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DEVELOPMENT OF A MATHEMATICAL MODELLING TOOL FOR PREDICTING CONTAMIANAT CONCENTRATION IN GROUNDWATER AT VICNITY OF DUMPSITES

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Abstract**:** *The disposal of municipal solid waste (MSW) into primarily dumpsites in developing countries causes a number of potential public and Environmental health risks while there are various studies that have evaluated the contaminant that cause the risks Dumpsites are notorious for environmental pollution, posing significant risks to human health and the ecosystems. This study develops a conceptual model to investigate the impact of Age and waste quality on contaminant concentrations at dumpsites. A comprehensive review of existing literature and field observations informed the development of the model. A thorough examination of the relationships between leachate age and its level of toxicity, its impact as a result of seasonal variation and waste quality was undertaken in relation to contaminant concentration, key factors influencing contaminant concentration and a conceptual framework for predicting contaminant concentration in both space and temporal variation was performed with a view of enabling informed decision on contamination remediation at dumpsite. A mixed methods approach combined fields observations, laboratory analysis and mathematical modelling resulted in understanding contaminant concentration increases with dumpsite age due to leachate formation and transport, seasonal variation significantly impact contaminant concentrations with peaks levels during dry season and waste quality influences contaminant composition and concentration .The developed model integrates the contaminant source, leachate generation and seasonal variability with site –specific parameters and waste quality index. The study contributes to the understanding of contaminant dynamics at dumpsites informing waste management strategies, environmental monitoring programs and risks assessment and mitigation measures.*

Keywords: *Wastes Composition, Age, Composition, Contaminant, Model, Assessment*

INTRODUCTIONS

Contaminant transport modelling is a crucial tool widely used for predicting the fate and transport of contaminants in the environment. In the present study a model equation was developed to enable prediction of contaminant concentration at given time and distance at dumpsite. Contaminants transport models helps in identifying potential groundwater contamination risks and proper adequate and effective remediation strategies. The developed modelled equation is developed to simulate the transport of lead(Pb), Chromium (Cr) and Zinc(Zn) in groundwater at Dumpsites in Maiduguri. The developed modelled equation is based on the principle of Advection –Diffusion (ADE) which is widely used equation for contaminant transport and concentration in a porous media (Bear,1972, Fetter,2001). The

Advection –Dispersion (ADE) account for the transport and concentration of contaminant through Advection, dispersion and biodegradation.

The modeled equation is designed to incorporate site-specific parameters such as soil properties, groundwater flow rates and initial contaminant concentration. The developed modelled equation is validated with existing ADE models equation such as Ogota –Ban equation and Domenico equation where reasonable similarity in the results were observed with Ogota-Bank Equation yielding less results compared to the modelled equation which could be attributed to some observed overestimation of some parameters in the equation.

Graphical presentation of all the parameters were illustrated and discussed while cross-Validation and regression Analysis was conducted to ascertain the degree of fitness of the equation in its prediction. Conclusion was reached with the fact that Ogota -Bank Equation is good for predicting of some contaminant concentration while its performed fairly for some of the tested parameters whereas the developed modelled equation is good for the predictions of some of the parameters tested.

Model development for dumpsites refers to the process of creating a mathematical representation of the sites behaviors simulating the migration of contaminants through the soil, groundwater and air. This helps predict potential environmental impact and inform decision –making for site management and remediation

METHODOLOGY

Additional parameters may be required depending on site conditions and model complexity.

These outline parameters are used to develop and calibrate the model ensuring accurate simulations and reliable predictions.

The development of a model to determine a contaminant concentration requires the following basic and important steps as follows:

10. Identity contaminant of concern (e.g. Heavy Metals (HMs) organic pollutants etc.)
11. Characterize the dumpsite properties (e.g. soil profile, type, moisture content (MC) and temperature.
12. Determine contaminant sources and pathway e.g. leachate, runoff, air emissions
13. Select appropriate sampling methods
14. Develop a sampling plan (e.g. location, frequency, numbers of samples).
15. Analyze samples using appropriate laboratory methods
16. Use numerical models (e.g. fate and transport methods) to stimulate contaminant behavior.
17. Calibrate and validate model using field data.
18. Use model outputs to estimate contaminant concentrations and risks.

