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ORIGINAL PAPER

Characteristic curve modeling of plant species behavior in soils with heavy metals

Elizabeth J. Lam · Brian F. Keith · Jaume Bech · Fernando A. Alvarez · Vicente Zetola · Luis H. Pereira · Ítalo L. Montofré

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Abstract Many vegetal species can accumulate great amounts of metallic elements in their tissues. For this reason, they are called metal hyperaccumulators. An indicator of great interest in environmental sciences is the bioconcentration factor because it is recognized for establishing the potential accumulation of chemicals in organisms. Particularly in soil phytoremediation processes, it measures the capacity of a certain plant to capture metals, in terms of soil concentration. According to their behavior, four types of plants can be distinguished regarding soil concentration increase: indicator, excluder, accumulator, and hyperaccumulator. This study proposes a new model to categorize plants according to their behavior related to soil concentration increase, using several characteristic curves obtained from 1288 experimental measurements collected from different bibliographic sources. The metals analyzed were Cu, Fe, Pb, and Zn. The proposed model is obtained through linear regression and nonlinear transformations to model the expected behavior of plants in high concentration conditions. In particular, the basic equation of the model has three key components to represent the expected concentration in the plant root given the final soil concentration level, the type of species, and specific metal: a linear factor that determines the growth for low concentration values, an exponential factor that determines its decrease for high concentration values, and a logarithmic factor

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E. J. Lam (✉)
Chemical Engineering Department, Universidad Católica del Norte, 1270709 Antofagasta, Chile
e-mail: elam@ucn.cl

B. F. Keith
Department of Computing and Systems Engineering, Universidad Católica del Norte, 1270709 Antofagasta, Chile

J. Bech
Soil Science Laboratory, Faculty of Biology, Universidad de Barcelona, Barcelona, Spain

F. A. Alvarez
Administration Department, Universidad Católica del Norte, 1270709 Antofagasta, Chile

V. Zetola
Construction Management Department, Universidad Católica del Norte, 1270709 Antofagasta, Chile

L. H. Pereira
Aquaculture Department, Universidad Católica del Norte, 1270709 Antofagasta, Chile

Í. L. Montofré
Mining Business School, ENM, Universidad Católica del Norte, Antofagasta, Chile

Í. L. Montofré
Mining and Metallurgical Engineering Department, Universidad Católica del Norte, 1270709 Antofagasta, Chile

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that limits the maximum value that can be reached in practice and influences the decay for high concentration values. After fitting the experimental data using linear regression, the proposed model has a 0.084 R^2 determination coefficient and all of its parameters are considered significant. Furthermore, it shows that 60 of the 257 species assessed behave as accumulators and 10 of them as hyperaccumulators. The main contribution of this model is its ability to handle soils with high concentrations, where it would be hard for plants to achieve concentrations similar to or higher than the substrate containing them. Thus, the conventional criterion of the bioconcentration factor would incorrectly categorize a plant as an excluder. In contrast, this new model allows assessing plant effectiveness in a phytoremediation process of highly concentrated affected sites, such as mine tailings.

Keywords Phytoremediation · Bioconcentration factor · Heavy metals · Soil pollution · Characteristic curves

Introduction

Mining provides raw materials for other industrial sectors vital for the development of the population and global economy, thus having a potential economic, social, and environmental impact. The latter has caused the population's opposition because they perceive how the environmental quality of the zone is affected by a mining project (Lam et al., 2018, 2020; Mancini & Sala, 2018). The environment and its components have been severely affected by the presence of substances, which have become significant sources of environmental pollution mainly due to heavy metals (Carkovic et al., 2016; Chakraborty et al., 2017; Gong et al., 2018; Lam et al., 2017).

Soils are a non-renewable resource, their conservation being essential for ensuring food and a sustainable future. Two centimeters of fertile soil are generated over thousands of years (Montgomery, 2007). However, owing to anthropogenic activity, these soils could be potentially affected by the presence of heavy metals and metalloids. These metals and metalloids become highly environmentally important due to their toxicity, non-biodegradability, and bioavailability, bearing potential contamination risks for cultures, along with being a threat to people's health and safety (Kacholi & Sahu, 2018; Zwolak et al., 2019).

Depending on their use and activity developed, soils could be classified into three main groups: (1) Residential, (2) agricultural, and (3) industrial-mining. This is due to the discrepancy between the metal concentration levels expected from each of them. An industrial-mining soil is expected to contain more heavy metals and metalloids than those found in, for example, a residential or agricultural soil (Ashaiekh et al., 2019).

Phytoremediation has been used by many researchers to mitigate the impact of heavy metals and metalloids in the environment, including soil, water, and (to a lesser extent) air (Wei et al., 2021). Vegetal species highly tolerant to certain substances and negative environmental conditions have been found (Lam et al., 2018; Sarma et al., 2021; Tiwari & Lata, 2018). Plants growing in soils with high metal concentrations can be classified into four basic categories known as excluders, indicators, accumulators, and hyperaccumulators (Baker, 1981; Raskin et al., 1994). Excluder plants inhibit metal translocation from the root to the aerial section. Thus, the concentration found in the leaves is low. On the contrary, accumulator species can concentrate metal in their aerial section. Indicator species show a proportional relationship between metal concentration in the soil, absorption, and metal accumulation in the plant. So, the concentration in the leaves reflects that of the soil. In many cases, toxicity symptoms are visible in the plant (Baker, 1981).

Minguzzi and Vergnano (1948) found that the species *Alyssum bertolonii* (Desv) could accumulate more than 1% (10,000 mg/kg) nickel in its leaves, contrary to the usual levels for plants of the order 1–50 mg/kg. Brooks et al. (1977) called them "plants with unusually high nickel content" (greater than 1000 mg/kg dry material in a certain tissue of their aerial biomass) while introducing for the first time the term "hyperaccumulator". The criterion for choosing it was somehow arbitrary, based on the fact that a limited number of plants was able to accumulate levels higher than 1000 mg/kg, thus categorizing these plants as nickel hyperaccumulator species. Later, Baker and Brooks (1989) defined "hyperaccumulator species" as plants accumulating high metal concentrations in a tissue, in their natural habitat (Baker & Brooks, 1989; Diwan et al., 2008). As a whole, hyperaccumulator plants reach high metal concentrations in their leaves, that is, 10–100 times the usual concentrations (Chaney et al., 2020). Currently, the term hyperaccumulator refers to plants able to absorb 100 times more metals than the rest of the species (Baker & Brooks, 1989), thus establishing the following new criteria: over 10,000 mg/kg for Mn and Zn; over 1000 mg/kg for Co, Cu, Ni, As, Se, and Pb; and more than 100 mg/kg for Cd (Brooks et al., 1977, Baker et al., 2020).

The characteristic curve representing metal concentration behavior in plants versus metal concentration in the soil is shown in Fig. 1 (Adriano, 2001). For excluder species, metal concentration in the plant is lower than in the soil, while for indicator species, both concentrations tend to be the same. In accumulator and hyperaccumulator species, concentrations in the plant are much higher than in the soil or substrate containing them (Kaewtubtim et al., 2016; Mganga et al., 2011).

