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Auteurs: Ivan Viveros Santos, Annie Levasseur, Cécile Bulle, Louise Deschênes, & Anne-Marie Boulay

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Modelling the influence of climate change on characterization factors for copper terrestrial ecotoxicity

Ivan Viveros Santos ^{a,*}, Annie Levasseur ^b, Cécile Bulle ^c, Louise Deschênes ^a, Anne-Marie Boulay ^a

^a CIRAIG, Chemical Engineering Department, Polytechnique Montréal, P.O. Box 6079, Montreal, QC H3C 3A7, Canada

^b Department of Construction Engineering, École de Technologie Supérieure, 1100 Notre-Dame Ouest, Montreal, Quebec H3C 1K3, Canada

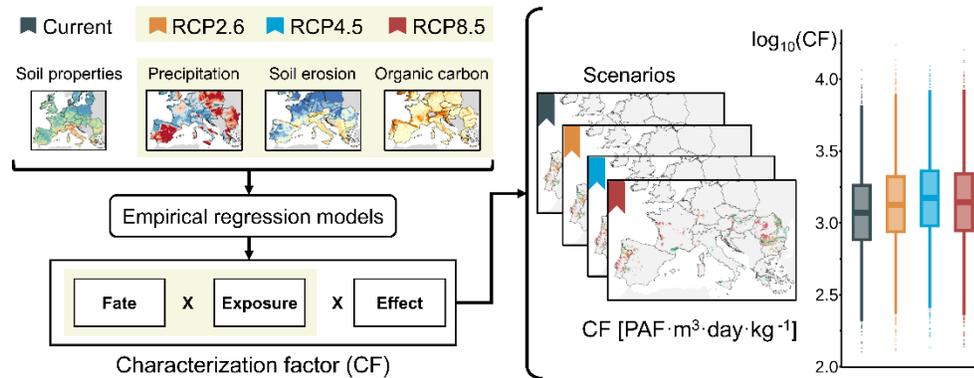
^c CIRAIG, ESG UQAM, Strategy, Corporate & Social Responsibility Department, Montreal, QC H3C 3P8, Canada

* Corresponding author: E-mail address: ivan.viveros-santos@polymtl.ca

Abstract

The use of copper-based preparations is a long-standing practice in viticulture to control vine fungal diseases, which has led to high copper concentrations in vineyard soils and impacts on off-target terrestrial organisms. Under projected climate change, some of the mechanisms and properties of soils that influence the extent of metals ecotoxicity impacts are projected to be altered, namely soil erosion, rainfall, temperature, and organic carbon content. In this context, and within the framework of life cycle assessment, this study aims to simulate the influence of projected changes in soil organic carbon, soil erosion, and rainfall on characterization factors (CFs) for copper terrestrial ecotoxicity across non-calcareous European vineyard soils. We employed empirical regression models to account for metal speciation and bioavailability as determined by soil characteristics. CFs were computed for a current scenario and mid-term future scenarios by 2050 determined across three Representative Concentration Pathways (RCP2.6, RCP4.5, and RCP8.5). Although future scenarios suggest that CFs may either increase or decrease, CFs are projected to increase for a larger share of the European vineyard surface, which may lead to higher terrestrial ecotoxicity impacts. The RCP4.5 scenario projects the highest increases in CFs, with a 27% rise in the median CF in comparison with the current scenario. Whereas the RCP8.5 and RCP2.6 scenarios project a 19% and 14% increase in median CFs, respectively. The changes in CFs were determined principally by the changes in copper bioavailability driven by projected changes in soil organic carbon. However, the spatial variability of CFs was larger than the temporal variation, with a variation of roughly 2 orders of magnitude across the analyzed scenarios. This study highlights the relevance of integrating spatial

differentiation and the influence of projected climate change in the characterization modelling of copper terrestrial ecotoxicity.



Keywords: Life cycle impact assessment, terrestrial ecotoxicity, speciation, climate change, regionalization, interactions.

Highlights:

- Method accounting for the interaction of climate change and terrestrial ecotoxicity.
- Neglecting the influence of projected climate change potentially underestimates copper terrestrial ecotoxicity.
- Projected changes in soil organic carbon content control changes in future CFs.

