Mathematical Model for Estimation the Concentration of Heavy Metals in Soil for Any Depth and Time and its Application in Iraq

L. N. M. Tawfiq*, Kareem A. Jasim and E. O. Abdulhmeed*****

College of Education for Pure Science Ibn Al-Haitham, Baghdad University.

* Author to whom correspondence should be addressed; Email: dr.lumanaji@yahoo.com

**kaj_1964@yahoo.com and ***feelactive@gmail.com

Abstract

The aim of this paper is to develop a model equation that can estimate the concentration of heavy metal in the soil for any depth and times. The model equation was developed can be considered as a good representation of the concentration of heavy metals in soil depending on the practical results. That the study which applied in Baghdad city in Iraq.

Keywords: Mathematical model, Soil layers, Heavy metals.

1. Introduction

Generally, nutritional metals do occur naturally in fruits and vegetables as essential trace elements needed for good health, but they could be toxic when their concentrations exceed limits of safe exposure; sixteen chemical elements are known to be important to a plant's growth and survival [1]. The sixteen chemical elements are divided into two main groups: nonmineral and mineral. The nonmineral nutrients are hydrogen (H), oxygen (O), and carbon (C), these nutrients are found in the air and water. The 13 mineral nutrients, which come from the soil, are dissolved in water and absorbed through a plant's roots. Heavy metals are that elements having specific gravity that is at least five times the specific gravity of water which is expressed as 1 at 4°C and refers to metallic elements with an atomic weight greater than iron (55.8 g/mol) [2].

Mathematical Models are simplified representations of some real world entity can be in equations or computer code are intended to mimic essential features while leaving out inessentials, that is, models describe our beliefs about how the world functions. Mathematical modeling aims to describe the different aspects of the real world, their interaction, and their dynamics through mathematics [3].

In this paper we study and develop a model equation that can estimate the concentration of heavy metal in the soil. Several worker have already investigated the mobility of heavy metal in the soil amended with sewage sludge and concluded that only relatively small amount of metal were available for transport in the soil water immediately after sludge application [4].

Giordano and Mortvedt [5] show that under excessive leaching condition, movement of heavy metal in soil is somewhat greater from inorganic than from complexes sources found in sewage sludge.

This research work, therefore aimed at developing a mathematical model equation that estimate the concentration of heavy metals in the soil. This aim can be achieved through the realization of the following objectives:

- Collection of data showing the concentration of heavy metals at different percentage of the soil with respect to distance and time.
- Development of mathematical model equations for the concentration of heavy metals in the soil.
- Simulation of the model equation using computer software programmed, MathLab 2014 professional.

  Compare the simulated result with the experimental data.

2. Mathematical Model of Heavy Metals in Soil

2.1. Assumptions

The assumptions involved in this modelling of the heavy metals in the soil are thus:

1) Porous medium is homogeneous, isotropic, and saturated
2) There is no dispersion in the directions transverse to the flow direction.

2.2. Mathematical Modelling

In this section we develop mathematical model of heavy metals material through soils, by using the classical convection-dispersion equation which defined as [6]:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - V_x \frac{\partial C}{\partial x} - \frac{\rho_b}{\theta} \frac{\partial S}{\partial t} \tag{1}$$

Where;

$$S = k_d . C \tag{2}$$

C: solute concentration (mg/L)

K_d is the distribution coefficient (cm^2/Kg)

θ: soil water content

V_x: Darcy's flux (cm/hr)

D_L: hydrodynamic dispersion coefficient (cm^2/hr)

x: soil depth (cm)

t: t ime (day)

p: Solid density

Equation (1) can then be written as:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - V_x \frac{\partial C}{\partial x} - \frac{\rho_b}{\theta} \frac{\partial}{\partial t}(K_d C) \quad (3)$$

Since k_d is a constant, so rewrite equation (3) as following:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - V_x \frac{\partial C}{\partial x} - \frac{K_d \rho_b}{\theta} \frac{\partial C}{\partial t} \quad (4)$$

And rearranging we get:

$$\frac{\partial C}{\partial t} + \frac{K_d \rho_b}{\theta} \frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - V_x \frac{\partial C}{\partial x} \quad (5)$$

