

Modeling and simulation of cadmium transport influenced by high degree of saturation and porosity on homogeneous coarse depositions

Abstract

This paper monitors the effect from degree of saturation and porosity on the migration rate of cadmium in homogeneous coarse formation. The study expresses the rate of coarse homogeneity reflecting on the deposition of cadmium in deltaic depositions. Other studies were carried out on a particular soil formation that could not predict comprehensive migration rate of cadmium concentration in coarse depositions. These were monitored on deltaic location where coarse depositions are predominant thus degree of saturation and porosity were observed to influence cadmium concentration in the study area. Porosity and degree of saturation were the major effect that determine their variation of cadmium concentration, the derived solution was subject to simulation, these values express linear concentration of cadmium, but with variations at different depth to phreatic bed, the study has expressed the influences from porosity and degree of saturation reflecting on cadmium concentration, experts in pollution transport will definitely apply this tool to monitor the formation characteristics influences on cadmium transport in deltaic depositions.

Keywords: modeling, cadmium, Transport, saturation, porosity and coarse depositions

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Introduction

Experts have observed Cadmium as one of the most toxic metals with carcinogenic and teratogenic impacts. The main foundation of Cd contamination in agricultural soils is the extensive application of mineral phosphorous fertilizers, fungicides and sewage sludge.¹⁻³ Experts have observed that Cadmium is bound to permanently charged surfaces of clay minerals, to surfaces of hydroxyl groups along the edges of clay particles, it also includes to phyllosilicate clays,⁴ to Fe and Al (hydro)oxides, and to phenol and carboxyl groups of soil organic matter.⁵ There are several factors that pressure cadmium mobility in agricultural soils are e.g. tillage practices, duration of the cadmium-soil interaction, soil type and layering, water flow and solute transport distribution between the macrospore and matrix domain, rain/irrigation intensity, total and active CaCO₃ content, organic matter content, as well as pH value of the soil solution.⁶⁻¹⁰ It has been assumed that the movement of heavy metals requires the metal to be in the soil solution. For that reason, physical mixture through ploughing of the soil surface during repeated cultivation is the main factor that contributes to an increase in the concentration of heavy metals beneath the zone of application. The preferential paths for water flow and solute transport in the unsaturated zone of soil are the hydrologically effective (= surface vented) macrospores: biopores (e.g. earthworm, ant, and root holes), inter-aggregate pores, and desiccation cracks.^{6,11-15} Soil is a natural body consisting of layers (soil horizons) of mineral constituents of variable thicknesses different from the parent materials in their morphological, physical, chemical, and mineralogical characteristics.^{16,17-22} Soil is also a multiphase mineral and organic porous media consisting of three phases: solid, liquid and gaseous. The solid phase consists of particles of various distribution generated by partitioning of rocks by different environmental (erosion, transport, deposition), thermal and chemical processes. There are three main types of soil particles distinguished: sand, silt and clay. The

relative amounts of each fraction in the soil sample, sorted according to its size (particle diameter) are presented by particle size distribution or grain size distribution.²³ Soil particles are usually packed loosely, with different, even unique three dimensional spatial orientation, thus creating a soil solid structure filled with empty pores, which may be occupied by fluids – liquids or /and gases. The fraction of void space in the porous material/soil is defined by porosity ratio.²⁴⁻²⁶

Developed model

$$\theta_w V \frac{\partial C}{\partial t} = \Phi \frac{\rho}{\rho_w} V \frac{\partial C}{\partial x} \quad (1)$$

$$\theta_w V X T = \Phi \frac{\rho}{\rho_w} V X T$$

Substituting solution $C = XT$ into (1), we have

$$\theta_w V X T^1 = \Phi \frac{\rho}{\rho_w} V X^{11} T \quad (2)$$

$$\theta_w V \frac{T^1}{T} = -\Phi \frac{\rho}{\rho_w} V \frac{X^{11}}{X} \quad (3)$$

$$\theta_w V \frac{T^1}{T} - \Phi \frac{\rho}{\rho_w} V \left[\frac{X^{11}}{X} \right] \quad (4)$$

$$\theta_w V \frac{T^1}{T} - \frac{X^{11}}{X} \quad (5)$$

Considering when $LnX \rightarrow 0$

$$\theta_w V T^1 = \Phi \frac{\rho}{\rho_w} V \frac{X^{11}}{X} - T = \lambda^2 \quad (6)$$

