ISSN 2348 – 8034
Impact Factor- 3.155

GLOBAL JOURNAL OF ENGINEERING SCIENCE AND RESEARCHES

NUMERICAL MODEL FOR ESTIMATION THE CONCENTRATION OF HEAVY METALS IN SOIL AND ITS APPLICATION IN IRAQ

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ABSTRACT
The aim of this paper is design numerical model which describes the spread of heavy metals in soil horizontally. The suggested models can be used to estimates the concentration of heavy metals in soil for any times. So, we can determine the contamination levels by some heavy metals such Copper, Lead, Zinc, Cadmium, Cobalt, and Nickel with the potential for this contamination sources with their impact.

Keywords- *Numerical model, Soil, Heavy metals.*

I. INTRODUCTION
Nonlinear phenomena are of fundamental importance in various fields of science and engineering. The nonlinear models of real-life problems are still difficult to solve either numerically or analytically.

There has recently been much attention devoted to the researches for better and more efficient solution methods for determining a solution, approximate or exact, analytical or numerical, to nonlinear models, especially, contamination model.

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].

Numerical 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 design numerical 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.

There are many researchers studied the contamination in soil by heavy metals by using traditionally methods such [6-10].

In this paper, we introduce an application for the suggested design of model equation which describe the soil contamination by heavy metals for different zones in Baghdad city.

II. NUMERICAL 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. Numerical Modelling

Let $(x_0, t_0), (x_1, t_1), \ldots, (x_m, t_n)$ is the given point in the (x, y)-plane, we have to find a polynomial passing through these points, where (x_i, t_j), $i = 0,1,2,\ldots.m$, and t_j, $j=0,1,2\ldots,n$, are given as a rectangular grid.

The polynomial of degree m in x, and n in t, can be constructed to interpolate through (x_i, t_j) as follow:

Let $\ell_i(x) = \prod_{\substack{k=0 \\ k\neq i}}^{m} \frac{(x-x_k)}{(x_i-x_k)}$, $\ell_j(t) = \prod_{\substack{j=0 \\ k\neq j}}^{n} \frac{(t-t_k)}{(t_j-t_k)}$

Let $\ell_{ij} = \ell_i(x)\ell_j(t)$, $0 \le i \le m$, $0 \le j \le n;$

So, we have $\ell_{ij}(x_k, t_s) = \begin{cases} 1 & i = k, j = s \\ 0 & otherwise \end{cases}$

Thus ℓ_{ij} represents a polynomial of degree m in x and n in t. Then, we get the two dimensions interpolating polynomial $P_{m,n}(x, t)$ that interpolates f(x,t) in the given data would be written as:

$$P_{m,n}(x, t) = \sum_{i=0}^{m} \sum_{j=0}^{n} f(x_i, t_j) \ell_{ij}(x, t),$$

$$= \sum_{i=0}^{m} \sum_{j=0}^{n} f(x_i, t_j) \prod_{\substack{k=0 \\ k\neq i}}^{m} \frac{(x-x_k)}{(x_i-x_k)} \prod_{\substack{j=0 \\ k\neq j}}^{n} \frac{(t-t_k)}{(t_j-t_k)} \qquad (1)$$

Now, we introduce theorem which guaranty the uniqueness of these polynomial and it's prove given in [11].

Theorem 3.1
There exist a unique polynomial $P_{m,n}(x, t)$ passing through given $(n+1)(m+1)$ data.

Note: The problem is well-posed; *i.e.*, it has a unique solution that depends continuously on the data.

Theorem 3.2
Suppose (x_i, t_j), $0 \le i \le m$, $0 \le j \le n$, are distinct points in the interval [a, b]×[c, d] and $f \in C^{m+n+2}$ ([a, b]×[c, d]). Then

$$R(x, t) = f(x, t) - P_{m,n}(x, t) = \frac{\partial^{m+1} f(\theta_1, t)}{(m+1)!\, \partial x^{m+1}} + \frac{\partial^{n+1} f(x, \theta_2)}{(n+1)!\, \partial t^{n+1}} - \frac{\partial^{m+n+2} f(\xi_1, \xi_2)}{(m+1)!\,(n+1)!\, \partial x^{m+1} \partial t^{n+1}}$$

It is clear that finding the error is practically difficult with the two dimensional interpolation. But we can determine the behavior of the errors.