Then we get:

$$\frac{\partial}{\partial t} C(1 + \frac{K_d \rho_b}{\theta}) = D_L \frac{\partial^2}{\partial x^2} C - V_x \frac{\partial}{\partial x} C \quad (6)$$

That is:

$$(1 + \frac{K_d \rho_b}{\theta}) \frac{\partial C}{\partial t} = D_L \frac{\partial^2}{\partial x^2} C - V_x \frac{\partial}{\partial x} C \quad (7)$$

Let

$$\rho = (1 + \frac{K_d \rho_b}{\theta}) \quad (8)$$

So, equation (7) can be written as:

$$\rho \frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - V_x \frac{\partial C}{\partial x}, \qquad 0 < x < \infty \quad t > 0 \quad (9)$$

And $\rho \approx 1$, then equation (9) can thus be written as (for simply $D_L = D$, $V_x = V$):

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial^2 x} - V \frac{\partial C}{\partial x} \quad (10)$$

Which is a second order linear PDE, with initial - boundary conditions:

$$C(x, 0) = C_{x,0} = C_0 \, e^{\frac{-Vx}{D}}$$

$$C(0, t) = C_\circ \text{ and } \frac{\partial C}{\partial x}(\infty, t) = 0.$$

Where;

$C_\circ$: Initial concentration (mg/L).

V: The average pore- water velocity, (cm/hr)

x: soil depth (distance) (cm).

t : time (day^{-1}).

The amount of each element retained by each soil s (mg / kg) was calculated from the initial concentration in solution (mg/ L) and the final concentration C in solution (mg/L).

2.3. Solving the Model Equation

We will use the Adomian Decomposition Method (ADM) to solve the equation (10),

First we consider the linear differential equation in an operator form by

$$L_t C = D\, L_{xx} C - V\, L_x C \qquad (11)$$

Where L, is the derivative symbol which assumed to be invertible.

Applying the inverse operator L^{-1} to both sides of equation (11), and using the initial condition: $C(x, 0) = C_{x,0} = C_0\, e^{\frac{-Vx}{D}}$

We get: $$C = C_0\, e^{\frac{-Vx}{D}} + D\, L_t^{-1} L_{xx} C - V\, L_t^{-1} L_x C \qquad (12)$$

Related to Adomian method, we define the solution C by an infinite series of components given by:

$$C = \sum_{n=0}^{\infty} C_{x,n}$$

Then the equation (12) can be written as:

$$\left(\sum_{n=0}^{\infty} C_{x,n}\right) = C_0\, e^{\frac{-Vx}{D}} + D\, L_t^{-1} L_{xx} \left(\sum_{n=0}^{\infty} C_{x,n}\right) - V\, L_t^{-1} L_x \left(\sum_{n=0}^{\infty} C_{x,n}\right) \qquad (13)$$

Where $c_{x,0}$, $c_{x,1}$, $c_{x,2}$, … can be determined as far as we like.

As given in our model, the zeros component $C_{x,0} = c_0\, e^{\frac{-Vx}{D}}$, then:

$$C_{x,1} = L_t^{-1} \left(D\, L_{xx}\, c_0\, e^{\frac{-Vx}{D}} - V\, L_x\, c_0\, e^{\frac{-Vx}{D}}\right)$$

$$= L_t^{-1} \left(c_0 \frac{V^2}{D}\, e^{\frac{-Vx}{D}} + c_0 \frac{V^2}{D}\, e^{\frac{-Vx}{D}} \right)$$

$$= 2t\, c_0 \frac{V^2}{D}\, e^{\frac{-Vx}{D}}$$

$$C_{x,2} = L_t^{-1} \left(D\, L_{xx} \left(2t\, c_0 \frac{V^2}{D}\, e^{\frac{-Vx}{D}}\right) - V\, L_x \left(2t\, c_0 \frac{V^2}{D}\, e^{\frac{-Vx}{D}}\right)\right)$$

$$= L_t^{-1} \left(2t\, c_0 \frac{V^4}{D^2}\, e^{\frac{-Vx}{D}} + 2t\, c_0 \frac{V^4}{D^2}\, e^{\frac{-Vx}{D}}\right)$$

