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ESTIMATETHE CONCENTRATION OF HEAVY METALS IN SOIL BY USING TRIGONOMETRIC CUBIC B-SPLINE METHOD AND ITS APPLICATION IN BAGHDAD, IRAQ

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ABSTRACT

The aims of this paper, is to estimate the concentration of heavy metals such cadmium, copper, nickel,lead, and zincin soilby using trigonometric cubic B-spline collocation method. In this work the usual finite difference scheme is applied to discretize the time derivative. Trigonometric cubic B-spline basis functions are used as aninterpolating function in the space dimension.Whereas the result is the concentration of heavy metals. This method is also suggested to estimate the concentration of heavy metals such cadmium, copper, nickel, lead, and zinc in soil of Baghdad city, Iraq. Thus we can estimate the contamination in soil by heavy metals. The result showed that the proposed method can successfully estimate the concentration of heavy metals in soilfor any depth.

***Keywords**: Trigonometric cubic B-spline basis functions, Cubic trigonometric B-spline collocation method Soil contamination, Heavy metals, Soil property.*

I. INTRODUCTION

Heavy Metals (HMs) occur naturally in soils formed by alteration and erosion processes of geological underground materials. Soil can contain increased amounts of heavy metals of varying concentrations, coming from different natural sources, but the major source of soil pollution by heavy metals is human activity-mainly industrialization and agriculture[1]. Soil contaminated with heavy metals have serious consequences for terrestrial ecosystems, agricultural production and human health [2]. Heavy metals contamination is considered as a negative effect of industrial activities which must be monitored assessed and managed [3].

For instance, several authors have studied how to estimate the contamination in soil or estimate the concentration of heavy metals without prices. A number of authors have studied this problem using parallel processing technique such [4-13].

In this work, a numerical collocation finite difference technique based on trigonometric cubic B-spline is presented for estimating the concentration of heavy metals such cadmium and nickel in soil. A usual finite difference scheme is applied to discretize the time derivative while trigonometric cubic B-spline is utilized as an interpolating function in the space dimension.

This paper suggests an effective, low cost and easily accessible method to estimate the concentration of heavy metals in soil and compared the results with the traditional laboratory devices: Inductively Coupled Plasma-Mass Spectrometry (ICP- MS) to illustrate the accuracy and the efficiency of the suggested technique.

II. TRIGONOMETRIC CUBIC B-SPLINE FUNCTION

In this section, the cubic trigonometric basis function is defined as follows [14, 15]

$$TB_i^4(x)=\frac{1}{z}\begin{cases} q^3(x_i), & x\in[x_i,x_{i+1}) \\ \mathrm{q}(x_i)\left(\mathrm{q}(x_i)\,\mathrm{p}(x_{i+2})+p(x_{i+3})\,\mathrm{q}(x_{i+1})\right)+p(x_{i+4})\,\mathrm{q}^2(x_{i+1}), & x\in[x_{i+1},x_{i+2}) \\ \mathrm{p}(x_{i+4})\left(\mathrm{q}(x_{i+1})\,\mathrm{p}(x_{i+3})+p(x_{i+4})\,\mathrm{q}(x_{i+2})\right)+q(x_i)\,\mathrm{p}^2(x_{i+3}), & x\in[x_{i+2},x_{i+3}) \\ p^3(x_{i+4}), & x\in[x_{i+3},x_{i+4}] \end{cases} \quad (1)$$

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Where,

$$q(x_i)=\sin\left(\frac{x-x_i}{2}\right),\ p(x_i)=\sin\left(\frac{x_i-x}{2}\right),\ z=\sin\left(\frac{h}{2}\right)\sin(h)\sin\left(\frac{3h}{2}\right)$$

Where as $h=(b-a)/n$ and $TB_i^4(x)$ is a piecewise cubic trigonometric function with some geometric properties like continuity, non-negativity and partition of unity [16,17]. The values of $TB_i^4(x)$ and its derivatives at nodal points are required and these derivatives are tabulated in Table 1.

