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# An extension of the characteristic curve model of plant species behavior in heavy metal soils

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**Abstract** This article proposes a mathematical model to characterize phytoremediation processes in soils contaminated with heavy metals. In particular, the proposed model constructs characteristic curves for the concentrations of several metals (As, Cd, Cu, Fe, Pb, Sb, and Zn) in soils and plants based on the experimental data retrieved from several bibliographical sources comprising 305 vegetal species. The proposed model is an extension of previous models of characteristic curves in phytoremediation processes developed by Lam et al. for root measurements using the bioconcentration factor. However, the proposed model extends this approach to consider roots, as well as aerial parts and shoots of the plant, while at the same time providing a less complex mathematical formula compared to the original. The final model shows an adjusted R2 of 0.712, and all its parameters are considered statistically significant. The model may be used to assess samples from a given plant species to identify its potential as an accumulator in the context of soil phytoremediation processes. Furthermore, a simplified version of the model was constructed using an approximation to provide an easy-to-compute alternative that is valid for concentrations below 37,000 mg/kg. This simplified model shows results similar to the original model for concentrations below this threshold and it uses an adjusted factor defined as $[]_{plant}/\sqrt{[]_{soil}}$ that must be compared with a threshold depending on the metal, type of

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measurement, and target (e.g., accumulator or hyperaccumulator). The full model construction shows that 90 out of the 305 species assessed have a potential behavior as accumulators and 10 of them as hyperaccumulators. Finally, out of the 1405 experimental measurements, 1177 were shown to be accumulators or hyperaccumulators. In particular, 85% of the results coincide with the reported values, thus validating the proposed model.

**Keywords** Phytoremediation · Accumulation factor · Heavy metals · Soil pollution · Characteristic curves

## Introduction

Increased heavy metal concentration in different mediums, such as water and soil, is mainly due to anthropogenic industrial, mining, and agricultural activities (Lam et al. 2016; Samarghandi et al. 2007; Welch, 1995). There are several factors that must be considered when evaluating metal concentrations in the soil. In particular, most heavy metals tend to be more mobile and, therefore, are more available at acid pH, except for arsenic, molybdenum, and chromium, which are more available at alkaline pH (Lam et al. 2017, 2018). On the contrary, at basic pH, metals are slightly mobile in soils and tend to accumulate on the surface, the most biologically active horizon, thus increasing vegetal accessibility. Additionally, the composition of primary minerals must be considered, as it conditions the chemical composition of the soil (Kabata-Pendias, 1993; Mile & Mitkova, 2012; Nyandat, 1980). Moreover, the presence of soluble and active heavy metal forms (Alloway, 1995; Moral et al. 2005; Nelson et al. 1981) must also be considered in the evaluation process.

High metal and metalloid concentrations in soils create potential risks (Kumar et al. 2019; Lam et al. 2022). In general, heavy metals are toxic for human beings and cumulative, i.e., they cannot be eliminated by the body, making their presence in the environment even worse (Cao et al. 2021; Jaishankar et al. 2014; Kaur et al. 2018). Unlike organic wastes, heavy metals do not degrade, making their elimination more difficult (Lam et al. 2022; Singh et al. 2011; Yao et al. 2012).

Some plant species have developed physiological and biochemical mechanisms that minimize the harmful effects of some substances, such as heavy metals (Lasat, 2002; Zhang et al. 2006). In particular, some species accumulate metals in the rhizosphere or perform translocation to different vegetal organs (Salt et al. 1994; Susarla et al. 2002; Tangahu et al. 2011). In this way, a technology known as phytoremediation was born. Phytoremediation is defined as a group of strategies that use vegetal species and their associated mechanisms to extract, accumulate, immobilize or transform environmental contaminants (Poschenrieder and Coll, 2003; Ghosh y Singh, 2005; Pilon-Smits, 2005). It can be used in water, soil, and air with heavy metal contents. This technology has become particularly interesting due to its cost-effectiveness and ability to be used in situ (Abou-Shanab et al. 2011, Alaboudi et al. 2018).

Phytoremediation can be mainly applied in contaminated water and soil (Lam et al. 2018; Wei et al. 2021). In soils contaminated with heavy metals, the use of plants helps accumulate or immobilize these potentially toxic substances (Simiele et al. 2020). As a whole, heavy metals at high concentrations have highly toxic effects, being considered potential environmental pollutants (Page et al. 1982). Two strategies used by plants to remove heavy metals from the soil have been identified: phytoextraction and phytostabilization (Alaboudi et al. 2018; Egendorf et al. 2020) and, to a lesser extent, phytovolatilization (Awa & Hadibarata, 2020; Khalid et al. 2017; Yao et al. 2012).

Plants growing in metalliferous soils have developed physiological and biochemical mechanisms to minimize toxic effects caused by metals (Ahemad, 2019; McIntyre, 2003). For example, they use mechanisms for controlling accumulation in roots and metal translocation to different vegetal organisms. Plants use strategies to face metals, either through exclusion or sequestering with chelating agents (Evangelou et al. 2007; Kazakou et al. 2008) or by controlling metal entrance to the root and its translocation (Thakur et al. 2016).

Baker (1981) classified plants for the first time, based on their strategies to capture and transport metals from the soil to the plant. Considering $C_{leaf}/C_{root}$ ratio, he categorized them as accumulators and excluders. Then, Baker and Walker (1990) proposed a new classification: metal excluders and non-excluders, excluders being plants limiting metal concentration in shoots. Later, concentration limits for other metals such as Zn, Mn, and Cd were introduced to categorize these plants (Baker & Walker, 1990; Pollard et al. 2014). According to Pollard et al. (2014), hyperaccumulator species can be regarded only as one subset of a larger metal-tolerant plant category. However, the exact relationship between metal tolerance and metal hyperaccumulation has not been fully solved (Masarovičová et al. 2010). Plants may be categorized according to the extent of metal capture and transport from the soil to the plant. Thus, species behave as excluders, indicators, accumulators, or hyperaccumulators (Massoura et al. 2004; Tognacchini et al. 2020). Determining if a species is potentially a hyperaccumulator requires reliable indicators and criteria.

Among these indicators is the accumulation factor defined as$AF = \frac{[]_{leaf}}{[]_{soil}}$, (Baker et al. 1994), later reported as$\frac{[]_{shoot}}{[]_{root}}$, (Fitz and Wenzel, 2002) and as$\frac{[]_{plant}}{[]_{soil}}$, (Kumar et al. 2009; Selvaraj et al. 2013; Ghosh & Singh, 2005; Yoon et al. 2006).

AF is an important indicator to select species for phytoextraction processes (Sakakibara et al. 2010). The definition of indicators depends on the author. In addition, experimental phytoremediation data available in the literature are diverse. Some authors provide experimental data on metal concentrations measured in the aerial/shoot tissues (Alaboudi et al. 2018; Nazir et al. 2011; Yoon et al. 2006). Others refer to concentrations in roots (Nazir et al. 2011; Yoon et al. 2006) and still others to those in leaves (Salazar & Pignata, 2014; Willscheret al. 2017).

