

EXPERIMENTAL INVESTIGATION, MODELING AND SIMULATION OF THE ABSORPTION RATE OF IRON (Fe) IONS INTO ROOTS OF JUTE VEGETABLE FROM POLLUTED SOIL

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ABSTRACT

Contamination of agricultural soils with heavy metal ions poses a significant threat to both the environment and human health. This research focuses on conducting an experimental investigation and developing modeling framework to understand and predict the absorption rates of iron (Fe) ions in jute vegetable (Corchorus olitorius) grown on polluted soil. The study involved collecting soil samples from polluted agricultural fields and conducting greenhouse experiments with jute vegetable plants. Various soil properties, such as pH, organic matter content, and initial metal ion concentrations, were analyzed. The jute plants were carefully grown under controlled conditions, and the concentrations of Fe ions in both the soil and plant tissues were monitored over a designated period. The obtained experimental data were used to develop a modeling framework that describes the absorption rates of the metal ions in jute vegetable plants. The modeling approach incorporated factors such as age of the plant, initial metal ion concentrations, plant growth parameters, and environmental conditions. Statistical analysis and regression techniques were employed to derive the model equations, and the accuracy and reliability of the models were assessed using validation datasets and statistical indices. The research outcomes contribute to a deeper understanding of the absorption mechanisms and kinetics of Fe ions in jute vegetable plants cultivated in polluted soils. The developed models provide valuable tools for predicting and managing heavy metal contamination in agricultural systems. This model can aid in assessing the risks associated with heavy metal accumulation in jute vegetable crops and guide the development of effective mitigation strategies. The findings of this study have implications for policymakers, agricultural practitioners, and environmental scientists involved in soil management and food safety. By better understanding the behavior of heavy metal ions in jute vegetable plants, this research helps to establish guidelines for sustainable land management practices and safe food production in areas affected by soil pollution.

Keywords: Absorption, Kinetics, Bioaccumulation and Phytoremediation, modelling

1 INTRODUCTION

The term “heavy metals” refers to any metallic element that has a relative density greater than 5g/cm^3 . Heavy metals include; Lead (Pb), Cadmium (Cd), Zinc (Zn), Mercury (Hg), Arsenic (As), Silver (Ag), Chromium (Cr), Copper (Cu), Iron (Fe), Manganese (Mn) and the Platinum group elements. They are non-biodegradable and persistent environmental contaminants, initially, they are deposited on the soil surface, then absorbed by the apoplast of plant roots and further distributed and accumulated into their edible and non-edible parts, posing an imminent danger to the food chain [1, 2]. The uptake of metal ions from the soil depends on different factors such as their solubility, soil pH, plant growth stages, fertilizer

and soil [3]. A very less amount of heavy metals can also be taken up by vegetables through atmospheric deposition [4]. Vegetables are major part of human platter as they have high amounts of fibers, minerals, vitamins, and antioxidants. Therefore, heavy metals contamination of vegetables cannot be ignored due to their significance in food quality assurance. Furthermore, the food chain pyramid is the track by which biologically toxic trace metals are accumulated in humans and other animals [5, 4]. Heavy metals come in the food chain from a variety of sources. Cd, for example, is taken up from the soil by the roots and transferred to the body of plant. In the instance of Pb, the heavy metal is absorbed by plants through air pollution, whereas As and Hg can be received from dirt water. Some heavy metals having a capacity to accumulate in the tissues (liver, feathers, muscles, kidney, and other organs) of upper customers during the transit from one segment of the food chain to the next. Metal ions are liberated into the soil, water, and air from their parental materials. These HMs are found in soil in decipherable, non-soluble, and moderately soluble forms, with the soluble forms being most harmful since they are quickly captivated by plants through roots before spreading all over the whole plant's organs. Metal toxicity is caused through the disruption of cellular metabolic processes [6, 7, 8, 9]. Hazardous metals are changed to persistent oxidation states in the acid standard and combine with particular proteins and enzymes when they reach the stomach from contaminated foods. The stabilized metal compounds interact with cysteine's sulfhydryl groups (-SH) as well as methionine's Sulphur atoms (-SCH₃), causing protein molecules to breakdown [8, 10].

