

# Predictive modelling of the long-term accumulation of trace metals in tropical soils amended with organic wastes – field trial validation

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## Abstract

The relevance of models early developed under temperate climate and with a generic parameterization for simulating long-term accumulation of trace metals in soil amended with organic wastes in tropical areas is questionable. This study therefore aimed at adjusting the parameterization of an accumulation model to the specific conditions of the tropical island of la Reunion and validating the model against mid-term field trials. The usual parameterisation based on generic multiples regression equations taken from the literature substantially over-predicted trace metals concentration in the edible organs of plants and in the soil solution determined from local data set and thus overestimated trace metals output from the upper soil layer by plant uptake and leaching. The generic multiples regression equations were therefore substituted by distribution patterns based on the local data set to adjust model parameterization to the specific conditions of la Reunion. The adjusted model predicted fairly well trace metals accumulation in the upper soil layer amended with organic wastes compared with the generic model that tended to slightly underestimated trace metals accumulation. Further validation of the adjusted model against two additional field trials is currently in progress. This will open perspectives for applying the model to the assessment of long term recycling of organic wastes at the island scale.

## Introduction

Due to the ongoing growth of the world's population, the production of agricultural, industrial and urban wastes increase. Agricultural recycling of waste as fertilizer and soil amendment is a good alternative to settle this issue. However the environmental impact of such agricultural recycling practices had to be control since it can result in significant accumulation of inorganic contaminants such as trace metals. This ascertainment is especially notable for long-term and repeated applications [1].

Several models were already developed to predict the accumulation of trace metals in soils amended with organic wastes [2, 3]. If the relevance of simulation outputs was addressed theoretically, it was however barely or even not at all assessed operationally on the mid- or long-term through field monitoring. Furthermore none of the studies above-cited were conducted on tropical areas, thus questioning the ability of the genericity of the models.

This study therefore aimed at adjusting the parameterization of an accumulation model to the specific conditions of the tropical island of la Reunion and validating the model against mid-term field trials.

## Material and Methods

### Modelling

The model formalism based on a mass balance of trace metals inputs and outputs in the upper layer of soil in which organic matter is mixed by ploughing according to Baize [4]. Trace metals concentration,  $C_{st}$ , ( $\text{mg kg}^{-1}$  DW) in the upper soil layer at a given time period (year or cropping cycle) was calculated as follows:

$$C_{st} = C_{st,1} + (I - O) / (10 \rho dp) \quad \text{Eq. (1)}$$

where,  $\rho$ , is the density of soil layer ( $\text{kg m}^{-3}$ ) and,  $dp$ , is the ploughing depth of soil (m).

The trace metals input,  $I$ , ( $\text{g ha}^{-1}$ ), from organic waste ( $I_{ow}$ ), mineral fertilizers ( $I_{mf}$ ), and pesticides ( $I_p$ ) was calculated as follows:

$$I = I_{ow} + I_{mf} + I_p \quad \text{Eq. (2)}$$

Every inputs were calculated as follows:

$$I = A C / 1000 \quad \text{Eq. (3)}$$

where,  $A$ , ( $\text{kg ha}^{-1} \text{ year}^{-1}$ ) is the amount of products added for each cropping cycle and  $C$  ( $\text{mg kg}^{-1}$ ) is the concentration of trace metals in the products.

Trace metals output,  $O$ , ( $\text{g ha}^{-1}$ ) via trace metals uptake by plants  $O_p$  ( $\text{mg kg}^{-1}$ ) and trace metals leaching  $O_l$  ( $\mu\text{g l}^{-1}$ ) to deeper soil layers or the geological material was calculated as follows:

$$O_p = C_p M / (1000) \quad \text{Eq. (4)}$$

and

$$O_l = 10 F Cl \quad \text{Eq. (5)}$$

where,  $C_p$ , is the concentration of trace metals in plants ( $\text{mg kg}^{-1}$ ),  $M$ , is the dry mass of plants ( $\text{kg ha}^{-1}$ ),  $Cl$ , is the concentration of trace metals in soil solution ( $\text{mg m}^{-3}$ ) and,  $F$ , is the precipitation excess (m) that leached down trace metals in soil [5].