Metal phytoextraction efficiency largely depends on the translocation of large amounts of metal assimilated by the roots to the harvestable parts of the plant (Zayed & Terry, 2003). According to Yoon et al. (2006), for species to be considered suitable for phytoremediation, AF must be greater than 1 (Usman et al. 2019). Hyperaccumulators have AF greater than 1, sometimes reaching 50–100 (Cluis, 2004). However, high metal concentrations in soil could result in AF < 1 (Ali et al. 2013). AF > 1 indicates that the plant can be subjected to phytostabilization, i.e., contaminant mobility within the non-saturated (vadose) zone is reduced by the accumulation of roots or immobilization within the rhizosphere, thus reducing soil contamination (Bolan et al. 2011).

This paper proposes a mathematical model based on empirical data and generates a formula that can be used as an indicator in the phytoremediation of soils containing heavy metals. Furthermore, an approximate heuristic using a new factor definition based on the empirical model is provided for lower concentrations. The proposal in this article is an extension of the model developed by Lam et al. (2022), originally restricted to modeling the metal concentration in the root of the plant, based on the final metal concentration in the soil in a phytoremediation process. Instead, the extended model considers not only the root of the plant but also measurements in shoots, reducing the complexity of the original model and achieving similar results. This paper aims to develop a new characteristic curve model for the concentrations of several metals (As, Cd, Cu, Fe, Pb, Sb, and Zn) in soils and plants, based on experimental data from several bibliographical sources. The model coefficients proposed were estimated empirically, using a database of metal concentrations in phytoremediation processes for different types of soils, including experimental soils in a laboratory, and mining, industrial, and agricultural soils. This diverse set of soil samples allowed the development of a model for handling a wide range of metal concentrations. Furthermore, the database includes 305 vegetal species, which allowed generating new characteristic curves and criteria to classify phytoremediation strategies. Finally, an even simpler criterion is proposed using some approximations. This secondary criterion can be used in lower concentrations and could provide data from many contexts.

## Materials and methods

### Experimental data

The model was constructed using an experimental data set containing 2,678 experimental points. These data points correspond to the final concentration measurements of metals in soils and plants from different species subjected to phytoremediation processes. In particular, the data contain concentrations of As, Cd, Cu, Fe, Pb, Sb, and Zn in the soil and from the root or shoot of the plants. These experimental values were taken from different bibliographic sources and are an extended version of the data set used by Lam et al. (2022), which only considered root-level data. The database includes 305 different plant species and is categorized by the type of soil (mining, industrial, laboratory, and agricultural). Table 1 shows a summary of this database.

In Table 1, N represents the amount of experimental data, $\Delta C_{F\text{-soil}}$ represents the final soil concentration ranges of each metal, $\Delta C_{F\text{-root}}$, and $\Delta C_{F\text{-shoot}}$ represents the final concentration ranges of each metal in the plant (either in the root or shoot). The concentrations shown in Table 1 correspond to the values reported by the different bibliographic sources referenced in this work. In most cases, the original sources do not provide the initial soil concentration value. Thus, the proposed model does not consider this value in the analysis.

Table A1 in Appendix A presents all the plant species used in this work in more detail for the different metals that were analyzed with this model (As, Cu, Cd, Fe, Pb, Sb, and Zn). In total, there are 305 species belonging to 220 genders and 101 families.

## Characteristic curves

This paper proposes a new mathematical model to describe the behavior of the final metal concentration in a plant following a phytoremediation process. In particular, the model is used to define a series of characteristic curves to model the phytostabilization capabilities of the plant species and classify them into four different categories: excluder, indicator, accumulator, and hyperaccumulator species.

In the literature, this categorization is usually specific to the plant species, regardless of the environmental conditions. However, Lam et al. (2022) reported a recent effort to develop a condition-dependent model that considers the environmental concentration levels. Thus, under this new paradigm, plant species would be considered as hyperaccumulators or accumulators for certain environmental conditions, rather than this being an intrinsic property of the plant species, as it does not only depend on it, but rather on its environment and the species.

In practice, a curve accurately representing the behavior of different species in low and high heavy metal concentrations is useful for scientists and practitioners to figure out whether a species is an excluder, indicator, accumulator, or hyperaccumulator. Following Lam et al. (2022), a plant species is considered an excluder if the experimental results for the species are below the excluder characteristic curve. The species is considered an indicator if it falls between excluder and accumulator curves, the indicator curve being used only for reference. The species is considered an accumulator if the results surpass the accumulator curve, but not the hyperaccumulator curve. The species is defined as a hyperaccumulator if the results surpass the hyperaccumulator curve.

As noted by Lam et al. (2022), the characteristic curves must meet some mathematical conditions to adequately model the behavior of plant species in different environments. In particular, let $[]_{plant}$ the final concentration of the metal of interest in the plant (either in the shoot or roots), and $[]_{soil}$ the final concentration of the metal of interest in the soil. The model must conform to the following constraints:

- Curves must be non-negative and include the point (0, 0).
- For low soil concentrations, the accumulator and hyperaccumulator curves should be stricter than the basic reference line (i.e., $[]_{plant} = []_{soil}$). This implies higher requirements to be classified as an accumulator or hyperaccumulator when concentrations are low.

**Table 1** As, Cu, Fe, Pb, Sb, and Zn concentrations of 305 vegetal species

| Metal | N | $\Delta C_{F\text{-soil}}$ mg/kg | $\Delta C_{F\text{-root}}$ mg/kg | $\Delta C_{F\text{-shoot}}$ mg/kg | Soil Type | N° of species |
|---|---|---|---|---|---|---|
| As | 6 | 33.75–2,860 | – | 27.0–1,430 | a | 6 |
| Cu | 814 | 3.638–190,80 | 0.421–40,800 | 0.059–7,600 | a,b,c,d | 214 |
| Cd | 75 | 0.15–32.1 | 0.1–44.4 | 0.1–53.2 | a | 13 |
| Fe | 250 | 6.83–308,500 | 0.39–51,800 | 1.05–27,278.7 | a,b,c,d | 60 |
| Pb | 737 | 0.084–1,113,000 | 0.03–20,250 | 0.0036–27,950 | a,b,c,d | 207 |
| Sb | 20 | 9.7–31.1 | – | 0.29–3.49 | a | 3 |
| Zn | 776 | 1.65–46,500 | 0.01–9900 | 0.2–27,278 | a,b,c,d | 212 |

a Mining, b industrial, c experimental at the laboratory, d agricultural

- For high concentrations, the hyperaccumulator and accumulator curves should have lower values, compared to the reference line. This implies lower requirements to be classified as an accumulator or hyperaccumulator.
- For extremely high values, all curves should tend to zero, as the conditions would not be adequate at all for plant survival. This implies much lower requirements to be classified as an accumulator or hyperaccumulator.

Based on these constraints, this paper proposes a mathematical model for these characteristic curves. Particularly, this model is an extension of previous work by Lam et al. (2022), who proposed the form described in Eq. 1, using the bioconcentration factor logarithm (ratio between root-level concentration and soil concentration).

$$\ln\left(\frac{[]_{plant}}{[]_{soil}}\right) = A + B\sqrt{[]_{soil}} + C\ln\left(\ln\left([]_{soil} + 1\right) + 1\right) \tag{1}$$

Although these characteristic curves provide a good description of the average behavior of different plant species in multiple scenarios, it is a highly complex over-engineered solution, when trying to achieve the desired shape and properties of the function. Thus, the original model must rely on a hand-crafted function that is neither easy to manipulate nor easily generalizable, using a composite logarithm term and an unnecessary square root. However, similar behavior can be achieved through a much more parsimonious model. This work shows such a model and constructs a new set of characteristic curves, having some additional benefits and advantages over the original model.