1. Introduction

Copper-based fungicides are widely used in organic and conventional viticulture to control fungal diseases, namely downy mildew (*Plasmopara viticola*) (Droz et al., 2021). Initiated in the late 19th century, the use of copper-based fungicides is a long-standing practice in viticulture, because of the high effectiveness of copper under rainy conditions and its relatively low market cost (Tamm et al., 2022). The application rate and timing of copper-based fungicides are closely related to hydroclimatic conditions, agricultural practices, vine variety, and policies (Droz et al., 2021). An average fungicide application rate of 8.1 kg·ha⁻¹ has been estimated by Panagos et al., (2018) for permanent crops (among which viticulture), which is higher than that for arable land (0.54 kg·ha⁻¹) (Panagos et al., 2018) and higher than the maximum application rate established by the European Union regulations (4 kg·ha⁻¹) (Droz et al., 2021). The continuous application of copper-based fungicides has led to high copper content in vineyard soils in comparison with other land uses (Ballabio et al., 2018a; Droz et al., 2021), leading to impacts on terrestrial and aquatic organisms (Bart et al., 2017; Fernández et al., 2015; Ruyters et al., 2013).

Life Cycle Assessment (LCA) is a holistic method to evaluate the potential environmental impacts related to a product or service across its entire life cycle from resource acquisition to its end of life (ISO, 2006a, 2006b). In the context of LCA, the impacts on terrestrial and aquatic organisms resulting from the emissions of chemicals are evaluated under the ecotoxicity impact category (Fantke et al., 2017; Peter Fantke et al., 2018). LCA studies on wine production have reported copper as the dominant contributor to the ecotoxicity impacts due to the application of copper-based fungicides in viticulture (Falcone et al., 2016; Vázquez-Rowe et al., 2012). Nevertheless, the high contribution of metals to ecotoxicity impacts is not restricted to viticulture. A study addressing the question as to whether the inclusion of speciation (i.e., the different pools of metal in soil) changes the rank contribution of metals to terrestrial ecotoxicity assessed roughly 13000 unit processes of the ecoinvent database employing three life cycle impact assessment methods. The authors concluded that even when metal speciation is integrated into the characterization of terrestrial ecotoxicity, metals remain the main contributors to this impact category and that the difference

in results among different impact methods is explained by variations in the coverage of chemicals (Sydow et al., 2020).

Recent efforts in LCA were devoted to enhancing the assessment of metals ecotoxicity-related impacts by including metal speciation in the computation of characterization factors (CFs) (Dong et al., 2014; Gandhi et al., 2010; Owsianiak et al., 2013; Plouffe et al., 2016). Within LCA, CFs are applied to convert and aggregate life cycle inventory interventions (i.e., emissions or resource consumption) into scores of potential impacts. Regarding terrestrial ecotoxicity, two main methodological frameworks have been developed to derive CFs including metal speciation driven by soil properties. One method employed empirical regression models to compute the different pools of metal in soil (Owsianiak et al., 2013), whereas a second approach used the geochemical speciation model WHAM 6.0 for the same purpose (Plouffe et al., 2016). Both methodological approaches break down the CF into a fate factor (FF) describing the distribution of the substance in the environment, a bioavailability factor (BF) corresponding to the fraction of the total metal that is available for uptake by organisms, and an effect factor (EF) representing the potentially affected fraction of species (PAF) by the available metal pool (Owsianiak et al., 2013; Plouffe et al., 2016). Owsianiak et al., (2013) also introduced an accessibility factor (ACF) in the computation of CFs, which represents the fraction of reactive metal over total metal. In consequence, the BF is expressed by the fraction of free ions of the reactive metal in soil. Moreover, Owsianiak et al., (2013) derived a multiple linear regression (MLR) for the calculation of CFs for copper, with soil organic carbon being the controlling factor due to its influence on metal fate. Besides, the proposed MLR was shown to be improved by integrating soil pH, which influences metal bioavailability. In addition, it has been reported that the key factors explaining 45% of the copper content in European vineyards are precipitation, aridity, and soil organic carbon (Droz et al., 2021).

In the context of copper-based fungicides use in viticulture, subsequent studies derived CFs for copper terrestrial ecotoxicity including metal speciation (Peña et al., 2018; Villanueva-Rey et al., 2019; Viveros Santos et al., 2018). Peña et al. (2018) and Viveros Santos et al. (2018) computed site-dependent CFs for non-calcareous soils, that is, CFs at a relatively low spatial resolution inherited from the Harmonized World

Soil Database, which is a 30 arc-second raster database. However, both studies aimed at computing CFs for large geographical areas. Peña et al. (2018) concentrated on European vineyards and found a spatial variability of CFs over 1.5 orders of magnitude. Viveros Santos et al. (2018) focused on non-calcareous soils of the world and reported a spatial variability of CFs derived with WHAM 6.0 of 5.5 orders of magnitude. On the other hand, Villanueva-Rey et al. (2019) calculated spatially differentiated CFs for wine-growing regions in Northern Spain and Portugal and found a spatial variability of 1.6 orders of magnitude between the lowest and highest value of CFs.