In line with these, there are various numerical model for contaminants transports which includes:

6. Advection Dispersion Equation (ADE)
7. Darcy's law
8. Contaminant Transport Equation (CTE)
9. HYDRUS

10. MODFLOW

Base on the site specific parameters obtained and reference to exiting similar equations, such as Ogata-Bank and Domenico Equations, a new simplified numerical solution using the Advection-Dispersion Equation (ADE) to determine contaminant concentration at the dumpsites in Maiduguri.

The simplified and user-friendly equation is give as:

$$C(x,t) = (x,t) = \left(\frac{Co}{4x\ X\ x1}\sqrt{\text{CD} - \text{DY} * \text{DZ}) * \text{t}}\right) \text{x exp(- (}$$

$$(x - \text{vt})^2 / 4 \text{ x Dxxt) + (y}^2/(4\text{XDy x t)}$$

$$+ (\text{Z}^2/ (4\text{x DZ x t}) + (\text{V } x \text{ x}) / (2\text{x Dx }) +$$

$$(\text{Kd x exp x V}) /(\text{R + n})$$

(x,t) =Contaminant concentration at Distance x and t

Co = Initial contaminant concentration

Dx, Dy, Dz = Longitudinal, to verse and vertical dispersivities

V = groundwater velocity

X, y, z = Coordinates

ts = Time since contamination started

tf = Time Contamination Stop

Kd = partition coefficient

p = Bulk density

R = Retardation factor

n = Effective porosity

The following assumption are made as often found in modelling of any kind.

Assumptions:

e. Contaminant transport is dominated by Advection and Dispersion
f. Soil properties are homogenous and isotropic
g. Groundwater flow is steady and uniform
h. Contaminant decay is negligible.

To set up a numerical solution, we can discrete the equation using Finite Difference (FD) or Finite Element (FE) methods.

Let assume a ID solution for simplicity. We can divide the distance (X) into smaller segments (ΔX) and time t into smaller intervals (Δt)

The detailed developed Equation for the determination of contaminant concentration is as follows:

$C(x,t) = (\frac{Co}{4x \text{ ^ } x}\sqrt{5\ r\ t\ )}$ x exp(- (x – v x t)²/ (4 x 5 x t)–

(V x X) /(2 x D) - (Kd x e x v) / (R x n)+

(L x I x A) / (W x b x I< x i)

:

2. Defining the ADE
   $\partial e/\partial t$ = D ∂^2 C/ ∂x^2 - V∂C/∂x

   Where,
   C = Concentration
   T = Time
   D = Dispersion Coefficient
   X = Distance

b) Applying initial and final boundary conditions

(x, o) = Co (Initial Concentration

(x, t) = Co (Boundary Conditions at X=0)

(δ, t) = 0 (Boundary condition at X = δ

Using the method of separation of variables

(x, t) = X (x) T (t)

Separating the variables and integrating

X(x) = A e^ (Vx/2D) + Be^ (-v x/2D)

T (t) = Ce^ C-Dt)

Applying the boundary conditions to determine constants:

A = Co

B = O

C = C_D

Combining X (x) and T (t) to get the general solutions.

C (x, t) = C_o x e^ C-Dt) x e^ (Vx/2D)

Using the Finite Difference methods to discretize the solution

C(x, t) = C (i, n) = C_o x e^ (-Dn Dt) x

e^ (Vi Dx /2D)

Where

i = Spatial index

n = Time Index

Dx = Spatial Step

Dt = Time Setup

Solving for C (i, n) at each time step and spatial location.

These steps lead to the numerical solution of the ADE

The mathematical steps used to derive the Advection Dispersion Equation (ADE)

8) Define the Advection-Dispersion Equation (ADE) The ADE describes the transport of a contaminant in a porous medium.