## Proposed model

The basic model proposed here is defined as the relationship between the $[]_{plant}$ logarithm and a function designed to meet the aforementioned requirements, following a much simpler approach than the original model of Lam et al. (2022).

$$\ln\left([]_{plant}\right) = b_0 + b_t + b_m + b_s + b_1[]_{soil} + b_2 \ln\left([]_{soil}\right), \text{ with } []_{soil} \geq 0,$$

where $b_0$ is the basic growth rate of the curve growth (i.e., like the slope of a line), $b_t$ is the influence of the species, $b_m$ is the influence of the relevant metal, and $b_s$ is the influence of the type of measurement (shoot or root). In this case, certain metals are grouped together due to their similar behavior (Group 1: As/Fe/Zn, Group 2: Cu/Pb/Cd, and Group 3: Sb); $b_1$ is the influence of the linear term $[]_{soil}$, and $b_2$ is the influence of the logarithmic term. Unlike Lam et al. (2022), this model does not consider an adjusted logarithm with a + 1 term. In the edge case of zero values, by solving for $[]_{plant}$ and taking limits as $[]_{soil}$ approaches zero, it is possible to show that this curve passes through the origin.

In this model, $b_1$ must take negative values to meet the aforementioned requirements and $b_2$ should take positive values. These assumptions are confirmed when adjusting the curve with real data.

For interpretability purposes, it is useful to make algebraic arrangements and solve for $[]_{plant}$, which gives the following formula:

$$[]_{plant} = \underbrace{e^{b_0+b_t+b_m+b_s}[]_{soil}^{b_2}}_{(1)} \underbrace{e^{b_1[]_{soil}}}_{(2)}, \text{ with } []_{soil} \geq 0. \tag{2}$$

Component (1) represents a power factor with a positive coefficient $b_2$ and determines the growth rate in low concentration values. The constant factor could be considered as the “slope” of this factor, determined by the basic growth rate of the function, the type of plant, the metal analyzed, and the type of measurement. Since $e^{b_0+b_t+b_m+b_s} > 0$, this value is never zero. Furthermore, in practice, the value of $b_2$ is between 0 and 1. Thus, this power factor grows slower than a linear function. Component (2) represents an exponential factor with a negative coefficient $b_2$. This component determines the decrease rate for high concentration values, leading to the eventual convergence to zero as the values of soil concentration tend to infinity, as required by the defined constraints of the model.

## Linear model

The empirical values of the coefficients were determined using linear regression. During pre-processing, the concentration logarithms were computed to be used in the model. The fitting process is described below.

First, the linear regression model was obtained by using $y = \ln\left([]_{plant}\right)$ as the response variable and the following variables as the predictor variables:

- The value of the final metal concentration in the soil $\left([]_{soil}\right)$.
- The logarithm of the final metal concentration in the soil $\left(\ln[]_{soil}\right)$.
- The type of metal (Group 1: As/Fe/Zn, Group 2: Cu/Pb/Cd, and Group 3: Sb).
- The type of measurement: root or shoot of the plant.
- The plant species (305 different species).

Following the methodology of Lam et al. 2022, this model was fit in two stages. First, species were grouped into clusters, based on the linear model coefficients without any further pre-processing. Next, the final model was obtained by using the final clusters as features instead of the full 305 species. This clustering is done for both statistical and simplification purposes since considering all species separately would make it more complex and ineffective in practice.

The initial linear fit has a value of $R^2_{adj} = 0.725$ and a $p$ value $< 0.001$. However, as expected, most variables associated with the species are considered non-significant with $\alpha = 0.05$. Thus, the model is reduced following the clustering approach mentioned above. As the goal is to determine characteristic curves to describe behaviors of different groups of species, clustering them together for modeling purposes makes sense. To do this, the coefficient values corresponding to each species can be used as a reference.

Figure 1 shows the distribution of the species coefficients in the basic model. This curve seems to follow a normal distribution. This is confirmed using a goodness-of-fit test based on D'Agostino and Pearson's (1973) tests using skew and kurtosis to test for normality $(p = 0.62)$. This normal distribution has an average of $\overline{b_{specie}} = 0.484$ and a standard deviation of $s_{specie} = 1.198$. However, as

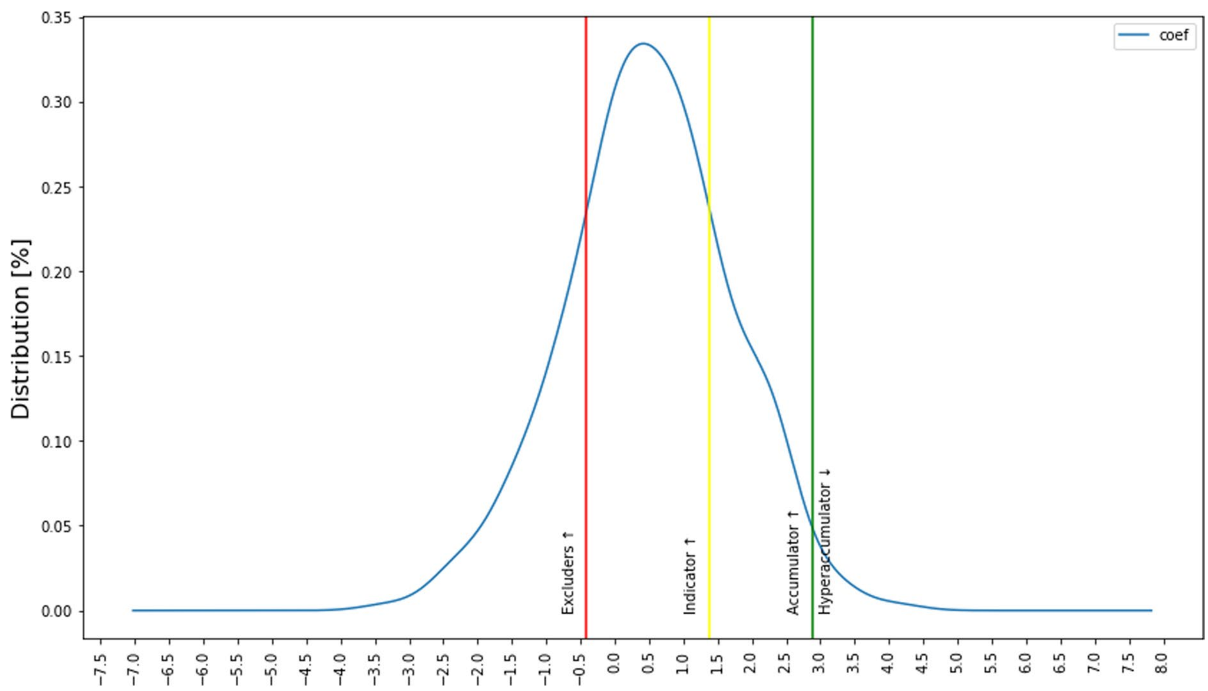


**Fig. 1** Coefficient distribution associated with the plant species term in the basic linear model. Vertical lines show the threshold associated with each type of species

shown by a small bump near 2.0, there are slightly more results on the right side of the curve. 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 corresponding to species with accumulator behavior. This behavior was also observed in the original model of Lam et al. (2022). Thus, the results in this extended data set suggest that this trend still holds when considering both roots and shoot concentration measurements.