$$= \frac{4\,t^2}{2} c_0 \frac{V^4}{D^2} e^{\frac{-Vx}{D}}$$

$$C_{x,3} = L_t^{-1}\left(D\, L_{xx}\left(\frac{4\,t^2}{2} c_0 \frac{V^4}{D^2} e^{\frac{-Vx}{D}}\right) - V\, L_x\left(\frac{4\,t^2}{2} c_0 \frac{V^4}{D^2} e^{\frac{-Vx}{D}}\right)\right)$$

$$= L_t^{-1}\left(2t^2 c_0 \frac{V^6}{D^3} e^{\frac{-Vx}{D}} + 2t^2 c_0 \frac{V^6}{D^3} e^{\frac{-Vx}{D}}\right)$$

$$= 8\frac{t^3}{3!} c_0 \frac{V^6}{D^3} e^{\frac{-Vx}{D}}$$

And so on for other components. Consequently, the solution in a series form is given by:

$$C = C_{x,0} + C_{x,1} + C_{x,2} + C_{x,3} \ldots\ldots$$

$$= c_0 e^{\frac{-Vx}{D}} + 2t\, c_0 \frac{V^2}{D} e^{\frac{-Vx}{D}} + \frac{4\,t^2}{2} c_0 \frac{V^4}{D^2} e^{\frac{-Vx}{D}} + 8\frac{t^3}{3!} c_0 \frac{V^6}{D^3} e^{\frac{-Vx}{D}} + \ldots.$$

That is:

$$C = c_0 e^{\frac{-Vx}{D}} \{ 1 + (\tfrac{t}{D})(2v^2) + \frac{1}{2!}\left(\frac{t}{D}\right)^2 (2v^2)^2 + \frac{1}{3!}\left(\frac{t}{D}\right)^3 (2v^2)^3 + \ldots \}$$

i.e., $C = c_0 e^{\frac{-Vx}{D}} e^{\frac{2tV^2}{D}}$

Thus $$C = c_0 \exp\left(\frac{-Vx}{D} + \frac{2V^2}{D} t\right) = c_0 \exp\left\{\frac{V}{D}(-x + 2Vt)\right\} \quad (14)$$

Thus, equation (14) represents the closed form solution of the model equation.

Now, we choose D = 0.5 m^2/d and V = 5.14 × 10^{-6} ms^{-1} $= 44.4096 \times 10^{-2}\ \frac{m}{d}$, depending on results of [7, 8].

Therefore, $C = c_0 \exp\left\{\frac{44.4096\times 10^{-2}}{0.5}\left(-x + 2\left(44.4096 \times 10^{-2}\right)t\right)\right\}$

$$C = c_0 \exp\{0.888192(-x + 0.888192t)\}. \quad (15)$$

3. Application the Mathematical Model

3.1. Location of the Study Area

The study area is located in central Iraq, within the sector of the stable sedimentary plain which represents the western part of the pavement is stable. Where is located between latitudes (33° 44-33° 25) and longitudes (44° 29-44° 16), and Baghdad city includes nine municipal units, five of which are located in Rusafa and four in the Karkh district and each unit containing a number of municipal districts, and associated with all units of the municipal network of highways. The area of the Municipality of Baghdad municipality towards its units (869,031) km^2, [9]. The rates of decline of the earth's surface 0.1 m/km to the south, as the average height between (32-36) meters above sea level, see Figure 1.

The study area is also characterized by the presence of industrial sites, communities and agricultural land, with an area of land inhabited, including the postcard beaches of the limits of industrial facilities (67%), while the land area is uninhabited, including agricultural land (33%), [10].