Table 1. Maximum concentration limits of some trace elements in soils and vegetables [11]

Chemical Element	Maximum allowable limits in soils (µg/g)	Maximum allowable limits in vegetable (µg/g)
As	20	20
Cd	3	0.1
Co	50	50
Cr	100	30
C	100	73
Fe	50,000	435
Mn	2,000	500
Ni	50	67
Pb	100	0.3
Se	10	30
Zn	300	100

Although, uptake of some heavy metals and their accumulation potential in some commonly grown vegetables has been studied, however, very limited research has been conducted on the uptake of Iron (Fe) ions by jute (*Corchorus olitorius*). No known study has modeled the absorption rate of Iron (Fe) ions by Jute (*Corchorus olitorius*) vegetable. The absence of studies on the modeling uptake of Fe ions by Jute (*Corchorus olitorius*) vegetable in Nigeria and in Adamawa State represents a gaping hole in vital scientific information, considering that the vegetable is a widespread consumable vegetable or plant in Africa and is grown in Nigeria and Adamawa State mostly on soils which potentially contains high levels of Iron (Fe) and other metal ion [12]. It is necessary to find a fast-reliable way to evaluate how the iron concentrations changes with time throughout the Jute vegetable growth period. The concentration and time data obtained will be used to develop a kinetic model that will fit the rate of uptake of iron from the polluted soil with time. The developed model could be used to process growth and uptake data for a rapid assessment of time and concentration parameter for the deployment of Jute plant as hyperaccumulator of iron for phytoremediation purposes. For the absorption mechanism in Jute plant, the following dynamics was preferred to other candidate functions. Rate of absorption.

$$r_A = \frac{dC_A}{dt} = KC_A^n \tag{1}$$

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.

1.1 Model Development

The above model is a special case of Fick's law [13, 14] 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 the heavy metal 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. This study focuses on the development of mathematical models for the absorption rate of Fe in Jute vegetable (*Corchorus Olitorius*) from soil and water. Determination of Fe concentration in the soil and roots of Jute plant (*Corchorus Olitorius*) at different stages of growth of the vegetable using Atomic Absorption Spectroscopy (AAS). The absorption mechanism and development of a mathematical model for the process of absorption of Fe by jute plant (*Corchorus Olitorius*) from polluted soils and water is also covered in the study.

2 MATERIALS AND METHODS

2.1 Materials

2.2 Soil Sample Preparation.

The soil samples air dried to a constant weight. The heavy metal in the soil samples were evaluated using the soil testing method by [15]. The dried soil samples were ground with a pestle and mortar to pass through 2-mm mesh sieve. 1g each of the sieved soil samples weighed into a beaker was digested in a mixture of 50 ml concentrated nitric acid (HNO_3) and 1 ml concentrated sulphuric acid (H_2SO_4) and 1ml concentrated perchloric acid (HClO_4) on hot plate with gentle boiling. At completion of digestion, the samples were evaporated to dryness. The residue was then mixed with 10ml of 0.1M nitric acid and filtered into 100 ml standard flask using Whatman No 1 filter and made up to mark with distilled water.

2.2 Vegetable Sample Preparation

The concentration of heavy metals in vegetable samples were determined using analytical methods of soil testing and plant analysis as described by [16] The vegetable samples were reduced to fine powder on a grinder prior to drying at 60°C in an oven to a constant weight. 3.0 g of the fine powdered vegetable samples were weighed into conical flasks and digested in a mixture of 3 ml concentrated perchloric acid (HClO_4), and 25 ml concentrated nitric acid (HNO_3), and 10 ml of hydrogen peroxide (H_2O_2) at 120°C for 4 hours, 130°C for 5 hours, the resultant mixture mixed with H_2O_2 and heated again for 10 minutes on a hot plate in a fume cupboard. The resulting solution was made up to 50 ml with distilled deionized water.