Following the same approach as Lam et al. (2022), this information is then used to empirically define a series of thresholds. In particular, a new variable called "Type of Species" is defined using the criteria shown in Table 2. This new variable takes the place of the variable indicating the plant species. Based on these results, a new linear model is developed in the same way as before, but now utilizing this variable.

## Results

### Characteristic curves

This section shows the resulting curves. Results are first exemplified for Cu, Cd, and Pb, based on root concentration. A second example with the shoot concentrations and Sb is presented later.

The final model is $R^2_{adj} = 0.712$. There were only marginal losses in $R^2_{adj}$ by grouping the species. The *F* value of the model is 847.5, with a *p* value < 0.001. Table 3 shows the coefficients of the model and their associated *p* values.

Table 3 also shows the values used as a baseline in the linear model (i.e., their coefficients are set to zero). In particular, indicator species were determined as the baseline for the type of species, which makes sense, given their definition. For metals, the model uses As, Fe, and Zn as the baseline. For the type of measurements, root measurements were used as the baseline.

**Table 2** Definition of the "Type of Species" variable by their thresholds, based on the methodology of Lam et al. (2022)

| Type of species | Lower threshold definition | Upper threshold definition | Lower threshold value | Upper threshold value |
|---|---|---|---|---|
| Hyperaccumulator | $\overline{b_{specie}} + 2 \cdot s_{specie}$ | $+\infty$ | 2.28 | $+\infty$ |
| Accumulator | $\overline{b_{specie}} + 0.75 \cdot s_{specie}$ | $\overline{b_{specie}} + 2 \cdot s_{specie}$ | 1.38 | 2.28 |
| Indicator | $\overline{b_{specie}} - 0.75 \cdot s_{specie}$ | $\overline{b_{specie}} + 0.75 \cdot s_{specie}$ | −0.41 | 1.38 |
| Excluder | $-\infty$ | $\overline{b_{specie}} - 0.75 \cdot s_{specie}$ | $-\infty$ | −0.41 |

**Table 3** Final linear model coefficients and their *p* values

| Coefficients | Value | *p*-value |
|---|---|---|
| Intercept ($b_0$) | 1.8247 | < 0.001 |
| Type of species ($b_t$)—Excluder | −1.3088 | < 0.001 |
| Type of species ($b_t$)—Indicator | 0 | N/A (Baseline) |
| Type of species ($b_t$)—Accumulator | 1.6837 | < 0.001 |
| Type of species ($b_t$)—Hyperaccumulator | 3.0213 | < 0.001 |
| Type of measurement ($b_s$)—Root | 0 | N/A (Baseline) |
| Type of measurement ($b_s$)—shoot | −0.3796 | < 0.001 |
| Metal ($b_m$)—As/Fe/Zn | 0 | N/A (Baseline) |
| Metal ($b_m$)—Cu/Pb/Cd | −0.7262 | < 0.001 |
| Metal ($b_m$)—Sb | −2.7866 | < 0.001 |
| Coefficient $[]_{soil}$ ($b_1$) | $-2.834.\times10^{-06}$ | < 0.001 |
| Coefficient $ln([]_{soil})$ ($b_2$) | 0.5928 | < 0.001 |

To illustrate the model, Fig. 2 shows Cu, Cd, and Pb curves. For the other metals, changing the coefficient corresponding to the models shown in Table 3 would be sufficient.

Figure 2 shows the characteristic curves of Cu, Cd, and Pb for high concentrations. The indicator and excluder curves are close to the X-axis, while the excluder curve is practically indistinguishable from it. However, the hyperaccumulator and accumulator curves exhibit the desired behavior (i.e., they grow quickly and then slowly decrease, tending to zero).

In this zoomed-out view, the hyperaccumulator line behaves very similar to the reference line at the start and then provides a more lenient criterion as it starts to slow down and decline. However, on further inspection, the hyperaccumulator line is actually above the reference line up to about 20,000 mg/kg of final soil concentration threshold.

Moreover, compared to the original model proposed by Lam et al. (2022), these curves achieve similar global maxima. Following the original methodology and using the complex characteristic curves provides similar values. However, as mentioned above, the new model is more parsimonious (i.e., it provides a simpler explanation) and there is no loss of descriptive capabilities.

Figure 3 shows the characteristic curves of moderately high concentrations. Here, the threshold where behavior changes for the hyperaccumulator curve is clear. Following this logic, similar behavior can be expected for the accumulator curve.

Figure 4 shows the characteristic curves of moderately low concentrations. The accumulator curve is more demanding than the reference line in low concentrations, but it becomes less demanding as the concentration in the soil rises, as shown by its intersection with the reference line at around 1000 mg/kg. The indicator curve in blue represents the expected average plant behavior, while the excluder curve shows the plants with a very bad performance when compared to the others. In this zoomed-out view, both of these curves are still fairly close to the X-axis and do not provide much information.

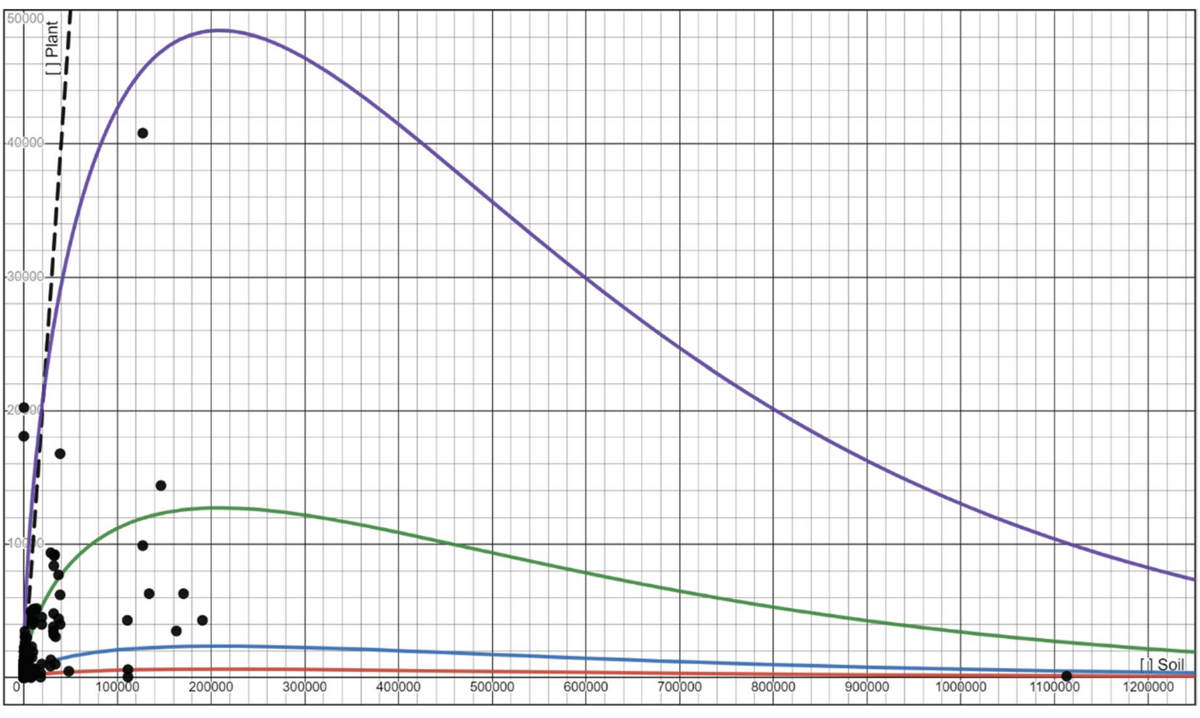


**Fig. 2** Characteristic curves for high concentrations. The X-axis shows the final soil concentration [mg/kg] and the Y-axis shows the final plant concentration [mg/kg]. The dashed line represents the reference straight line of Y = X. The dots represent the Cu, Cd, and Pb samples used to construct the model