$\partial c/\partial t = D\partial^2$ C/∂x^2 - V∂c/∂x

Where,

C = Concentration of the contaminant mg/L

T = Time (Days)

D = Dispersion Coefficient (m^2 /d)

V= Velocity of the ground water flow (m/day)

X = Distance from the source (m)

9) Apply initial and final boundary emotions
   - Initial Conditions: $((x, o) = C_o$Inital concentration
   - Boundary condition at X = O ; e(o, t) = C_o (Constant Concentration at the source.
   - Boundary Condition at X = δ
     C(δ, t) = 0 (Concentration approves zero from the source)

10) Use the method of separation of variables assume a solution of the form;
    e($(x, t) = (x)\ T(t)$

Substitute this into the ADE

X (x) T(t) = DX (x) T (t) - VX $^1(x)$ T (t)

Separate the variables

T(t) / T (t) = DX^{ii} (X) /X (x) - VX$^i(x)$ /X (x)

11) Solve the following differential equation (ODE)

Solve the ODEs for X(x) and T (t) :

X (x) = Ae^ (v x12D) + Be^ (- ^ Vx /2D)

T (t) = Ce^ (-^ Dt)

12) Apply boundary conditions to determine constants

A = C_o

B = O

C = C_o

13) Combine X(x) and T(t) to get the general solution

Combine the solutions for X (x) and T(t) to get the general solution:

((x, t) = C_ox e^ (-Dt) x e^ (Vx/2D)

14) Discretize the solution using Finite Difference.

Discretize the solution using the Finite Difference to obtain a numerical solution:

((x, t) = C(i, n) = C_o x e^ (-^ (Dn Dt) x e^ (vi Di Dx/2D)

Where

i = spatial index

n = Time Index

Dx = Spatial Step

Dt = Time Steps

These are the steps used in arriving at the development of the equation (model) for the solution of the ADE to generate the model.

Using the model developed;

The concentration of the contaminant at certain distance can be evaluated accordingly as follows:

Table 1.0 Lead (pb) at 1825 days)

Distance (x)m	Conc (mgIL
5m	0.843
10m	0.654
15m	0.513
20	0.403
25m	0.316

Table 2.0 Lead concentration at 3650days

Distance (xx)m	Conc.(mg/ L)
5m	0.351
10m	0.251
15m	0.181
20	0.131
25m	0.095

Table 3.0 Chromium (r) at (1825 days)
Initial concentration (Co) = 0.987 mg/L

Distance $(x)m$	Conc (mg/ L)
5m	0.587
10m	0.453
15m	0.354
20	0.277
25m	0.216

Table 4.0 Chromium at 3560 days
Initial Concentration C_o2.86 mgIL

Distance (m)	Conc mg/L
5m	0.245
10m	0.179
15m	0.131
20	0.097
25m	0.072

COMPARATIVE ANALYSIS OF THE MODEL EQUATION AND OGOTA-BANK EQUATION

The ogota-bank equation is also another tool used widely to determine contaminant concentration at disposal sites.it is in view of this that a comparative analysis of both methods using same results was undertaken with a view of validating the model developed.

Given same environmental conditions to determine the level of concentration of Lead(Pb), Chromium(Cr) and Zinc (Zn) at the dumpsite and peculiar parameters for the Lead (Pb) is also given as follows.

Co =1.42 mg/L (initial concentration)

V = Velocity (0.1m/day (average groundwater flow velocity

D =0.5m/day (longitudinal dispersion coefficients)

ts= 1825days (start time)

tf= 3650days (end time)

Distances measured at 5,10,15,20 and 25m from source

Using Ogota bank equation

C (x, t) = Co/2 *erfc {x-v (tf-ts)0/2*erfc(D*(tf-ts))

Table 3.7 Calculations Using Ogota –Bank Equation

Table 7.0 Lead (Pb)

Distances (m)	C(x,t)	Concentration(mg/L)
5	C(5,3650)	0.411
10	C(10,3650)	0.231
15	C(15,3650)	0.134
20	C(20,3650)	0.079
25	C(25,3650)	0.047