A factor to consider is the substrate concentration level. For example, a certain plant could behave as an accumulator and also as a hyperaccumulator if the site has low concentrations because the plant can contain a higher concentration of a certain metal than the one contained in the substrate. However, if the same plant is exposed to a site with a very high concentration of the same metal, the plant may extract the same as or a higher metal concentration than in the less contaminated substrate. Nevertheless, since the substrate concentration is so high, the plant concentration cannot be equated to the substrate concentration. So, the plant would be categorized as an excluder in this scenario.

In this context, the bioconcentration factor (BCF) is one of the most important indicators for measuring phytoremediation process efficiency (Hrynkiewicz et al., 2018), which indicates the ability of a plant to absorb metals from contaminated soil and is defined as the ratio of final metal concentration between the root and the soil (Lam et al., 2017, 2018).

For instance, if a soil shows a 2A Pb final concentration level and a given plant is able to extract from the soil a 3A concentration, then the plant will be categorized as an accumulator or hyperaccumulator since BCF will be 3/2, i.e., greater than 1. Considering a different scenario, where the final substrate concentration is 6A and the same plant is able to extract from the soil the same 3A concentration, then the plant will be categorized as an excluder in this new environment since the BCF will be 3/6, i.e., lower than 1. The questioning to this statement is: then, the plant behavior should be defined according to the

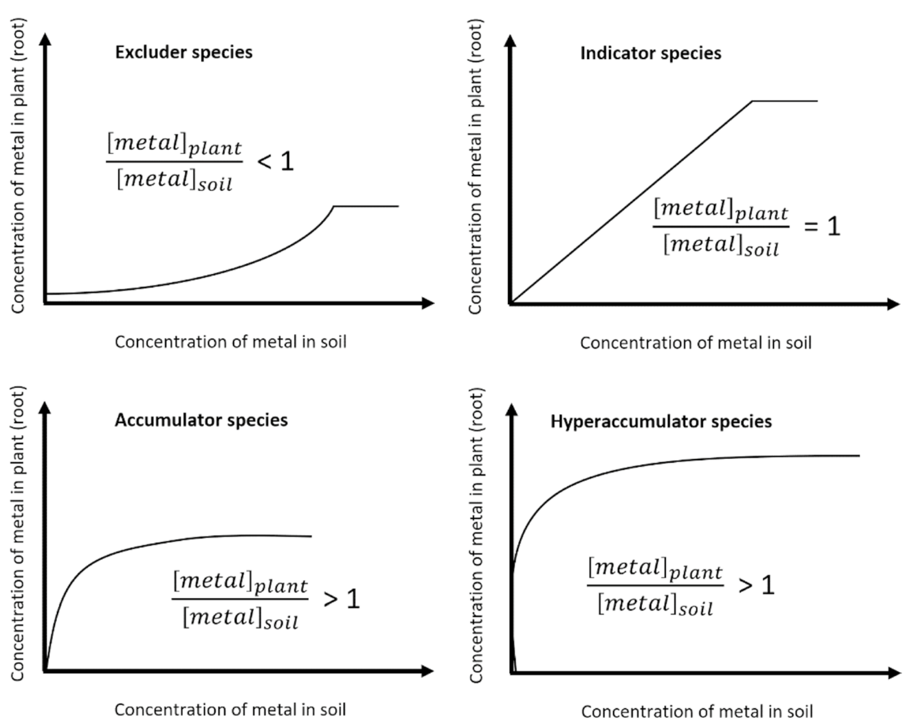

Fig. 1 Characteristic plant curves for different metal extraction strategies (excluder, indicator, accumulator, and hyperaccumulator species), Adriano, 2001

environment and, then, the correct way of referring to it would be, "the species is potentially an accumulator of a certain metal in a certain environment", without identifying the plant as a potential accumulator (excluder, indicator, hyperaccumulator). Examples of the expected behavior of plants in each scenario are shown in Fig. 1. For high metal concentrations, the plant will reach such a saturation level that a constant concentration value will be observed in the plant in all cases. The term concentration saturation will be used when the plant cannot translocate more metals to the leaves. This analysis shows that a plant cannot be categorized as an excluder, indicator, accumulator, or hyperaccumulator of a given metal since this will depend on the concentration of the environment.

As discussed by Azlan et al. (2014) and Kamari et al. (2014), BCF is a measure of a plant's ability to accumulate metals from the soil. According to Baker (1981) and Rezvani and Zaefarian (2011), the following criteria must be considered: if $BCF < 1$, the plant is an excluder; if $1 < BCF < 10$, the plant is an accumulator; and if $BCF > 10$, the plant is a hyperaccumulator. Plants with a BCF value > 1 are suitable for phytoextraction (Kamari et al., 2012, 2014).

This paper presents a BCF mathematical model, which depends on substrate metal concentration. Coefficients were estimated by using a metal concentration database in the phytoremediation processes of different types of soils: experimental at the lab, industrial-mining, and agricultural. These soils consider a wide range of concentrations for the heavy metals assessed. In addition, the database generated contained 257 vegetal species to develop new characteristic curves and, therefore, new criteria to categorize the plants. The new criteria proposed here are expected to be more reliable than the traditional criteria mentioned above since it considers the true substrate concentrations.

In particular, the aim of this paper is to develop a characteristic curve of Cu, Fe, Pb, and Zn concentrations in substrates and plants. To do this, experimental data were analyzed from different bibliographic sources related to experimental, agricultural, industrial, and mining soils subjected to phytoremediation processes. We note that the set of analyzed metals was chosen because of their environmental significance in contaminated soils and the availability of data in the reviewed articles. There are other potentially relevant elements, such as Cd and As, but there were not enough data in the reviewed articles to construct a statistically significant model for these elements.

Materials and methods

Experimental data

Experimental data corresponding to 1288 final concentration measurements of soils and plants subjected to phytoremediation processes were collected. These experimental points were taken from different bibliographic sources and correspond to 257 vegetal species planted in contaminated sites, categorized as mining, industrial, experimental at the lab, and agricultural by the corresponding authors. All of the plant concentrations used in this work are based on root concentrations. Table 1 shows a summary of the data used in this paper.

In Table 1, N is the amount of experimental data used, $\Delta C_{F\text{-}Soil}$ is the final concentration range of metal in the soil, and $\Delta C_{F\text{-}Plant}$ is the final concentration range of metal in the plant root. Plant concentrations shown in Table 1 correspond to those reported in the different bibliographic sources based on root concentration values.