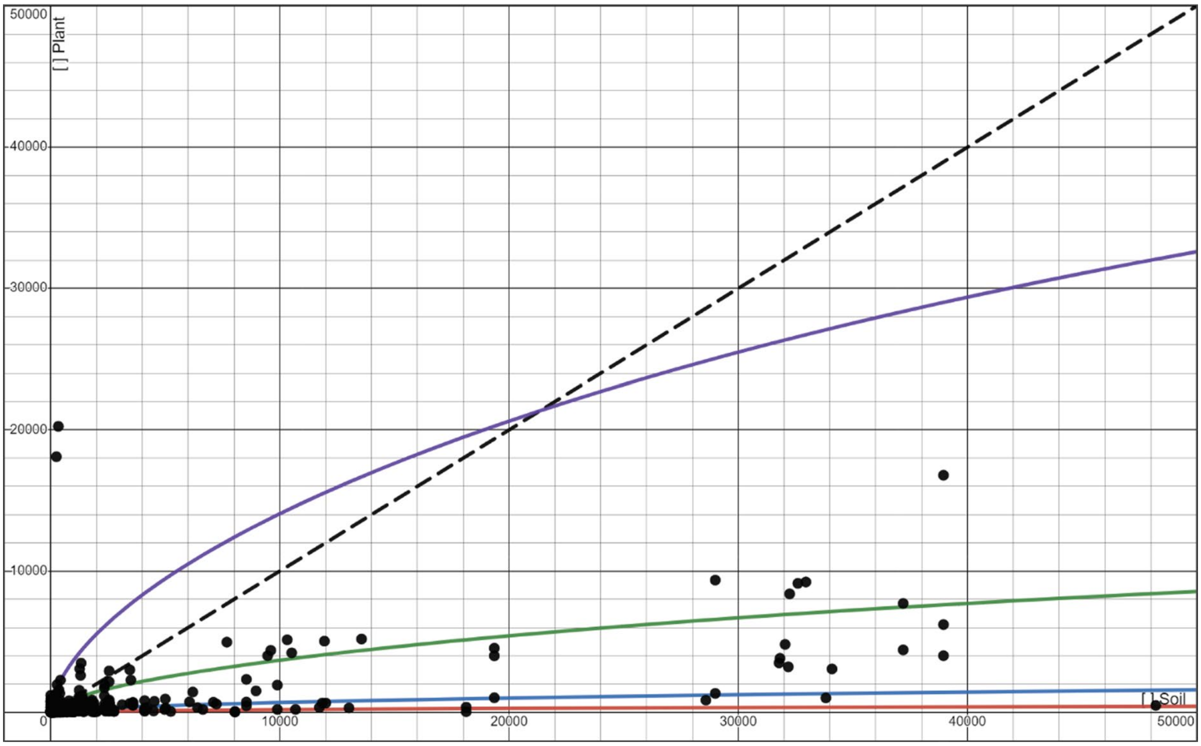


**Fig. 3** Characteristic curves for moderately high concentrations. The X-axis shows the final soil concentration [mg/kg] and the Y-axis shows the final plant concentration [mg/kg]. The dashed line represents the reference straight line of Y = X. The dots represent the Cu, Cd, and Pb samples used to construct the model

Figure 5 shows the characteristic curves of low concentrations. This view clearly shows that for lower concentrations, the proposed model is more demanding than the reference line. However, compared to the original model of Lam et al. (2022), at this level, the hyperaccumulator and accumulator curves were practically undistinguishable from the Y-axis. Thus, the original model was much more stringent in its requirements. In contrast, the model proposed here provides a mid-point between the strictness of the original model for low values and the laxness of the classic straight-line criteria. Furthermore, it is more realistic for higher values, the same way as the original model.

## Usage example

To exemplify how these curves could be used in practice, the methodology is applied to a series of five experimental samples of Zn. Data were taken from Lázaro (2008). The viability of the species as accumulators or hyperaccumulators will be analyzed in accordance with the established criteria of the model proposed here. Furthermore, a comparison will be made with the original model of Lam et al. (2022).

Table 3 shows the results obtained using the coefficients for indicators, accumulators, and hyperaccumulators. These values are then compared with the sample $[]_{plant}$. In the first example, an 800 mg/kg sample $[]_{shoot}$ is higher than the predicted hyperaccumulator $[]_{plant}$ threshold, thus the *Cistus landanifer* is classified as a potential hyperaccumulator of Zn in these conditions. In contrast, the *Thymus mastichina* value is just above the hyperaccumulator threshold. It may be argued that more experiments could be useful to effectively determine whether it is behaving as a hyperaccumulator or only as an accumulator.

The results of the original model compared to the proposed model are different, with the proposed model being more lenient. This is the expected behavior for lower concentrations, as discussed in the previous subsection.

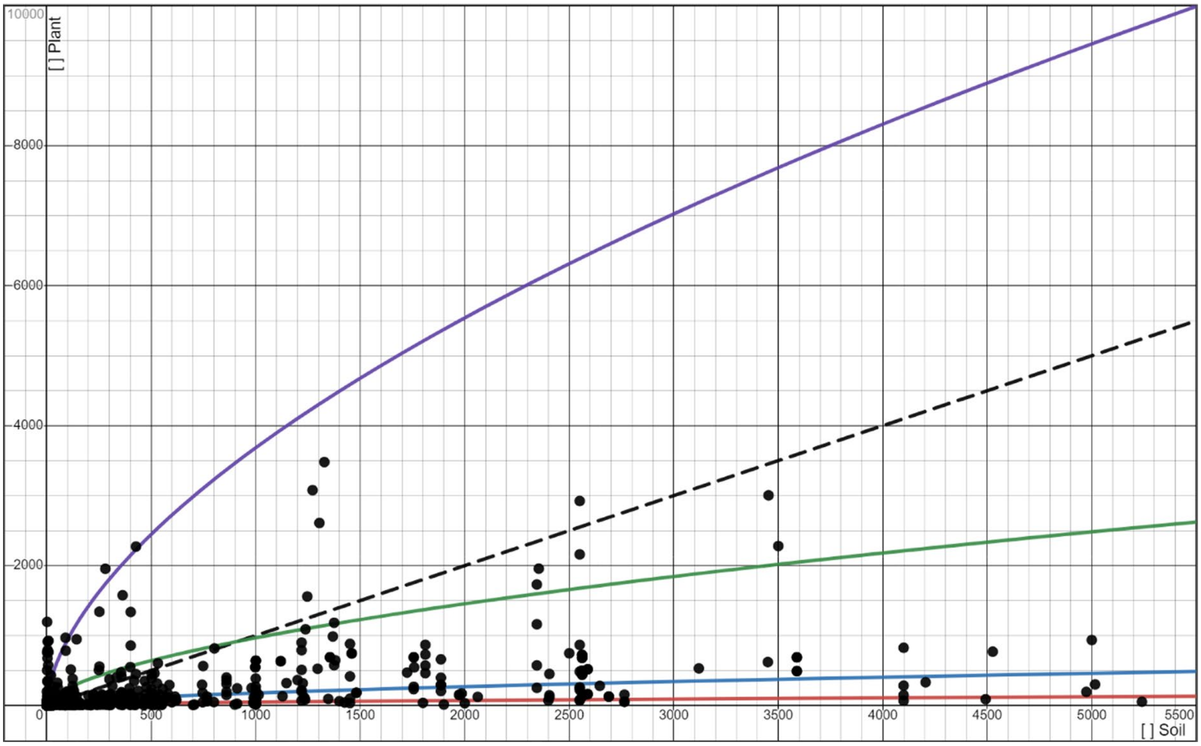


**Fig. 4** Characteristic curves for moderately low concentrations. The X-axis shows the final soil concentration [mg/kg] and the Y-axis shows the final plant concentration [mg/kg]. The dashed line represents the reference straight line of Y = X. The dots represent the Cu, Cd, and Pb samples used to construct the model

