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Geochemical Speciation and Potential Mobility of Heavy Metals in Agricultural Soils of Cross River State, Nigeria: A Visual MINTEQ Modelling Approach

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Abstract

This study evaluated the geochemical speciation, aqueous behaviour, and potential mobility of selected heavy metals in agricultural soils from twelve farm locations across the Yakurr and Biase Local Government Areas of Cross River State, Nigeria, using the Visual MINTEQ geochemical modelling software. Soil samples were collected from Ekori, Adim, Akpet, Umon, Abini, Agwagune, Mkpani, Idomi, Inyima, Ugep, Nko, and Abaribara, and analysed for Cu, Ni, Zn, Cr, Mn, Fe, Pb, Cd, and As using atomic absorption spectrophotometry. The measured physicochemical parameters exhibited substantial spatial variability, with soil pH ranging from 4.0 to 6.9 and moisture content ranging from 70% to 99%. Elevated concentrations of Ni, Pb, Cd, and As were observed at Idomi, Inyima, and Ugep, while Cu concentrations remained below the WHO drinking water guideline across all locations. Visual MINTEQ modelling revealed that under the prevailing near-neutral water chemistry (pH 6.29-6.77), the investigated metals occurred predominantly as dissolved free ions and carbonate complexes. The calculated ionic strength ranged from 0.00134 to 0.00584 mol/L, while free-ion activities varied considerably among farms. Malachite saturation indices were consistently negative (−0.9 to −4.1), indicating undersaturation and a low likelihood of spontaneous copper mineral precipitation. The model further indicated that Cd, Pb, and Cu could persist in dissolved forms under the existing geochemical conditions, thereby increasing their potential availability for transport and biological uptake. These results show that total metal concentrations alone do not adequately describe environmental mobility, as aqueous speciation, pH, ionic strength, and mineral saturation strongly influence metal behaviour. The findings underscore the potential risk of continued metal mobility and groundwater contamination in the investigated agricultural environments, highlighting the need for integrated geochemical assessments in environmental monitoring programmes.

Keywords: Heavy metals; Visual-MINTEQ; Geochemical speciation; mobility; groundwater, mineral saturation.

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Introduction

Aquatic environments, including rivers, lakes, wetlands, estuaries, and groundwater systems, play a critical role in the mobility, bioavailability, and toxicity of metals (Osae *et al.,* 2025). Of particular concern are redox-active metals such as iron (Fe), manganese (Mn), chromium (Cr), arsenic (As), and mercury (Hg), whose redox reactions significantly influence solubility and mobility, thereby determining whether metals are retained in the sediment phase or released into the water column (Dendievel *et al.,* 2022; Qiao *et al.,* 2023). The migration pathways and ultimate fate of redox-sensitive elements in aquatic environments are rendered complex by the interaction of geochemical, hydrological, and biological processes (Xue *et al.,* 2026). Changes in dissolved oxygen concentrations, pH, organic matter composition, and biological activity can readily induce rapid redox reactions, particularly at the water-sediment interface and in groundwater flow systems (Dong *et al.*, 2023). These processes are further complicated by spatial variability in sediment composition and temporal variability in hydrological conditions, making it challenging to determine metal transport behaviour based solely on field measurements (Ferreira *et al.,* 2023). In response to these complexities, geochemical modelling approaches have been developed as useful predictive tools. Traditionally, geochemical models have been based on thermodynamic equilibrium approaches, using mass action laws and thermodynamic data to predict the distribution of metal species and mineral saturation under equilibrium conditions (Di Bonito *et al.,* 2024). Although these approaches provide useful insights into potential chemical species distributions, they may not adequately model non-equilibrium redox reactions, which are time-dependent in natural aquatic systems (Mundra *et al.,* 2025). Modern geochemical models have incorporated spatially distributed reaction kinetics and dynamic redox reactions, allowing for more realistic simulations of heterogeneous systems (Shao *et al.,* 2021; Jiang *et al.*, 2023).