Table 8.0 Comparing this results with the modelled equations for Lead(Pb)

Distance(m)	Modelled equation	Ogota-bank equation	% difference
5	0.825	0.411	50.3
10	0.475	0.231	51.4
15	0.282	0.134	52.5
20	0.169	0.079	53.3
25	0.102	0.047	54.1

The percentage difference observed between the two solutions ranges from 50.3% to 54.1 % indicating that the Ogota- Bank solution yields lower contaminants concentrations than the modelled equation

Calculating same for Chromium (Cr) and Zinc (Zn) using the Ogota –Bank equation

For Chromium (Cr)

Co =0.987 mg/L All other parameters remained the same since it's a same porous medium 1

Using Ogota =Bank Equation `

Table 9.0 C (x, t) =(Co/2) *erfc{(x-v(tf-ts)/ (2* sqrt(D*tf-ts)}

X(m)	C(x,t)	Conc. mg/L
5	C(5,3650)	0.573
10	C(10,3650)	0.324
15	C(15,3650)	0.192
20	C(20,3650)	0.115
25	C(25,3650)	0.069

Table 10.0 Modelled result and Ogota –Bank equation

X(m)	Modelled Result (mg/L)	Ogota-Bank (mg/L)	% differences
5	1.183	0.573	51.5
10	0.673	0.324	51.9
15	0.394	0.192	51.4
20	0.235	0.115	51.1
25	0.141	0.069	51.1

Table 11.0 Equally calculating for Zinc (Zn) using Ogota-Bank equation and comparing it with modelled results table 10.0

X(m)	Modelled Result mg/L	Ogota –Bank mg/L	% Differences
5	1.925	1.653	14.1
10	1.098	0.931	15.1
15	0.643	0.545	15.2
20	0.382	0.324	15.2
25	0.229	0.194	15.3

The percentage difference observed between the two solutions range from 14.1% to 51.9% indicating that the Ogota –Bank equation solution yields lower contaminant concentrations than the modelled equation for both chromium and Zinc.

VALIDATION OF THE MODEL

It is necessary to validate the developed model using regression analysis for both the modelled equation results and the Ogota- Bank equations. The R^2 (R-squared) values were obtained as follows:

LEAD (Pb)

Modelled results vs ogota –Bank equation.

R-squared (R^2) =0.943

CHROMUIM (Cr)

Modelled results Vs Ogota- Bank equation

R-squared (R^2) =0 813

ZINC (Zn)

Modelled results vs Ogota –Bank equation

R-squared (R^2) =0.959

The R-squared values indicates the goodness of fit between the two methods. A higher R-squared value means a better fit table 12.0.

PARAMETER	R-squared (R^2)	COMMENTS
Lead(Pb) mg/L	0.934	Good fit
Chromium (Cr) mg/L	0.813	Fair fit
Zinc (Zn)mg/L	0.959	Excellent fit.

These results suggest that the Ogota-Bank equation is a good predictor for Lead (Pb) and Zinc (c Zn), but less accurate for chromium (Cr),

However, R-Squared(R^2) method alone is not sufficient to conclude the validity of a model. Other necessary factors like residual analysis and cross-validation can be useful.in view of these, the residual analysis was performing to established a solid ground for the validity of the model.

The standard deviations Results:

- Lead: (0.103) approximately 10% of the mean predicted values and its indicates a relatively small amount of variation in the residual suggesting a good fit with most residuals within + or minus 0.2%mg/L.
- Zinc (Zn) (0.09) approximately 9% of the mean predicted value) indicating a relatively small amount of variation in the residuals thereby suggesting a good fit with most residuals within plus or minus 0.2mg/L.

- Chromium (Cr) (0.143) approximately 25% of the mean predicted value indicating a moderate amount of variation in the residuals., thereby suggesting a potential issue with the model fit, with some residuals exceeding plus or minus 0.3mg/L

Using similar equation by Domenico equation for contaminant concentration which is given as follows: \

$$C(x, t) = Co/2 * erfc(V - vt) / 2sqrt(Dx - t))$$

Using above equation with the developed model yielded same results which is an indication that the developed model performs reasonably well.