Notification: Many authors specialize the formula (1) for small numbers of data, before asserting that certain shortcomings make it a bad choice for practical computations. Among the shortcomings sometimes claimed are these:

1. Each evaluation of $P(x, t)$ requires (n^2) and (m^2).
2. Adding a new pair $((x_{m+1}, t_{n+1}), f_{m+1,n+1})$ requires a new computation from scratch.
3. The computation is numerically unstable.

Now, we applied suggested design to estimate the concentration of heavy metals in soil.

III. SAMPLING

The Capital of Iraq Baghdad City (33°14'-33°25'N, 44°31'-44°17'E), is characterized by arid to semi-arid climate with dry hot summers and cold winters; the mean annual rainfall is about 151.8 mm. For the purpose of collection of soil samples, the study area was divided in to five main types of land use viz. residential, commercial, agricultural, main roads and industrial; and two main source areas, within each land use type viz. roadside and open areas.

The samples are carefully collected from each source area in different land using types with a stainless steel spatula. They were air–dried in the laboratory, homogenized and sieved through a 2mm polyethylene sieve to

ISSN 2348 – 8034
Impact Factor- 3.155

remove large debris, stones and pebbles, after they were disaggregated with a porcelain pestle and mortar. Then these samples were stored in clean self–sealing plastic bags for further analysis.

Metal determinations were done by Atomic Absorption Spectrometry (AAS 6300, Shimadzu, Japan), X– ray fluorescence analysis (XRF) or Inductively Coupled Plasma-Mass Spectrometry (ICP-MS).

The samples are carefully chosen from each source area depending on the suggested technique.

IV. RESULTS FROM SUGGESTED DESIGN

Now, we applied the suggested model to study a concentration of heavy metals in Baghdad city. In this case, the data and information on soil 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 residential, commercial, agricultural, main roads and industrial; as shown in Figure 1.

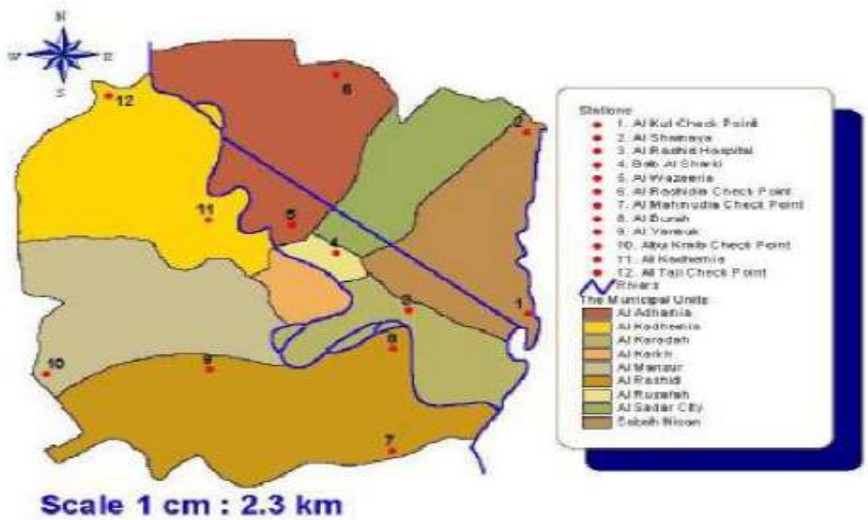

Figure 1: Map of Baghdad city showing study stations

Now, we applied suggested design to estimate the concentration of heavy metals in Baghdad soils but in this case we use the data for concentrations of previous years (1998 – 2014) from ministry of agriculture and the data for concentrations of 2015 are calculated in laboratory by using ICP-MS device where the composition and properties of selected soil is given in Table (1), and the results are illustrated as follow:

1- For spreading the Cu, which illustrated in Figure (2), represents kink waves which rise or descend from one asymptotic state to another and approaches a constant at infinity.