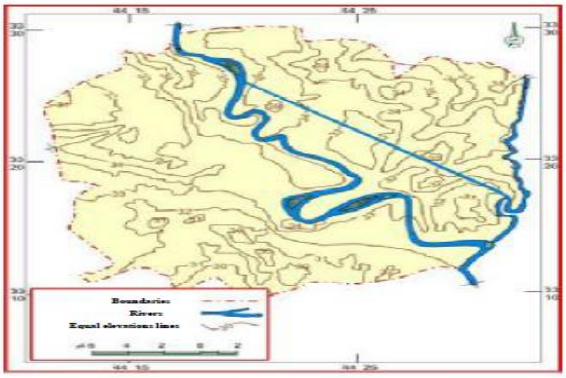

Figure 1: Map of Baghdad city showing rate of earth slop

3.2. Methods and Materials

The data and information on soil contaminants is selected from 12 stations located on different parts of the city of Baghdad for the purpose of collecting samples of soil have been distributed on a regular basis so as to cover most areas of the city, with a focus on the type of each area as commercial, industrial or residential, as shown in Figure 2.

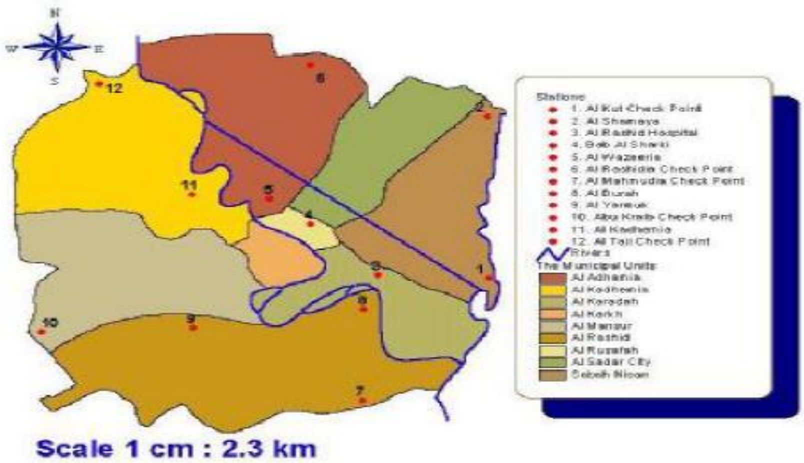

Figure 2: Map of Baghdad city showing study stations

Now, in the equation (15) if, substituting the initial concentrations (C_0) of heavy metals, then we get the concentrations of this heavy metals for time t(d) and depth x(m). The practical results illustrated in Figure (3), where t = 0, …, 5000 day and x = 0, 10, 20 cm, then the figure represent the concentrations of heavy metals in soil of Baghdad city for years from 2004 to 2016.

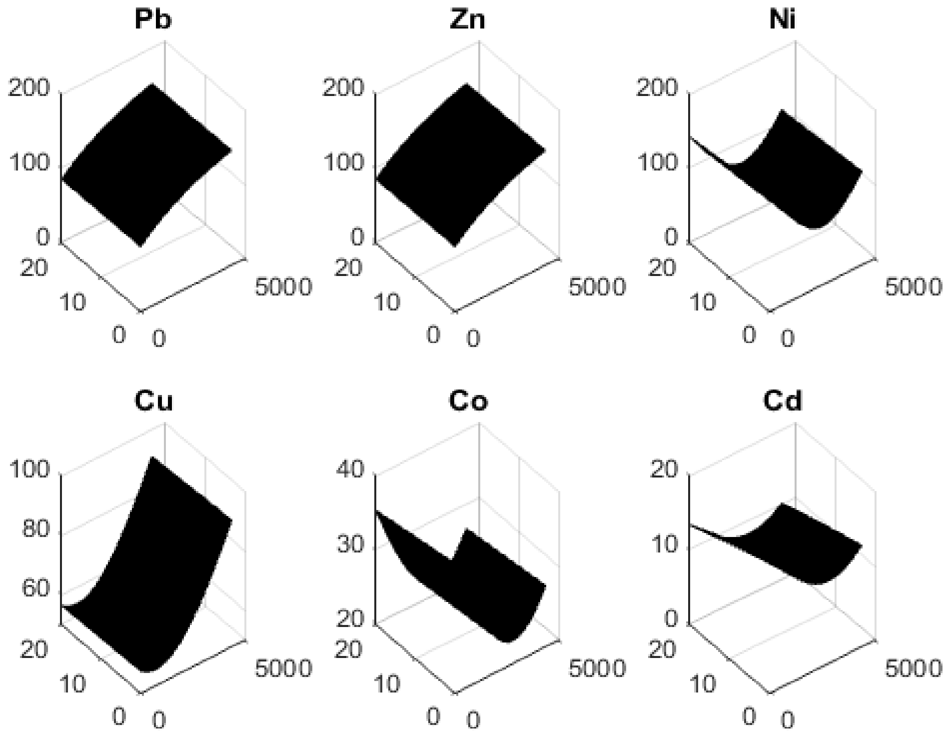

Figure3: Concentrations of heavy metals for time t(d) and depth x(m) in Baghdad city.

