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To cite this article: Luma Naji Mohammed Tawfiq *et al* 2019 *J. Phys.: Conf. Ser.* **1294** 032020

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Estimate the Rate of Contamination in Baghdad Soils By Using Numerical Method

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Abstract. The aim of this paper is to evaluate the rate of contamination in soils by using accurate numerical method as a suitable tool to evaluate the concentration of heavy metals in soil. In particular, 2D –interpolation methods are applied in the models of the spread the metals in different direction. The paper illustrates the importance of the numerical method in different applications, especially environment contamination. Basically, there are many roles for approximating functions. Thus, the approximating of function namely the analytical expression may be expressed; the most common type being is polynomials, which are the easy implemented and simplest methods of approximation. In this paper the divided difference formula is used and extended in two dimensions (2D) to evaluate the concentration of metals in soil to estimate the rate of contamination in Baghdad city, Iraq.

Keywords: Interpolation method, divided difference, contamination, Heavy metals.

1. Introduction

An important aspect in the numerical methods subject is the approximation of the different values, operation designated as interpolation, which is employed in most of the branches of the science, engineering [1], economics [2], etc.

The problems of polynomial interpolation for the approximate functions of several independent variables are necessary but the methods are less well developed than in the case of functions of a single variable. In many problems in engineering and science, the data given as a sets of discrete points, so required interpolating which must have many important properties such as: continuity and orthogonally, moreover it is easy to evaluate; it should be easy to integrate and differentiate [3].

The application of numerical method in soil contamination is firstly beginning in 2015 by Tawfiq, et al., [4, 5] and the modification of the method introduced in [6, 7]. Then she developed the method to evaluate the concentration of heavy metals by parallel processing technique for more details see [8-10]. In this paper the extending of divided difference method in 2D are introduced then applied to estimate the rate of contamination depending on calculating the concentration of heavy metals in some zone in Baghdad city, then estimate the in that soil.



2. Numerical Method

The interpolation can be performed by approximating the unknown law of variation with an analytical function. The problem of function approximation arise when are known only the numerical values of function or when the function is very complicated.

Generally, a problem solved by interpolation can be formulated depending on continuous real valued function f .

Let $f(x)$ given at the distinct point $x_i, i= 0,1,2,\dots,n$, define the zeros divided difference of f with respect to x_i as $f[x_i] = f(x_i)$, The first divided difference of the f with respect to x_i and x_j denoted $f[x_i, x_j]$ defined as [11]:

$$f[x_i, x_j] = \frac{f[x_j] - f[x_i]}{x_j - x_i}$$

The second divided difference denoted $f[x_i, x_{i+1}, x_{i+2}]$ and is defined as:

$$f[x_i, x_j, x_k] = \frac{f[x_j, x_k] - f[x_i, x_j]}{x_k - x_i}$$

Similarly the n th divided difference relative to $x_0, x_1, \dots, x_{n-1}, x_n$, is given by

$$f[x_0, x_1, \dots, x_{n-1}, x_n] = \frac{f[x_1, x_2, \dots, x_n] - f[x_0, x_1, \dots, x_{n-1}]}{x_n - x_0}$$

The value of $f[x_0, x_1, \dots, x_n]$ is independent of the order number x_0, \dots, x_n .

i.e., $f[x_i, x_j, x_k] = f[x_j, x_i, x_k] = f[x_k, x_j, x_i]$

Now, we generalized the formula of divided difference in 2D, i.e., x, y - plane.

Consider the points (x_i, y_j) are distributed as rectangular grid such: $x_i, i= 0, 1, 2, \dots, m$ and $y_j, j= 0, 1, 2, \dots, n$, then we can get a polynomial of degree m in x and n in y as:

$$P_{m,n}(x, y) = \sum_{i=0}^m \sum_{j=0}^n w_{i-1}(x) w_{j-1}(y) f[x_0, x_1, \dots, x_i, y_0, y_1, \dots, y_j] \quad (1)$$

Where; $w_{i-1}(x) = \prod_{k=0}^{i-1} (x - x_k)$, $w_{j-1}(y) = \prod_{k=0}^{j-1} (y - y_k)$, $w_{-1}(x) = 1$ and $w_{-1}(y) = 1$.

3. Suggested Modification

For generating the approximations that has as it basis the divided difference at x_0, x_1, \dots, x_n , this required method uses the connection between divided difference and the derivative of f .