2.2.1 Analytical Procedure for Absorbance

The absorption spectrophotometer with air – acetylene burner, appropriate hollow cathode lamp and wavelength corresponding the element -Iron (Fe) was set at optimum condition. The samples and standard solution of known concentrations was aspirated into the Atomic Absorption Spectrophotometer and the absorbance were obtained from a readout device. Samples were also analyzed repeatedly to ensure the precision and accuracy of analysis. The absorbance of a series of standard solution for Fe was plotted against the concentrations, and a standard curve was obtained. The concentration of Fe in the sample solutions corresponding to their absorbance were then obtained from their standard curves.

3 RESULTS AND DISCUSSION

The variation in concentration of Fe in different parts of Jute vegetable is presented in Figure 1. The levels of Fe in the different parts of jute vegetable are shown in figures 4 below. In the absorption mechanism of heavy metals, once a heavy metal ion is absorbed through the roots of the vegetable and transported to the xylem vessels, there is possibility of movement through the whole plant. The rate and extent of movement within the plant depends on the molecular weight of the metal concerned, the plant species and the age of the plant. The concentration ranking of the chosen heavy metals in the different parts of the vegetable under study is as thus, Roots > Stem > Leaves. From the ranking, generally in this study,

Fe ions were retained mostly in the stem compared to leaves and root parts of the vegetable which is consistent with the findings by Bonanno [17] which states that, it could be as a result of the lower molecular weight of the heavy Fe ions compares to the roots of the vegetable. It was observed from the study that the concentration ranking of Fe ion within the stem of the vegetable under study remains almost the same irrespective of its concentration level in the plant. This observation is in agreement with the statement made by [18] that the rate and extent of movement of metals within plants depends on the metal concerned (its molecular weight), the plant organ and the age of the plant.

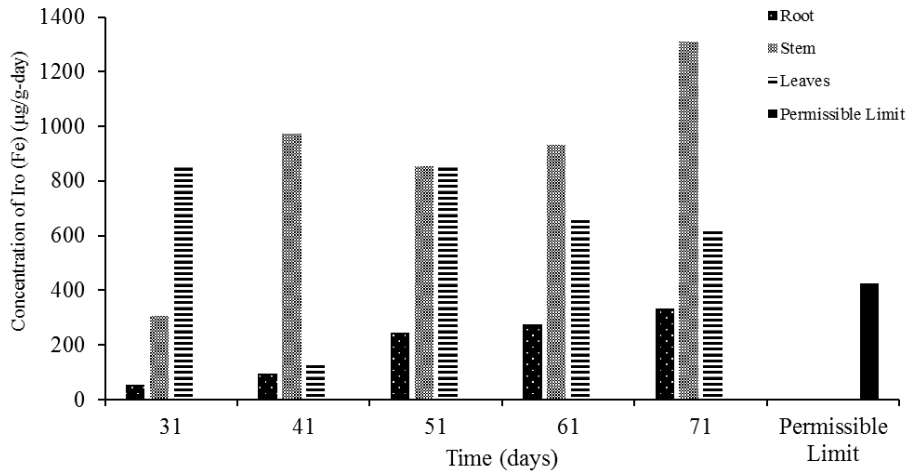


Figure 1. Variation of Iron (Fe) concentration in different parts of the vegetable with time

In Figure 1 above, Fe^{2+} appears to be concentrated in all parts of Jute plant. Its concentration is relatively more in leaves and stems. It can be seen from Figure 1 that Fe^{2+} tends to accumulate in the stems, followed by leaves and then roots in Jute plant. It can be seen from the distribution of Fe^{2+} in parts of Jute (Figure 1) that higher concentrations of the metal ions are found in the stems. This however, is a new finding as far as this work and plant is concerned as it does not agree with any findings in the literature. The concentrations of Fe^{2+} in the leaves and stems of the vegetable are above the [19] maximum permissible level of 425 $\mu\text{g/g}$ in plants as shown in Table 1. This implies that the vegetable is not safe for human and animal consumption. Generally, concentrations of Fe^{2+} clearly show higher concentrations in stems than leaves and then roots. In general, Stems > Leaves > Roots.

