Empirical knowledge to improve terrestrial ecotoxicity characterisation of trace elements with USEtox

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Abstract

USEtox is the consensus model for toxicity in LCA, yet it does not provide characterisation for terrestrial ecotoxicity. Owsianiak et al. (2013) suggested a new framework able to account for soil physical-chemical properties to characterise terrestrial ecotoxicity for trace elements. The performance of this USEtox-based Owsianiak framework was herein tested in the context of soil contamination by copper (Cu) and zinc (Zn) following the application of livestock faeces. To do so, one French soil sample exhibiting properties representative of the main average properties of European soils was incubated under laboratory controlled conditions alone or with the application of 31 swine or poultry faeces collected from experimental pens where livestocks was fed with different rate of Cu and Zn complements. The main endpoints of Cu and Zn availability in soils calculated in the Owsianiak framework were determined analytically on each of the 32 experimental treatments, namely: i) reactive Cu and Zn extracted with 0.43 M HNO_3, ii) total Cu and Zn in extracted soil solutions, and iii) free ionic Cu and Zn in extracted soil solutions. The single value for the intermediate endpoints (i.e. fate, accessibility, bioavailability, and effect factors) and the comparative toxicity characterisation factor calculated with the Owsianiak framework for Cu using the initial soil properties were within the range of values computed by Owsianiak et al. for a variety of global soils, thereby validating the hypothesis about the representativeness of the chosen soil. From an experimental point of view, the application of swine and broiler faeces to the soil induced substantial changes in soil pH and dissolved organic carbon concentration compared to the non-amended control soil. These chemical alterations of soil solution chemistry in faeces-amended soils induced a significant decrease of Cu^{2+} activity for 19 out of 31 faeces compared to the non-amended soil. These observed variations suggests consequently that intermediated endpoints determined for each experimental treatment will likely show some discrepancies with those determined theoretically with the Owsianiak framework, thereby opening the discussion to suggest some potential improvements.

Keywords: bioavailability; exposure; fate; speciation; trace metals

Introduction

Organic waste (OW) is increasingly being used as a source of nutrients for crops and organic matter for soils, via agricultural recycling. OW-borne contaminants, including trace elements (TE), are transferred to soils when OW is spread. Once in the soil, the fate of TE depends on several factors, which include its original chemical forms (i.e. speciation) in OW which itself depends on the treatment (e.g. composting, anaerobic digestion, storage) OW may undergo before spreading and the soil physical-chemical properties (e.g. pH).

USEtox is the consensus model for toxicity in LCA, yet it does not provide characterisation for terrestrial ecotoxicity, due to the complexities of its modelling, the paucity of terrestrial toxicity data, and other constraints (e.g. the concentration threshold for considering a TE as a contaminant or as a micronutrient). USEtox research has contributed evolving models for the estimation of terrestrial ecotoxicity (e.g. Owsianiak et al. 2013; Plouffe et al. 2016).

In such context, the SUMINAPP project (https://www.suminapp.eu/) produced empirical research on the fate and bioavailability (two key elements for the characterisation of trace elements in USEtox), and integrated the results within the Owsianiak et al. (2013) approach to i) validate it and reduce the uncertainty of its results by comparison with experimental characterisations, and ii) identify neglected mechanisms that should be integrated in a future terrestrial ecotoxicity framework.

Material and methods

Two strategies were followed. First, the USEtox-based Owsianiak et al. (2013) framework (comparative toxicity = fate x exposure[= accessibility x bioavailability] x effect) was applied to measured data from a specific soil from the French Qualiagro experimental site (Noirot-Cosson et al. 2016), which physical-chemical properties compatible with those of the "standard" USEtox soil.

Second, the predicted constituencies of the comparative toxicity characterisation factor were contrasted with results from laboratory tests on the Qualiagro soil. The soil was incubated for 26 d under laboratory controlled conditions alone (i.e. the non-amended soil) or with 31 animal faeces (see Tella et al. (2016) for experimental details). The faeces consisted of swine (8 and 11 from pigs and piglets, respectively) or broiler (7) faeces sampled from experimental pens where alternative dietary (i.e. Cu and Zn feed complements) treatments and an aging process (with or without) were tested.