#### *Field experiment for model validation*

To validate our model, trace metals concentration in the upper soil layer of three field experiments performed in la Reunion were simulated, and then compared with field measurements. The three field experiments were monitored for seven to eight years and consisted in: (i) five market-garden crops species (i.e. *Brassica oleracea*, *Daucus carota*, *Lactuca sativa*, *Lycopersicon esculentum* et *Phaseolus vulgaris* L.) grown twice a year in an andic cambisol [6] amended with pig slurry compost, poultry litter compost or NPK fertilizer, (ii) a pastureland crop (*Stenotaphrum dimidiatum* L.) grown in an andic cambisol amended or not with pig slurry and (iii) sugarcane (*Saccharum officinarum* L.) grown in a nitrisol [6] amended with pig slurry, rhum vinasse or NPK fertiliser. Cadmium (Cd), copper (Cu), nickel (Ni) and zinc (Zn) concentration were measured at each cropping cycle in the edible organs of plants or in shoots for *S. dimidiatum*, soil and organic wastes and only one time in mineral fertilizer and pesticides. Meteorological station at each site provided one measurement per day of potential evapotranspiration and rainfall (mm).

## **Results and Discussion**

Even if the model was run for Cd, Cu, Ni and Zn, only the results obtained for Zn are presented hereafter.

Calibrations of the model for the field trials with sugarcane and pastureland are currently in progress therefore only calibration of the model for the market-garden crops trials is presented hereafter.

#### *Trace metals concentration in plant*

For the estimation of trace metals uptake by market-garden crops ( $O_p$ ), the relevance of two methodologies was assessed:

- (i) the calculation of the median of the distribution pattern of trace metals concentration in plants measured in the field experiment;
- (ii) the calculation of trace metals concentration in plants using a multi-linear regression model with the following formalism:

$$C_p = a \ln C_{st} + b \text{pH} + c \quad \text{Eq. (6)}$$

where the coefficients  $a$ ,  $b$  and  $c$  were determined either according to Efrogmson et al. [7] (Regression 1) or by developing a specific regression with the field experiment data set (Regression 2).

The application of both regression models 1 and 2 in order to estimate Zn concentration in market-garden crops was not relevant. The distribution pattern of Zn concentration modelled by regression 1 was compared to that of Zn concentration measured in the field experiment (Tab. 1). Computed medians for market-garden crops in regression 1 were  $108 \text{ mg.kg}^{-1}$  in modeled values while ranging from 18 to  $64 \text{ mg kg}^{-1}$  in measured one. On average, values determined by regression 1 were between 2 and 6 times higher those measured. Cu, Ni and Zn concentration in soil of la Réunion are relatively

high but comes from natural pedo-geochemical background. However despite these high concentrations, trace metals mobility and phytoavailability are low [8]. This presumably explain with the regression 1 depicted as a generic equation by Efromson et al. [7] did not work with the specific soil conditions occurring in la Réunion. We attempted to re-parameterize Eq. (6) with filed data. If this regression model (regression 2) was per se able to estimate trace metals concentration in the range of those measured, regression 2 was not able to predict adequately the variability of field measurements even when a regression model was built up independently for each plants species (results not showed). Consequently, we adopted the medians of trace metals concentration in each plants species as the predictor of Cp in the accumulation model.

**Tab 1. Distribution of Zn concentration (mg kg<sup>-1</sup>) in market-garden crops measured or modelled by multiple regressions.**

	Lettuce		Cabbage		Tomato		Carrot		Bean	
	measured	modeled								
Min	34	94	14	94	11	92	14	87	22	64
Q1	52	103	18	101	15	102	20	103	31	101
<b>Med</b>	<b>63</b>	<b>108</b>	<b>20</b>	<b>108</b>	<b>18</b>	<b>108</b>	<b>25</b>	<b>108</b>	<b>35</b>	<b>107</b>
Q3	78	112	25	113	22	112	34	112	38	111
Max	132	122	49	121	43	121	60	121	50	121

#### Trace metals concentration in the soil solution

For the estimation of trace metals leached (*Ol*), the relevance of two methodologies was assessed:

- (i) the calculation of the median of the distribution pattern of trace metals leached measured in the field experiment;
- (ii) the calculation of trace metals leached using a multi-linear regression model with the following formalism:

$$Cp = a \log CTE + b \log SOM + c \text{pH} + d \quad \text{Eq. (7)}$$

where the coefficients a, b and c were determined either according to Sauvé et al. [10] (Regression 3).