We note that in most of the reviewed articles, the initial soil concentration value is not indicated. We note that the initial soil concentration would be useful information in general, as this information could

Table 1 Cu, Fe, Pb, and Zn concentrations of 257 vegetal species

Metal	N	$\Delta C_{F\text{-}Soil}$ mg/kg	$\Delta C_{F\text{-}Plant}$ (Root) mg/kg	Soil origin	N° species
Cu	402	0.6–190,800	0.421–40,800	a,b,c,d	246
Fe	125	10.83–308,500	0.39–51,800	a,b,c,d	60
Pb	377	0.084–1,113,000	0.03–20,250	a,b,c,d	239
Zn	384	1.65–46,500	0.01–9,900	a,b,c,d	243

a Mining, *b* industrial, *c* experimental at the lab, *d* agricultural be used to determine whether intervention is required to begin with. However, since most of the reviewed works did not include this information, the proposed model only uses final soil concentrations and plant (root) concentrations. This approach ensures that the model works with most of the available data. However, it should be noted that it might be possible to develop an improved model if sufficient data with initial soil concentrations were available.

Table A in online appendix shows the names of the species, gender, and family of the metals assessed, totaling 257 species belonging to 200 genders and 83 families.

Characteristic curve

This paper defines a model describing the behavior of characteristic curves that relate the final soil concentration to the final root concentration in a phytoremediation process.

These characteristic curves describe the average behavior of different plant species in various scenarios. Particularly, characteristic curves for different types of metals and species categories are considered: excluder, indicator, accumulator, and hyperaccumulator. This categorization is specific for the plant, regardless of the environment.

To define the different accumulation capacities between species, a curve properly representing the behavior of low and high heavy metal concentrations must be found. These curves are used for determining whether a species is an excluder, indicator, accumulator, or hyperaccumulator. Particularly, if the results for a species lie below the excluder curve, it is considered an excluder. If the results lie between the excluder and accumulator curves, it is considered an indicator, the indicator curve being only a reference. If the results lie between the accumulator and hyperaccumulator curves, it is considered an accumulator. If the results lie over the hyperaccumulator curve, it is considered a hyperaccumulator.

Let $[]_{\mathrm{root}}$ be the final concentration of the metal of interest in the plant root and $[]_{\mathrm{soil}}$ be the final concentration of the metal of interest in the soil. The characteristic curve describing the relationship between these terms should have the following characteristics:

- All the curves should be positive and begin at the origin.
- For low concentrations, the hyperaccumulator curve should be similar to the straight line of reference $[]_{\mathrm{root}} = 10[]_{\mathrm{soil}}$ (BCF = 10).
- For low concentrations, the accumulator curve should be similar to the straight line of reference $[]_{\mathrm{root}} = []_{\mathrm{soil}}$ (BCF = 1).
- For high concentrations, the hyperaccumulator and accumulator curves should take values lower than their corresponding straight lines of reference.
- For extremely high values, all the curves should tend to zero, assuming that the conditions are not adequate for plant survival.

A relationship is defined between the natural logarithm of BCF $\left[\frac{[]_{\mathrm{root}}}{[]_{\mathrm{soil}}}\right]$ and a function particularly designed for the behavior described in the requirements above. In particular,

$$\ln\left(\frac{[]_{\mathrm{root}}}{[]_{\mathrm{soil}}}\right) = b_0 + b_t + b_m + b_1\sqrt{[]_{\mathrm{soil}}} + b_2\ln\left(\ln\left([]_{\mathrm{soil}} + 1\right) + 1\right), \text{ with } []_{\mathrm{soil}} \geq 0,$$

where b_0 is the basic growth rate of the curve (similar to the slope of a straight line), b_t is the species influence on the growth rate, and b_m is the influence of the target metal on the growth rate. In this case, two metal categories with similar behavior (Cu/Pb and Fe/Zn) are considered; b_1 is the influence of the square root term, and b_2 is the influence of the logarithmic compound term. This logarithmic term is adjusted for ensuring the absence of indefinite values, in the extreme case that $[]_{\mathrm{soil}} = 0$).

Note that b_1 must take negative values to meet the requirements previously determined. In practice, b_2 also takes a negative value when adjusting the curve with real data.

To interpret these coefficients, it is useful to make algebraic arrangements to clear $[]_{\mathrm{root}}$. So, the following function is obtained

$$[]_{\text{root}} = \underbrace{e^{b_0+b_i+b_m}[]_{\text{soil}}}_{(1)} \underbrace{e^{b_1\sqrt{[]_{\text{soil}}}}}_{(2)} \underbrace{\left(\ln\left([]_{\text{soil}}+1\right)+1\right)^{b_2}}_{(3)}, \text{ con } []_{\text{soil}} \geq 0. \quad (1)$$

Component (1) is a linear function factor and determines the growth of low concentration values. Note that $e^{b_0+b_i+b_m} > 0$ by definition of the exponential function. Thus, this component is never null. Component (2) is an exponential function factor, whose coefficient b_1 is negative, and determines its decrease for high concentration values. Component (3) is a logarithmic factor, whose exponent b_2 is negative. It is used for penalizing the function value, limiting the maximum value that could be reached in practice. In addition, it influences the function decay for high values.

Once these functions and their coefficients are defined, the statistical procedure for fitting data to these characteristic curves is described.

Linear model

To determine the values of the coefficients defined above, linear regression was used after making data changes to follow the model proposed by the characteristic curves previously defined. This process is described below. First, linear regression was made by intercepting the natural logarithm of BCF $\left[\ln\left(\frac{[]_{\text{root}}}{[]_{\text{soil}}}\right)\right]$ and the following variables:

- Square root of the final metal concentration in the soil $\left(\sqrt{[]_{\text{soil}}}\right)$.
- Compound logarithm displaced from the final metal concentration in the soil $\left(\ln(\ln\left([]_{\text{soil}}+1\right)+1\right)$.
- Type of metal (2 categories: Cu/Pb and Fe/Zn).
- Plant species: 257.

This linear fit shows a value of $R^2_{\text{adj}} = 0.665$ and a general p value of $9.76 \cdot 10^{-175}$. Nevertheless, most variables associated with the species are considered non-significant with $\alpha = 0.05$. Thus, the model must be simplified to keep only significant variables. Also, the base model provides specific data for each species, thus making it very complex and little useful in practice. Hence, changes must be made to the model in order to simplify it.

Since the objective is to find characteristic curves for the different species behaviors (e.g., accumulator), the species with similar behavior are grouped. To do this, the coefficient values associated with each species can be analyzed after fitting the baseline linear model.

Figure 2 shows the distribution of the coefficients associated with each species in the baseline linear model. The curve is similar to a normal distribution, with an average $\overline{b_{\text{specie}}} = 1.420$ and a standard deviation of $s_{\text{specie}} = 1.361$. However, between 2.5 and 3.5 and 4.5 and 6 approximately, there is a number of concentrated values greater than expected in a normal distribution. The difference is only observed on the right side of the distribution. This behavior is similar to p values reported in other studies, which usually accumulate near 0.05, further than expected (Perneger & Combescure, 2017) because publications usually show positive results; in this case, accumulator species in the range 2.5–3.5 and hyperaccumulators in the range 4.5–6.