Suppose that the distinct numbers x_0, x_1, \dots, x_n are given together with the values of f and f' at these numbers, define a new sequence: $z_0, z_1, \dots, z_{2n+1}$ by $z_{2i} = z_{2i+1} = x_i, \forall i= 0,1,\dots, n$; and construct the divided difference table in the form of Table (1) that uses $x_0, x_1, \dots, x_{2n+1}$.

Since $z_{2i} = z_{2i+1} = x_i, \forall i$ we cannot define $f[z_{2i}, z_{2i+1}]$ by divided difference formula, however, if we assume that the reasonable substitution in this situation is $f[z_{2i}, z_{2i+1}] = f'(z_{2i}) = f'(x_i)$, we can use the entries: $f'(x_0), f'(x_1), \dots, f'(x_n)$, in place of undefined first divided differences:

$$f[z_0, z_1], f[z_2, z_3], \dots, f[z_{2n}, z_{2n+1}].$$

The remaining divided differences are produced as usual divided differences and are employed in divided difference formula. Table (1) illustrates the entries that are used for the first three divided difference columns when determining by suggested manner $x_0, x_1 \bar{a} x_2$. In the same manner, the remaining entries are generated as in the Table (1). The modify polynomial is then obtained by

$$P_{2n+1}(x) = f[z_0] + \sum_{i=1}^{2n+1} f[z_0, z_1, \dots, z_i](x - z_0)(x - z_1) \dots (x - z_{i-1}). \quad (2)$$

Then equation (2) can be generalized as the following two variables formula

$$P_{2m+1, 2n+1}(x, y) = f[z_0, v_0] + \sum_{i=1}^{2m+1} \sum_{j=1}^{2n+1} f[z_0, z_1, \dots, z_i; v_0, v_1, \dots, v_j](x - z_0) \dots (x - z_{i-1})(y - v_0) \dots (y - v_{j-1}) \quad (3)$$

For simplification,

$$P_{2m+1, 2n+1}(x, y) = \sum_{i=0}^{2m+1} \sum_{j=0}^{2n+1} f[z_0, \dots, z_i, v_0, \dots, v_j] w_{i-1}(x) w_{j-1}(y) \quad (4)$$

For all $i = 1, 2, \dots, m \bar{a} j = 1, 2, \dots, n$

Where; $z_{2i} = z_{2i+1} = x_i \bar{a} v_{2j} = v_{2j+1} = y_j$.

Table 1: Suggested modification of divided difference

z	$F(z)$	First divided difference	Second divided difference
z_0	$f[z_0] = f(x_0)$	$f[z_0, z_1] = f'(x_0)$	
z_1	$f[z_1] = f(x_0)$	$f[z_1, z_2] = \frac{f[z_2] - f[z_1]}{z_2 - z_1}$	$\frac{f[z_0, z_1, z_2]}{z_2 - z_0} = \frac{f[z_1, z_2] - f[z_0, z_1]}{z_2 - z_0}$
z_2	$f[z_2] = f(x_1)$	$f[z_2, z_3] = f'(x_1)$	$\frac{f[z_1, z_2, z_3]}{z_3 - z_1} = \frac{f[z_2, z_3] - f[z_1, z_2]}{z_3 - z_1}$
z_3	$f[z_3] = f(x_1)$	$f[z_3, z_4] = \frac{f[z_4] - f[z_3]}{z_4 - z_3}$	$\frac{f[z_2, z_3, z_4]}{z_4 - z_2} = \frac{f[z_3, z_4] - f[z_2, z_3]}{z_4 - z_2}$
z_4	$f[z_4] = f(x_2)$	$f[z_4, z_5] = f'(x_2)$	$\frac{f[z_3, z_4, z_5]}{z_5 - z_3} = \frac{f[z_4, z_5] - f[z_3, z_4]}{z_5 - z_3}$
z_5	$f[z_5] = f(x_2)$		

Now, the suggested modification can be generalized in two variables, for illustration we construct Table (2) as the same manner of Table (1) but in two variables.