The main endpoints of Cu and Zn availability in soils calculated in the Owsianiak framework were determined analytically on each of the 32 experimental treatments, namely: i) reactive Cu and Zn extracted with 0.43 M HNO_3, ii) total Cu and Zn in extracted soil solutions, and iii) free ionic Cu and Zn in extracted soil solutions as measured for Cu with an ion selective electrodes or estimated for Zn by modelling using WHAM (Tipping et al. 2011) and chemical properties measured in soil solutions.

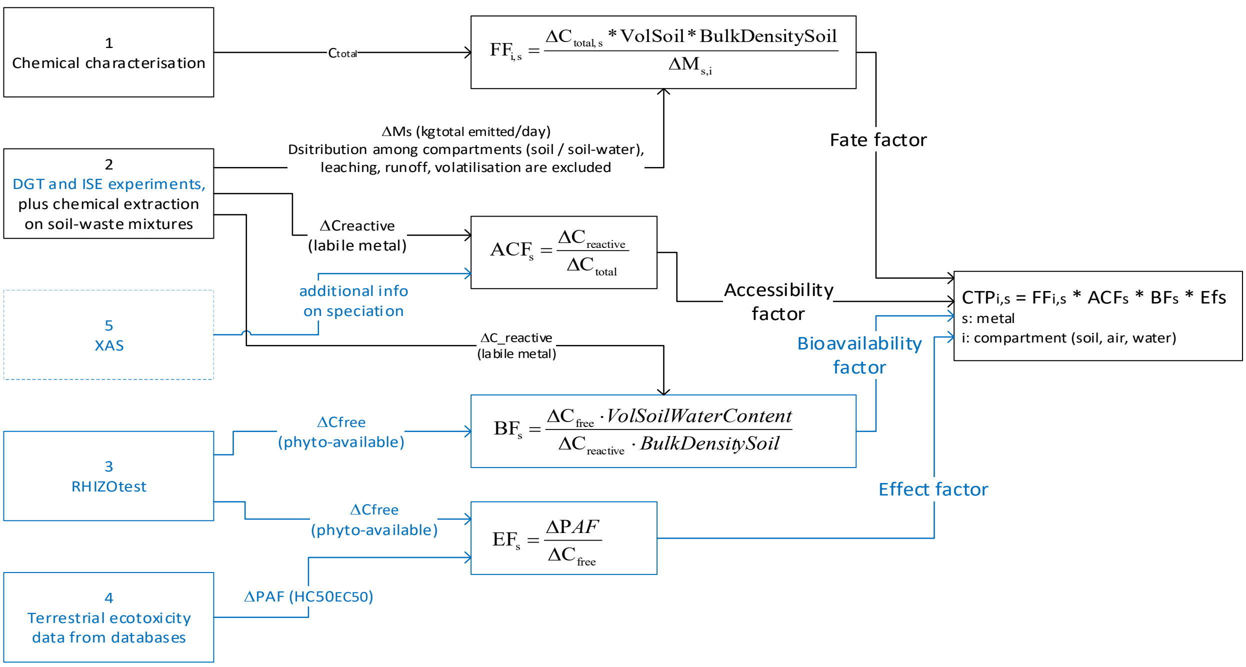

Fig. 1. Data sources to inform terrestrial ecotoxicity of trace elements with USEtox (elements in blue represent work in progress)

Consequently, the intermediate endpoints (i.e. fate, accessibility, bioavailability, and effect factors) and the comparative toxicity characterisation factor calculated with the Owsianiak framework for Cu and Zn using the initial and fixed soil properties was compared to those determined on each of the 32 experimental treatments. Fig. 1 summarises the different ecotoxicity determination elements.

