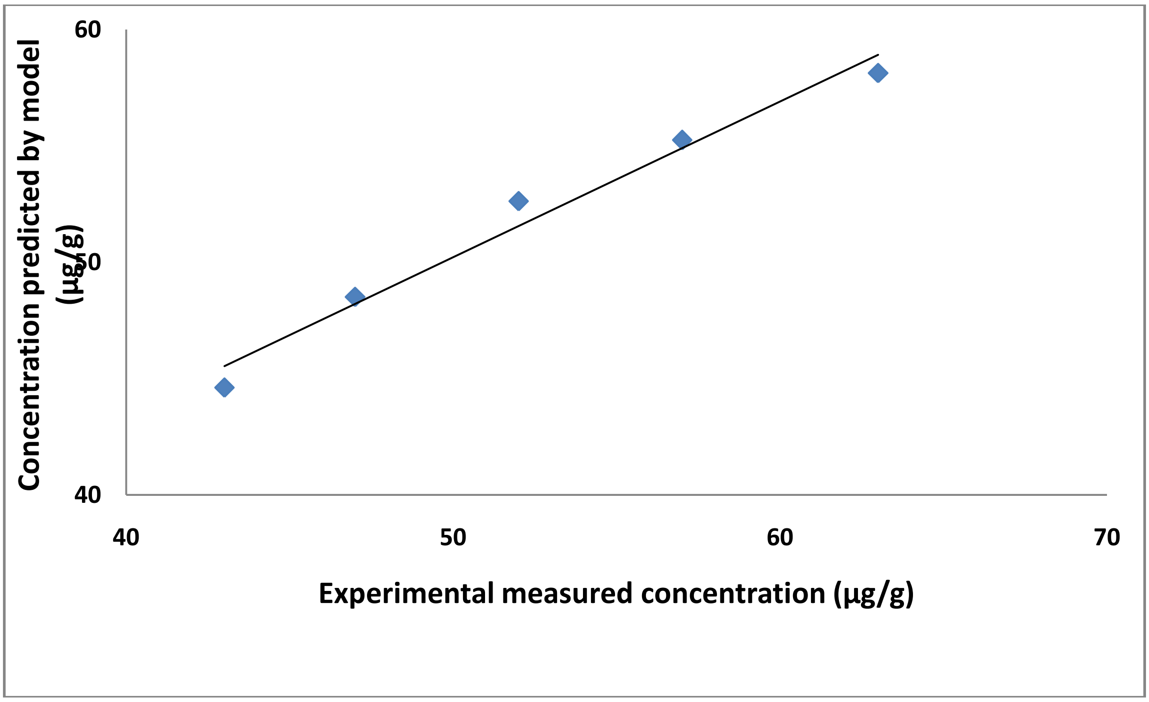

Figure 3: Variation of Zn concentrations predicted by model with experimental measuredvalues

The concentrations of Zn at the early stage (0 – 30 days) of the root development when the concentration was difficult to measure experimentally, and other periods (40, 50, 60, 70, 80 and 90 days) which are outside the experimental values were simulated using the developed model equations. The results of the predicted are shown in Fig. 4. It was observed that the trend of the predicted values were similar to that of the experimental measured values.