Visual MINTEQ is a stand-alone geochemical modelling software for simulating aqueous speciation, mineral solubility, adsorption, and metal complexation in water and soil systems, providing a graphical user interface (GUI) for specifying water chemistry, pH, or redox conditions, and selecting thermodynamic databases (Zhang *et al.,* 2022; Wu *et al.,* 2023). The program can compute metal speciation, solubility equilibria, sorption, precipitation/dissolution, and ion interactions under specific conditions such as pH, temperature, and ionic strength. Visual MINTEQ has been widely applied in environmental studies to understand the behaviour of metals in water and soil systems (Nuamah *et al.,* 2026). For instance, Irunde *et al.* (2022) used MINTEQ to examine how arsenic adsorption varies with pH and adsorbent dose in water from the Lake Victoria

Basin, demonstrating that the model could predict arsenic removal efficiency under varying conditions.

Despite these advances, limited research has been conducted on the geochemical speciation and mobility of heavy metals in agricultural soils of southeastern Nigeria, particularly within the Cross River State region. Agricultural activities, combined with the region's tropical climate, high rainfall, and significant hydrological fluctuations, create conditions conducive to metal mobilisation and potential groundwater contamination. Given that agricultural soils in this region are subject to both anthropogenic influences (fertiliser application, agrochemical use) and natural processes (weathering, organic matter decomposition), understanding the geochemical controls on metal speciation and mobility is essential for assessing environmental risks. Therefore, this study aimed to: (1) determine the concentrations of selected heavy metals (Cu, Ni, Zn, Cr, Mn, Fe, Pb, Cd, and As) in agricultural soils from twelve farm locations in Yakurr and Biase Local Government Areas of Cross River State, Nigeria; (2) apply Visual MINTEQ to model the aqueous speciation, free-ion activities, and mineral saturation states of these metals under prevailing geochemical conditions; and (3) evaluate the potential mobility of metals and their implications for groundwater contamination risk.

Materials and Methods

2.1 Description of Study Area

The research was conducted in the Yakurr and Biase Local Government Areas of Cross River State, Nigeria, a tropical region characterised by high annual rainfall, elevated temperatures, and significant hydrological fluctuations. The study area encompasses twelve sampling points: Ekori, Adim, Akpet, Umon, Abini, Agwagune, Mkpani, Idomi, Inyima, Ugep, Nko, and Abaribara. The geographical coordinates of sampling points ranged between latitudes 5.24°N and 6.71°N and longitudes 7.10°E and 9.44°E, reflecting the spatial distribution across the region. These sampling locations comprise agricultural environments influenced by both anthropogenic activities (agricultural practices, potential contamination sources) and natural processes (weathering and organic matter deposition). The tropical climate, presence of organic matter, and spatial variations in oxidation-reduction potential make this area particularly suitable for investigating metal geochemistry in waterlogged ecosystems.

2.2 Sample Collection and Field Measurements

Soil samples were collected from twelve different farm locations within the study area to ensure adequate spatial representation. Sampling was conducted using clean, acid-washed containers to minimise contamination and maintain sample integrity for accurate analysis. Field measurements of physicochemical parameters, including pH, temperature, electrical conductivity (EC), total dissolved solids (TDS), and oxidation-reduction potential (ORP), were performed in situ using a calibrated multiparameter meter (Hanna Instruments HI98194). These measurements were performed immediately upon sample collection to capture the natural state of the samples

without post-collection alteration. The geographical coordinates of each sampling point (Table 1) were recorded using a GPS device (Garmin eTrex 10) for proper documentation, sample identification, and future replication.

2.3 Sample Preparation and Heavy Metal Analysis

Soil samples were air-dried at ambient temperature, homogenised, and sieved through a 2-mm mesh to remove debris and ensure uniformity. A representative subsample (approximately 5 g) was digested using a mixture of hydrochloric acid (HCl) and nitric acid (HNO3) following standard digestion protocols (USEPA Method 3050B). The digestion process involved heating the sample-acid mixture to complete digestion, producing a clear solution suitable for analysis. Heavy metal concentrations (Cu, Ni, Zn, Cr, Mn, Fe, Pb, Cd, and As) were determined using an Atomic Absorption Spectrophotometer (PerkinElmer AAnalyst 400). The analytical procedure involved the following steps:

(i) Instrument Calibration: The AAS instrument was calibrated and optimised according to manufacturer specifications for each metal of interest using standard solutions of known concentrations to generate calibration curves with high linearity ($R^2 > 0.995$).