Table 1: Values of $TB_i^4(x)$ and its derivatives.

x	x_i	x_{i+1}	x_{i+2}	x_{i+3}	x_{i+4}
TB_i	0	p_1	p_2	p_1	0
TB_i'	0	p_3	0	p_4	0
TB_i''	0	p_5	p_6	p_5	0

Where as

$$p_1=\frac{\sin^2\left(\frac{h}{2}\right)}{\sin(h)\sin\left(\frac{3h}{2}\right)},\ p_2=\frac{2}{1+2\cos(h)},\ p_3=-\frac{3}{4\sin\left(\frac{3h}{2}\right)},\ p_4=\frac{3}{4\sin\left(\frac{3h}{2}\right)}$$

III. DISCRIPTION OF NUMERICAL METHOD

This section discusses the cubic trigonometric B-spline collocation method for solving numerically the

$$\alpha C_t=\beta C_{xx}-\gamma C_x \tag{2}$$

With the initial and boundary condition

$$C(x,0)=w\quad a\le x\le b \tag{3}$$

$$C(a,t)=f\quad 0\le t\le T$$

$$C_x(b,t)=0 \tag{4}$$

Whereas α ,β and γ are constants,the solution domain $a\le x\le b$ is equally divided by knots x_i into n subintervals $[x_i,x_{i+1}]$, $i=0,1,2,...,n-1$ where $a=x_0<x_1<...<x_n=b$. Our approach for (2) equation using cubic trigonometric B-spline is to seek an approximate solution as [19]

$$C_j(x,t)=\sum_{j=-3}^{n-1}S_j(t)TB_j^4(x) \tag{5}$$

whereas $S_j(\mathrm{t})$ is to be determined for the approximated solutions $C_j(x,t)$ to the exact solution at the point (x_j,t_i) .The approximations C_j^i at the point (x_j,t_i) over subinterval $[x_i,x_{i+1}]$ can be defined as

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$$C_j^i = \sum_{k=j-3}^{j-1} S_k^i TB_k^4(x) \tag{6}$$

Whereas $j = 0,1,2,...,n$. So as to get the approximations to the solution, the values of $B_{3,j}(x)$ and its derivatives at nodal points are required and these derivatives are tabulated using approximate functions (4) and (6), the values at the knots of C_i^j and their derivatives up to second order are

$$\begin{cases} (C)_j^i = p_1 S_{j-3}^i + p_2 S_{j-2}^i + p_1 S_{j-1}^i, \\ (C_x)_j^i = p_3 S_{j-3}^i + p_4 S_{j-1}^i \\ (C_{xx})_j^i = p_5 S_{j-3}^i + p_6 S_{j-2}^i + p_5 S_{j-1}^i \end{cases} \tag{7}$$

Approximation for the solutions of equation (1) at t_{j+1} th time level can be given as: $\alpha(\frac{C^{n+1}-C^n}{\Delta t}) = \theta(\beta(C_{xx}^{n+1}-C_{xx}^n)-\gamma(C_x^{n+1}-v_x^n))(1-\theta)(\beta(C_{xx}^{n+1}-C_{xx}^n)-\gamma(C_x^{n+1}-C_x^n))$ (8)

The subscripts n and $n+1$ are successive time levels, $n = 0,1,2,..$ and Δt is the time step.
The equation (8) with putting the values of nodal values C and derivatives using (7) becomes the following difference equation with variable S_j , $j = -3,...,\mathrm{n}-1$ and noted the equation a Crank-Nicolson when $\theta = \frac{1}{2}$

$$a_1 S_{j-3}^{n+1} +_1 a_2 S_{j-2}^{n+1} + a_3 S_{j-1}^{n+1} = b_1 S_{j-3}^n + b_2 S_{j-2}^n + b_3 S_{j-2}^n \tag{9}$$

$$\begin{cases} a_1 = \alpha p_1 + \Delta t\theta\lambda p_3 - \Delta t\theta\beta p_5 \\ a_2 = \alpha p_2 - \Delta t\theta\beta p_6 \\ a_3 = \alpha p_1 + \Delta t\theta\lambda p_4 - \Delta t\theta\beta p_5 \\ b_1 = \alpha p_1 - \Delta t(1-\theta)\lambda p_3 + \Delta t(1-\theta)\beta p_5 \\ b_2 = \alpha p_2 + \Delta t(1-\theta)\beta p_6 \\ b_3 = \alpha p_1 - \Delta t(1-\theta)\lambda p_4 + \Delta t(1-\theta)\beta p_5 \end{cases} \tag{10}$$

From equation (10), we have a system consists of (N+1) linear equation known with (N+3) unknowns $\delta_{-3}, \delta_{-2}, \delta_{-1}, ...\delta_{n-1}$ to get a unique solution needed for adding two equations obtained from BC (4).

$$\begin{aligned} p_1 S_{j-3}^i + p_2 S_{j-2}^i + p_1 S_{j-1}^i = f \qquad & j = 0 \\ p_3 S_{j-3}^i + 0 S_{j-2}^i + p_4 S_{j-1}^i = 0 \qquad & j = N \end{aligned} \tag{11}$$

From equations (9-10) the system consists $N+3 \times N+3$ in the following form:

$$M_{N+3xN+3} S_{1xN+3}^{n+1} = N_{N+3xN+3} S_{1xN+3}^n + b \tag{12}$$

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IV. METHODS & MATERIALS

4.1. 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.