Considering the cut points empirically observed (about 2.5 for accumulators and 4.5 for hyperaccumulators), an auxiliary indicator variable "Type of species" is defined, according to the following criteria:

- "Type of species" is classified as a hyperaccumulator if the coefficient associated with the sample species is over 4.14 ($\overline{b_{\text{specie}}} + 2 \cdot s_{\text{specie}}$).
- "Type of species" is classified as an accumulator if the coefficient associated with the sample species lies between 2.44 and 4.14 (from $\overline{b_{\text{specie}}} + 0.75 \cdot s_{\text{specie}}$ to $\overline{b_{\text{specie}}} + 2 \cdot s_{\text{specie}}$).
- "Type of species" is classified as an indicator if the coefficient associated with the sample species lies between 0.40 and 2.44 ($\overline{b_{\text{specie}}} \pm 0.75 \cdot s_{\text{specie}}$).
- "Type of species" is classified as an excluder if the coefficient associated with the sample species is lower than 0.4 ($\overline{b_{\text{specie}}} - 0.75 \cdot s_{\text{specie}}$).

These values are in line with the high-frequency sectors shown in Fig. 2. This new variable is used for replacing the variable indicating the specific plant species. In using this variable, a linear model is constructed in the same way as before.

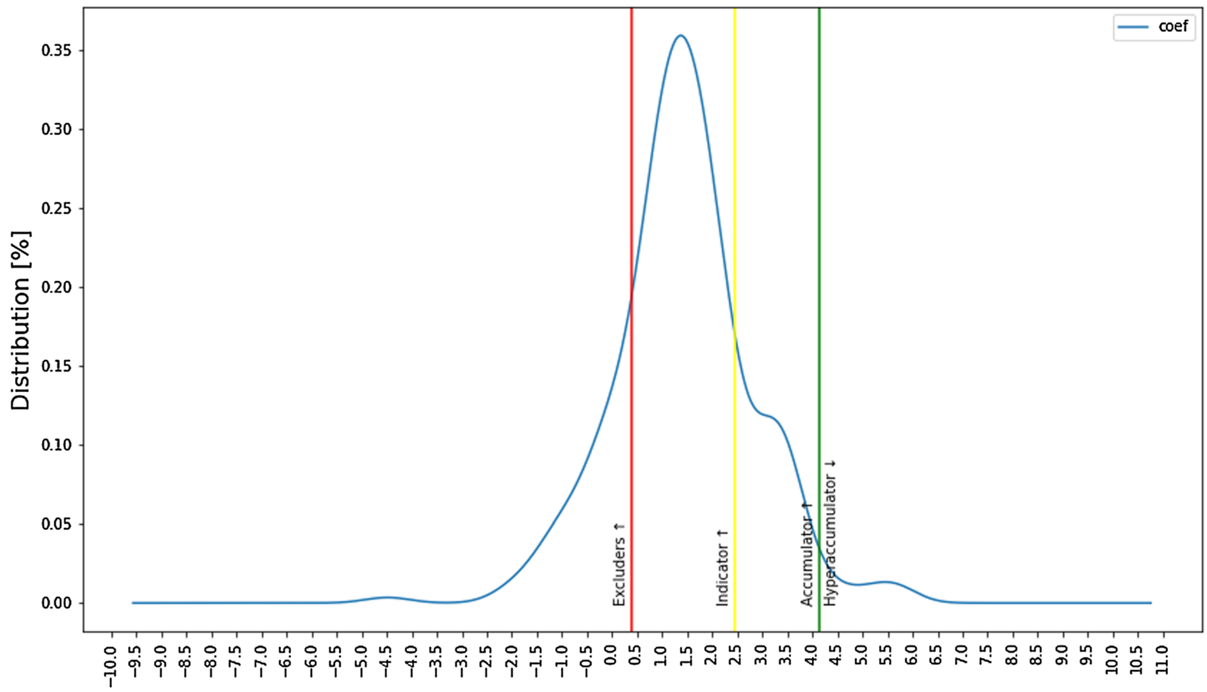

Fig. 2 Coefficients associated with plant species in the baseline linear model. Lines show the threshold associated with each type of species

Table 2 Final linear model coefficients, using root concentration data

Coefficients	Value	*p*-value
Intercept (b_0)	2.8464	<0.001
Type of species (b_t)—Excluder	-1.5607	<0.001
Type of species (b_t)—Indicator	0	N/A (Baseline)
Type of species (b_t)—Accumulator	1.9338	<0.001
Type of species (b_t)—Hyperaccumulator	3.8239	<0.001
Metal (b_m)—Cu/Pb	0	N/A (Baseline)
Metal (b_m)—Fe/Zn	0.5093	<0.001
Coefficient $\sqrt{[]_{soil}}$ (b_1)	-0.0035	<0.001
Coefficient $\ln(\ln\left([]_{soil}+1\right)+1$ (b_2)	-2.1090	<0.001

Results

Characteristic curves

This section shows the resulting curves. Results are exemplified for Cu and Pb, based on root concentration.

The model has $R^2_{adj}=0.664$. There were practically no losses of R^2_{adj} in grouping the species. The F value of the model is 424.4, with a p value of $3.23\cdot10^{-300}$. Table 2 shows the coefficients and their associated p values.

Table 2 shows that indicator species were determined as the baseline for the type of species and Cu and Pb as the baseline for the types of metals. So, their associated coefficients equal zero. Figure 3 shows the characteristic curves of Cu and Pb for high concentrations. The indicator and excluder curves are practically indistinguishable from the Y-axis.

We note that in the case of Fe and Zn, it would be sufficient to add the coefficient corresponding to the metals as shown in Table 2 (approximately 0.5). Using the Fe/Zn parameter in the model would shift the curves up and change the scales, but the overall behavior of the curves would remain the same. Thus, the general descriptions of Figs. 3, 4, 5,and 6, which contain the Cu/Pb curves, would also be applicable to the Fe/Zn curves.

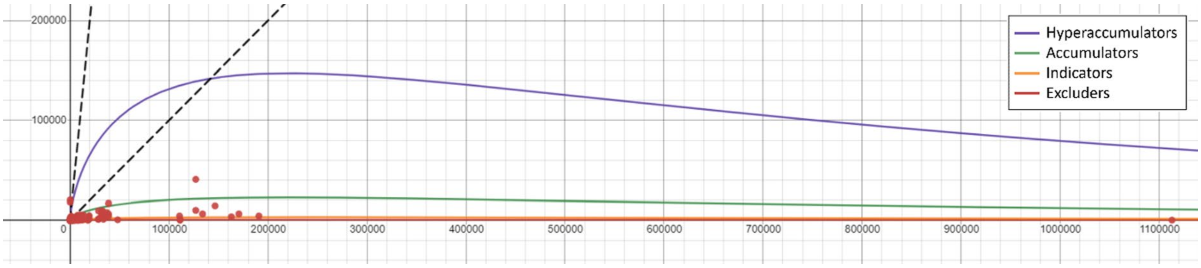

Fig. 3 Characteristic curves of high concentrations. The X-axis is the final soil concentration [mg/kg], and the Y-axis is the final plant concentration [mg/kg]. The dashed lines represent the traditional criteria of BCF > 1 and BCF > 10. The dots represent the samples used for constructing the model