Table 2: Suggested modification of divided difference in two variables

(x_i, y_j)	$f[x_i, y_j]$	First divided difference	Second divided difference
(x_0, y_0)	$f[x_0, y_0]$	$\frac{\partial}{\partial x} \frac{\partial}{\partial y} f[x_0, y_0]$	
(x_1, y_0)	$f[x_1, y_0]$	$\frac{f[x_1, y_0] - f[x_0, y_0]}{(x_1 - x_0)}$	$\frac{f[x_1, y_0] - f[x_0, y_0]}{(x_1 - x_0)}$
(x_0, y_1)	$f[x_0, y_1]$	$\frac{f[x_0, y_1] - f[x_0, y_0]}{(y_1 - y_0)}$	$\frac{f[x_1, y_0] - f[x_0, y_0]}{(x_1 - x_0)}$
(x_1, y_1)	$f[x_1, y_1]$	$\frac{f[x_1, y_1] - f[x_1, y_0]}{(y_1 - y_0)}$	$\frac{f[x_1, y_1] - f[x_0, y_1]}{(x_1 - x_0)}$
(x_0, y_0)	$f[x_0, y_0]$	$\frac{\partial}{\partial x} \frac{\partial}{\partial y} f[x_0, y_0]$	
(x_1, y_0)	$f[x_1, y_0]$	$\frac{f[x_1, y_0] - f[x_0, y_0]}{(x_1 - x_0)}$	$\frac{f[x_1, y_0, y_1] - f[x_0, x_1, y_0]}{(y_1 - y_0)}$
(x_0, y_1)	$f[x_0, y_1]$	$\frac{f[x_0, y_1] - f[x_0, y_0]}{(y_1 - y_0)}$	$\frac{f[x_1, y_0, y_1] - f[x_0, x_1, y_0]}{(y_1 - y_0)}$
(x_1, y_1)	$f[x_1, y_1]$	$\frac{f[x_1, y_1] - f[x_1, y_0]}{(y_1 - y_0)}$	$\frac{f[x_1, y_0, y_1] - f[x_0, x_1, y_0]}{(y_1 - y_0)}$
(x_0, y_0)	$f[x_0, y_0]$	$\frac{\partial}{\partial x} \frac{\partial}{\partial y} f[x_0, y_0]$	
(x_1, y_0)	$f[x_1, y_0]$	$\frac{f[x_1, y_0] - f[x_0, y_0]}{(x_1 - x_0)}$	$\frac{f[x_1, y_0] - f[x_0, y_0]}{(x_1 - x_0)}$
(x_0, y_1)	$f[x_0, y_1]$	$\frac{f[x_0, y_1] - f[x_0, y_0]}{(y_1 - y_0)}$	$\frac{f[x_1, y_1] - f[x_0, y_1]}{(x_1 - x_0)}$
(x_1, y_1)	$f[x_1, y_1]$	$\frac{f[x_1, y_1] - f[x_1, y_0]}{(y_1 - y_0)}$	$\frac{f[x_1, y_1] - f[x_0, y_1]}{(x_1 - x_0)}$
(x_0, y_0)	$f[x_0, y_0]$	$\frac{\partial}{\partial x} \frac{\partial}{\partial y} f[x_0, y_0]$	
(x_1, y_0)	$f[x_1, y_0]$	$\frac{f[x_1, y_0] - f[x_0, y_0]}{(x_1 - x_0)}$	
(x_0, y_1)	$f[x_0, y_1]$	$\frac{f[x_0, y_1] - f[x_0, y_0]}{(y_1 - y_0)}$	
(x_1, y_1)	$f[x_1, y_1]$	$\frac{f[x_1, y_1] - f[x_1, y_0]}{(y_1 - y_0)}$	

Practically, as in Figure (1), we need to find the value of the function $f(x, t)$ at the red spot which equals to the sum of the product of each coloured spot by the area of the same colour rectangle, divided by the area of all four rectangles.

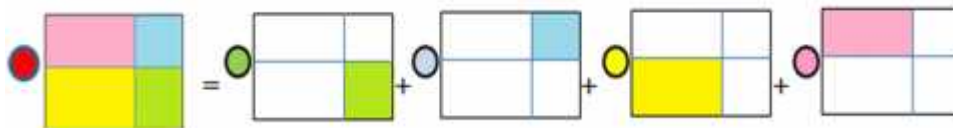


Figure 1: Practical representation of 2-D Interpolation

Now, we applied suggested interpolation method to evaluate the concentration of heavy metals in soil zones of Baghdad city.