4.2. 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. It 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 towards its units is (869,031) km^2. The rates of decline of the earth surface is 0.1 m/km to the south, as the average height between (32-36) meters above sea level.

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%), [18].

4.3. Samples

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 1.

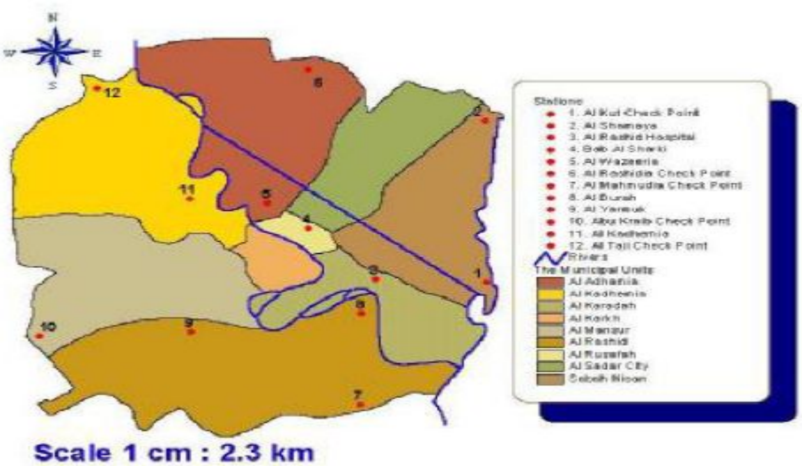

Figure 1: Map of Baghdad city showing study stations

4.4. Applied suggested method

So far, We already applied suggested method to estimate the concentration of cadmium (Cd) in the soil as follow: For crank-Nicolson scheme put $\theta = 0.5$

$$\alpha S^{n+1} - \theta \Delta t\,(\beta S_{xx}^{n+1} - \gamma S_x^{n+1}) = \alpha S^n + (1-\theta)\Delta \mathrm{t}\,(\beta S_{xx}^n - \gamma S_x^n) \quad (12)$$

From equation (12) we have the system consists (N+1) linear equation Known with (N+3) unknowns $S_{-3}, \mathrm{S}_{-2}, \ldots \mathrm{S}_{n-1}$ to get a unique add two equation We get from BC

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$$C(0,t) = f = 0.06 \Rightarrow p_1 S_{j-3}^{n+1} + p_2 S_{j-2}^{n+1} + p_1 S_{j-1}^{n+1} = 0.06$$

$$C_x(100,t) = 0 \quad \Rightarrow p_3 S_{j-3}^{n+1} + 0 S_{j-2}^{n+1} + p_4 S_{j-1}^{n+1} = 0$$

Now have the following system:

$$M_{(N+3)\times(N+3)}\, s_{(1+N)\times(N+3)}^{n+1} = N_{(N+3)\times(N+3)}\, s_{(1+N)\times(N+3)}^{n} + b$$

To get the initial state from initial condition and getting on S^0 as following:

$$(C_j^0)_x = w_0'(x_j) = 0 \Rightarrow p_3 S_{j-3}^{n+1} + 0 S_{j-2}^{n+1} + p_4 S_{j-1}^{n+1} = 0 \text{ where j=0}$$

$$C_j^0 = w_0(x_j) = 0.06 \Rightarrow p_1 S_{j-3}^{n+1} + p_2 S_{j-2}^{n+1} + p_1 S_{j-1}^{n+1} = 0.06 \text{ where j=0,1..,N} \qquad (13)$$

$$(C_j^0)_x = w_0'(x_j) = 0 \Rightarrow p_3 S_{j-3}^{n+1} + 0 S_{j-2}^{n+1} + p_4 S_{j-1}^{n+1} = 0 \text{ where j=N}$$

Thus, the system of equations in (13) can be represented as a matrix of order $N+3 \times N+3$, of the form: $AF^0 = d$

Where

$$\begin{bmatrix} p_3 & 0 & p_4 & 0 \ldots\ldots & & & 0 \\ p_1 & p_2 & p_1 & 0 \ldots 0 & & & 0 \\ 0 & p_1 & p_2 & p_1 & 0 \ldots 0 & & 0 \\ . & & & & & & \\ . & & & & & & \\ 0 & & & & p_1 & p_2 & p_1 \\ 0 \ldots\ldots\ldots\ldots & & & & p_3 & 0 & p_4 \end{bmatrix} \begin{bmatrix} S_{-3}^0 \\ S_{-2}^0 \\ 0 \\ . \\ . \\ S_{n-1}^0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0.06 \\ 0.06 \\ . \\ . \\ 0.06 \\ 0 \end{bmatrix}$$

That calculates the concentration of cadmium (Cd) in the soil with depth 1000 cm, the results illustrated in Figure (2). Also, estimate the concentration of Nickel (Ni) in soil with depth 1000 cm by suggested method and the results illustrated in Figure (3).