$$\theta_w V \frac{T^1}{T} = \lambda^2 \tag{7}$$

$$\frac{X^{11}}{X} = \lambda^2 \tag{8}$$

$$\Phi \frac{\rho_b}{\rho_w} V = \lambda^2 \tag{9}$$

This implies that equation (10) can be expressed as:

$$\Phi \frac{\rho_b}{\rho_w} V \frac{X^{11}}{X} = \lambda^2 \tag{10}$$

$$\Phi \frac{\rho_b}{\rho_w} V \frac{X^2}{X} = \lambda^2 \tag{11}$$

$$\theta_w V \frac{d^2 y}{dx^2} = \lambda^2 \tag{12}$$

$$\theta_w \frac{\rho_b}{\rho_w} V \frac{d^2 y}{dx} = \lambda^2 \tag{13}$$

$$\theta_w \frac{d^2 y}{dx^2} = \lambda^2 \tag{14}$$

$$d^2 y = \left[\frac{\lambda^2}{\theta_w V} \right] dx^2 \tag{15}$$

$$d^2 y = \left[\frac{\lambda^2}{\theta_w V} \right] dx^2 \tag{16}$$

$$\int d^2 y = \int \frac{\lambda^2}{\theta_w V} dx^2 \tag{17}$$

$$dy = \frac{\lambda^2}{\theta_w V} x dx \tag{18}$$

$$\int dy = \int \frac{\lambda^2}{\theta_w V} X dx + C_1 \tag{19}$$

$$y = \frac{\lambda^2}{\theta_w V} + C_1 + C_2 \tag{20}$$

$$y = 0 \tag{21}$$

$$\Rightarrow \frac{\lambda^2}{\theta_w V} X^2 C_{1x} + C_2 = 0 \tag{22}$$

Applying quadratic expression, we have

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \tag{23}$$

Where $a = \frac{\lambda^2}{\theta_w V}$, $b = C_1$ and $c = C_2$

$$X = \frac{-(C_1) \pm \sqrt{(C_1)^2 - 4 \left(\frac{\lambda^2}{\theta_w V} \right) C_2}}{2 \frac{\lambda^2}{\theta_w V}} \tag{24}$$

$$X = \frac{-C_1 + \sqrt{C_1^2 - 4C_2 \frac{\lambda^2}{\theta_w V}}}{2 \frac{\lambda^2}{\theta_w V}} \tag{25}$$

$$X = \frac{-C_1 + \sqrt{C_1^2 - 4C_2 \frac{\lambda^2}{\theta_w V}}}{2\theta_w V} \tag{26}$$

$$X = \frac{-C_1 + \sqrt{C_1^2 - 4C_2 \frac{\lambda^2}{\theta_w V}}}{2\theta_w V} \tag{27}$$

$$X = \frac{-C_1 - \sqrt{C_1^2 - 4C_2 \frac{\lambda^2}{\theta_w V}}}{2 \frac{\lambda^2}{\theta_w V}} \tag{28}$$

Substituting equation (20) to the following condition and initial values condition.

$$t = 0, C = 0 \tag{29}$$

$$\text{Therefore, } X_{(x)} = C_1 e^x - e^{-mx} + C_2 M^{em2x} \tag{30}$$

$$C_1 \text{Cos}M_{1x} + C_2 \text{Sin}M_{2x} \tag{31}$$

$$y = \frac{\lambda^2}{\theta_w V} + C_1 + C_2 \tag{32}$$

$$C(x,t) = \left[C_1 \text{Cos}M_1 \frac{\lambda^2}{\theta_w V} x + C_2 \text{Sin}M_2 \frac{\lambda^2}{\theta_w V} x \right] \tag{33}$$

But if $x = \frac{v}{t}$

Therefore, equation (33) can be expressed as:

$$C(x,t) = \left[C_1 \text{Cos}M_1 \frac{\lambda^2}{\theta_w V} \frac{v}{t} + C_2 \text{Sin}M_2 \frac{\lambda^2}{\theta_w V} \frac{v}{t} \right] \tag{34}$$

Materials and methods

Standard laboratory experiment where performed to monitor the rate of cadmium concentration at different formation, the soil deposition of the strata were collected in sequences base on the structural deposition at different study area, this samples collected at different location generated variation of cadmium concentration at different depth producing through the application of ASS from different strata, the experimental result are applied to compared with theoretical values for model validation

Results and discussion

Results and discussion are presented in tables including graphical representation of cadmium concentration at different Depth and Time (Tables 1–4) (Figures 1–4).