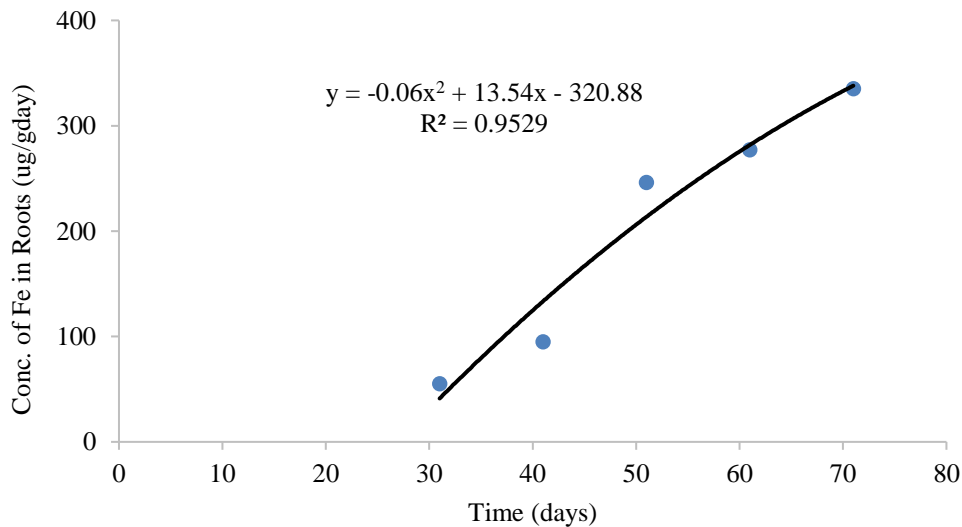


Figure 2. Variation of Iron (Fe) concentration in Jute Roots with time

Figure 2 presents the relationship between root uptake of Fe^{2+} and time taken/maturity. There was a significant ($p \leq 0.05$) increase in the concentration of Fe in the vegetable roots. The study observed that, the lowest Fe^{2+} concentration was recorded in the roots. This however, tends to disagree with the findings of [20, 21, 22, 23] who in their studies, discovered low metal accumulation in fruity and leafy parts of vegetable crops, and higher concentrations in other vegetative parts (the roots). This may possibly be due to poor metal ions mobility within the plants and also lower molecular weight. The relationship is a second order polynomial with correlation ratio of $R^2 = 0.9525$. The empirical equation relating the concentration of Fe^{2+} in roots with time is a polynomial of second degree and correlation coefficient of $R^2 = 0.9529$.

$$C_{Fert} = -0.06t^2 + 13.54t - 320.88 \tag{2}$$

Therefore,

$$\frac{dC_{Fert}}{dt} = -0.12t + 13.54 \tag{3}$$

Applying the absorption kinetics:

$$R_{Fert} = \frac{dC_{Fert}}{dt} = K_{Fert} C_{Fert}^n \tag{4}$$

The rate of Iron uptake, $R_{Fert} = \frac{dC_{Fert}}{dt}$ at different times is obtained using Equation (3) and given in Table 2. Taking the \ln of both sides,

$$\ln R_{Fert} = \ln K_{Fert} + n \ln C_{Fert} \tag{5}$$

The plot of $\ln R_{Fert}$ against $\ln C_{Fert}$ in Equation (5) gives a linear relationship with slope n and intercept $\ln K_{Fert}$ as seen below (Figure 3).