4. Sampling

The study area, Bab Al- Muadham, is located in the center of Baghdad. It has 3 central districts and near Mohammed Al- Kasim highway: residential land, commercial land and industrial land. Six sites were selected for study within Bab Al-Muadham area as illustrated in Figure 2. The distances of sampling sites from Mohammed Al- Qasim highway were (300,

600,750, 900, 900, and 950m). At each site, Soil samples were collected at a range of depths (0 -5), (5-10), (10-15), (15-20), & (20-25) cm, the soil was generally taken from (0-25) cm of the topsoil because much of the nutrient uptake by plants is from this depth (given in Table3). Samples were preserved in cleaned polyethylene bags and finally transported directly to the laboratory.

These samples represent the initial data which used to get interpolation function that is substituting in divided difference formula (1).



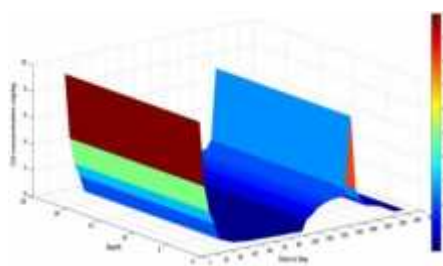
Figure 2: Locations of samples Sites in Bab Al- Muadham city, Baghdad

Table 3: Concentrations of HMs for different zones in Bab Al- Muadham city.

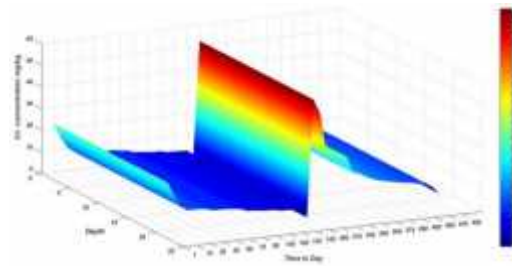
Zone	Depth(cm)	Pb	Cu	Zn	Ni	Cd	Fe	Mn	EC	PH
1	0-20	139.52	23.82	370	-	10	-	-	-	-
2	0-20	29.32	17.5	190	-	5	-	-	-	-
3	0-20	27.78	12.5	170	-	3	-	-	-	-
4	0-20	27.77	10	141	-	2	-	-	-	-
5	0-20	24.05	10	120	-	0.75	-	-	-	-
6	0-20	19.71	9.96	120	-	0.6	-	-	-	-
7	0-20	18.48	9.35	100	-	0.43	-	-	-	-
8	0-20	18.8	8.6	50	-	0.29	-	-	-	-
9	0-20	17.65	8.5	-	-	0.25	-	-	-	-
10	0-20	17.5	8.5	-	-	0.2	-	-	-	-
11	0-20	15.89	8	-	-	0.15	-	-	-	-
12	0-20	15.10	7.71	-	-	0.14	-	-	-	-
13	0-20	15.04	6.49	35	62.5	0.13	-	-	5700	8.25
14	0-20	13.68	6.32	24	57.5	0.11	-	-	5130	7.9
15	0-20	12	5.96	16	55	0.10	-	-	1300	7.9
16	0-20	11.71	5.52	15.5	54	0.08	-	-	868	7.7
17	0-20	11.6	5.32	15	43.5	0.06	-	-	803	7.68
18	0-20	11	4.78	14.5	36.5	0.05	-	-	346	7.6
19	0-20	10	4.70	11	27.3	0.05	-	-	335	7.44
20	0-20	10	4.49	10	27	0.05	-	-	321	7.17