There is a growing interest in assessing future-oriented scenarios employing LCA to foresee the potential environmental impacts of new technologies and products (Bisinella et al., 2021; Sacchi et al., 2022), or to evaluate them under projected environmental conditions altered by climate change (Sala et al., 2017). Particularly, since agriculture is highly dependent on climate, some LCA studies have addressed the potential impact of projected climate change on the environmental performance of some crops, namely corn, soybean, spring barley, and wine grapes (Cosme and Niero, 2017; Garba et al., 2014; Lee et al., 2020; Viveros Santos et al., 2023). These studies simulated the impact of climate change at the life cycle inventory level, considering the variation of crop yield due to climate and extreme events, as well as changes in agricultural practices such as the application rate of pesticides and fertilizers. However, it is expected that the fate, exposure, and effect of pollutants will be altered under future environmental conditions (Noyes and Lema, 2015; Stahl Jr. et al., 2013). In this regard, research has been conducted to develop CFs under future scenarios. For instance, CFs for assessing water use-related impacts were developed to integrate the impact of climate change on water availability in near- and mid-term future scenarios in Spain. It was found that future decreases in water withdrawals compared to the current situation would lead to lower impacts related to freshwater resources accessibility (Núñez et al., 2015). Moreover, CFs for marine eutrophication were parameterized to simulate the influence of projected environmental conditions on the fate, exposure, and effect of nitrogen emissions. While the effect factors are projected to increase by around 7% for marine eutrophication, the decreases in fate and exposition factors will result in a decrease in CFs of around 22% by 2050 for the North Sea and Baltic Sea (Cosme and Niero, 2017).

The terrestrial ecotoxicity of metals is site-dependent owing to the influence of soil properties and climate conditions on metal speciation (Owsianiak et al., 2013; Plouffe et al., 2016). Besides, some soil properties and mechanisms that affect the ecotoxicity impact of metals such as organic matter, moisture, rainfall, microbial activity, and soil erosion are susceptible to climate change (Biswas et al., 2018; Fu et al., 2018; Noyes and Lema, 2015; Pham et al., 2021). Projected soil erosion rates indicate a potential increase of 13% to 22.5% by 2050 compared to the current situation in Europe (Panagos et al., 2021), which might increase the runoff of contaminants (Biswas et al., 2018), and of particular concern in sloping vineyards (Pham et al., 2021). Moreover, projected changes in the frequency and intensity of rainfall will also impact the runoff and leaching of pollutants (Biswas et al., 2018). In addition, the projected changes in soil organic carbon (SOC) may modify the mobility of copper in vineyard soils, which will vary spatially given that projections indicate increases in SOC stocks in some parts of Europe by 2050, but also point to decreases principally in southern Europe (Droz et al., 2021; Yigini and Panagos, 2016). Some studies have also reported the adverse effects of increasing air temperature and drier conditions on the performance of soil invertebrates in metal-polluted soils. Still, the authors stressed the need to conduct more research to disentangle the effect of changing environmental conditions on species sensitivity from induced changes in metal speciation (Fu et al., 2018; González-Alcaraz and van Gestel, 2016).

Given that some soil properties and mechanisms affecting the fate, mobility, and bioavailability of metals in soils are projected to change under future environmental conditions, as derived from climate change scenarios, the purpose of this exploratory study is to simulate the influence of expected changes in soil organic carbon, soil erosion rates, and precipitation on future CFs for copper terrestrial ecotoxicity. Sets of CFs were calculated for current and mid-term future scenarios by 2050. The latter scenarios were based on projections of the above-mentioned parameters derived according to the Global Climate Model (GCM) IPSL-CM5A-LR across three Representative Concentration Pathways (RCP2.6, RCP4.5, and RCP8.5). This study addresses both the spatial and temporal dimensions of the characterization modelling of copper terrestrial ecotoxicity. Hence, on the one side, this study contributes to the ongoing efforts in LCA to account for spatially differentiated impacts. On the other side, it provides CFs for studies that aim

to assess the environmental impacts of product systems under future scenarios, which is particularly relevant to agricultural systems. Furthermore, this study proposes an approach to account for the interaction of impact categories, which are normally characterized independently in the framework of LCA.

2. Methods

2.1. Study area and temporal scenarios

The study area corresponds to the European vineyard surface (Figure A1b), representing approximately 26% of land dedicated to permanent crops and 1.7% of the total agricultural land of the European Union. The European vineyard area is defined by a layer retrieved from the CORINE Land Cover project of the European Environment Agency (2017) (Figure A1b). Despite the low share of agricultural land under vineyards, a large amount of copper-based fungicides sold in the EU is used extensively in permanent crops (vineyards, olive groves, and fruit trees). Furthermore, in the EU, vineyard soils have the highest median copper concentration ($26.09 \text{ mg}\cdot\text{kg}^{-1}$) in comparison to other land uses ($11.58 \text{ mg}\cdot\text{kg}^{-1}$) (Figure A1) (Ballabio et al., 2018b).