We implemented the Owsianiak approach in Excel, and were able to compute predicted values for the comparative toxicity characterisation factors for Cu and Zn using Qualiagro soil characteristics.

Results and discussion

The application of swine and broiler faeces to the Qualiagro soil induced substantial changes in the solution chemistry and Cu and Zn availability of soils compared to the non-amended soil (Fig. 2). Soil pH tended to either increase or decrease with the application of 13 out of 31 faeces, with a significant increase observed for three aged pig faeces (Fig. 2a). Soil DOC increased significantly for all faeces applications compared to the non-amended soil and up to four-fold with some piglet faeces applications (Fig. 2b). These chemical alterations of soil solution chemistry in faeces-amended soils induced a significant decrease of Cu^{2+} activity for 19 out of 31 faeces compared to the non-amended soil. All these modifications of chemistry and Cu speciation in the solution of faeces-amended soils were in agreement with recent results obtained under realistic field conditions (Laurent et al. 2020). Accordingly, this experiment seems adequate to evaluate the robustness of the USEtox-based Owsianiak framework in the context of OW-amended soils.

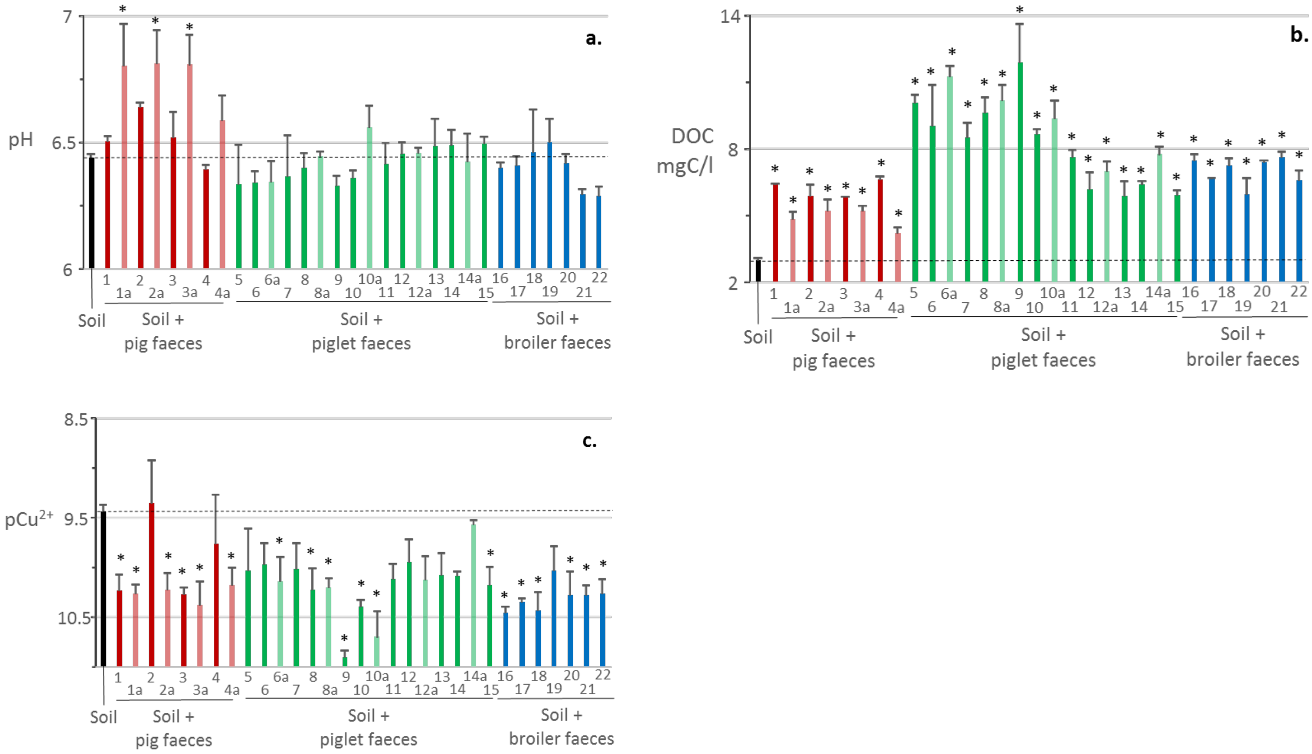

Fig. 2. Acidity (pH, a.), dissolved organic carbon (DOC) concentration (b.), and free ionic copper activity (pCu^{2+}, c.) measured in the non-amended soil (soil) and in the soil amended with 31 swine or poultry faeces. Some faeces were aged (a). Dashed lines correspond to the mean value measured in the control. Stars correspond to faeces applications that had a significant effect (ANOVA with Fisher, then HSD Tuckey tests; $p \leq 0.05$) on pH, DOC, and pCu^{2+} compared to the control soil