21	0-20	4.8	4.45	9.5	26	0.01	-	-	260	7.05
22	0-20	2.25	0.2	0.8	20.5	0.01	-	-	97	7.0
23	0-20	81		47	-	0.85	-	-	-	-
24	0-20	90		59.1	-	1.1	-	-	-	-
25	0-20	101.2		63.2	-	1.5	-	-	-	-
26	0-20	125		71.5	-	1.7	-	-	-	-
27	0-20	150		78	-	1.86	-	-	-	-
28	0-20	192		85.5	-	1.96	-	-	-	-
29	0-20	300		89.5	-	2	-	-	-	-
30	0-20	340		90.5	-	2	-	-	-	-
31	0-20	410		98.2	-	2.6	-	-	-	-
32	0-20	690.60	54.25	388.38	155.76	8	-	-	2000	8.34
33	0-20	682.71	47.25	243.98	140.20	2.4	-	-	1165	8.34
34	0-20	600.60	37.45	213.00	139.18	1.5	-	-	576	8.31
35	0-20	512.71	28	149.74	136.50	1.00	-	-	515	8.30
36	0-20	450.60	27.28	123.70	112.2	0.90	-	-	485	8.22
37	0-20	400.60	26.16	101.60	110.15	0.80	-	-	471	8.21
38	0-20	80.3	26.14	78.00	92	0.7	-	-	369	8.03
39	0-20	72	18.35	41.00	67.5	0.65	-	-	356	7.3
40	0-20	65	17.5	38	66	0.25	-	-	263	7.27
41	0-20	51.1	15.65	37.7	63.34	0.05	3133.44	759.76	-	7.78
42	0-20	50	14.29	30.5	52	0.04	2998.41	659.00	-	7.73
43	0-20	39.5	13.25	25	47.75	0.03	2977.93	589.76	-	7.53
44	0-20	37.32	12.72	22.87	43.5	-	2884.73	581.32	-	7.47
45	0-20	34.5	12	20	39.20	-	2681.04	541.17	-	7.41
46	0-20	32.34	11.36	18.94	39.18	-	2233.43	470.60	-	6.92
47	0-20	27.27	11	18.8	38.09	-	1422.56	153.26	-	6.89
48	0-20	26.13	10.4	18	36.09	-	1327.50	100.60	-	6.89
49	0-20	25.34	9.7	15.78	36.09	-	1305.81	98.92	-	6.89
50	0-20	25.34	9.30	15	28.85	-	1013.13	89.18	-	6.78
51	0-20	7.65	7.30	9.7	25.6	-	1011.54	86.54	-	6.73
52	0-20	6.3	4	8.35	20.5	-	884.73	79.00	-	6.67
Mean	0-20	118.86	13.30	77.35	61.27	1.28	1989.5	350.75	1124.2	7.53

Now, if, the initial value of concentrations of heavy metals (C_0) is given in Table (3) substituting in the equation (1), then we get the concentrations of this heavy metals for time $t(d)$ and depth $x(m)$. The practical results is illustrated in Figure (3), when the figures represent the concentrations of heavy metals such: Cd, Cu, Fe, Mn, Ni, Pb, Zn and Cr respectively in soil of Bab Al- Muadham city.