Table 2. The rate of Fe uptake of jute root with time

Time in days	Rate (R_{Fert}) in $\mu\text{g/g-day}$
31	17.26
41	18.46
51	19.66
61	20.86
71	22.06

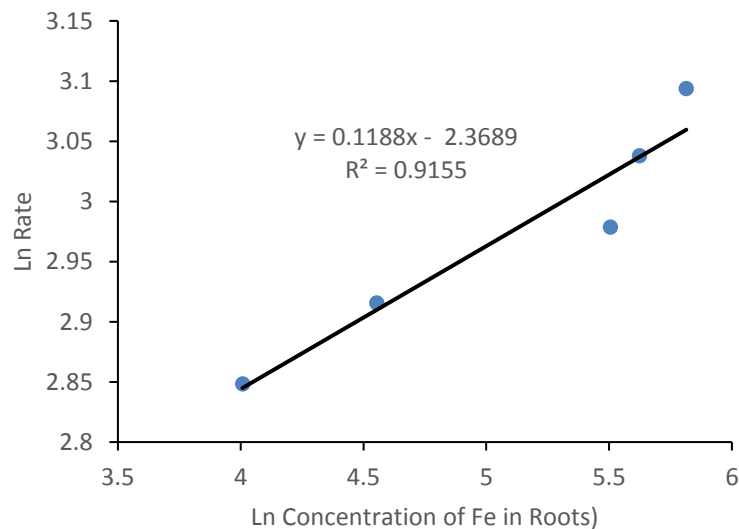


Figure 3. Variation of Ln rate of absorption of Fe with Ln concentration in jute roots with time

From Figure 4, slope $n = 0.12$ and intercept $\ln K_{Fert} = -2.3689$. Therefore,

$$K_{Fert} = e^{-2.3689} = 0.0936 \left(\frac{\mu g}{gday} \right) \tag{6}$$

From the empirical model, the rate of absorption is of the order 0.12 since $n = 0.12$ and therefore the absorption model is given by:

$$R_{Fert} = \frac{dC_{Fert}}{dt} = K_{Fert} C_{Fert}^{0.12} \tag{7}$$

Integrating Equation (6) gives the solution:

$$C_{Fert} = 0.0833 C_{Ferto}^{0.12} + e^{0.0936t} \tag{8}$$

Substituting C_{Fert} into Equation (8) gives the Iron absorption model of jute roots.

$$R_{Fert} = K_{Fert} (0.0833 C_{Ferto} + e^{0.0936t})^{0.12} \tag{9}$$

Therefore,

$$R_{Fert} = 0.0936 (0.0833 C_{Ferto} + e^{0.0936t})^{0.12} \tag{10}$$

The rate of absorption of Iron in Jute root as seen above is fractional or decimal rate (i.e. $R_{Fert} < 1$). This rate form predicts that the reactant concentration (soil concentration) will fall to zero and then become negative at some finite time, also, as a consequence of this feature, in real systems, the observed fractional order will shift upward to unity as reactant (soil concentration) is depleted [24]. Also, the experimental and model predicted values of Iron contained in Table 4 showed some level of agreement. This is because the percentage difference lies within 50% (0.9 to 33.5). Iron has fair absorption rate by roots of Jute vegetable. The plot of the predicted concentration against the experimental concentrations also gave a linear relationship with a high correlation coefficient which also confirms that both data are in agreement (Figure 4).

Table 3. Comparison between the experimental and model predicted Fe concentrations

Time (days)	Conc. of Fe (Experimental) ($\mu g/gday$)	Conc. of Fe (Prediction) ($ug/gday$)	% Difference
31	55	41.2	33.5
41	95	133.4	28.8
51	246	213.6	15.2
61	277	281.8	1.7
71	335	338	0.89

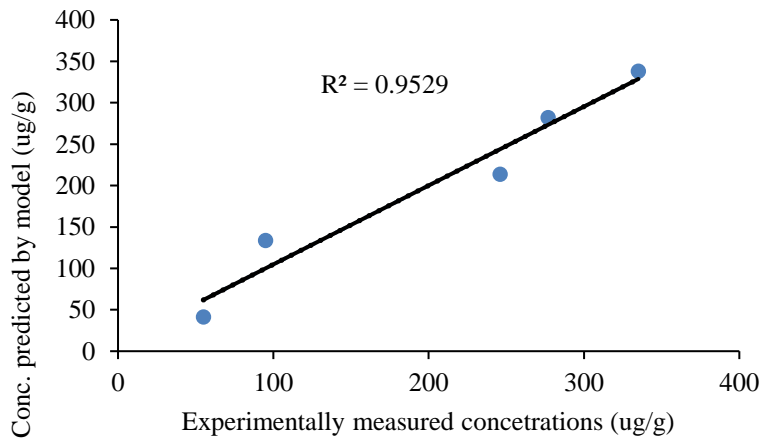


Figure 4. Variation of Fe concentration predicted by model with experimentally measured values