To assess the effect of projected changes in soil organic carbon, soil erosion rates, and precipitation on the characterization modelling of copper terrestrial ecotoxicity, CFs were computed for two temporal scenarios:

- Current scenario: A scenario based on historical or recent datasets of climate and soil properties to determine CFs for the current state of the environment. This is a common practice in environmental modelling, namely in LCA (P. Fantke et al., 2018; Kounina et al., 2014) and environmental risk assessment (Stahl Jr. et al., 2013) to evaluate the potential environmental impacts of emissions.
- Midterm future scenario: A prospective scenario by 2050, according to data availability on projections of soil organic carbon, soil erosion rates, and precipitation. Moreover, the selected time horizon is aligned with the 20-year midterm period (2041-2060) defined by the Intergovernmental Panel on Climate Change (IPCC) to project the impact of climate change (IPCC, 2021).

Based on available data, we considered projections of soil organic carbon, soil erosion rates, and precipitation according to three Representative Concentration Pathways (RCP) spanning from the trajectory of ambitious greenhouse gas (GHG) emissions mitigation (RCP2.6) to the less aggressive one (RCP8.5) and including an intermediate trajectory of GHG emissions mitigation (RCP4.5).

2.2. Characterization factors for copper terrestrial ecotoxicity

The characterization model for metals terrestrial ecotoxicity utilized in this study is based on a methodological framework that employs multiple linear regressions to compute metal speciation and bioavailability in soil (Owsianiak et al., 2013). According to Equation 1, the characterization factor $CF_{i,s}$ ($\text{PAF} \cdot \text{m}^3 \cdot \text{day} \cdot \text{kg}_{\text{total emitted}}^{-1}$) of total metal s emitted to the environmental compartment i is composed of a fate factor $FF_{i,s}$ (day) for total metal s in soil, an accessibility factor ACF_s ($\text{kg}_{\text{reactive}} \cdot \text{kg}_{\text{total}}^{-1}$) that expresses the fraction of reactive metal over total metal s in soil, a bioavailability factor BF_s ($\text{kg}_{\text{free}} \cdot \text{kg}_{\text{reactive}}^{-1}$) that quantifies the free ion fraction of the reactive metal s in soil, and an effect factor EF_s ($\text{PAF} \cdot \text{m}^3 \cdot \text{kg}_{\text{free}}^{-1}$) that represents the potentially affected fraction (PAF) of soil organisms by the free ion metal in soil.

$$CF_{i,s} = FF_{i,s} \cdot ACF_s \cdot BF_s \cdot EF_s \quad (1)$$

In line with previous studies that derived CFs for metals terrestrial ecotoxicity (Owsianiak et al., 2013; Peña et al., 2018; Villanueva-Rey et al., 2019; Viveros Santos et al., 2018), we applied the methodological approach based on empirical regression models to account for metal speciation and bioavailability in soil; since the purpose of our study was to calculate the relative impact of projected changes in soil organic carbon, soil erosion rates, and precipitation on future CFs for copper terrestrial ecotoxicity. We assumed that the relative change in characterization factors between current and future scenarios would be in the same range regardless of the methodological framework used to calculate them. Besides, using empirical regression models streamlined computing CFs for copper terrestrial ecotoxicity according to the format (raster) of the available layers of soil properties for both current and future scenarios (2.5.4). In section A2

of the supplementary materials, we present the empirical regression models used for calculating the different pools of copper in soil (metal speciation) and the equations for computing the different intermediate factors of Equation 1.

To integrate the effect of expected changes in soil properties and climatic conditions altered by climate change on future CFs for copper terrestrial ecotoxicity, we used projections of soil organic carbon, soil erosion rates, and precipitation. The selection of these parameters is justified by their influence on the fate and bioavailability of metals in soil (Droz et al., 2021; Owsianiak et al., 2013). The projected changes in parameters were integrated into the computation of CFs for copper terrestrial ecotoxicity employing empirical regression models. Table 1 summarizes the influence of the parameters affected by climate change on the intermediate factors of CFs (as per Equation 1).

Table 1. Changes that were introduced in the characterization modelling to simulate the influence of projected environmental conditions on CFs for copper terrestrial ecotoxicity.