(ii) Sample Analysis: Digested samples were aspirated into the AAS, and absorbance readings were recorded at specific wavelengths for each metal.

(iii) Quality Control: Analytical quality was assured through the analysis of certified reference materials, reagent blanks, and duplicate samples. Results were expressed as mean ± standard deviation (SD) for triplicate analyses.

2.4 Geochemical Modelling Using Visual MINTEQ

Visual MINTEQ (version 3.1) was used to compute the equilibrium speciation of chemical species in aqueous solutions. The program can compute metal speciation, solubility equilibria, sorption, precipitation/dissolution, and ion interactions under specified conditions of pH, temperature, and ionic strength. The program is based on the application of thermodynamic laws to determine the activity of dissolved species under a given set of conditions, whether in a natural water system or a laboratory system.

The following input parameters were used for the Visual MINTEQ modelling:

(i) Chemical Composition: Measured concentrations of major ions (Ca2+, Mg2+, Na+, K+, Cl-, SO42-, HCO3-, CO32-) and heavy metals (Cu, Ni, Zn, Cr, Mn, Fe, Pb, Cd, As) were entered as total dissolved concentrations.

(ii) pH: Measured in situ pH values were used as input.

(iii) Temperature: Measured in situ temperatures (23.5–36.8°C) were used.

(iv) Ionic Strength: Ionic strength was calculated using the Davies equation:

$$logyi = -Azi\left(\left(\frac{\sqrt{I}}{I + \sqrt{I}}\right) - 0.3\,I\right)$$

where γi is the activity coefficient, zi is the ion charge, I is the ionic strength, and A is the Debye–Hückel constant (0.508 at 25°C).

(v) Thermodynamic Database: The MINTEQ thermodynamic database

(version 4.0) was used, which includes equilibrium constants for aqueous complexes, minerals, and sorption reactions.

The model output included: (i) aqueous speciation of metals (free ion activities, complexed species); (ii) saturation indices (SI) for mineral phases (e.g., malachite, cerussite); and (iii) distribution of metal species as percentages of total dissolved concentration.

2.5 Data Analysis

Descriptive statistics were calculated for all measured parameters. Metal concentrations were compared with World Health Organisation (WHO) drinking water guidelines to assess regulatory exceedances. Spatial distribution maps were generated using ArcGIS software. Saturation indices were interpreted as follows: SI > 0 indicates supersaturation (precipitation possible), SI = 0 indicates equilibrium, and SI < 0 indicates undersaturation (dissolution favoured).

Results

Table 1 shows variations in soil fertility and environmental conditions across the twelve farm locations. Soil fertility ranged from 142 at Akpet farm to 711 at Abaribara farm, indicating that Abaribara, Abini, Umon, and Idomi farms have more fertile soils, while Akpet and Inyima farms may require soil nutrient improvement. Soil moisture was generally high (70–99%), suggesting favourable conditions for crop growth. The soil pH ranged from 4.0 to 6.9, indicating that most soils were acidic, with Abini and Umon farms being strongly acidic and likely requiring liming to improve crop performance. Soil temperatures varied between 23.5°C and 36.8°C, while sunlight intensity and humidity also differed considerably among the locations. Overall, the results indicate that although the farms generally possess adequate moisture and suitable environmental conditions for agriculture, differences in fertility and soil acidity highlight the need for location-specific soil management practices to enhance crop productivity.