Cd



Cu

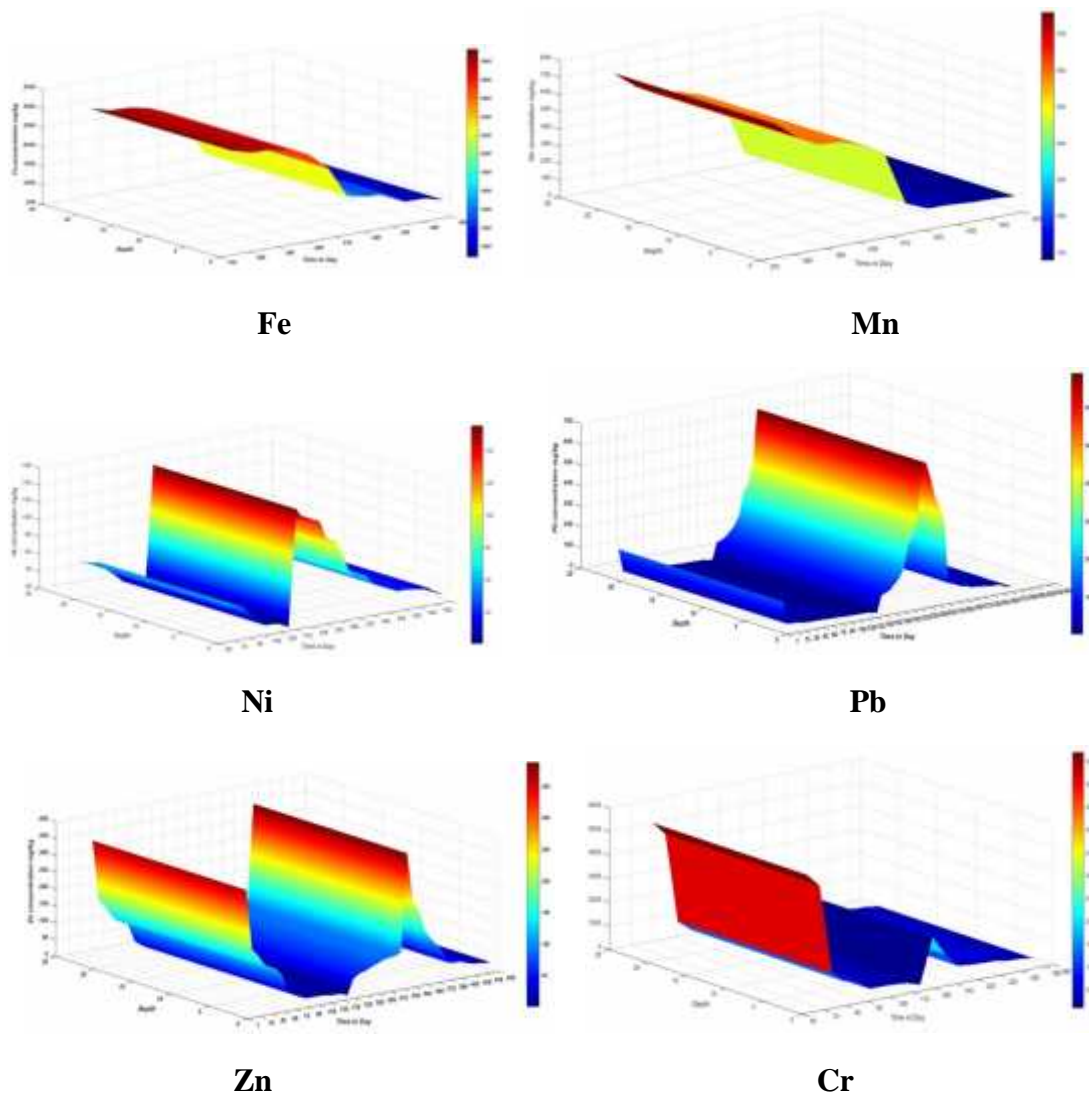


Figure 3: Concentration of HM in Bab Al- Muadham city

5. Factors Controlling the Distribution of Heavy Metals in the Soil

Many factors and variables govern trace metal behavior in soils and sediments in complex ways [12]. These factors are: Organic matters (O.M.), Clay minerals, Iron oxides and pH [13]. Mineral and organic soils can bind metals to different extents. Organic matter, Fe oxides, and clay content are the most significant soil properties influencing sorption reaction.

In this paper, we study the effect of pH using suggested method since, pH plays an important role in the mobility of heavy metals in the soil which controlled directly by the solution of metals hydroxides, in addition pH affects the solution of organic matters and the charge on the iron and aluminum oxides, increasing of pH for soil increase the ability of soil to catch the metals on the soil surface through absorption process [14]. High pH soils may have an inadequate availability of Fe, Mn, Cu, Zn, and especially of Br and phosphorus [15]. Trace elements in soils depends on contaminants concentration, chemical speciation, water movement and soil matrix properties such as mineralogy, pH and redox potential, the solubility of trace elements increases with decrease pH value of soil towards acidity [16].

The value of soil pH in this study ranging (6.0- 7.6) with average (6.8) which illustrated in Figure 4, the values of pH in the soil samples were over (8.0) in the two highest soil samples in the concentration of heavy metals and the two lowest soil samples in the concentration of heavy metals. So it can not consider as an important factor that controlling the mobility of heavy metals in the soil of Bab Al- Muadham city.