4 MODEL SIMULATION

The concentrations of Fe ions at the early stage (0 to 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 equation. The results of the predicted values are shown in Figures 8. It was observed that the trend of the predicted results is similar to that of the experimental measured values. This clearly shows that the Fe ions absorption model equation can be used to simulate and hence predict the concentrations of Fe ions in Jute roots at any given time of its growth period. Also, the Fe ions follow the same absorption mechanism as reported by [18]. Figure 5 clearly shows that the vegetable roots start developing at day twenty-seven (27), before then, it was not possible to measure the concentration of Fe^{2+} in Jute's roots due to the fact that the roots had not started developing then. However, from day twenty-seven (27) and beyond the concentration can be conveniently measured with the aid of the developed model as can be seen from the graph.

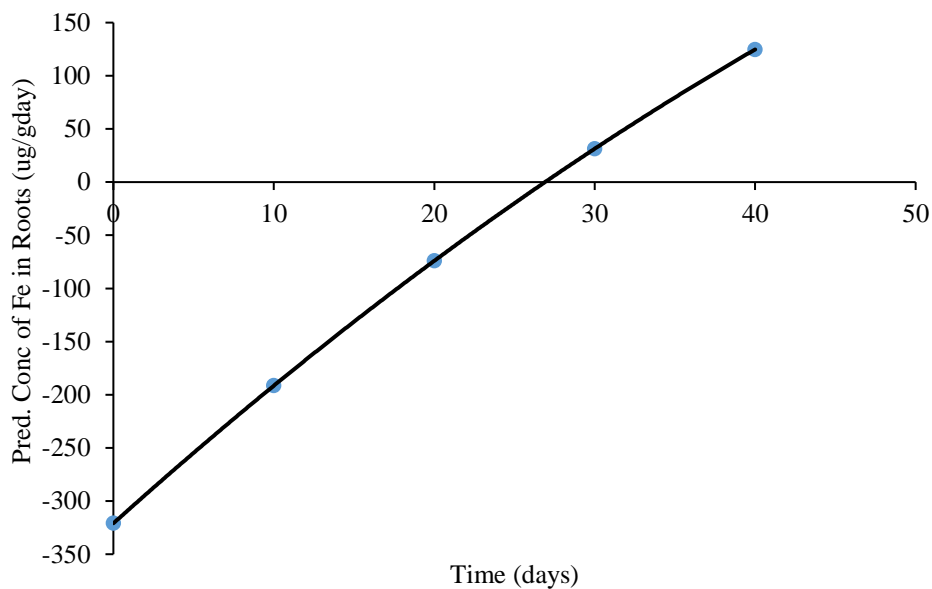


Figure 5. Variation of Fe concentration with time using the model for prediction

5 CONCLUSIONS

The following conclusions could be made from the study. The absorption kinetic model for Fe was found to be: $R_{Fert} = 0.0936 (0.0833C_{Ferto} + e^{0.0936t})^{0.12}$. The concentrations of iron ions in the roots of Jute vegetable increased with time of growth. It was found that Jute vegetable is a high accumulator of Fe. Therefore, growing Jute vegetable in a loamy soil for consumption under conditions of high levels of Fe application is not advisable. The rate of absorption of Iron in Jute root is a fractional or decimal rate (i.e $R_{Fert} < 1$). The mass transport coefficient was found to be $0.0936 \left(\frac{\mu g}{gday}\right)$. The validation of the experimental results of concentration of iron in Jute roots with the values predicted by the developed model is in fair agreement with variations ranging within 30 to 40 %.

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