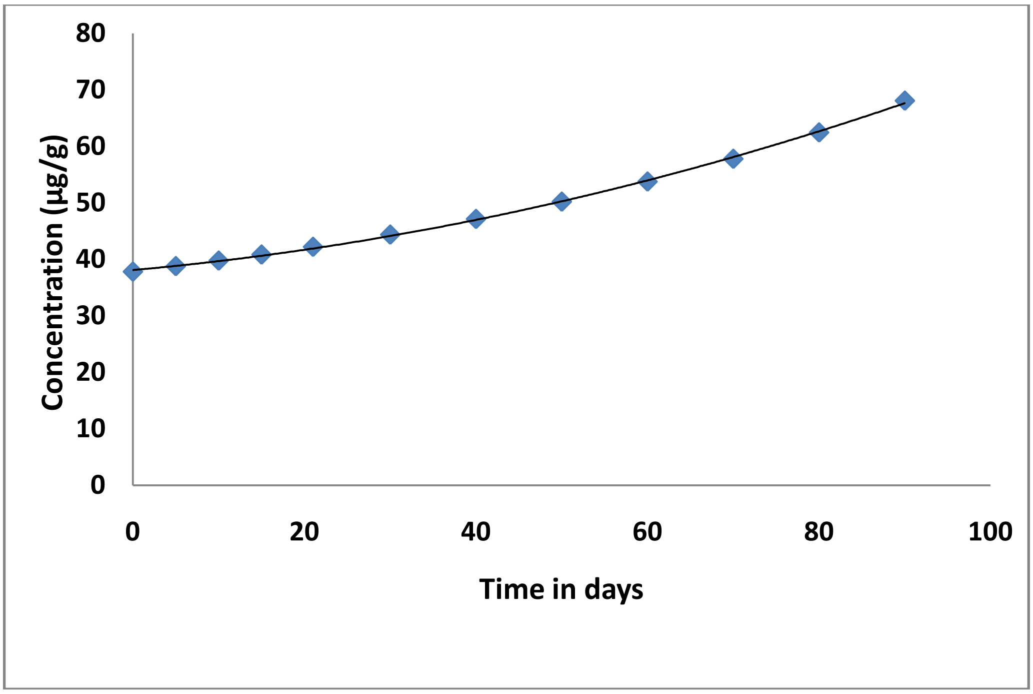

Figure 4: Variation of Zn concentration with time using the model for prediction

The model was validated by plotting the model and experimental values with time as shown in Fig. 5 below. The model values agreed with the experimental measured values which shows that the model developed can be used to predict the concentration of Zinc in roots of Bushgreen plant grown on a polluted soil at any time within the growth period.

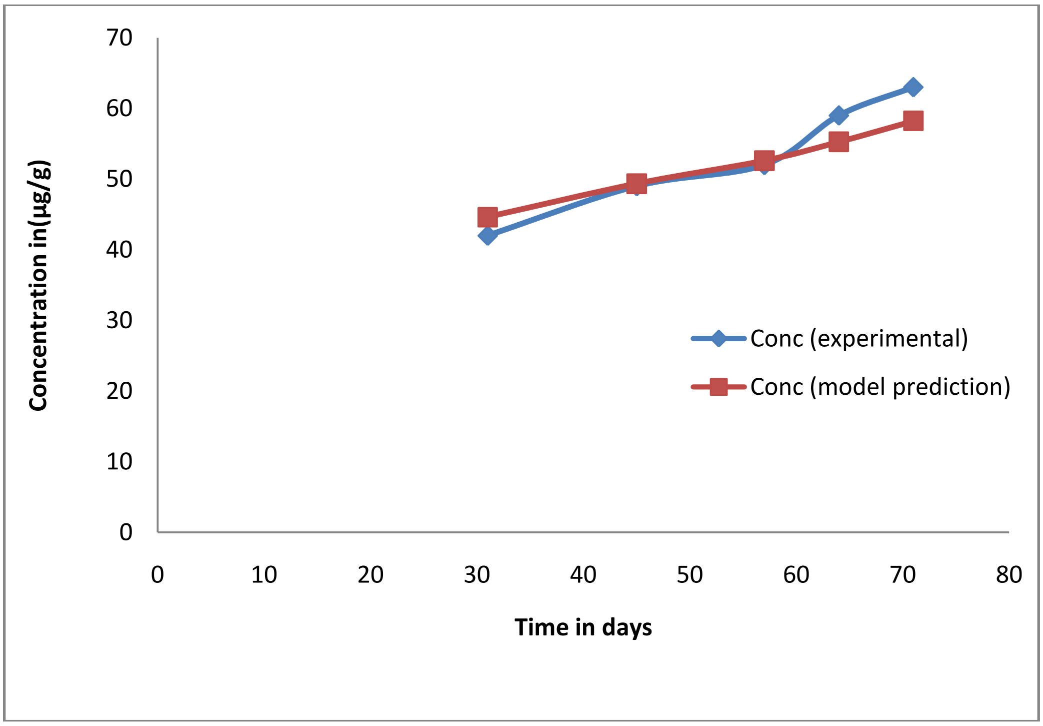

Figure 5: Variations of the experimental and model values with time

V. Conclusions

From the study the following conclusions could be made:
The rate of absorption of Zinc by roots of Bushgreen vegetables followed second order kinetics
A model equation was developed for the absorption of Zinc by Bushdreen roots grown on a polluted soil
The model developed was validated and the values obtained from the model agreed with the experimental values between 92.41 to 99.29 percent.
The developed model was also used to simulate the concentrations of Zinc at the stage of roots development when the concentrations cannot be measured experimentally and value outside the measured experimental values and the trend were the same.

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