Parameter influenced by projected climate change (source)	Affected parameter	Equation (Model)	Affected factor of Equation 1
Projections of soil erosion (Panagos et al., 2021)	Transfer rate from soil to freshwater	Equation A1 (USEtox)	FF _{i,s}
Projections of precipitation (Fick and Hijmans, 2017; Petrie et al., 2021)	Transfer rate from soil by leaching	Equation A1 Equation A2 (USEtox)	FF _{i,s}
Projections of soil organic matter (Yigini and Panagos, 2016)	Cu _{total dissolved} K _d	Equation A7 Equation A10 (USEtox)	FF _{i,s}
	Cu _{reactive}	Equation A6	ACF _s , BF _s
	Cu _{free}	Equation A8	BF _s

Fate factors of copper in agricultural soil (FF_{i,s}) were computed for a direct emission to this compartment using USEtox, the UNEP/SETAC scientific consensus multimedia model for characterizing

the (eco)toxicological impacts of chemicals in LCA (Fantke et al., 2017). USEtox considers a steady-state modelling framework for resolving the mass balance of pollutants in the different environmental compartments included in its nested model. Accordingly, in this study, the fate factors of copper were derived for a direct emission of 1 kg/day of copper to agricultural soil. The landscape parameters of USEtox were modified to account for current and projected values of soil erosion rates and average annual precipitation. Moreover, we considered soil-water partitioning coefficients (K_d) computed for each mapping unit according to Equation A10. K_d ($L \cdot kg^{-1}$) is the ratio of the total soil metal content ($mg \cdot kg^{-1}$) and the total dissolved metal concentration ($mg \cdot L^{-1}$). In USEtox, K_d is a substance-specific parameter required for computing the fate of metals in soil, because it influences runoff from soil (Equation A1) and leaching to deeper soil layers (Equation A2) (Fantke et al., 2017). In section A1.2 of the supplementary materials, we present a preliminary sensitivity analysis of fate factors to partitioning coefficients, average annual precipitation, and soil erosion, as computed with USEtox. This brief sensitivity analysis aimed to confirm that USEtox allows accounting for changes on average annual precipitation, soil erosion, and partitioning coefficients in fate factors for copper emissions.

In the computation of future CFs for copper terrestrial ecotoxicity, soil organic carbon, soil erosion rates, and precipitation were the only parameters that we considered as influenced by climate change in the future, whereas other soil properties were considered constant. The latter assumption is in line with the studies that generated maps of projected SOC stocks and soil erosion rates (Panagos et al., 2021; Yigini and Panagos, 2016). Soil pH influences metal speciation and this soil property is also vulnerable to changing environmental conditions driven by climate change. Nonetheless, the dynamic of pH in the soil is moderate in comparison to other environmental compartments such as freshwater and the ocean, because of the buffer effect of soil minerals. Yet, in some circumstances such as those of increased rainfall, soil pH may be altered due to the leaching of basic cations, leading to acidic soils (Biswas et al., 2018). However, to the best of our knowledge, there are no projections on future soil pH estimated according to environmental conditions influenced by climate change. Furthermore, the temporal resolution of USEtox hinders the modelling of time-specific events such as heavy rainfall.

The EFs ($\text{PAF} \cdot \text{m}^3 \cdot \text{kg}_{\text{free}}^{-1}$) were computed following the USEtox approach, as per Equation 2, where ΔPAF is the incremental change in the potentially affected fraction of species (PAF) per free ion concentration in soil (ΔC_{free}), $\text{HC50}_{\text{EC50}}$ is the geometric mean of distinct median effective concentration (EC_{50}) values, that is the concentration that leads to an observed effect in 50% of organisms (P. Fantke et al., 2018). In keeping with previous studies addressing the calculation of CFs for metals terrestrial ecotoxicity (Owsianiak et al., 2013; Viveros Santos et al., 2018), terrestrial biotic ligand models (TBLMs) were employed to compute EC_{50} of six different endpoints (Table A2) (Thakali et al., 2006). TBLMs have been considered an adequate method to compute site-dependent EFs including metal speciation, but their range of applicability is limited to non-calcareous soils. The TBLMs for computing EC_{50} values for copper take as parameters the activities of hydrogen and magnesium. The latter parameter was computed following the modelling of cation exchange described in Owsianiak et al., (2013). Hydrogen and magnesium activities were considered constant; therefore, for a given mapping unit, the EF is the same for both current and future scenarios. The use of TBLMs allowed integrating metal speciation and bioavailability but precluded including the effect of changes in temperature on the extent of effect factors. However, it is still challenging to disentangle the influence of changing environmental conditions on species sensitivity from the changes caused by modifications of metal speciation (Fu et al., 2018; González-Alcaraz and van Gestel, 2016). The inclusion of ACFs and BFs in the computation of future CFs permitted to consider the influence of changes in organic matter content on bioavailability, but the potential impact of changing temperature on the sensitivity of terrestrial organisms was not included.

$$EF = \frac{\Delta PAF}{\Delta C_{\text{free}}} = \frac{0.5}{\text{HC50}_{\text{EC50}}} \quad (2)$$