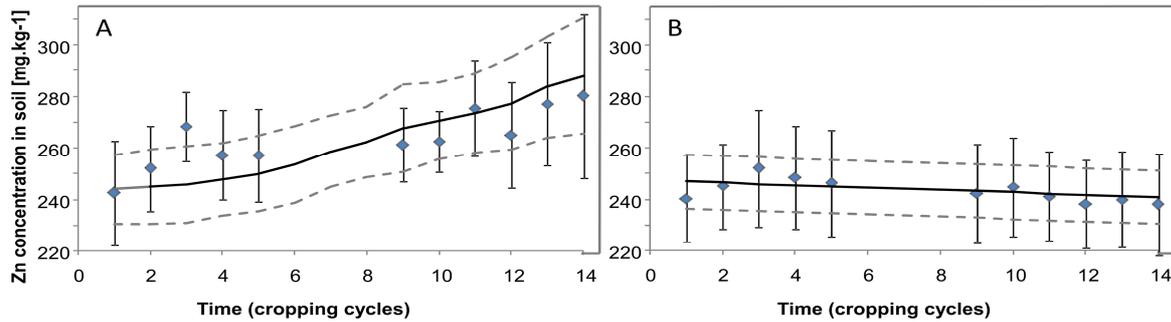
The application of regression 3 in order to estimate Zn concentration in soil solution was not relevant. The distribution of Zn concentration given in regression 3 was compared to that measured in the field experiment (Tab. 2). The median of Zn concentration in solution was equal to 442  $\mu\text{g l}^{-1}$  in regression 3 while it was 111  $\mu\text{g l}^{-1}$  in measured one. On average, modeled values were between 4 times higher than measured ones. Here again, the high pedo-geochemical background in trace metals in the soil of la Réunion associated with a rather low mobility presumably explains that the regressions developed by Sauvé et al. [10] did not work herein. We therefore chose to use the median of trace metals concentration in soil solution as the predictor of trace metals leached.

**Fig 2. Distribution of Zn leached ( $\mu\text{g l}^{-1}$ ) in Colimaçon soil layer measured or modelled**

	Zn leached ( $\mu\text{g l}^{-1}$ )	
	measured	modeled
Min	50	63
Q1	76	178
<b>Med</b>	<b>111</b>	<b>442</b>
Q3	185	574
Max	889	1043

#### Model validation

Using the medians of trace metals concentration in plants and in the soil solution, the adjusted model was run to predict Zn total accumulation in soil of the market-garden crop field experiment. A low but continued increase in Zn concentration in soil amended by the pig slurry compost and the poultry litter compost was observed during the 14 cropping cycles (Fig. 1.A). Soil Zn concentration increased respectively from 242 and 241  $\text{mg kg}^{-1}$  at the beginning of the experiment to 280 and 270  $\text{mg kg}^{-1}$  after the fourteenth cropping cycles. For both amendment modalities, the increase is well predicted by our model, which predicts a concentration of 288  $\text{mg kg}^{-1}$  and 290  $\text{mg kg}^{-1}$  in the soils amended with pig slurry compost and poultry litter compost, respectively, at the end of the experiment. In the soil layer soil amended by mineral fertilizer, Zn concentration tended to slightly decreased from 245 to 240  $\text{mg kg}^{-1}$ . The model simulated pretty well this tendency (Fig. 1.B). These results suggest that the adjusted model would be adapted to the specific climatic and soil conditions of la Réunion.



**Fig. 1** Measured (symbols) or modelled (curve) total Zn concentration ( $\text{mg.kg}^{-1}$ ) in soil layer amended by pig slurry compost (A) or NPK fertilizer (B) during 14 cropping cycles. Values are means of replicates ( $n=4$ ) with bars standing for standard error for measured values and dashed curve standing for standard error for modeled values.

## Conclusion and perspectives

We validate our model against a mid-term field trial with market-garden crops in the specific climatic and soil conditions of la Réunion. The adjustment of our model with specific data from the field experiment avoided the overestimation of trace metals output from trace metals uptake by plants or trace metals leached and thus the underestimation of total trace metals accumulation on the soil layer. Our adjusted model will be also assessed soon for two additional field experiments representative of agricultural practices in la Réunion. After this validation step, the model could be applied to compare different scenarios of organic wastes recycling at the island scale and to further assess the ecotoxicological issue of trace metals accumulation in agricultural soils on a long-term perspective.

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