3.3. Results and Discussion

Figure 2, illustrate the results of the concentrations of take elements in soils and areas of Baghdad, which calculated from equation (15), and Figure 4, illustrates the comparison for concentration of heavy metals in Baghdad soil with previous studies, we see that:

- **Lead (Pb)**: We can deduce that the soil of some areas of Baghdad under the influence of lead contaminated divorced and industrial plants such as the smelter and battery plant in Abu Ghraib and Waziriya and brick factories polluting to the air and soil existing in the Adhammaai region, as well as the impact of vehicles with gasoline, which took increasing dramatically, leading to increased air pollution in lead and thus contamination of soil, as well as the impact of foundries and workshops with public and private sector in the city areas.
- **Zinc (Zn):** The reason for increased concentrations of zinc in the soil of the city of Baghdad to increase the acidic soil because the easy assimilation of zinc, as well as a result of increased soil organic matter, and has indicated several studies have suggested that increased concentrations of zinc in the soil due to the influence of vegetation as well as the impact of human activities and of laboratories and foundries and the use of Nutraceuticals and pesticides in the soil.
- **Copper (Cu):** We see that the soil of some area is contaminated with copper significantly and there is also this element pollution in other areas such as Waziriya and Rashid Hospital. The cause of increased concentrations of copper in the soil of the city dates back to adsorption by clay minerals and its transmission over long distances with the river sediment as well as increasing organic materials, and increased copper in the soil due to industrial activities such

as workshops, foundries and smelting operations in addition to the impact of irrigation water and drainage.

- **Nickel (Ni):** We see that the soil of some areas contaminated nickel. The cause of increased concentrations of nickel in the soil due to adsorption processes by clay minerals and to the al Qaeda presence in the rocks and sedimentary rocks, and organic materials play an important role in increasing concentrations of nickel in the soil. Industrial activities also play an equally important role in increasing concentrations of nickel in the soil through the spread of the electrical industry and laboratories as well as batteries, workshops and foundries with the private sector and deployed in the city.
- **Cobalt (Co):** We conclude that some of the city contaminated soils crusts. The increase in the concentrations of cobalt in the soil are the result of several factors, including the origin and composition of soil and weathering processes and the impact of human activities as well as the impact of irrigation water.
- **Cadmium (Cd):** We see that the soil contaminated with cadmium city. Increasing concentrations of cadmium in the soil due to the increase of organic matter in the soil and the presence in the rock base and as a result of industrial activities as well as the use of conditioners, pesticides, and the impact of water drainage.