The characterisation factors computed with the Owsianiak approach by using the initial and fixed soil properties are within the range of values computed by Owsianiak et al. for a variety of soils all around the world (Fig. 3). These results consequently support the hypothesis about the representativeness of the chosen soil as compared to the world soil database considered by Owsianiak et al. (2013) when implementing its new USEtox framework.

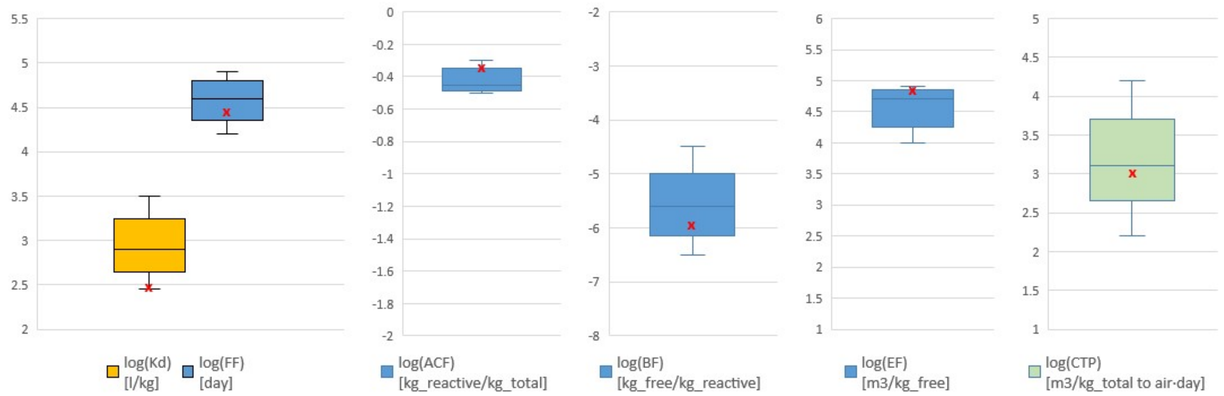

Fig. 3. Range of results obtained by Owsianiak et al. (2013) vs. our computed values (x) for Cu using the Qualiagro soil (no reference results were available for Zn)

Perspectives

Due to COVID19-related delays, the final part of the dataset on soil Cu and Zn availability has not to date been statistically treated. However, the results already treated showed that the application of livestock faeces to soil induced substantial changes in the chemistry and Cu speciation of soil solutions compared to the non-amended soil. These variations thus suggests that fate, accessibility, and bioavailability factors determined for each experimental treatment will likely show some discrepancies with those determined theoretically with the Owsianiak framework. Once the last experimental data will be treated, the whole dataset will be used to compare the CTP of the default Owsianiak framework results with the 32 CTPs based on measured values of total Cu and Zn concentration in soil solution as the main parameter used to compute the fate factor, of reactive Cu and Zn concentration in soil as the parameter used to compute the accessibility factor, and of Cu^{2+} and Zn^{2+} activity as the main parameter used to compute the bioavailability factor. Such results would enable us to open the discussion for suggesting some potential improvements of the Owsianiak framework.

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