2.3. Analysis and attribution of the changes in characterization factors

Projected changes in CFs ($\Delta\text{CF}_{\text{I,S}}$) can be associated with the changes in FFs, ACFs, and BFs according to the derivative of Equation 1:

$$\begin{aligned}\Delta CF_{i,s} &= \frac{dCF_{i,s}}{dFF_{i,s}} \Delta FF_{i,s} + \frac{dCF_{i,s}}{dACF_s} \Delta ACF_s + \frac{dCF_{i,s}}{dBF_s} \Delta BF_s + \frac{dCF_{i,s}}{dEF_s} \Delta EF_s \\ &= ACF_s \cdot BF_s \cdot EF_s \cdot \Delta FF_{i,s} + FF_{i,s} \cdot BF_s \cdot EF_s \cdot \Delta ACF_s + FF_{i,s} \cdot ACF_s \cdot EF_s \cdot \Delta BF_s\end{aligned}\quad (3)$$

where $FF_{i,s}$, ACF_s , and BF_s are the corresponding values of these intermediate parameters for the current scenario; Δ represents the projected changes in intermediate parameters compared to the current period, and the EF was assumed constant for a given mapping unit. The largest term on the right side in Equation 3 would be interpreted as the dominant factor in $\Delta CF_{i,s}$.

2.4. Spatial differentiation of characterization factors

To evaluate the influence of spatial differentiation and facilitate their use by LCA practitioners, the computed CFs for copper terrestrial ecotoxicity at the native resolution of 500 m were aggregated into three lower spatial resolutions: wine-growing regions, European regions, and European countries. The spatial differentiation at the level of wine-growing regions allows using site-dependent CFs in cases where the site of emission is known. The second spatial differentiation considered was at the level of European regions, which are defined by the NUTS2 level. The NUTS classification (Nomenclature of Territorial Units for Statistics) corresponds to the European Union system for defining administrative units at different spatial levels, namely countries, regions, provinces, and municipalities (European Commission, 2022). The spatial differentiation at the level of European regions was chosen since it is frequently employed for formulating policies, in addition, several environmental indicators have been reported at this scale (Ballabio et al., 2018a; Panagos et al., 2021, 2018). The spatial differentiation at the country level was considered because the available datasets from life cycle inventory databases are generally at this level, which may simplify connecting spatialized elementary flows to regionalized CFs (Patouillard et al., 2020).

While some impact methods in LCA, such as IMPACT World+, recommend aggregating CFs at native resolution into lower spatial resolution based on emission or extraction data as a proxy for the probability of emissions or extractions occurring in a given point of space (Bulle et al., 2019), we performed the aggregation according to an area-weighted average (Equation 4). The reason for this modelling choice is

the lack of detail on sales of fungicides per category (Panagos et al., 2018). Still, European vineyards rely heavily on copper-based fungicides (Ballabio et al., 2018a; Droz et al., 2021). Moreover, the aggregation criterium used in this study is consistent with previous studies that computed CFs for copper terrestrial ecotoxicity (Villanueva-Rey et al., 2019; Viveros Santos et al., 2018). In Equation 4, CF_i is the characterization factor of the overlapped vineyard soil i , and A_i represents the surface of vineyards within a given aggregation region (wine-growing regions, NUTS2, or country). The aggregations of CFs at different spatial resolutions were performed using the R package *exactextractr* (Baston, 2020).

$$CF_{area-weighted\ average} = \frac{\sum_{i=1}^n CF_i \cdot A_i}{\sum_{i=1}^n A_i} \quad (4)$$

2.5. Data source

2.5.1. Current and future soil organic matter in Europe

Current (2010) and future (2050) soil organic carbon (SOC) stocks in Europe were obtained from the study by Yigini and Panagos (2016), through the European Soil Data Centre (ESDAC) (Panagos et al., 2012). The map of current SOC stocks was derived utilizing the regression kriging geostatistical technique, which relied on 22,300 soil samples (0-20 cm) from the LUCAS Topsoil Database and data on terrain, climate, land cover use, and other soil properties, namely soil texture and available water capacity as environmental predictors (Yigini and Panagos, 2016). Regarding the projections of future SOC stocks, the researchers hypothesized that, by 2050, soil organic carbon is controlled primarily by climate, land cover, and inherent soil properties. Accordingly, maps of future SOC stocks were derived by using the fitting regression derived from the base model and projections of climate and land cover. The researchers acknowledge that soil organic carbon content is driven predominantly by the balance between net primary production (NPP) from vegetation and the degradation rate of organic matter. Nevertheless, it is projected that climate change will affect SOC levels in the long term, whereas the impact of land-use change and land management practices will have a greater impact in the short term (Yigini and Panagos, 2016).