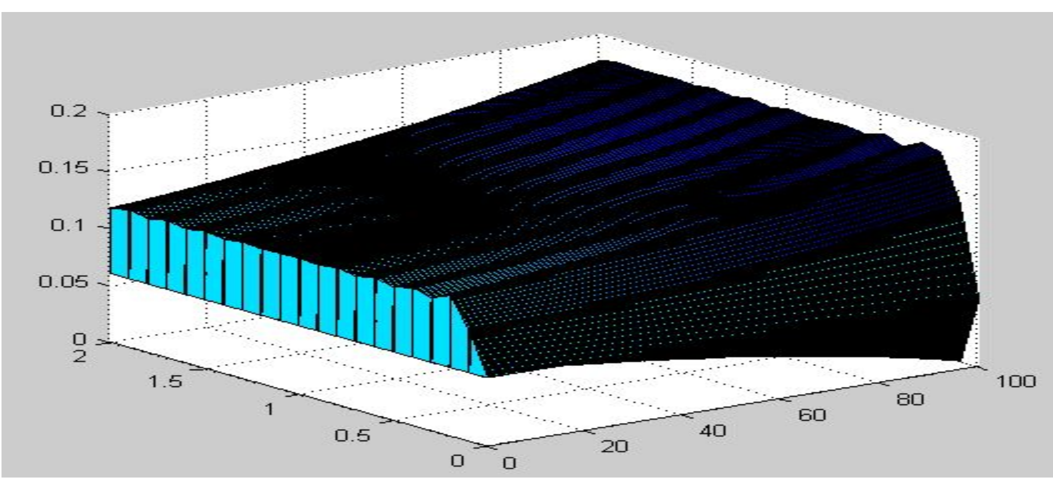

Figure2: Concentrations of Cd in soil of Baghdad

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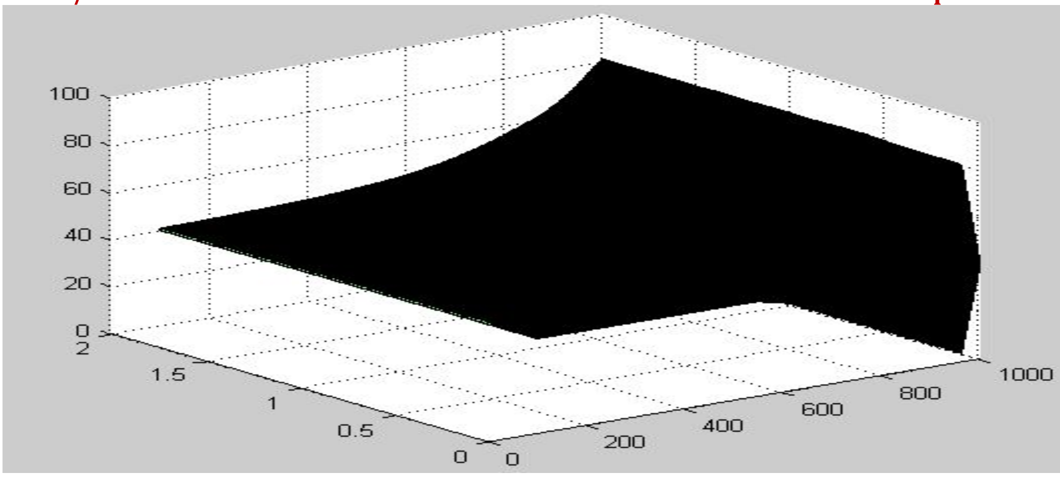

Figure3: Concentrations of Ni in soil of Baghdad

V. RESULTS & DISCUSSION

The suggested method is used to estimate the concentration of heavy metals such cadmium (Cd) and nickel (Ni). Moreover, the applied suggested method to estimate the concentration of other heavy metals such: copper (Cu), zinc (Zn) and lead (Pb). Figure 4-6, illustrate the results of the concentrations of taking elements in soils and areas of Baghdad, which calculated from suggested method.