Table 1: Soil physicochemical characteristics of the twelve sampled farm locations

S/N	Name of farm area	Fertility	Moisture	pH	Temperature	Sunlight	Humidity
1	Ekori farm	448	70	6.5	30.2	1078	89
2	Nko farm	416	76	6.0	36.3	3785	81
3	Akpet farm	142	99	6.2	24.6	7800	62
4	Umon farm	660	96	4.5	36.8	5342	51
5	Abini farm	702	99	4.0	34.2	5543	58
6	Agwagune farm	546	99	5.0	33.9	1697	57
7	Mkpani farm	472	94	5.5	23.5	5677	72
8	Idomi farm	647	84	6.7	30.4	1176	84
9	Adim farm	444	70	6.5	30.2	7810	92
10	Ugep farm road	421	94	6.9	30.2	7810	81
11	Inyima farm	147	86	6.5	31.6	5742	64
12	Abaribara farm	711	82	6.8	36.2	1746	77

Table 2: Heavy metal profile and physicochemical properties of soils from selected farms (mg/kg; mean ± SD)

Farms	Cu	Hg	As	Ni	Zn	Mo	V	Cr	Mn	Fe	B	Pb	Cd
Idomi	0.5437±0.56	ND	0.1191±0.15	1.8397±0.31	0.1231±0.30	0.0033±0.60	0.0482±0.40	0.2059±0.69	0.0404±0.62	0.0514±0.62	0.2850±0.80	0.0982±0.40	0.0304±0.15
Inyima	0.2575±0.25	ND	0.0564±0.30	0.8714±0.45	0.0583±0.10	0.0016±0.36	0.0228±0.42	0.0976±0.70	0.0191±0.45	0.1191±0.41	0.1350±0.60	0.0465±0.40	0.0144±0.20
Ugep	0.2861±0.60	ND	0.0627±0.40	0.9683±0.25	0.0648±0.40	0.0017±0.72	0.0253±0.45	0.1084±0.46	0.0213±0.42	0.1213±0.32	0.1500±0.51	0.0517±0.35	0.0160±0.26
Abaribara	0.0028±0.40	ND	ND	0.0091±0.20	0.0134±0.40	0.0005±0.36	ND	0.0040±0.40	0.0012±0.40	0.0112±0.31	0.0012±0.45	0.0016±0.40	0.0042±0.20
Mkpani	0.0056±0.35	ND	ND	0.0181±0.36	0.0269±0.31	0.0010±0.31	ND	0.0080±0.66	0.0024±0.40	0.0124±0.41	0.0025±0.46	0.0033±0.36	0.0084±0.25
Abini	0.0061±0.40	ND	ND	0.0199±0.25	0.0295±0.61	0.0010±0.45	ND	0.0087±0.42	0.0026±0.38	0.0227±0.45	0.0027±0.46	0.0036±0.55	0.0093±0.25
Akpet	0.0040±0.31	ND	ND	0.0130±0.31	0.0193±0.40	0.0007±0.44	ND	0.0057±0.35	0.0017±0.32	0.0217±0.22	0.0018±0.40	0.0023±0.50	0.0061±0.18
Nko	0.0051±0.21	ND	ND	0.0166±0.46	0.0245±0.30	0.0009±0.31	ND	0.0073±0.70	0.0022±0.45	0.0122±0.65	0.0023±0.56	0.0030±0.40	0.0078±0.18
Ekori	0.0098±0.56	ND	ND	0.0314±0.40	0.0467±0.50	0.0017±0.40	ND	0.0138±0.40	0.0041±0.51	0.0131±0.49	0.0043±0.51	0.0057±0.40	0.0147±0.26
Agwagune	0.0056±0.56	ND	ND	0.0180±0.42	0.0267±0.47	0.0009±0.50	ND	0.0079±0.25	0.0023±0.60	0.0123±0.59	0.0025±0.70	0.0032±0.40	0.0084±0.28
Umon	0.9970±0.31	ND	ND	0.0227±0.31	0.0337±0.40	0.0012±0.44	ND	0.0100±0.35	0.0030±0.32	0.0230±0.42	0.0031±0.40	0.0041±0.50	0.0106±0.18
Adim	0.0035±0.21	ND	ND	0.0115±0.46	0.0171±0.30	0.0006±0.31	ND	0.0051±0.70	0.0015±0.45	0.0115±0.62	0.0016±0.56	0.0021±0.40	0.0054±0.18