RESULT AND DISCUSSION

LEAD (Pb) mg/L

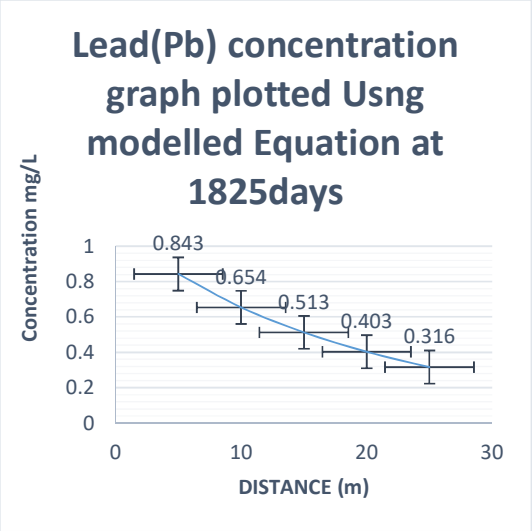
Lead (Pb) is a toxic bluish –white metal that can contaminate groundwater near Dumpsites through various pathways which may include leaching from waste disposal, corrosion of lead –containing materials and from industrial wastes. The presence of observed lead (Pb) concentration can be attributed to the presence of Batteries, electronics and construction materials as observed by khan et al.,2020 and Kumar et al., 2018.it was hereby also observed that the presence of lead(Pb) at the dumpsites can be attributed to the presence of old batteries, construction materials and substantial quantities of E-wastes. The proximity of the dumpsites to human settlement which is as closed as 5m away has substantially contributed to the uncontrolled disposal of these harmful solid wastes materials at the dumpsites. The graph shows that the magnitude of lead concentration reduces with Distance from the dumpsite.

The maximum allowable limit by WHO for lead (Pb) is 0.01mg/L while EPA recommended action level at 0.015mg/L

PRESENCE OF LEAD AT DUMPSITES:

- Battery Disposal: -Lead –acid batteries are significant source of Lead (Pb) contamination at Dumpsites as observed by Khan et al.,2020.
- Electronics wastes(E-wastes). Lead (Pb) is used in electronic wastes such as computers, Television
  and mobile phones which are often disposed up at dumpsites in his part of the World (Singh etal.,2018)
- Construction materials: -Lead –based paints, Soldering and plumbing materials can contribute to c Lead(Pb) contamination in Dumpsites (Huang et al.,2019)
- Industrial Waste: -Lead processing industries such as Smelting and refining can generate Lead- containing wastes that ends up in Dumpsites (Sharma et al.,2019)

From the graph, it shows that the concentration levels are high with the few years of the Dumpsites lifespan but gradually reduce ces with time and distance.



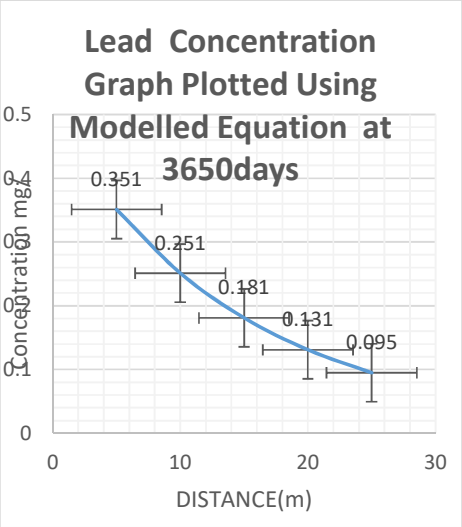
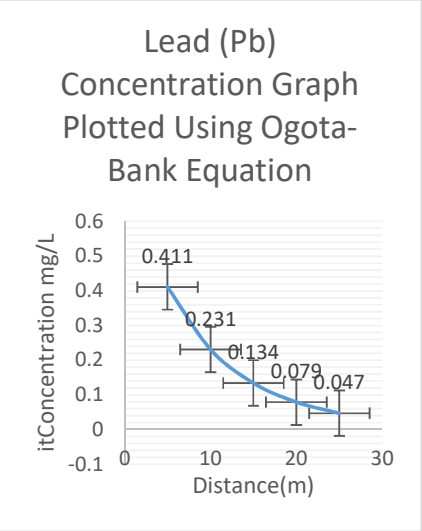