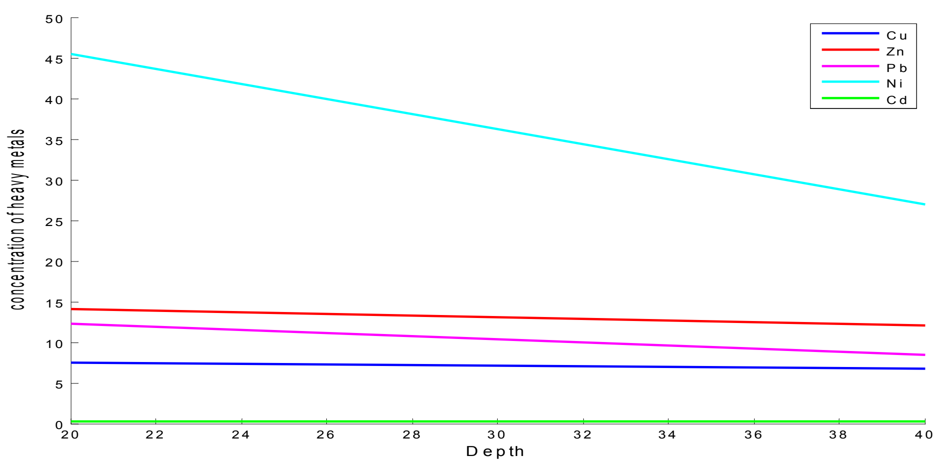

Figure 4: Concentration of heavy metals inAgricultural lands for Baghdad city

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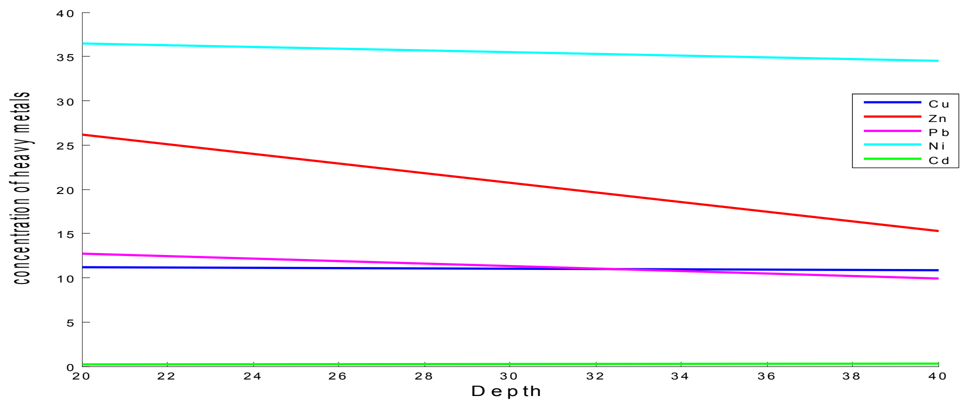

Figure 5: Concentration of heavy metals inIndustrial lands for Baghdad city

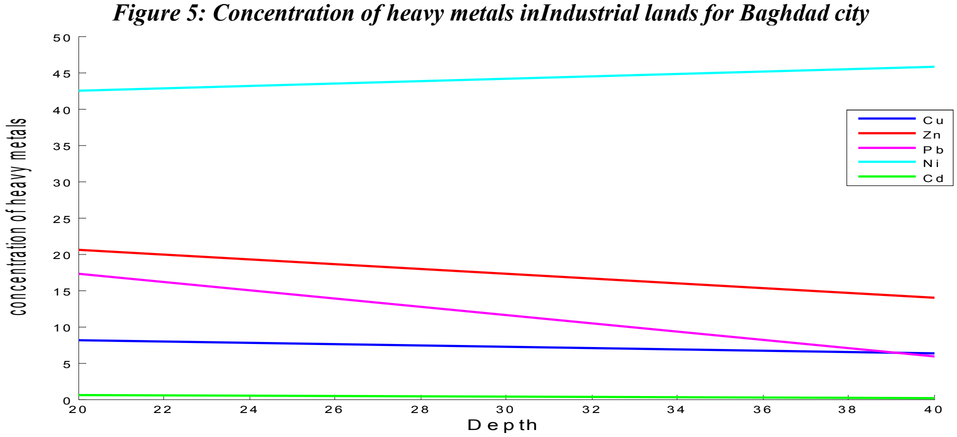

Figure 6: Concentration of heavy metals in Commercial lands for Baghdad city

VI. CONCLUSIONS

In this paper, we discussed thetrigonometric cubic B-spline collocation methodto estimate the concentration of heavy metals(Cd, Ni, Cu, Zn, and Pb) in soil for different depth. This way is better than using the laboratories as laboratories cost a lot of many, time and effort. The practical results show:

- The average of the concentrations of heavy metals in soil for different zones in Baghdad are increasing 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:

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

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