The projections of SOC are available according to four global climate models (GCMs) and four RCP scenarios. Since the main purpose of our study is to compute the relative magnitude of change in CFs for

copper terrestrial ecotoxicity, we considered the projected SOC stocks derived from the GCMIPSL-CM5A-LR, in line with a previous study that addressed the impact of climate change on the environmental performance of viticulture (Viveros Santos et al., 2023). Besides, to assure consistency across the parameters influenced by climate change considered in this study, we selected the projections under the RCP2.6 and RCP8.5 scenarios in line with Viveros Santos et al., (2023), and included the intermediated scenario RCP4.5.

Because soil organic matter (OM) and dissolved organic carbon (DOC) are required for calculating metal speciation (Equations S6, S7, S8), we first produced maps of soil organic carbon content ($SOC\%$) employing the *raster* package in R (Hijmans et al., 2022), using the maps of SOC stocks (SOC_{stock}) expressed in tonnes·ha⁻¹, the soil sampling depth ($d = 20$ cm), and a map of soil bulk density (ρ_b) in g·cm⁻³. The latter computations were performed according to Equation 5, which was used in the study by Yigini and Panagos (2016). The map of bulk density was taken from the study by Ballabio et al. (2017) and downloaded from the ESDAC portal (Panagos et al., 2012).

$$SOC\% = \frac{SOC_{stock}}{\rho_b \times d} \quad (5)$$

Based on the derived maps of SOC (%), we generated maps of soil organic matter content (OM) (Figure S3) considering the relationship $OM = 1.72 \cdot SOC$, that is, assuming that organic matter (OM) contains 58% of organic carbon, which is in line with previous studies that computed site-dependent CFs for metals terrestrial ecotoxicity accounting for speciation and bioavailability (Plouffe et al., 2016; Viveros Santos et al., 2018). Finally, in line with Viveros Santos et al. (2018) and Owsianiak et al. (2013), we computed maps of DOC (mg/l) according to an empirical regression (Equation A3) reported by Römken et al. (2004).

2.5.2. Current and future soil erosion rates in Europe

The maps of current (2016) and projected soil erosion rates (2050) in Europe used in this study were computed by Panagos et al. (2021) and made accessible by ESDAC (Panagos et al., 2012). The authors

applied the European version of the Revised Universal Soil Loss Equation (RUSLE), incorporating rainfall erosivity change, projections of land-use change, and expected changes in management practices promoted by European policy. Future rainfall erosivity was estimated by employing 19 GCMs according to three RCP scenarios. Even though the researchers reported high variability in changes in soil erosion between the GCMs, the maps of projected soil erosion are provided as an average composite of the 19 GCMs employed under each RCP. Therefore, for projected soil erosion rates, we were not able to select data derived according to a specific GCM.

The datasets of soil loss rate in $\text{Mg}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$ were converted into units of $\text{mm}\cdot\text{yr}^{-1}$ to make them suitable for computing fate factors with USEtox (Figure A5). Hence, the layers of soil loss rate ($\text{Mg}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$) were divided by the bulk density ($\text{Mg}\cdot\text{m}^{-3}$) and multiplied by a unit conversion factor of 0.1 ($\text{ha}\cdot\text{mm}\cdot\text{m}^{-3}$).

2.5.3. Current and future precipitation in Europe

We obtained monthly total precipitation (mm) datasets from WorldClim 2.0 data portal for the current scenario (1970-2000) and the future scenarios by 2050 under RCP2.6, RCP4.5, and RCP8.5 as modelled by the GCM IPSL-CM6A-LR (Fick and Hijmans, 2017; Petrie et al., 2021). The spatial resolution of the retrieved maps is 30 seconds (1 km^2 resolution). The prospective scenario by 2050 corresponds to the average climate of the period 2041-2060, which is consistent with the studies that simulated the projections of SOC stocks (Yigini and Panagos, 2016) and soil erosion by 2050 (Panagos et al., 2021) that were used in this study. Since the datasets of precipitation are inputs for the computation of fate factors with USEtox (Equations S1 and S2), layers of average annual precipitation ($\text{mm}\cdot\text{yr}^{-1}$) were calculated in Python employing the *Rasterio* package (Gillies et al., 2013) (Figure A7).

2.5.4. Auxiliary soil data

Table 2 lists the sources of the layers of soil properties that were considered constant under both current and future scenarios. These layers were downloaded from the ESDAC portal (Panagos et al., 2012).