The study from graphical representation shown in figure I express how the deposition of cadmium linearly increasing with change in depth at different depositions to the optimum rate recorded at

36m, the formation at this level experience progressive increase of concentration, these are reflected on predominant homogeneous structure of the strata, comparison between predictive and experimental values developed favorable fits, while figure two observed similar condition as exponential phase were experienced in the deposition of cadmium in different formation, the optimum values were also observed at 36 metres, comparing figure two to one, the concentration are much higher, it implies that the degree of porosity are higher than figure one. Both parameters developed favorable fits for model validation, while figure 3 developed linear increase to the optimum level recorded at 200 days, these condition implies that the system considered the migration at different time, the depositions of cadmium were observed to migrate to phreatic zone with higher concentration at two hundred days, the reality were observed from the degrees of porosities deposited at different depths, validation were observed to developed best fits between the predictive and experimental values. Figure four monitor the system at progressive transport to deeper depth, these were to determine their rate of increase or decrease in concentration, homogeneous rate of concentration were observed, but with slight heterogeneous experiences on experimental values that validated the predictive results.

Table 1 Predictive and experimental values for cadmium concentration at different depth

Depth [M]	Predictive cadmium concentration [Mg/L]	Experimental cadmium concentration [Mg/L]
3	2.87E- 06	2.80E- 06
6	4.74E- 06	5.50E- 06
9	6.62E- 06	6.20E- 06
12	8.49E- 06	8.01E- 06
15	1.03E- 05	1.13E- 05
18	1.22E- 05	1.23E- 05
21	1.41E- 05	1.50E- 05
24	1.59E- 05	1.47E- 05
27	1.78E- 05	1.64E- 05
30	1.97E- 05	1.91E- 05
33	2.16E- 05	2.06E- 05
36	2.35E- 05	2.25E- 05

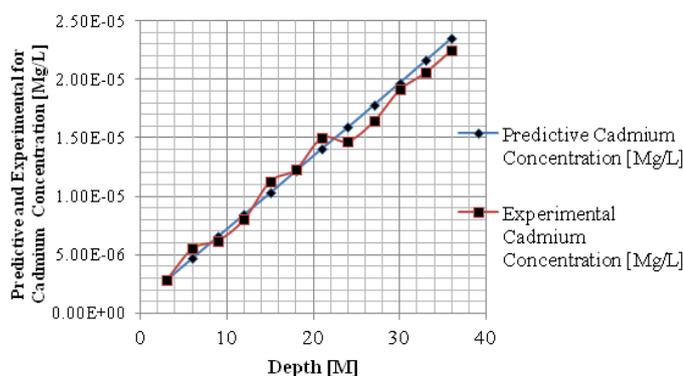


Figure 1 Predictive and experimental values for cadmium concentration at different depth.

Table 2 Predictive and experimental values for cadmium concentration at different depth

Depth [M]	Predictive cadmium concentration [Mg/L]	Experimental cadmium concentration [Mg/L]
3	1.63E- 01	1.65E- 01
6	3.33E- 01	3.11E- 01
9	4.89E- 01	4.45E- 01
12	6.52E- 01	6.52E- 01
15	8.15E- 01	8.18E- 01
18	9.77E- 01	9.54E- 01
21	1.40E+00	1.52E+00
24	1.30E+00	1.37E+00
27	1.47E+00	1.52E+00
30	1.63E+00	1.69E+00
33	1.79E+00	1.82E+00
36	1.95E+00	2.03E+00

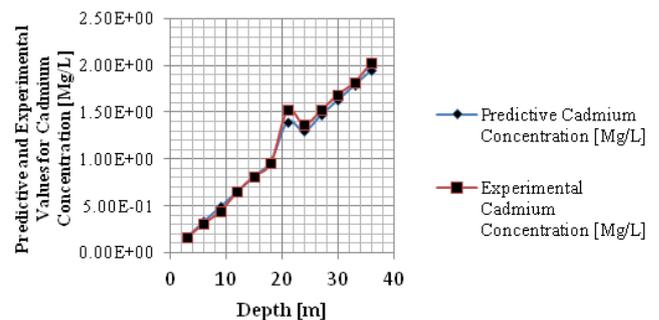


Figure 2 Predictive and experimental values for cadmium concentration at different depth.