Considering traditional assessment criteria, all these plant species would be considered Zn accumulators, or even hyperaccumulators, as the ratio $\frac{[]_{plant}}{[]_{soil}} \gg 1$. Thus, these results are consistent with traditional criteria.

Finally, let us consider an example with Fe and Zn, using a *Bidens triplinervia* sample and a *Plantago orbignyana* sample taken from Durán Cuevas et al., which was also used in Lam et al. (2022) for assessment purposes. In this case, both models show the same results, which makes sense as their behavior should be similar in high concentrations. The biggest differences occur in low concentrations.

## Species classification

Following the methodology by Lam et al. (2022), it is possible to use the criteria defined in Sect. 1.3 to construct a rough categorization of the plant species based on how they were grouped when creating the characteristic curves. Tables 4 and 5 show the species identified as accumulators and hyperaccumulators while constructing the model.

The species listed in Tables 4 and 5 should be studied further to confirm their accumulator or hyperaccumulator properties. However, the model does not consider any extra treatments applied or unusual situations that could impact the final concentration values of either the soil or the plant. Thus, there might be other factors influencing the results of this experiment (e.g., amendments).

## Limitations of the model and other considerations

As the original model of Lam et al. (2022), one of the key shortcomings of the model is that it only considers final concentrations without taking into account initial values. For further improvement of this model, it would be useful to incorporate the initial and final concentrations to evaluate the capabilities of a plant species. However, the reference

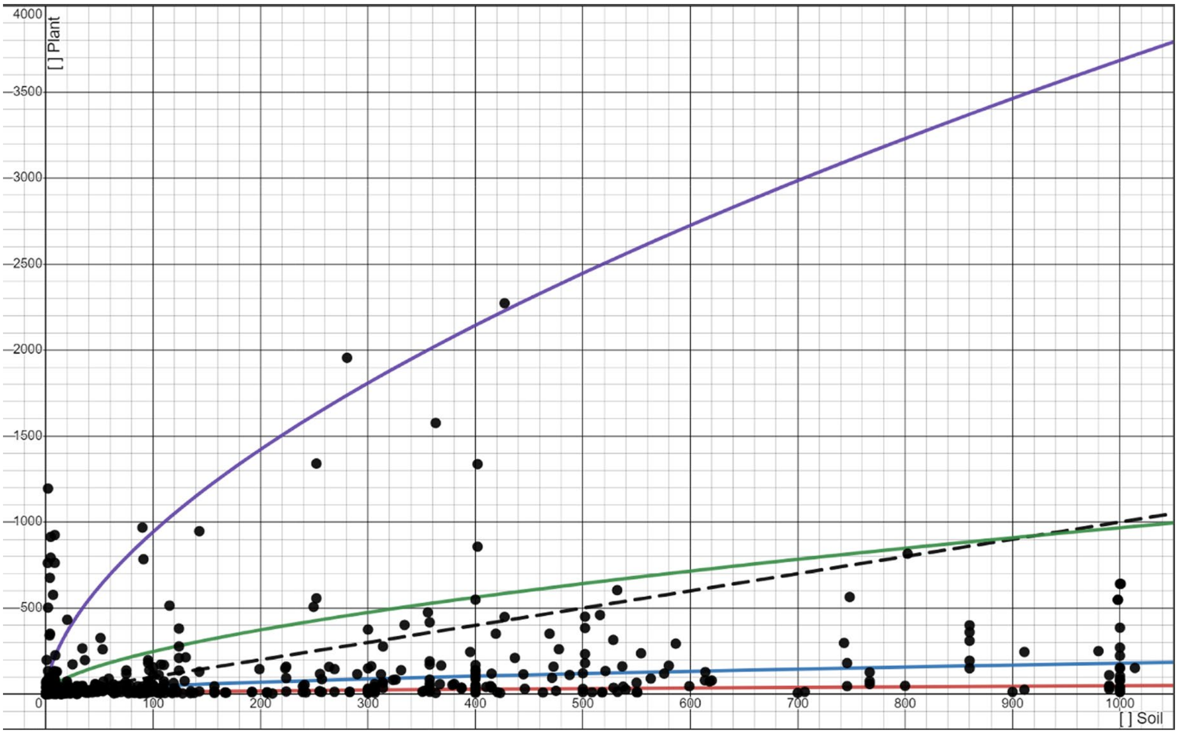


**Fig. 5** Characteristic curves for low concentrations. The X-axis shows the final soil concentration [mg/kg] and the Y-axis shows the final plant concentration [mg/kg]. The dashed line represents the reference straight line of Y = X. The dots represent the As, Fe, and Zn samples used to construct the model

papers used to construct the database relied on the final concentration values, following the common usage and definition of both the bioconcentration and the accumulation factors to evaluate plant species. The model was based on available data.

Furthermore, the proposed model is based on the average behavior of multiple species, assuming a normal distribution. This assumption holds well with current data according to the goodness-of-fit test, but it should be verified if the model is extended or adapted.

Moreover, the model does not consider other conditions (e.g., other plant treatments beyond phytoremediation). Initially, the type of soil (industrial, agricultural, laboratory, and mining) was considered in the model. However, further analysis of the resulting linear model parameters shows that this information is redundant.

Finally, the model would be initially valid for specific concentration ranges of the analyzed metals, particularly, As (33.75–2,860 mg/kg), Cu (3.638–190,800 mg/kg), Fe (6.83–308,500 mg/kg), Pb (0.084–113,000 mg/kg), Sb (0.29–3.49 mg/kg), and Zn (1.65–46,500 mg/kg). Using the model outside these parameters might result in erroneous findings. However, because these ranges and the model itself are based on varied experimental data, this should not be a constraint for most model implementations. All concentrations were measured in mg/kg. So, the model must always use the same units for consistency purposes.

Of the 305 species assessed, 90 behaved as accumulators under the experimental conditions; 11 showed this potential behavior for two metals, and four species showed accumulator characteristics for three metals.