2- For spreading the Cd, which illustrated in Figure (3), represents kink waves.

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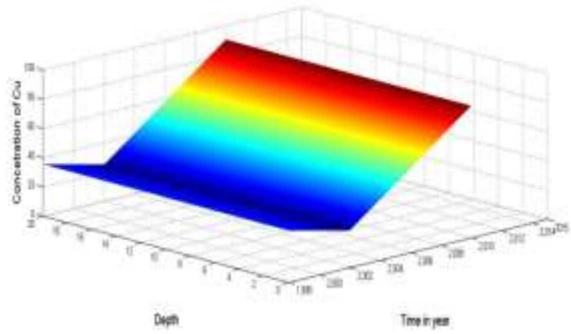

Figure 2: The wave solution for concentration of Cu in soil of Baghdad.

3- For spreading the Zn, which illustrated in Figure (4), represents Peakons are peaked solitary wave solution. In this case, the wave solution is smooth except for a peak at a corner of its crest or for bottom. Peakons are the points at which spatial derivative changes sign so that peakons have a finite jump in first derivative of the solution C(x, t). This means that peakons have discontinuities in the *x*-derivative but both one-sided derivatives exist and differ only by a sign [12].

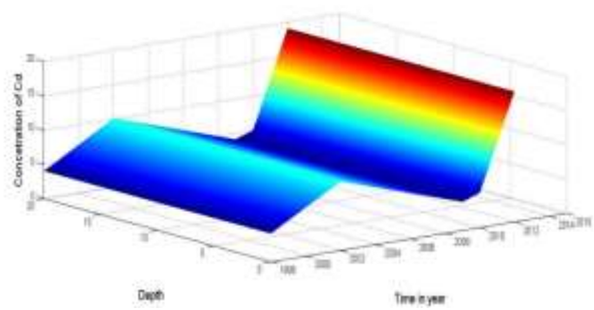

Figure 3: The wave solution for concentration of Cd in soil of Baghdad

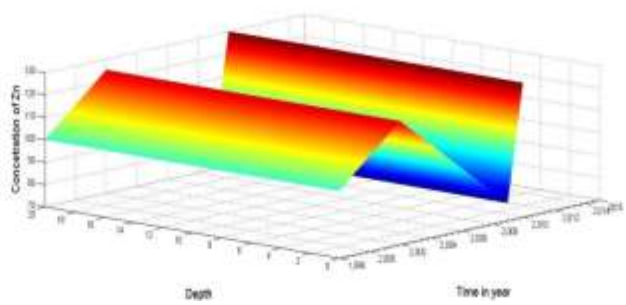

Figure 4: The wave solution for concentration of Zn in soil of Baghdad

4- For spreading the Pb, which illustrated in Figure (5), represents kink waves in the first part which defined on the interval [1998, 2011] and represents peakon waves in the second part defined on remainder interval.

5- For spreading the Co, which illustrated in Figure (6), represents represents kink waves.

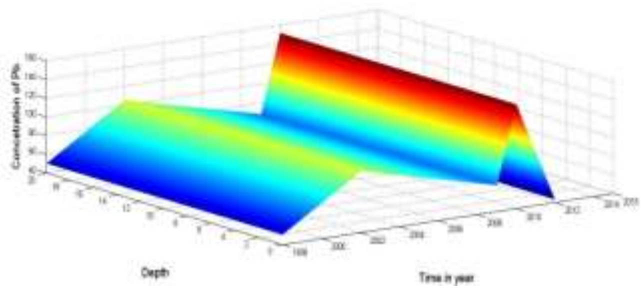

Figure 5: The wave solution for concentration of Pb in soil of Baghdad

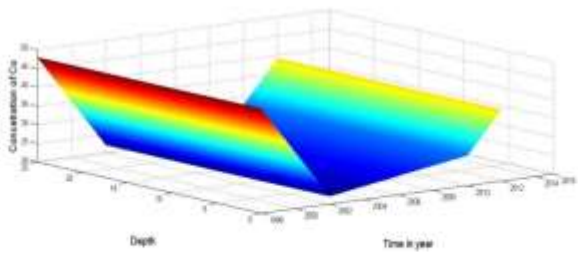

Figure 6: The wave solution for concentration of Co in soil of Baghdad

6- For spreading the Ni, which illustrated in Figure (7), represents kink waves.