Figure 2.0 shows lead concentration at the start and decommissioned period



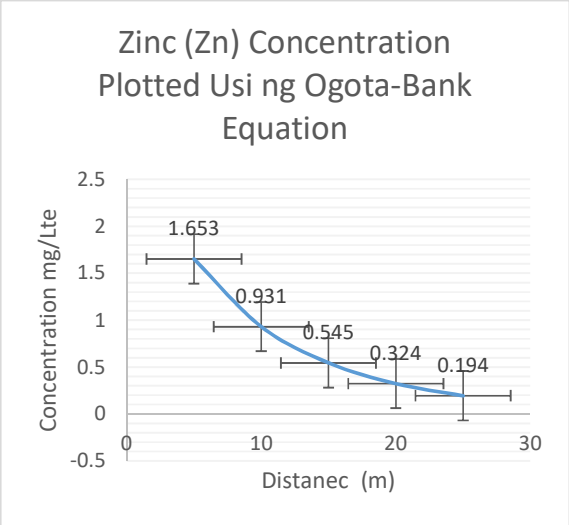


Figure 5.0 shows the Lead (Pb) and Zinc (Zn) concentration graph plotted from Ogota Results

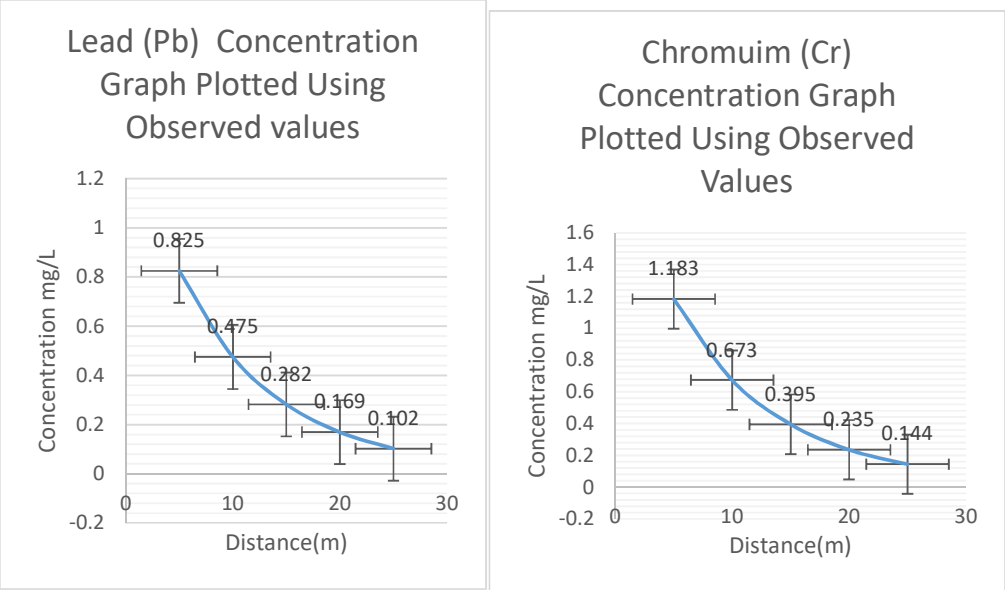


Figure 6.0 shows the Lead (Pb) and Chromium(Cr) concentration plotted using Observed results