Table 3 Predictive and experimental values for cadmium concentration at different time

Time Per Day	Predictive cadmium concentration [Mg/L]	Experimental cadmium concentration [Mg/L]
10	7.14E- 05	8.58E- 05
20	1.43E- 05	1.41E- 05
30	2.14E- 05	2.27E- 05
40	2.86E- 05	2.73E- 05
50	3.41E- 05	3.49E- 05
60	4.10E- 05	4.15E- 05
70	4.77E- 05	4.66E- 05
80	5.45E- 05	5.66E- 05
90	6.13E- 05	6.72E- 05
100	6.82E- 05	6.68E- 05
110	7.49E- 05	6.94E- 05

Table continued...

Time Per Day	Predictive cadmium concentration [Mg/L]	Experimental cadmium concentration [Mg/L]
120	8.17E- 05	8.03E- 05
130	8.86E- 05	8.88E- 05
140	9.54E- 05	9.42E- 05
150	1.02E- 04	1.09E- 04
160	1.09E- 04	1.19E- 04
170	1.15E- 04	1.31E- 04
180	1.23E- 04	1.33E- 04
190	1.29E- 04	1.39E- 04
200	1.36E- 04	1.41E- 04

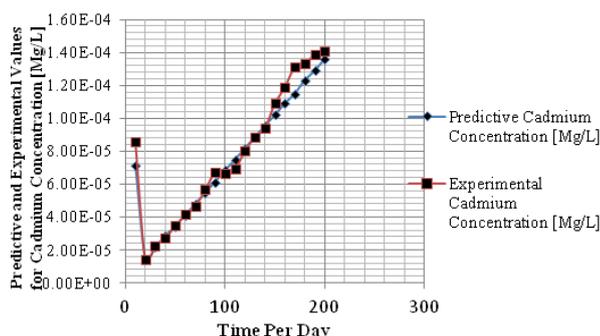


Figure 3 Predictive and experimental values for cadmium concentration at different time.

Table 4 Predictive and Experimental values for cadmium concentration at different depth

Depth [M]	Predictive cadmium concentration [Mg/L]	Experimental cadmium concentration [Mg/L]
3	3.85E- 04	3.66E- 04
6	7.71E-04	7.44E- 04
9	1.15E- 03	1.12E- 03
12	1.54E- 03	1.45E- 03
15	1.92E- 03	1.88E- 03
18	2.31E- 03	2.22E- 03
21	2.71E- 03	2.57E- 03
24	3.10E- 03	3.22E- 03
27	3.47E- 03	3.54E- 03
30	3.85E- 03	3.77E- 03
33	4.24E- 03	4.34E- 03
36	4.62E- 03	4.67E- 03
39	5.01E- 03	5.11E- 03
42	5.40E- 03	5.35E- 03
45	5.78E- 03	5.66E- 03
48	6.17E- 03	6.22E- 03
51	6.55E- 03	6.44E- 03
54	6.94E- 03	6.88E- 03
57	7.32E- 03	7.37E- 03
60	7.71E- 03	7.55E- 03

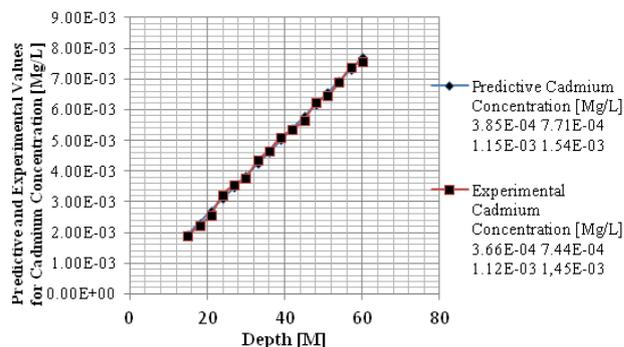


Figure 4 Predictive and experimental values for cadmium concentration at different depth.

Conclusion

The study has definitely defined the deposition of cadmium in homogeneous coarse formation, the structure in the study area were monitored applying *insitu* method of sample collection, the study express the behavior of cadmium deposition in the study location, increase in cadmium depositions were as a result of structural deposition of coarse formation, these were observed from porosity reflection rate in deltaic depositions, linear concentration were experienced in the simulation values, but variation of cadmium concentration were observed, the study has express the behavior of cadmium concentration in coarse structure, the predominant formation characteristics such as degree of saturation and porosity has express its influences on cadmium migrations. The study has evaluated the variation pressure from degree of saturation and porosity base its depositions on cadmium transport in coarse formations.

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Conflict of interest

The authors declare there is no conflict of interest.

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