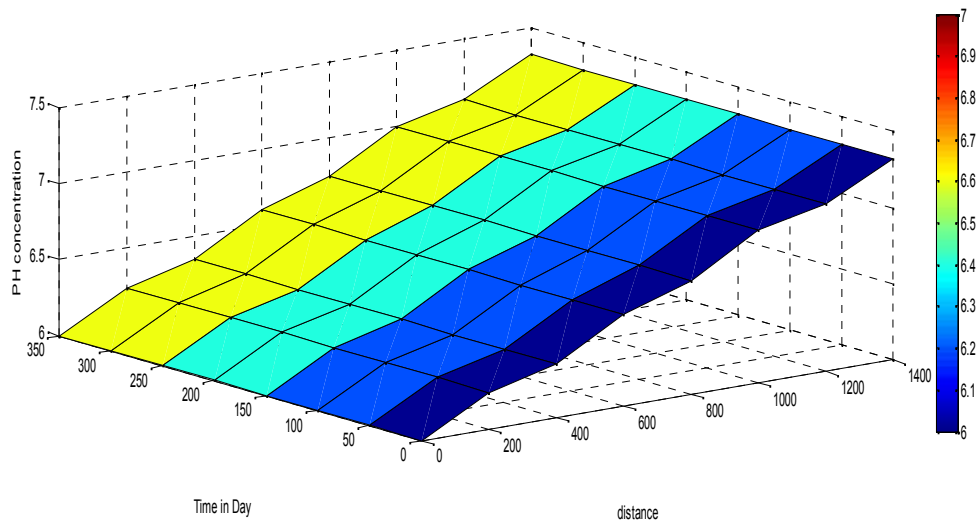


Figure 4: Results of PH by suggested method

6. Error Estimate and Default Weights

Every known software package scales either the maximum relative defect or relative error. The weights used to scale the maximum defect. In this research we modify this package to consist: interpolation simulink named "pythINSIM", which defined as :

$$\frac{\|C_I(x, t) - C_S(x, t)\|_{\infty}}{\|1 - C_S(x, t)\|_{\infty}}$$

Where; $C_I(x, t)$ is the value of concentration of heavy metals getting from laboratory inspecting, and $C_S(x, t)$ is the value of concentration of heavy metals getting from suggested method.

Also two dimensions interpolation simulink named "pythTDINSIM" defined as:

$$\frac{\|C_I(x, y, t) - C_S(x, y, t)\|_{\infty}}{\|1 - C_S(x, y, t)\|_{\infty}}$$

and multivariate interpolation simulink named "pythMDINSIM" which defined as:

$$\frac{\|C_I(x, y, z, t) - C_S(x, y, z, t)\|_{\infty}}{\|1 - C_S(x, y, z, t)\|_{\infty}}$$

The application of these packages for the results by suggested method is given in Table (4).

Table 4: Maximum defect

Heavy metals	pythINSIM
Cr	0.00483
Cu	0.0009
Fe	0.00204
Ni	0.00183
Pb	0.00087
Zn	0.00012
pH	0.0074

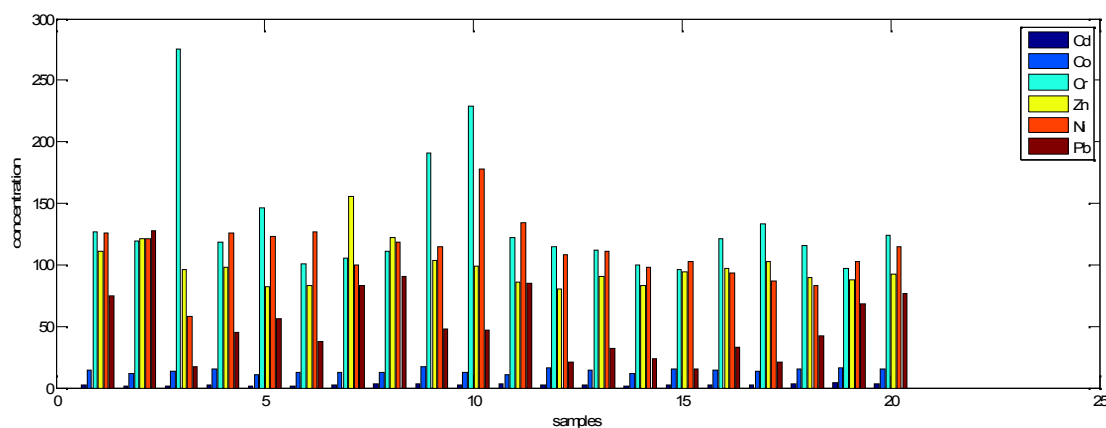
7. Conclusions

The theory of the result shows that there is a connection level of agreement between the practical and simulated results. This demonstrates that suggested modification for interpolation in 2 or more dimensions is more efficient, easy implemented and rapid compared with the other methods, also can be considered to be a good representation of that application.

The results which obtained from the present work show that the average of the concentrations of metals in soil for any time and zones in Bab Al- Muadham city are increase with the time, posing a great risk to the environment contamination.

There are different causes for increasing the contamination by 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 heavy metals 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. To illustrate the rate of contamination in the Bab Al- Muadham soils see Figure (5). The advantages of the suggested modification is: Directly uses for given data, easy implementation, and can be update easy.

**Figure 5:** Concentrations of heavy metals in the Bab Al- Muadham soils

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