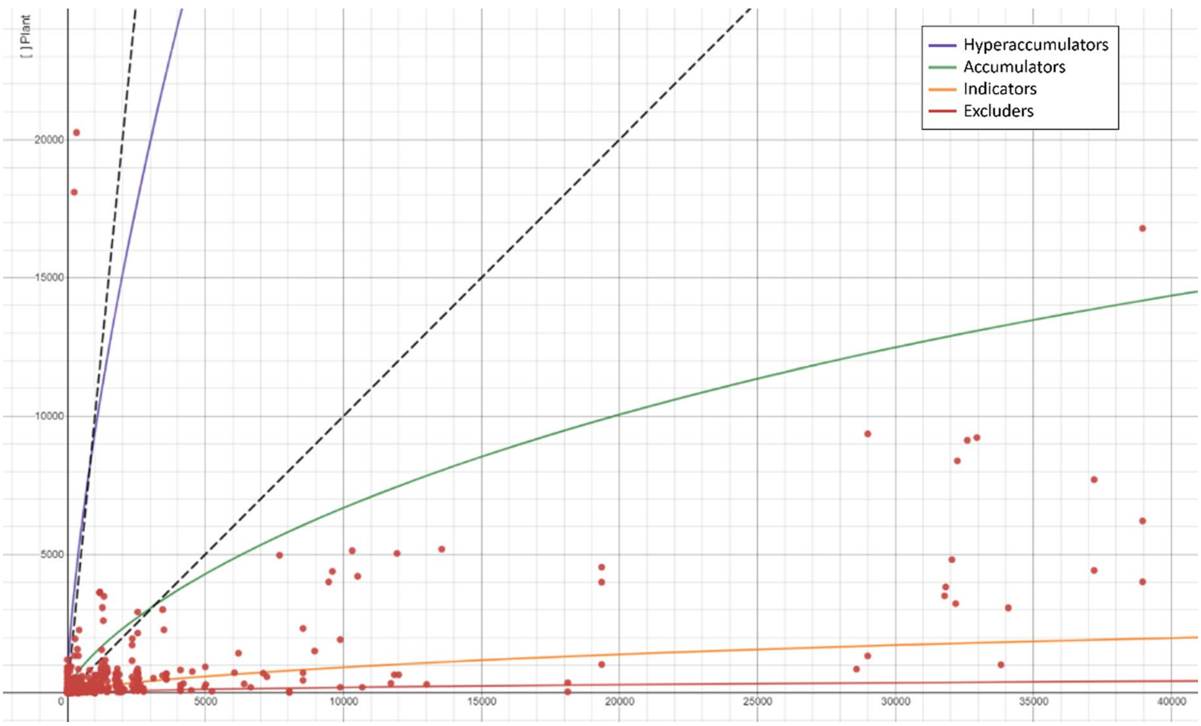

Fig. 4 Characteristic curves of moderately high concentrations. The X-axis represents the final soil concentration, while the Y-axis represents the final plant concentration [mg/kg]. The dashed lines represent the traditional criteria of BCF > 1 and BCF > 10. The dots represent the samples used for constructing the model

Figure 4 shows the characteristic curves of moderately high concentrations. The hyperaccumulator curve is relatively similar to the corresponding straight line of reference. The accumulator curve behaves similarly to its reference line at the beginning, but it increases much more slowly afterward.

Figure 5 shows the characteristic curves of moderately low concentrations. The accumulator and hyperaccumulator curves are more demanding than their straight lines of reference in moderately low concentrations. The indicator curve represents the general average plant behavior, while the excluder curve shows the plants with a very bad performance as compared to the others.

Figure 6 shows the characteristic curves of low concentrations. The hyperaccumulator curve is undistinguishable from the Y-axis, while the accumulator curve is more similar to the straight line

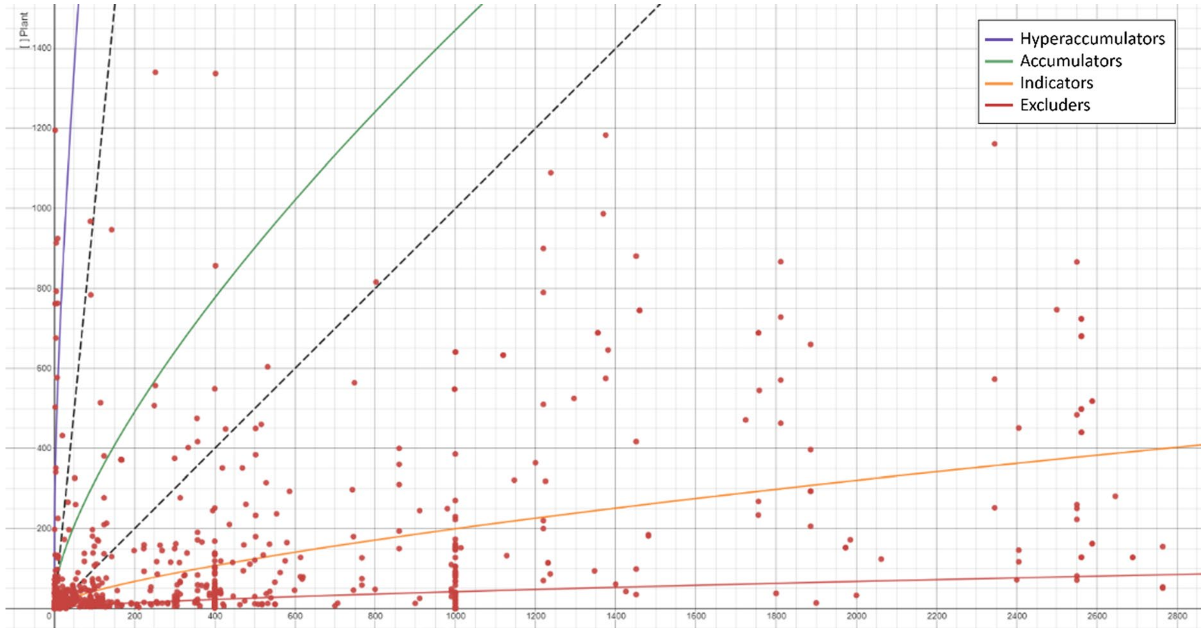

Fig. 5 Characteristic curves of moderately low concentrations. The X-axis represents the final soil concentration [mg/kg], and the Y-axis represents the final plant concentration [mg/kg]. The dashed lines represent the traditional criteria of BCF > 1 and BCF > 10. The dots represent the samples used for constructing the model