Regarding species with accumulator potential, the number of species per metal in descending order is Pb (58/201 species), Cd (3/12 species), Zn (47/211 species), Fe (13/59 species), and Cu (30/209 species). Regarding species with hyperaccumulator potential, the number of species per metal in descending

**Table 4** Accumulator species, according to their initial grouping in the base model for characteristic curves

| Accumulator species | | |
|---|---|---|
| *Abutilon indicum*[5] | *Chaerophyllum macropodum*[5] | *Hibiscus nicranthus*[5] |
| *Acacia albida*[5] | *Chenopodium album*[3] | *Imperata cylindrica*[5] |
| *Acanthus ebracteauts*[5] | *Chenopodium botrys*[5] | *Indigofera cuneata*[5] |
| *Achillea tenuifolia*[5] | *Cirsium congestum*[4] | *Ipomoea pes-caprae*[5] |
| *Aerva lanata*[5] | *Cistus ladanifer*[7] | *Juncus arcticus*[3, 7] |
| *Alnus nepalensis*[5,7] | *Cortaderia rudiuscula*[5, 7] | *Lactuca sativa*[2, 5, 7] |
| *Alyssum serpyllifolium*[7] | *Cousinia sp*[5] | *Lavandula stoechas*[7] |
| *Amaranthus dubius*[3] | *Cucurbita moschata*[7] | *Lepidium bipinnatifidum*[5] |
| *Añamosana marina*[5] | *Cynachum tubulosum*[5] | *Medicago sativa*[3, 4] |
| *Atriplex deserticota*[3] | *Cynodon dactylon*[5] | *Mullinum spinosum*[3] |
| *Baccharis amdatensis*[5, 7] | *Derris trifoliata*[5] | *Nonnea pérsica*[7] |
| *Baccharis latifolia*[7] | *Deschampsia cespitosa*[3,4, 7] | *Paederia foetida*[5] |
| *Bidens triplinervia*[5, 7] | *Digitaria sanguinalis*[4, 7] | *Papaver piptostigma*[5, 7] |
| *Brachiaria reptans*[5] | *Eragrostis aethiopica*[5] | *Parthenium hysterophorus*[5] |
| *Brickellia vernicifolia*[4, 5, 7] | *Erigeron berterianum*[3] | *Peganum harmala*[5] |
| *Bromus tectorum*[7] | *Eryngium campestre*[5] | *Pelargonium graveolens*[7] |
| *Canna indica*[5] | *Euphorbia hirta* [7] | *Pelargonium hortorum*[7] |
| *Carduus tenuiflorus*[5] | *Euphorbia macroclada*[4, 7] | *Pelargonium peltatum*[7] |
| *Cenchrus equinatus*[3] | *Gentiana pennelliana*[3,5] | *Persicaria barbata*[3] |
| *Centaurea persica*[7] | *Gomphrena celosioides*[7] | *Phragmites australis*[3] |
| *Centaurea virgata*[5] | *Helianthus annuus*[3, 7] | *Pinus spp*[3, 5, 7] |
| *Pinus yunnanensis*[5] | *Raphanus sativus*[3, 7] | *Setaria incrassata*[5] |
| *Piriformospora indica*[3] | *Rorippa globosa*[2] | *Solidago altissima*[3] |
| *Plantago amplexicaulis*[5] | *Rubus fruticosis*[3] | *Stipa barbata*[5] |
| *Plantago orbignyana*[5, 7] | *Santolina semidentata*[7] | *Stipa hohenackeriana*[5] |
| *Pluchea carolinensis*[4, 7] | *Sarcocornia fruticosa*[3] | *Taraxacum mongolicum*[2] |
| *Polyalthia longifolia*[3, 5] | *Scariola orientalis*[5] | *Thymus mastichina*[7] |
| *Portulaca oleracea*[3, 5] | *Schinus polygamus*[3] | *Tilia spp*[3, 5] |
| *Pteris vittata*[5] | *Scrophularia scoparia*[3] | *Verbascum speciosum*[4, 5, 7] |
| *Pteropyrum aucheri*[5] | *Senecio sp*[5] | *Zea mays*[3] |

[1]As, [2]Cd, [3]Cu, [4]Fe, [5]Pb, [6]Sb, [7]Zn

**Table 5** Hyperaccumulator species, according to their initial grouping in the base model for characteristic curves

| Hyperaccumulator species | | |
|---|---|---|
| *Cardaria draba*[3] | *Euphorbia macroclada*[3] | *Reseda lutea*[3] |
| *Chaerophyllum* macropodum[3] | *Gomphrena celosioides*[5] | *Sonchus tenerrimus*[6] |
| *Cirsium congestum*[3] | *Plantago amplexicaulis*[6] | |
| *Euphorbia hirta*[5] | *Reseda alba*[5] | |

[1]As, [2]Cd, [3]Cu, [4]Fe, [5]Pb, [6]Sb, [7]Zn

order is (10 in total): Sb (2/3 species) followed by Cu (5/209 species) and Pb (3/201 species). No species show hyperaccumulation potential for As, Cd, Fe, or Zn. Table 6 shows the results obtained using the traditional AF criterion and the proposed model.

Here, N is the number of experimental data used and NC corresponds to the number of matches obtained between both methodologies. Experimental data analysis shows that differences occur at very high or very low concentrations of metals in the soil, which is the expected behavior since the proposed model is stricter for lower concentrations and less strict for higher concentrations.

**Table 6** Comparison of results obtained with the AF criterion and the proposed model

a Mining, b industrial, c experimental at the laboratory, d agricultural

| Metal | N | AF Method | | Proposed model | | Matches | |
|---|---|---|---|---|---|---|---|
| | | Accumulator/Hyperaccumulator | | Accumulator/ Hyperaccumulator | | NC | % |
| | | YES (AF > 1) | NO (AF < 1) | YES | NO | | |
| As | 6 | 0 | 6 | 0 | 6 | 6 | 100 |
| Cu | 439 | 80 | 359 | 40 | 399 | 379 | 86 |
| Cd | 37 | 12 | 25 | 3 | 34 | 23 | 62 |
| Fe | 125 | 6 | 119 | 13 | 112 | 118 | 94 |
| Pb | 378 | 85 | 293 | 64 | 314 | 300 | 79 |
| Sb | 10 | 0 | 10 | 2 | 8 | 8 | 80 |
| Zn | 410 | 102 | 308 | 47 | 363 | 343 | 84 |

**Table 7** Threshold values in mg/kg for the simplified model

| Type of measurement | Metal | Excluder | Indicator | Accumulator | Hyperaccumulator |
|---|---|---|---|---|---|
| Root | As, Fe, and Zn | 1.675 | 6.201 | 33.395 | 127.230 |
| | Cu, Cd, and Pb | 0.810 | 3.000 | 16.155 | 61.547 |
| | Sb | 0.103 | 0.382 | 2.058 | 7.841 |
| Shoot | As, Fe, and Zn | 1.146 | 4.242 | 22.847 | 87.043 |
| | Cu, Cd, and Pb | 0.554 | 2.052 | 11.052 | 42.106 |
| | Sb | 0.071 | 0.261 | 1.408 | 5.364 |

For example, Cd shows that concentrations are low in general. Thus, it is easy to get a plant concentration the same as or higher than the soils, which leads to an AF greater than 1; however, this does not necessarily mean that the plant is an accumulator or a hyperaccumulator.

## Approximation-based model

To further simplify computations, it is possible to define an approximation-based model working relatively well in lower concentration ranges rather than the full spectrum of concentration ranges shown in the experimental data. In this section, a heuristic or approximation-based model is proposed, rather than a more formal or statistical method. This method shares some of the benefits of the proposed model (stricter in lower concentrations, but more lenient in higher concentrations), but it is only designed for concentrations up to 37,000 mg/kg (it loses its approximation power as concentrations get higher).