Zinc (Zn) presences in the observed concentration is as a result of Batteries, galvanized materials and wastes from zinc-processing factories. Similar observation at Other Dumpsites was reported by Kumaret al., 2018.It was observed that the contamination pathway in most cases can be attributed to leaching of heavy metals 9HMs) into soil and groundwater from the wastes disposed at the Dumpsites. This assertion was supported by similar finding by Singh et al.,2018 as well as equally reported by Huang et al.,2018 that storm water carries heavy metals from dumpsites into surrounding areas. The decrease in concentration level with distance is attributed to dispersion and dilution which is the spread out of the heavy metals and mixing with water thereby reducing the concentration levels of the contaminants as observed in the Ogota-Bank equation model. The second reason for the reduced concentration is as a result of adsorption and retention, a known phenomenon where soil and sediments absorbs and retains heavy metals(Hms) thereby reducing mobility of the heavy metals as observed in the Domenico equation outputs and thirdly, natural attenuation which is the biological and chemical processes break down or the immobilization processes of heavy metals as observed in sim lar work by EPA (2020).

REASONS FOR PREDICTING LOWER CONCENTRATION BY THE OGATA-BANK EQUATION.

- Overestimation of dispersion coefficients: -Ogota-Bank equation assumes a constant dispersion coefficient which might be overestimated, leading to lower predicted concentration
- Under estimation of sources strength: - if the source strength (contaminant input) is underestimated, the predicted concentration will be lower
- Neglecting sorption or degradation :-Ogota-Bank equation assumes no sorption or degradation, which might not be the case in reality: -This can lead to lower predicted concentration

To address these issues, we can consider the following options:

- Refining the model with more accurate data and parameters
- Incorporating additional processes like sorption or degradation
- Using more advanced models for numerical methods
- Conducting sensitivity analyses to identify critical parameters.

By addressing these potentials causes, we can improve the accuracy of concentration predictions using Ogata-Bank equation

ENVIRONMENTAL IMPLICATIONS

The environmental implications of predicting lower contaminant concentration using Ogata-Bank and developed equations

V. Underestimation of risks: - Predicting lower concentration may lead to underestimation of the actual risks, potentially resulting in inadequate remediation or management strategies

VI. Insufficient treatment: - Lower predicted concentration might lead to insufficient treatment or removal of contaminant potentially causing ongoing environmental harm

VII. Inadequate regulation: - Regulatory standards might be set too low, allowing for higher actual concentration and potentially harming the environment and human health

VIII. Environmental damage: -Underestimating contaminant concentration can lead to prolonged exposure, causing environmental damage such as groundwater contaminations, soil pollution, surface water pollution and harm to aquatic life and ecosystems.

CONCLUSION

The developed modelled equation and the Bogota-Bank equations are valuable tools for predicting contaminant transport in porous media. The developing modelled g equation was able to cater for some of identified inadequacies of the Ogota-Bank equation which includes among other the overestimation of dispersion coefficients, neglecting of non-linear sorption kinetics and geochemical reactions, inadequate representation of heterogeneous aquifer properties and limited consideration of uncertainty and sensitivity analysis. From the three values obtained from the analysis and the observed values, the two parameters namely Lead (Pb) and the Chromium (Cr) are in a very elevated concentration which may be harmful to human and the ecosystem while the Zinc (Zn) concentration is relatively within the normal range which may not be too harmful. All the three parameters which were calculated using the modelled equation and Ogota –Bank equation exhibited similar trend in magnitude while the observed values which were used as initial concentration(Co) were very much similar in concentration with the values obtained from the modelled equation while the same modelled equation results were observed to be higher than the Ogota-bank results. The developed modelled equation has the capacity to incorporate identified limitation of both Ogota-Bank equation and Domenico equation which are both existing contaminant transport model equation for predicting contaminant concentrations in landfill/Dumpsites.

RECOMMENDATION

To enhance the accuracy and reliability of contaminant transport predictions in dumpsites, it's imperative to adopt the following recommendations: -

IV. Developing a modified equation that incorporates the identified limitations and improve upon the limitations of the Ogota-bank equations
V. Defining the Ogota- Bank equation to account r for non-linear processes, heterogeneous aquifer properties and geochemical reactions
VI. Validating and calibrating models using field data to ensure accuracy and reliability

These recommendations if adopted can result in the development of a more advanced and accurate contaminants transports models, ultimately supporting better environmental management and risks decisions.

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