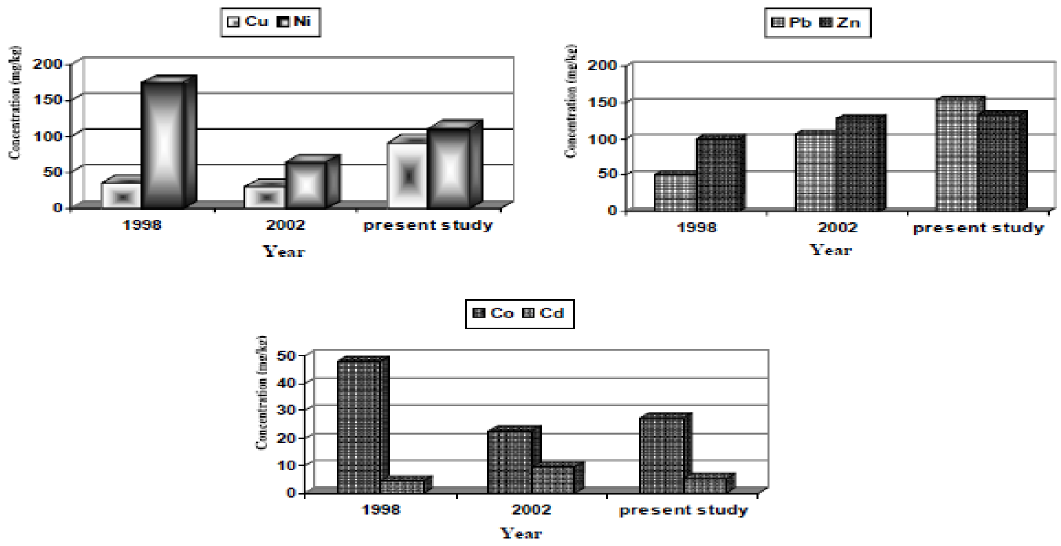

Figure 4: Comparison for concentration of heavy metals in Baghdad soil with previous studies

4. Conclusions

The analysis of the result shows that there is a very good level of agreement between the experimental and simulated results obtained. This can also be confirmed by the numerical analysis of the result by using interpolation.

In conclusion, the model can be considered to be a good representation of the estimating the concentrations of heavy metals in the soil.

The results of the analysis of lead in soil in Baghdad city, show the concentrations of this element has exceeded the permissible limits in some regions is due to the impact of divorced and industrial plants such as brick factories and smelters as well as the impact of divorced vehicles due to combustion. The results showed that concentrations of zinc in the soil did not exceed the permissible limits, indicating the presence of contamination of this element in the soil of Baghdad city. Also, observed by measuring the concentrations of Cu, Co, Ni, Cd it had exceeded the permissible limits, which indicates the existence of these elements in the soil of the city of Baghdad, and the reason for the increase in the concentrations of these elements is due to several reasons including the impact of industrial activities, but by less than in previous years due to suspension of many of these actors to work due to war conditions experienced by the country as well as the impact of adsorption by clay minerals and the presence of organic matter in the soil that play an important role in increasing concentrations of these elements as well as the weathering and irrigation and drainage.

References

[1] Ajmalkhan, M. U., and Showalter, A. M., (1999), Effect of salinity on growth, ion contact, and osmotic relation, Stapf. Journal of Plant Nutration, Vol. 22, No. 1, pp: 191-204.

[2] Kabata, A., and Pendias, H., (2001), Trace Elements in Soils and Plants, 3rd Edition, CRC press, Washington, D.C., 550 p.

[3] Bokil, V. A., (2009), "Introduction to Mathematical Modeling", Spring.

[4] Sidle R. C., and Kardos L. T., (1977), Aqueous release of heavy metals from two sewage sludges, Water Air Pollution, Vol. 8, pp. 453 459.

[5] Giordano, P. M., and Morvedt, J. J., (1979), Nitrogen effects on mobility and plant uptake of heavy metals in sewage sludge applied to soil columns, J. Env. Qual., Vol. 5, pp. 165-168.

[6] Selim, H. M., Amacher, M. C., and Iskandar, L. K., (1990), Modeling the Transport of Heavy Metals in Soils, Monograph 90-2,U.S. army corps of engineering.

[7] Meserecordias, W., L., Jasper, N., I., Karoli, N. N., and Patrick, A. N., (2014), Environmental Contamination by Radionuclides and Heavy Metals Through the Application of Phosphate Rocks During Farming and Mathematical Modeling of Their Impacts to the Ecosystem, International Journal of Engineering Research and General Science, Vol. 2, Issue 4, pp: 852 – 863.

[8] Bohun, C. S., (2010), Mathematical models for an undisturbed soil-column, Mathematics-in-Industry Case Studies Journal, Vol. 2, pp: 1-15.

[9] Maitham, A. S., (26-28 April 2010), Evaluation of Soil pollution by heavy metals in Baghdad city using GIS, The 1st International Applied Geological Congress, Department of Geology, Islamic Azad University, Mashad Branch, Iran, pp: 852-863.

[10] Hiti, M., (1985), The quality of groundwater within the city of Baghdad, MSc. thesis, College of Science, Baghdad University, Iraq.