Table 2 above presents the concentrations of selected heavy metals and physicochemical properties of soil samples collected from twelve farm locations. Copper, nickel, zinc, chromium, manganese, iron, boron, lead, cadmium, and arsenic were detected at varying concentrations, while mercury and vanadium were not detected in most samples. Arsenic was detected only at Idomi, Inyima, and Ugep, consistent with the exceedances reported in Table 4. Umon and Idomi farms exhibited relatively higher metal concentrations compared to other locations. Overall, the results indicate spatial variations in metal distribution and soil quality among the sampled farms.

Figure 1: Spatial Distribution Map of Sampling Locations

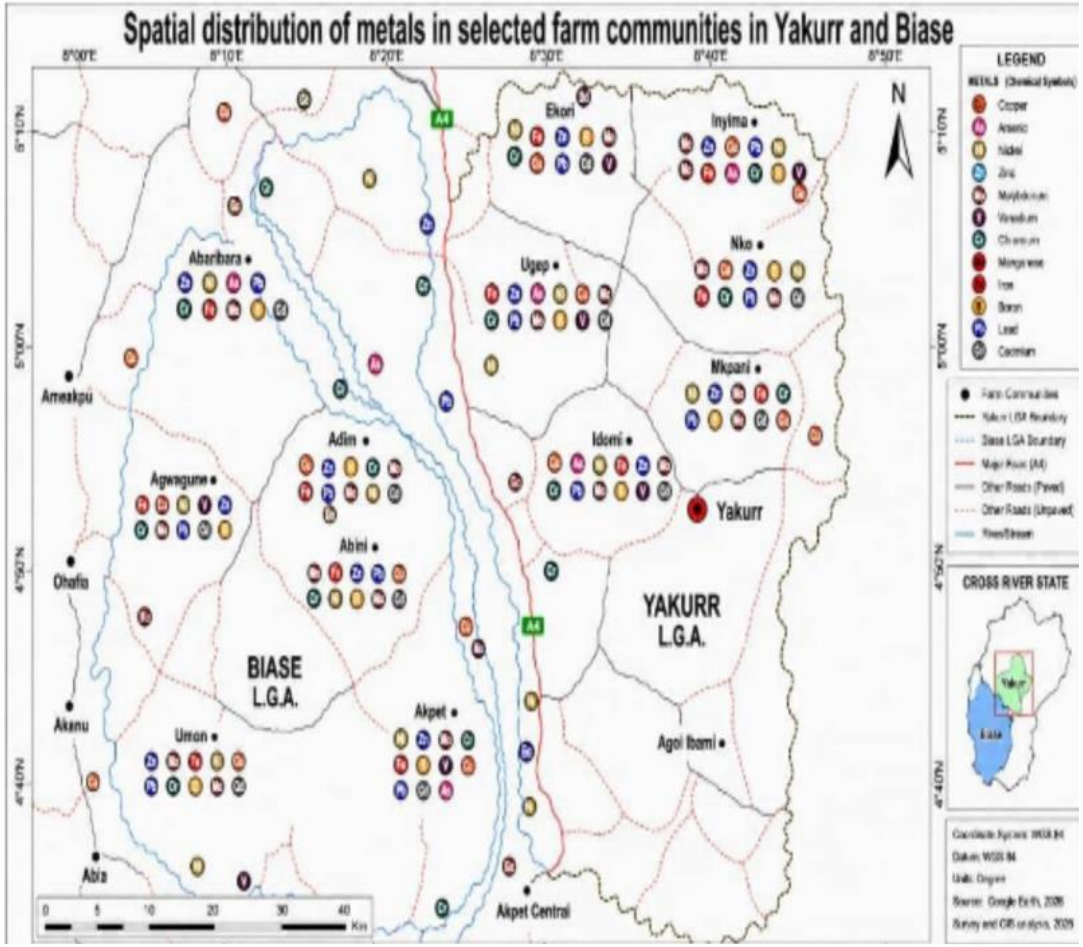

Table 3: MINTEQ-modelled free ion activities and saturation index (example for malachite)