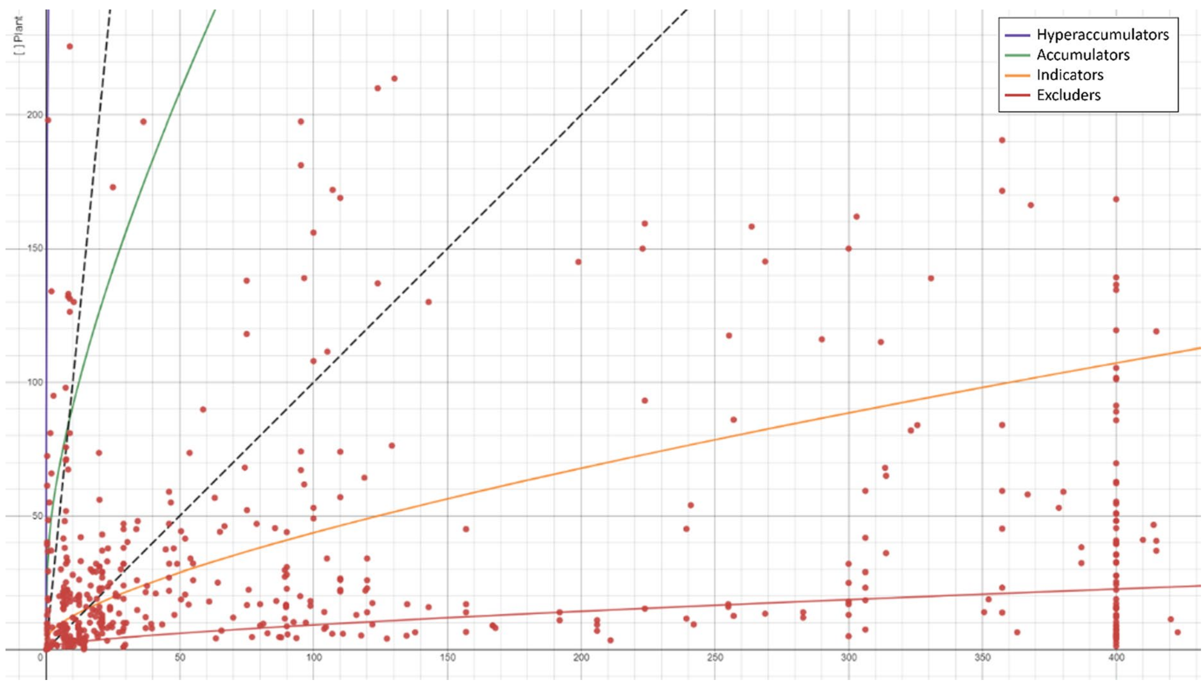

Fig. 6 Characteristic curves for low concentrations. The X-axis represents the final soil concentrations [mg/kg], while the Y-axis represents the final plant concentration [mg/kg]. The dashed lines represent the traditional criteria of BCF > 1 and BCF > 10. The dots represent the samples used for constructing the model

Table 3 Sample assessment of *Triticum aestivum* (Migueláñez, 2014), using the model proposed here

Metal	Sample $[]_{soil}$ mg/kg	Sample $[]_{root}$	Predicted indicator $[]_{root}$	Predicted accumulator $[]_{root}$	Predicted hyperaccumulator $[]_{root}$	Result
Pb	2.06	1195	7.25	50.14	331.90	Hyperaccumulator
Pb	4.62	914	9.53	65.88	436.13	Hyperaccumulator
Pb	802.36	816	169.52	1172.33	7760.89	Indicator
Pb	8.34	763	11.96	82.73	547.67	Hyperaccumulator
Pb	0.42	12.9	3.83	26.48	175.32	Indicator
Pb	2.06	1195	7.25	50.14	331.90	Hyperaccumulator

of reference for hyperaccumulators than that of accumulators. Thus, for low concentrations, the described model is stricter than the reference lines (BCF > 1 and BCF > 10), but it is more lenient for higher values.

Example of use

To exemplify how these curves could be used in practice, let's consider the experimental results of the 6 *Triticum aestivum* samples with Pb from Migueláñez (2014), shown in Table 3. Their viability as accumulators or hyperaccumulators is studied, according to the criteria established by the model proposed here. Equation (1) and the coefficients in Table 2 are used for each plant category. Table 3 shows the results obtained for predicted values, using the coefficients of the indicator, accumulator, and hyperaccumulator species. Then, these values are compared with the values of the "Sample $[]_{\text{root}}$" column. For the first example, 1195 mg/kg in the "Sample $[]_{\text{root}}$" column is greater than the predicted hyperaccumulator $[]_{\text{root}}$331.91 mg/kg. So, *Triticum aestivum* is classified as a Pb potential accumulator.

Table 3 shows that the plant species behaves as a hyperaccumulator in most samples. Therefore, it could be considered a hyperaccumulator. Additionally, the conditions promoting this specific behavior could be assessed.

If compared with the results of the conventional criterion, 5 of the 6 samples show a value of BCF > 10. Hence, they would be categorized as a Pb hyperaccumulator species, whereas one of the samples (802.36 mg/kg soil concentration) shows a BCF value between 1 and 10, classifying the plant as an accumulator of this heavy metal. The resulting criterion after applying the model proposed here classifies the plant as an indicator. The results obtained with the model proposed are coherent with the results obtained from conventional criteria.

As an additional example, let's consider the two following *Gentiana pennelliana* samples with Pb and Cu from Yoon et al. (2006), shown in Table 4.

According to the traditional criterion, these samples would be considered hyperaccumulators because BCF is greater than 10. However, using the model proposed in this study, they would only correspond to accumulators because the soil concentration is low and, therefore, the traditional criteria would overestimate the plant species capacity under these conditions. Instead, the model proposed is more demanding, as shown by the values predicted for each characteristic curve.

Table 4 Partial assessment of *Gentiana pennelliana* samples from Yoon et al. (2006), using the model proposed here

Metal	Sample $[]_{soil}$ mg/kg	Sample $[]_{root}$	Predicted indicator $[]_{root}$	Predicted accumulator $[]_{root}$	Predicted hyperaccumulator $[]_{root}$	Result
Pb	90	968	41.00	283.53	1877.00	Accumulator
Cu	20	432	17.80	123.13	815.12	Accumulator

Table 5 Partial assessment of *Bidens triplinervia* and *Plantago orbignyana* from Durán Cuevas et al. using the model proposed here

Metal	Sample $[]_{soil}$	Sample $[]_{root}$	Predicted indicator $[]_{root}$	Predicted accumulator $[]_{root}$	Predicted hyperaccumulator $[]_{root}$	Result
	mg/kg					
Fe	79,728	31,120	4287.25	29,649.52	196,280.74	Accumulator
Zn	30,656	3144	2846.54	19,685.91	130,321.32	Indicator

Finally, let's consider an example with Fe using a *Bidens triplinervia* sample and a *Plantago orbignyana* sample, shown in Table 5.

According to the traditional criterion, these samples would be considered excluders, as the BCF value is low (roughly 0.4 and 0.1 for the Fe and Zn samples, respectively). However, using the model proposed in this study, the *Bidens triplinervia* sample would actually be considered an accumulator, and the *Plantago orbignyana* sample would be considered an indicator. Thus, in both cases, the results differ from the traditional model because the soil concentrations are high and, therefore, the traditional criteria would underestimate the plant species' capacity under these conditions. Instead, the model provides a more lenient evaluation in cases where concentrations are high, as shown by the values predicted for each characteristic curve.