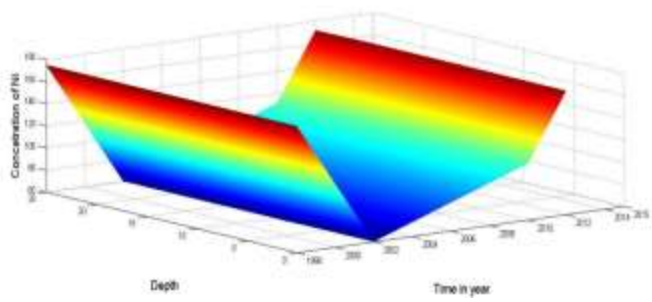

Figure 7: The wave solution for concentration of Ni in soil of Baghdad

Table 1: Composition and properties soil used in the present study.

Property	Soil
Particle size distribution (ASTM D 422)	
Sand (%)	1.5
Silt (%)	63.5
Clay (%)	35
Cation Exchange Capacity (meq/100g)	12.5
Initial pH	8.3
Background concentration of cadmium (mg/kg)	nill
Background concentration of nickel (mg/kg)	3.52
Background concentration of lead (mg/kg)	15
Organic matter (%)	0.49
Organic carbon (%)	0.16
Electrical conductivity EC (μS/cm)	593
Surface area (m^2/g)	22.776
Bulk density (g/cm^3)	1.1317
Porosity (n)	0.493
Specific weight	2.69
Soil classification	Silty clay loam

4.3. Traditional Remediation of Contaminated Soil

Traditional treatments for metal contamination in soils are expensive and cost prohibitive when large areas of soil are contaminated. Treatments can be done *in situ* (on-site), or *ex situ* (removed and treated off-site). Both are extremely expensive. Some treatments that are available include:
1. High temperature treatments (produce a vitrified, granular, non-leachable material).
2. Solidifying agents (produce cement-like material).
3. Washing process (leaches out contaminants).

The following management practices will not remove the heavy metal contaminants, but will help to immobilize them in the soil and reduce the potential for adverse effects from the metals – Note that the kind of metal (cation or anion) must be considered:

1. Increasing the soil pH to 6.5 or higher.
2. Draining wet soils.
3. Applying phosphate.
4. Carefully selecting plants for use on metal-contaminated soils.

V. DISCUSSION

The practical results show the following:

- The average of the concentrations of heavy metals in soil for different time and zones in Baghdad are increase with time, posing a great risk to the environment contamination.
- For the comparison among the concentrations of different regions: residential, industrial, commercial and agricultural regions, we see that:

soils agricultural < soils residential < soils commercial < soils industrial that is, the agricultural regions are the lowest while the 80 industrial regions are the highest for the concentrations of heavy metals.

- There are different causes for increasing the concentrations of heavy metals in soil such as: the big traffic jams resulting from the great number of cars lately which use gasoline that contains a lot of fourth lead Ethylene which cause big problems to the environment. This creates dangers to human beings. In addition, the increase in the amount of litter and how to get rid of industry waste in sewerage and the decrease in the green region which participate in lessening the damage of waste on the environment. As a result of increase in the population during the late years which results in converting the regions of vegetation to residential regions and the technological development which causes contamination because of the prolife ration of plants and workshops scattered everywhere. Add to all this, wars and their great contamination which are considered the most dangerous contaminates of the soil and environment. All these types of contaminates cause high rate of concentration of waste which exceeds the normal amount in soil, the increase of these metals has different types of danger on human health. The plants absorb these dangerous materials which in its turn go to human being through food consumption which they acquire because of eating these plants that have the dangerous metals.

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