Farm	Ionic strength (mol/L)	a(Cu2+) x 10^6 (M)	a(Pb2+) x 10^7 (M)	a(Cd2+) x 10^7 (M)	SI (malachite)
Idomi	0.00226	37.2	9.82	5.61	-1.2
Inyima	0.00138	17.1	4.60	2.63	-1.6
Ugep	0.00198	19.0	5.12	2.93	-1.5
Abaribara	0.00226	0.19	0.16	0.78	-4.1
Mkpani	0.00584	0.36	0.32	1.53	-3.8
Abini	0.00205	0.40	0.35	1.71	-3.7
Akpet	0.00205	0.26	0.23	1.11	-4.0
Nko	0.00134	0.34	0.30	1.45	-3.9
Ekori	0.00579	0.66	0.57	2.73	-3.5
Agwagune	0.00211	0.37	0.32	1.54	-3.8
Umon	0.00230	69.7	0.41	1.95	-0.9
Adim	0.00234	0.23	0.21	0.98	-4.0

In Table 3, there is a description of the ionic strength, metal ion activities, and the saturation index (SI) of malachite on the various farms. Ionic strength values range from 0.00134 to 0.00584 mol/L, which are quite low. This shows that the waters are relatively dilute, although there is a slight increase in ionic strength in some areas like Mkpani and Ekori. Metal ion activities show variations among themselves. Copper ion (Cu^{2+}) activity is quite high in Umon and Idomi when compared to the very low values in other places like Abaribara and Akpet. The lead (Pb^{2+}) and cadmium (Cd^{2+}) ions also behave similarly but in smaller amounts. The malachite SI values are negative (-0.9 to -4.1), which means that the water is unsaturated in relation to malachite.

Table 4: Regulatory exceedances (WHO drinking water guidelines)

Metal	Guideline (mg/L)	Farms exceeding guideline
Ni	0.07	Idomi (1.84), Inyima (0.87), Ugep (0.97)
Pb	0.01	Idomi (0.098), Inyima (0.047), Ugep (0.052)
Cd	0.003	All farms (0.004-0.030)
As	0.01	Idomi (0.119), Inyima (0.056), Ugep (0.063)
Cu	2.0	None (all <1.0)

Table 4 shows that several farms exceed WHO drinking water limits for toxic metals. Nickel, lead, cadmium, and arsenic are above guideline values in multiple locations, especially Idomi, Inyima, and Ugep, indicating significant contamination risks. In contrast, copper levels remain below the WHO limit across all farms, suggesting no regulatory concern for Cu.

Discussion

The detection of elevated metal concentrations across twelve farm locations signals a contamination problem that merits careful examination. The measured values for nickel, lead, cadmium, and arsenic in several samples depart substantially from regulatory benchmarks, indicating that these sites may be operating under environmental conditions that carry non-trivial ecological and human health implications. A meaningful understanding of the situation requires moving beyond simple concentration comparisons; the fate of these metals in the environment depends on their chemical speciation, their potential for transport through soil and groundwater, and the geochemical context in which they exist. The results presented here reflect a complementary modelling approach using Visual MINTEQ.

Geochemical Speciation and Metal Behaviour: The equilibrium modelling was performed using Visual MINTEQ, which simulates metal speciation and mineral saturation using its own thermodynamic database. A recent study by Paliulienė & Vasarevičius (2025) demonstrated that Visual MINTEQ can effectively model the dependence of

cadmium, lead, and copper speciation on soil pH and temperature, and the results from the present study are broadly consistent with that body of work. Free ion activities were calculated across all farms using measured pH and electrical conductivity (EC) as inputs. The farm with the highest ionic strength (I ~ 0.0058 mol/L at Mkpani and Ekori) also showed some of the highest free ion activities for several metals. The highest free copper activity (aCu^{2+} = 69.7 × 10-6 M) was observed at Umon, despite a relatively low total copper concentration (0.9970 mg/L). This indicates that the geochemical environment at this site favours a higher proportion of free, bioavailable copper ions relative to the total dissolved concentration. For Idomi (aCu^{2+} = 37.2 × 10-6 M) and Ugep (aCu^{2+} = 19.0 × 10-6 M), the measured free ion activities also correlate positively with total metal concentrations (Table 3).