Species classification

Based on the plant species grouped for defining the characteristic curves, a rough classification of the species corresponding to each type can be made, using the criteria proposed in this article. Only accumulator and hyperaccumulator species are shown in Table 6.

These species could be further assessed in future studies to validate their accumulator properties, particularly those the model categorizes as hyperaccumulators. The model excludes additional treatments and other special conditions that may influence the results of the final concentration. So, there may be other factors influencing these results and species classification, e.g., amendment-assisted phytoremediation, use of chelates, and others involved in the process.

Limitations of the model

One of the limitations of the model is that only the final concentrations are considered, not the initial ones. A more powerful model would include initial and final concentrations to determine the accumulation capacity of a plant species. However, given the BCF definition used in the literature and how the papers of reference report their results (i.e., final concentration values), a model was constructed considering only final values. Lastly, the model is based on the average behavior of multiple species and the assumption of normal behavior among them. In addition, it does not consider other conditions (e.g., other plant treatments). Initially, the type of soil assessed (industrial, agricultural, experimental at the lab, and mining) was considered. Later, the analysis of the resulting linear model showed that these data were redundant. Finally, the model would be initially valid for different concentrations ranges of Cu (0.6–190,800 mg/kg), Fe (10.83–308,500 mg/kg), Pb (0.084–113,000 mg/kg), and Zn (1.65–46,500 mg/kg). Using the model outside these ranges would yield invalid results. However, since these ranges and the model itself are based on a diverse set of experimental data, this should not be a limitation for most applications of the model.

Conclusions

This study proposes a model for classifying plant species into indicators, excluders, accumulators, and hyperaccumulators in the context of soil treatment through phytoremediation, using characteristic curves obtained from empirical data. The characteristic curves are constructed from a linear model relating BCF natural logarithm to soil concentration, expressed through a square root and a compound logarithm term, and the type of metal and plant. The

Table 6 Accumulators and hyperaccumulator species, according to their initial grouping in the base model for characteristic curves. The classification using the conventional BCF criteria is represented using yellow (BCF < 1, excluder or indicator), green (1 < BCF < 10, accumulator), and blue (BCF ≥ 10, hyperaccumulator)

Accumulators			Hyperaccumulators
Achillea tenuifolia[3]	*Eryngium campestre*[3]	*Plantago amplexicaulis*[3]	*Cardaria draba*[3]
Amaranthus dubius[1,3]	*Euphorbia hirta*[4]	*Portulaca oleracea*[1]	*Centaurea virgata*[1]
Arthronemun macrostachyum[1]	*Euphorbia macroclada*[1]	*Pteropyrum aucheri*[3]	*Cistus ladanifer*[4]
Bidens alba[3]	*Euphorbia macroclada*[2]	*Raphanussativus*[1,4]	*Cynachum tubulosum*[3]
Bidens triplinervia[2]	*Gentiana pennellian*[1,3]	*Reseda lutea*[3]	*Deschampsia cespitosa*[2]
Carduus tenuiflorus[3]	*Gomphrena celosioides*[3]	*Scoparia dulcis*[3]	*Euphorbia hirta*[3]
Casuarina equisetifolia[1]	*Hedychium coronarium*[3]	*Scrophularia scoparia*[1]	*Lolium strictum*[3]
Chloris radiata[3,4]	*Helianthus annuus*[1]	*Senecio sp*[3]	*Scrophularia scoparia*[3]
Cortaderia rudiuscula[4]	*Hibiscus nicranthus*[3]	*Setaria liebmannii*[3]	*Triticum aestivum*[3]
Cucurbita moschata[4]	*Indigofera cuneata*[3]	*Solanum nigrum*[1]	*Zea mays*[2]
Cynachum tubulosum[4]	*Hyptis alata*[3]	*Solanum torvum*[3]	
Cyperus luzulae[3]	*Juncus arcticus*[1,4]	*Steinchisma laxum*[3]	
Cyperu sodorantus[1]	*Lactuca sativa*[3]	*Tamarix ramosissima*[1,3]	
Dactylis glomerata[3]	*Medicago sativa*[2]	*Thelypteris sp*[3]	
Deschampsia cespitosa[1]	*Mimosa púdica*[3]	*Thymus mastichina*[3,4]	
Digitaria sanguinalis[2,3,4]	*Oldenlandia sp*[3]	*Thymus zygis*[3]	
Echinochloa colona[3]	*Papaver rhoeas*[3]	*Tripogandra serrulate*[3]	
Eleusine indica[3]	*Paspalum conjugatum*[3]	*Verbena sp*[3]	
Equisetum fluviatile[1,4]	*Peganum harmala*[3]	*Xanthium strumarium*[1]	
Eragrostis aethiopica[3,4]	*Pinus spp*[1]	*Zea mays*[4]	

[1]Cu, [2]Fe, [3]Pb, [4]Zn

model has some limitations, mainly because it does not consider the initial metal concentration in the substrate. In addition, behavior is based on the average behavior of multiple species and the assumption of normal behavior. Despite these limitations, the model shows a good performance. Particularly, the final model shows a 0.664 R^2 determination coefficient and all the variables used are regarded as significant. Therefore, this model can be used for assessing several samples from a specific plant to determine its potential as an accumulator in soil treatment through phytoremediation. The model construction shows that 60 out of the 257 species assessed have a potential behavior as accumulators and 10 of them as hyperaccumulators (Table 5).

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References

Adriano, D. C. (2001). *Trace elements in terrestrial environments: Biogeochemistry, bioavailability and risks of metals*. Springer.

Ashaiekh, M. A., Eltayeb, M. A., Ali, A. H., Ebrahim, A. M., Salih, I., & Idris, A. M. (2019). Spatial distribution of total and bioavailable heavy metal contents in soil from agricultural, residential, and industrial areas in Sudan. *Toxin Reviews, 38*(2), 93–105.

Azlan, K., Norjan, Y., Che Fauziah, I., Esther, P., Galuh, Y., (2014). The effects of micro-and nanohydroxyapatite application in metal contaminated soil on metal accumulation in Ipomoea aquatica and soil metal bioavailability. In: Proceeding of International Conference on Research, Implementation and Education of Mathematics and Sciences 2014 Yogyakarta State University.

Baker, A. J. (1981). Accumulators and excluders-strategies in the response of plants to heavy metals. *Journal of Plant Nutrition, 3*(1–4), 643–654.

Baker, A. J. M., & Brooks, R. R. (1989). Terrestrial higher plants that hyperaccumulate metallic elements—a review of their distribution ecology and phytochemistry. *Biorecovery, 1*, 81–126.