To derive this approach, first consider an alternative interpretation of this model which can be obtained through the following re-arrangement:

$$\frac{[]_{plant}}{[]_{soil}^{b_2}} = \underbrace{e^{b_0+b_t+b_m+b_s}}_{(1)}\underbrace{e^{b_1[]_{soil}}}_{(2)}$$

For lower concentrations, $e^{b_1[]_{soil}} \approx 1$. In fact, just at 37,000 mg/kg, it barely gets close to 0.9, i.e., the defined threshold for this model to be considered valid. If more tolerance is allowed, the model could be used with higher concentrations, but it would hurt its accuracy. Nevertheless, it is possible to further simplify the model by using this approximation.

$$\frac{[]_{plant}}{[]_{soil}^{b_2}} = e^{b_0+b_t+b_m+b_s}$$

Finally, for the last step, approximate $b_2 \approx 0.5$, which leads to a new simple ratio-based criterion. We call this criterion **Adjusted BCF** or **AF** (depending on whether the data used correspond to the root or the shoot, respectively), as shown in Eq. 3.

$$\frac{[]_{plant}}{\sqrt{[]_{soil}}} = e^{b_0+b_t+b_m+b_s} \quad (3)$$

**Table 8** Assessment of samples from Lázaro (2014), using the simplified approximate model. Results match with the originally proposed model, as concentrations are low

| Plant | Metal | Type of measurement | Sample $[]_{soil}$ | Sample $[]_{plant}$ | Adjusted AF | Result of Lam et al. (2022) methodology with shoot data | Result with the proposed model | Result with the simplified model |
|---|---|---|---|---|---|---|---|---|
| *Cistus ladanifer* | Zn | Shoot | 4.4 | 800 | 381.385 | Accumulator, but close to hyperaccumulator range | Hyperaccumulator | Hyperaccumulator |
| *Alyssum serpyllifolium* | | | | 395 | 188.309 | Accumulator | Hyperaccumulator | Hyperaccumulator |
| *Lavandula stoechas* | | | | 335 | 159.705 | Accumulator | Hyperaccumulator | Hyperaccumulator |
| *Thymus mastichina* | | | | 210 | 100.114 | Accumulator | Hyperaccumulator | Hyperaccumulator |
| *Santolina semidentata* | | | | 95 | 45.289 | Accumulator | Accumulator | Accumulator |

**Table 9** Partial assessment of *Bidens triplinervia* and *Plantago orbignyana* from Durán Cuevas et al., using the simplified approximate model. Results match partially with the originally proposed model, as concentrations are high (the Fe sample is above the 37,000 mg/kg threshold of the model validity)

| Metal | Type of measurement | Sample $[]_{soil}$ | Sample $[]_{plant}$ | Adjusted BCF | Result of Lam et al. (2022) methodology with shoot data | Result with the proposed model | Result with the simplified model |
|---|---|---|---|---|---|---|---|
| Fe | Root | 79,728 | 31,120 | 110.213 | Accumulator | Accumulator | Hyperaccumulator |
| Zn | Root | 30,656 | 3,144 | 17.957 | Indicator | Indicator | Indicator |

Equation 3 provides the following simpler threshold for concentrations below 37,000 mg/kg. These thresholds can be used with Adjusted BCF or AF to determine the type of species with a simpler formula. The thresholds for all relevant cases are shown in Table 7.

The application of these simplified threshold values with Adjusted AF or BCF is shown in Tables 8 and 9, repeating previous assessments with the simplified model. Results match with the originally proposed model, except when the concentration exceeds the 37,000 mg/kg validity threshold for the approximate model.

## Conclusions

This paper presents a model for categorizing plant species into indicators, excluders, accumulators, and hyperaccumulators in the context of soil treatment via phytoremediation, using characteristic curves derived from empirical data. The characteristic curves are built using a linear model relating metal concentrations in the plant (either in the roots or shoots) to soil concentration through both an exponential and a power term, implemented through linear regression. This model presents a simpler approach to the model of Lam et al. (2022), which relies on a complex hand-crafted function to model characteristic curves. The model has some limitations. Most notably, it does not take into account the initial metal concentration in the substrate. Furthermore, behavior is based on the average behavior of several species, as well as the assumption of normal behavior. Despite these constraints, the model performs well. Particularly, the final model shows an adjusted $R^2$ of 0.712, and all the variables used are regarded as significant. As a result, this model

**Table 10** Assessment of samples from Lázaro (2014), using the proposed model. The results differ from Lam et al. (2022) baseline model, showing how the proposed model is slightly more lenient for low concentration values

| Plant | Metal | Type of measurement | Sample $[]_{soil}$ mg/kg | Sample $[]_{plant}$ | Predicted indicator $[]_{plant}$ | Predicted accumulator $[]_{plant}$ | Predicted hyperaccumulator $[]_{plant}$ | Result of Lam et al. (2022) methodology with shoot data | Result with the proposed model |
|---|---|---|---|---|---|---|---|---|---|
| *Cistus ladanifer* | Zn | Shoot | 4.4 | 800 | 10.21 | 54.97 | 209.49 | Accumulator, but close to hyperaccumulator range | Hyperaccumulator |
| *Alyssum serpyllifolium* | | | | 395 | | | | Accumulator | Hyperaccumulator |
| *Lavandula stoechas* | | | | 335 | | | | Accumulator | Hyperaccumulator |
| *Thymus mastichina* | | | | 210 | | | | Accumulator | Hyperaccumulator |
| *Santolina semidentata* | | | | 95 | | | | Accumulator | Accumulator |

**Table 11** Partial assessment of *Bidens triplinervia* and *Plantago orbignyana* from Durán Cuevas et al., using the proposed model. Results coincide with Lam et al. (2022) baseline model, showing that both models have similar behaviors for high concentrations

| Metal | Type of measurement | Sample $[]_{soil}$ mg/kg | Sample $[]_{plant}$ | Predicted excluder $[]_{plant}$ | Predicted indicator $[]_{plant}$ | Predicted accumulator $[]_{plant}$ | Predicted hyperaccumulator $[]_{plant}$ | Result of Lam et al. (2022) methodology with root data | Result with the proposed model |
|---|---|---|---|---|---|---|---|---|---|
| Fe | Root | 79,728 | 31,120 | 1,075.472 | 3,981.105 | 21,440.021 | 81,684.097 | Accumulator | Accumulator |
| Zn | Root | 30,656 | 3,144 | 701.339 | 2,596.166 | 13,981.508 | 53,267.992 | Indicator | Indicator |

may be used to assess numerous samples from a given plant species to identify its potential as an accumulator in soil treatment via phytoremediation. A simplified version of the model was also constructed using approximations to provide an easy-to-compute version of the model for concentrations below 37,000 mg/kg. This simplified model shows results similar to the original model for concentrations below this threshold. The model construction shows that 90 out of the 305 species assessed have a potential behavior as accumulators and 10 of them as hyperaccumulators (Tables 10 and 11). Finally, out of the 1,405 experimental measurements, 1177 were shown to be accumulators/hyperaccumulators, that is, 85% of the results coincide with the reported values, thus validating the proposed model.

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**Human and animal rights** Since this study did not involve animal research, no consents were required to participate and publish data on animals. Therefore, the inclusion of these forms and other ethical issues related to the publication of this type of data does not apply to this study.

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