For lead, the highest free ion activities were observed at Idomi (aPb^{2+} = 9.82 × 10-7 M), followed by Ugep (5.12 × 10-7 M) and Inyima (4.60 × 10-7 M). At Ekori, despite a total lead concentration of only 0.0057 mg/L, the free lead activity was still measurable (aPb^{2+} = 0.57 × 10-7 M). Across the dataset, free ion activities varied by more than two orders of magnitude, highlighting that total metal concentration alone is a poor predictor of bioavailable or mobile metal fractions. The saturation index for malachite calculated using MINTEQ was consistently negative across all farms. This consistency increases confidence in the conclusion that copper will not precipitate spontaneously and will therefore remain available for transport and biological or plant uptake.

MINTEQ was used to evaluate the aqueous speciation and potential mobility of the investigated metals under the prevailing groundwater conditions. MINTEQ does not directly predict the distance or rate of contaminant migration. Rather, it determines the chemical forms of metals in solution and their tendency to remain dissolved or precipitate as mineral phases. Under the measured pH range of 6.29-6.77 and temperatures of 26.5-32.1°C, the MINTEQ results indicated that the metals occurred mainly as dissolved free ions and carbonate complexes. The absence of strong mineral precipitation, together with undersaturation with respect to relevant metal-carbonate minerals, suggests that the metals can remain available for movement with groundwater.

The MINTEQ results are particularly important for understanding the behaviour of Cd, Pb and Cu. Cadmium is expected to remain relatively mobile under near-neutral conditions because dissolved Cd species are not strongly removed through precipitation. Lead, although generally strongly retained by soil surfaces, may occur partly as dissolved carbonate complexes, which can increase its dissolved fraction under suitable chemical conditions. Copper may similarly form aqueous complexes that influence its dissolved concentration and mobility. Therefore, MINTEQ demonstrates that metal mobility is controlled not only by total concentration but also by aqueous speciation, pH, and mineral saturation. Changes in these conditions, particularly variations in pH or carbonate availability, could alter the proportion of metals present in mobile dissolved forms (Wang *et al.*, 2024). MINTEQ assessment indicates that the

investigated metals have the potential to remain dissolved and consequently become available for transport toward groundwater. However, MINTEQ alone cannot determine the actual travel distance or time required for a metal to reach the water table because it is primarily an equilibrium geochemical model. Its results are therefore best interpreted as an indication of chemical mobility and precipitation potential, rather than as direct evidence of contaminant migration rates. This distinction is important when assessing groundwater contamination risk, because dissolved metal species identified by MINTEQ may subsequently be transported through the subsurface depending on groundwater flow, dispersion, and interactions with soil surfaces.

Conclusions

Visual MINTEQ speciation modelling indicates that under the prevailing near-neutral pH conditions (6.29–6.77), the investigated metals occur predominantly as free divalent ions and carbonate complexes. The model shows that the waters are undersaturated with respect to malachite ($Cu_2(OH)_2CO_3$), cerussite ($PbCO_3$), and other relevant metal-carbonate minerals, indicating that significant mineral precipitation is unlikely under the existing conditions. Consequently, the metals are expected to remain largely dissolved and potentially available for transport and biological uptake. The formation of the neutral $PbCO_3^0$ complex is particularly important because it increases the dissolved fraction of lead and may enhance its mobility compared with predictions based solely on total lead concentration. Overall, the MINTEQ results suggest that the prevailing water chemistry favours the persistence of dissolved metal species, highlighting the potential for continued metal mobility and groundwater contamination if the existing geochemical conditions are maintained.

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