Baker, A. J., McGrath, S. P., Reeves, R. D., & Smith, J. A. C. (2020). Metal hyperaccumulator plants: a review of the ecology and physiology of a biological resource for phytoremediation of metal-polluted soils. *Phytoremediation of contaminated soil and water* (pp. 85–107). CRC Press.

Brooks, R. R., Lee, J., Reeves, R. D., & Jaffré, T. (1977). Detection of nickeliferous rocks by analysis of herbarium specimens of indicator plants. *Journal of Geochemical Exploration, 7*, 49–57.

Carkovic, A. B., Calcagni, M. S., Vega, A. S., Coquery, M., Moya, P. M., Bonilla, C. A., & Pastén, P. A. (2016). Active and legacy mining in an arid urban environment: Challenges and perspectives for Copiapo, Northern Chile. *Environmental Geochemistry and Health, 38*, 1001–1014. https://doi.org/10.1007/s10653-016-9793-5

Chakraborty, S., Man, T., Paulette, L., Deb, S., Li, B., Weindorf, D. C., & Frazier, M. (2017). Rapid assessment of smelter/mining soil contamination via portable X-ray fluorescence spectrometry and indicator kriging. *Geoderma, 306*, 108–119. https://doi.org/10.1016/J.GEODERMA.2017.07.003

Chaney, R. L., Li, Y. M., Brown, S. L., Homer, F. A., Malik, M., Angle, J. S., & Chin, M. (2020). Improving metal hyperaccumulator wild plants to develop commercial phytoextraction systems: approaches and progress. *Phytoremediation of contaminated soil and water* (pp. 129–158). CRC Press.

Diwan, H., Ahmad, A., & Iqbal, M. (2008). Genotypic variation in the phytoremediation potential of Indian mustard for chromium. *Environmental Management, 41*(5), 734–741.

Gong, Y., Zhao, D., & Wang, Q. (2018). An overview of field-scale studies on remediation of soil contaminated with heavy metals and metalloids: Technical progress over the last decade. *Water Research, 147*, 440–460.

Hrynkiewicz, K., Złoch, M., Kowalkowski, T., Baum, C., & Buszewski, B. (2018). Efficiency of microbially assisted phytoremediation of heavy-metal contaminated soils. *Environmental Reviews, 26*(3), 316–332.

Kacholi, D. S., & Sahu, M. (2018). Levels and health risk assessment of heavy metals in soil, water, and vegetables of Dar es Salaam, Tanzania. Journal of Chemistry, 2018.

Kaewtubtim, P., Meeinkuirt, W., Seepom, S., & Pichtel, J. (2016). Heavy metal phytoremediation potential of plant species in a mangrove ecosystem in Pattani Bay, Thailand. *Applied Ecology and Environmental Research, 14*(1), 367–382.

Kamari, A., Pulford, I. D., & Hargreaves, J. S. J. (2012). Metal accumulation in Lolium perenne and Brassica napus as affected by application of chitosans. *International Journal of Phytoremediation, 14*(9), 894–907.

Kamari, A., Mohd Yusoff, S. N., Putra, W. P., Ishak, C. F., Hashim, N., Mohamed, A., & Phillip, E. (2014). Metal uptake in water spinach grown on contaminated soil amended with chicken manure and coconut tree sawdust. Environmental Engineering & Management Journal (EEMJ), 13(9).

Lam, E. J., Cánovas, M., Gálvez, M. E., Montofré, Í. L., Keith, B. F., & Faz, Á. (2017). Evaluation of the phytoremediation potential of native plants growing on a copper mine tailing in northern Chile. *Journal of Geochemical Exploration, 182*, 210–217.

Lam, E. J., Gálvez, M. E., Cánovas, M., Montofré, Í. L., & Keith, B. F. (2018). Assessment of the adaptive capacity of plant species in copper mine tailings in arid and semiarid environments. *Journal of Soils and Sediments, 18*(6), 2203–2216.

Lam, E. J., Montofré, I. L., Álvarez, F. A., Gaete, N. F., Poblete, D. A., & Rojas, R. J. (2020). Methodology to prioritize chilean tailings selection, according to their potential risks. *International Journal of Environmental Research and Public Health, 17*(11), 3948.

Mancini, L., & Sala, S. (2018). Social impact assessment in the mining sector: Review and comparison of indicators frameworks. *Resources Policy, 57*, 98–111.

Mganga, N., Manoko, M. L. K., & Rulangaranga, Z. K. (2011). Classification of plants according to their heavy metal content around North Mara gold mine, Tanzania: implication for phytoremediation. Tanzania Journal of Science, 37.

Migueláñez, V. O. (2014). Diagnóstico ambiental de suelos contaminados por actividades mineras y evaluación de técnicas de estabilización para su recuperación (Doctoral dissertation, Universidad de Salamanca).

Minguzzi, C., & Vergnano, O. (1948). II Contenuto di nichel nelle ceneri di Alyssum bertolonii. *Atti Societá Toscana Scienze Naturali, 55*, 49–74.

Montgomery, D. R. (2007). Soil erosion and agricultural sustainability. *Proceedings of the National Academy of Sciences USA, 104*, 13268–13272. Provides evidence from 201 different field studies globally that the soil-erosion rates in no-till agriculture is similar to soil-production rates and can be considered as a sustainable agricultural practice.

Perneger, T. V., & Combescure, C. (2017). The distribution of p-values in medical research articles suggested selective reporting associated with statistical significance. *Journal of Clinical Epidemiology, 87*, 70–77.

Raskin, I., Kumar, P. N., Dushenkov, S., & Salt, D. E. (1994). Bioconcentration of heavy metals by plants. *Current Opinion in Biotechnology, 5*(3), 285–290.

Rezvani, M., & Zaefarian, F. (2011). Bioaccumulation and translocation factors of cadmium and lead in'Aeluropus littoralis'. *Australian Journal of Agricultural Engineering, 2*(4), 114–119.

Sarma, H., Islam, N. F., Prasad, R., Prasad, M. N. V., Ma, L. Q., & Rinklebe, J. (2021). Enhancing phytoremediation of hazardous metal (loid) s using genome engineering CRISPR–Cas9 technology. *Journal of Hazardous Materials, 414*, 125493.

Tiwari, S., & Lata, C. (2018). Heavy metal stress, signaling, and tolerance due to plant-associated microbes: An overview. *Frontiers in Plant Science, 9*, 452.

Wei, Z., Van Le, Q., Peng, W., Yang, Y., Yang, H., Gu, H., & Sonne, C. (2021). A review on phytoremediation of contaminants in air, water and soil. *Journal of Hazardous Materials, 403*, 123658.

Yoon, J., Cao, X., Zhou, Q., & Ma, L. Q. (2006). Accumulation of Pb, Cu, and Zn in native plants growing on a contaminated Florida site. *Science of the Total Environment, 368*(2–3), 456–464.

Zwolak, A., Sarzyńska, M., Szpyrka, E., & Stawarczyk, K. (2019). Sources of soil pollution by heavy metals and their accumulation in vegetables: A review. *Water, Air, & Soil Pollution, 230*(7), 1–9.