



## Heavy metal concentrations in plants and different harvestable parts: A soil–plant equilibrium model

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The model proposed in this study makes possible to characterize the nonlinear behavior of the soil–plant interaction with metal pollution.

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### ABSTRACT

A mathematical interaction model, validated by experimental results, was developed to modeling the metal uptake by plants and induced growth decrease, by knowing metal in soils. The model relates the dynamics of the uptake of metals from soil to plants. Also, two types of relationships are tested: total and available metal content. The model successfully fitted the experimental data and made it possible to predict the threshold values of total mortality with a satisfactory approach. Data are taken from soils treated with Cd and Ni for ryegrass (*Lolium perenne*, L.) and oats (*Avena sativa* L.), respectively. Concentrations are measured in the aboveground biomass of plants. In the latter case, the concentration of metals in different parts of the plants (tillering, shooting and earing) is also modeled. At low concentrations, the effects of metals are moderate, and the dynamics appear to be linear. However, increasing concentrations show nonlinear behaviors.

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### 1. Introduction

Increased attention has been focused on metals due to their harmful negative effect on the environment. In trace amounts, they are mostly necessary elements in living organisms; however, in higher concentrations they are toxic. Soil pollution by metals can be caused by fertilizers and pesticides. The use of industrial effluent and sewage sludge on agricultural soil has become a common practice in developing countries, as a result of which these toxic metals can be transferred and concentrated into plant tissues from the soil (Alloway, 1995). Industrial wastes are a major source of soil pollution from mining industries, chemical industries, metal processing industries, metallurgical operations, oil products and products of fossil fuel combustion (Van Assche and Clijsters, 1990; Kabata-Pendias, 2001).

The mobility and bioavailability of these elements depend on soil characteristics such as pH, organic matter, cation-exchange capacity, and soil redox potential (Adriano, 1986). Soil management can also change its physical, chemical, and biological characteristics; therefore, a different response of biological activity to metals toxicity may be observed. The activities of microorganisms that

promote plant growth can be also altered as a result of high metal concentrations (Wani et al., 2007).

At high concentrations, some metals have strong toxic effects and are regarded as environmental pollutants (Nedelkoska and Doran, 2000; Chehregani et al., 2005). Heavy metals are potentially toxic for plants. Phytotoxicity results in chlorosis, weak plant growth and yield depression, and may even be accompanied by reduced nutrient uptake, and disorders in plant metabolism (Dan et al., 2008).

In soils polluted by metals, plant growth can be inhibited by metal absorption. However, some plant species are able to accumulate fairly large amounts of metals without showing stress, which represents a potential risk for animals and humans (Oliver, 1997). Metal uptake by crops growing in contaminated soil is a potential hazard to human health due to transmission in the food chain (Brun et al., 2001; Gincchio et al., 2002; Friesl et al., 2006). There is also concern with regard to metal transmission through natural ecosystems (MacFarlane and Burchett, 2002; Walker et al., 2003). Parameters connected with metal uptake have been used as sensitive indicators of metal toxicity (Wilke, 1991; Nannipieri et al., 1997). The toxicity of metals in soil varies significantly according to the characteristics of the soil and the time elapsed after contamination by metals (Doelman and Haanstra, 1984; Speir et al., 1995). Data from studies on the toxic effect of metals on soils have been used to establish the concentrations at which metals affect soil biological processes for regulatory purposes (Giller et al., 1998).

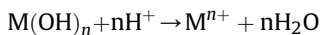
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Although a large number of experimental studies have been carried out to analyze the negative effects of the accumulation of metals in plants, little has been done to model mathematical formulas that are capable of generally relating the concentration of metals in the liquid phase of a soil and the concentration of metals present in plants. In this study, we model the relationship between the concentration of metals in soil and plants and in parts of plants (tillering, shooting and earing) with different concentration levels. Finally, we validate this relationship using recently published experimental results.

## 2. Modeling

It is widely accepted that the effects of metals on forest or agrosystem soils are complex, due to the fact that soil chemistry and its liquid phase involve a large number of reactions (Lindsay, 1979; Ulrich et al., 1980; Ulrich and Pankrath, 1983). We focus on the toxic effects of ions of metals, many of which become bioavailable in natural pH levels. De Leo et al. (1993) modeled the interaction between soil acidity and forest dynamics when aluminum is mobilized with acid deposition. Guala et al. (2009) simplified this model, in order to allow it to be validated experimentally. In this study we consider the model applicable to other metals in soil, modifying it in order to make it independent of acid deposition, assuming the mobility of other metals in natural pH levels in soil. The dominant reaction may be represented as:



In order to model the dynamic interaction, we have adapted the general mathematical expression of the model that describes the dynamics of soil acidity with respect to aluminum mobility and the characteristics of trees, according to the model proposed by De Leo et al. (1993), and modified by Guala et al. (2009). As a result, the new system gives us:

$$\begin{aligned} \frac{dB}{dt} &= B(h(B) - \mu(S)), \\ \frac{dS}{dt} &= \alpha A - h(B)S, \\ \frac{dA}{dt} &= \phi H - \beta A - \alpha AB/p, \\ \frac{dH}{dt} &= -\phi H/(m+n) - \beta H + W/p \end{aligned} \quad (1)$$

where  $B$  is the biomass of trees ( $\text{kg m}^{-2}$ ),  $n$  is the oxidative number of the metal,  $S$  is the metal concentration in trees ( $\text{mg kg}^{-1}$ ), and  $A$  and  $H$  are the available concentrations of metal  $M^{n+}$  ( $\text{mg L}^{-1}$ ) and proton  $H^+$  ( $\text{mg L}^{-1}$ ) in the soil solution, respectively.  $t$  is time,  $W$  is the proton flux to the soil during rainfall ( $\text{mgm}^{-2} \text{yr}^{-1}$ ),  $p$  is the available water for roots (mm) and  $\alpha$ ,  $\beta$  and  $\phi$  are the coefficients of absorption ( $\text{Lkg}^{-1} \text{yr}^{-1}$ ), leaching ( $\text{yr}^{-1}$ ) and reaction ( $\text{yr}^{-1}$ ), respectively.  $m$  is the atomic weight of the metal  $M$ .  $h(B)$  is the function of biomass net-growth and  $\mu(S)$  is the function of mortality or metabolic inefficiency of trees due to the concentration of  $M^{n+}$  they contain. While De Leo et al. (1993) used  $B$  to refer to the biomass of trees, Guala et al. (2009) showed that  $B$  may also indicate some other physiological characteristics, and that Equation (1) may also be applied to plants in general.

Although Equation (1) was originally proposed to specifically model the soil–plant interaction under the condition of aluminum mobility by acidity, we can reformulate the conditions of the last two equations for any deposited metal  $M^{n+}$ . In this case, we are not focusing directly on the mobility of aluminum due to the concentration of protons  $H$  as a result of acid deposition  $W$ , but on the availability of any deposited metal  $M^{n+}$  plus soil acidity conditions. As a result, under equilibrium conditions, the reformulated Equation (1) could be rewritten as:

**Table 1**

Ni concentration in the dry matter ( $\text{mg kg}^{-1}$ ) of several parts of oats (*Avena sativa* L.) (Poulik, 1997).

Ni total content ( $\text{mg kg}^{-1}$ )	Ni in tillering	Ni in shooting	Ni in earing
0	0	0	0.75
14	11.81	12.76	9.88
28	20.26	17.47	15.81
56	27.26	27.96	25.60
84	35.73	31.47	28.81
168	–	–	–

$$\begin{aligned} 0 &= B(h(B) - \mu(S)), \\ 0 &= \alpha A - h(B)S, \\ 0 &= \phi H - \beta A - \alpha AB/p, \\ 0 &= -\phi H/(m+n) - \beta H + W/p \end{aligned} \quad (2)$$

As significant amounts of metals may be available under natural acidity conditions in the liquid phase of soil and absorbed by plants instead of being fixed by the soil matrix, we may neglect the two last expressions of Equation (2) by focusing on the concentration of available metals  $A$  in the second equation of Equation (2).

As a result, the system in equilibrium is expressed as:

$$\begin{aligned} 0 &= B(h(B) - \mu(S)), \\ 0 &= \alpha A - h(B)S. \end{aligned} \quad (3)$$

Using Equation (3), it is possible to calculate the relationship between the concentration of available metals in soil  $A$  and the concentration of metals in plants  $S$ . The expression yields:

$$\alpha A = \mu(S)S$$

The net-growth function was assumed by De Leo et al. (1993) to be of the form  $h(B) = a/(1 + bB)$ , where coefficients  $a$ ,  $b > 0$  are constant; and the logistic form to be  $h(B) = r(1 - B/k)$  as proposed by Guala et al. (2009). Although it does not appear explicitly after Equation (3), in Equation (1) the definition of  $h(B)$  mutually determines the functional form of  $\mu(S)$ . Therefore, the functional form of growth  $h(B)$  should be considered. It is difficult to specify how metals in soils determine the metabolic inefficiency. Despite the fact that the quantitative relationship between the concentration of metals in soils and biomass production has already been documented for some years, metals do not seem to cause a significant risk far below a certain survival threshold, although the effects on different organs of the plant are detected.

In particular, the functional form of the metabolic inefficiency and eventual mortality  $\mu(S)$  is assumed by De Leo et al. (1993) as:

$$\mu(S) = \frac{c - fS}{e - S}$$

where in  $c, f, e > 0, S^e(0, e)$ ,  $S = e$  is the critical survival value. It does not mean that plants can resist until  $S = e$ ; this would be only possible if  $\mu(S)$  was 0 until  $S = e$ , which would mean that plants are completely insensitive to any concentration below  $e$ . Obviously, it is crucial to choose the values of the parameters correctly.

**Table 2**

Cd concentration in the dry matter ( $\text{mg kg}^{-1}$ ) of ryegrass (*Lolium perenne*, L.) in cultivated and uncultivated soil after 60 days (Moreno et al., 2006).

Cd total content ( $\text{mg kg}^{-1}$ )	Cd in uncultivated soil	Cd in plant	Cd in cultivated soil	Cd in plant
0	0.1	5.8	0.1	25.6
50	25.3	63.0	24.3	53.8
600	201	87.4	125	174
1000	329	130	242	198
2000	778	228	468	386
5000	1209	–	1030	721

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