Table 2. Source of auxiliary datasets of soil properties for the computation of copper speciation

Parameter	Unit	Database	Source
Bulk soil density	kg/l	-	(Ballabio et al., 2016)
Clay content	% (w/w)		
pH, measured in water	-	Maps of Soil Chemical properties at European scale based on LUCAS	(Ballabio et al., 2019)
Cation exchange capacity	cmolc/kg		
Calcium carbonate content	%		
Base saturation	%	Soil profile analytical database 14 (SPADE 14)	(Breuning-Madsen et al., 2018; Kristensen et al., 2019)
Exchangeable calcium	cmolc/kg		
Exchangeable magnesium	cmolc/kg		
Exchangeable sodium	cmolc/kg		
Exchangeable potassium	cmolc/kg		
Electrical conductivity of soil pore water	dS/m	LUCAS 2015 TOPSOIL data	(Fernández-Ugalde et al., 2020; Orgiazzi et al., 2018)
Copper content	mg/kg		(Ballabio et al., 2018b; Droz et al., 2021; Orgiazzi et al., 2018)

3. Results and discussion

3.1. Characterization factors under present and future scenarios

Fig. 1 (a) shows the distribution of regionalized CFs for copper terrestrial ecotoxicity across non-calcareous vineyard soils in European countries. Besides, Fig. 1 (b) illustrates the vineyard surface fraction for which CFs were calculated. Because the range of applicability of the TBLMs used for calculating EFs is restricted to non-calcareous soils, CFs were derived for around 30% of European vineyard soils. However, using TBLMs allowed us to account for metal speciation and bioavailability in the computation of EFs.

For the current scenario, the spatial variability of CFs spans 1.96 orders of magnitude between the minimum and the maximum values (considering a base-10 logarithmic scale), with a mean value of $1.46 \times 10^3 \text{ PAF} \cdot \text{m}^3 \cdot \text{day} \cdot \text{kg}^{-1}$. In comparison, Peña et al. (2018) reported similar findings on the geographical variability of CFs for copper terrestrial ecotoxicity in European vineyard soils, which was found to extend more than 1.5 orders of magnitude with a mean value of $2.34 \times 10^3 \text{ PAF} \cdot \text{m}^3 \cdot \text{day} \cdot \text{kg}^{-1}$. In contrast, Viveros Santos et al., (2018) derived CFs employing a method based on the geochemical speciation model WHAM 6.0 and found a spatial variability of around 5.5 orders of magnitude for non-calcareous soils of the world, with a median value of $1.73 \times 10^3 \text{ PAF} \cdot \text{m}^3 \cdot \text{day} \cdot \text{kg}^{-1}$.

The CFs for both current and future scenarios depict a similar trend with soil organic matter (Fig. A9). High organic matter content leads to low values of CFs because of the high affinity of copper for organic matter (Droz et al., 2021), which decreases copper mobility, and accordingly the associated FF. Conversely, high values of CFs occur where pH is low since copper solubility is dependent on soil pH values, and it tends to increase in acidic soils at a pH lower than six (Fig. A10). Furthermore, low FFs are related to low K_d values (Fig. A12), that is, in cases where copper concentration in the aqueous phase is high (Equation A10), which results in a higher influence on removal processes, namely runoff and leaching (Equations A1 and A2). This situation leads to potential increases in freshwater ecotoxicity; however, it is out of the scope of this study since this would require computing metal speciation according to freshwater properties (Dong et al., 2014) to be consistent with the modelling approach to account for metal speciation in the computation

of CFs for terrestrial ecotoxicity. Moreover, high values of CFs are associated with low annual precipitation because of a lesser contribution of the removal processes (leaching and runoff) (Fig. A11).

Low area coverage of CFs was obtained for Spain, Greece, and Italy, with 11% on average of their vineyard surface modelled. We obtained intermediate area coverage for France (31%), Germany (33%), and Bulgaria (36%) and larger coverage for Slovenia (55%), Romania (64%), and Portugal (86%) (Fig. 1 (b)). In section 3.3, we present CFs aggregated at three different spatial resolutions that could be used as an approximation of missing CFs for a particular vineyard. For instance, an aggregated CF at the country level could be used with the corresponding spatial variability set by the range of the minimum and maximum values to approximate the associated uncertainty of ignoring the corresponding CF for that vineyard.

As shown in Fig. 1 (a), the lowest spatial variability of CFs was obtained for Luxembourg under current and future scenarios, extending over 0.65 orders of magnitude within a 95% interval (2.5th and 97.5th percentiles). This is explained by the low vineyard surface of this country, corresponding to roughly 0.04% of the total European vineyard surface. Likewise, under the current scenario, CFs for Czechia exhibited a reduced spatial variability (0.78 orders of magnitude) in agreement with its low share of the total European vineyard surface (0.31%). Nevertheless, the spatial variability of the CFs for Czechia is projected to increase under future scenarios to 0.87 orders of magnitude. Spain has roughly a 21% share of the total European vineyard surface; however, because of the low vineyard surface modelled for this country, CFs showed a low spatial variability under the current and future scenarios (0.87 and 0.91 orders of magnitude, respectively). Furthermore, despite the largest share of France of the European vineyard surface (32%), the spatial variability of the CFs for this country is low under the current scenario (1.04 orders of magnitude), which is explained in part by the low vineyard surface fraction modelled (31%).

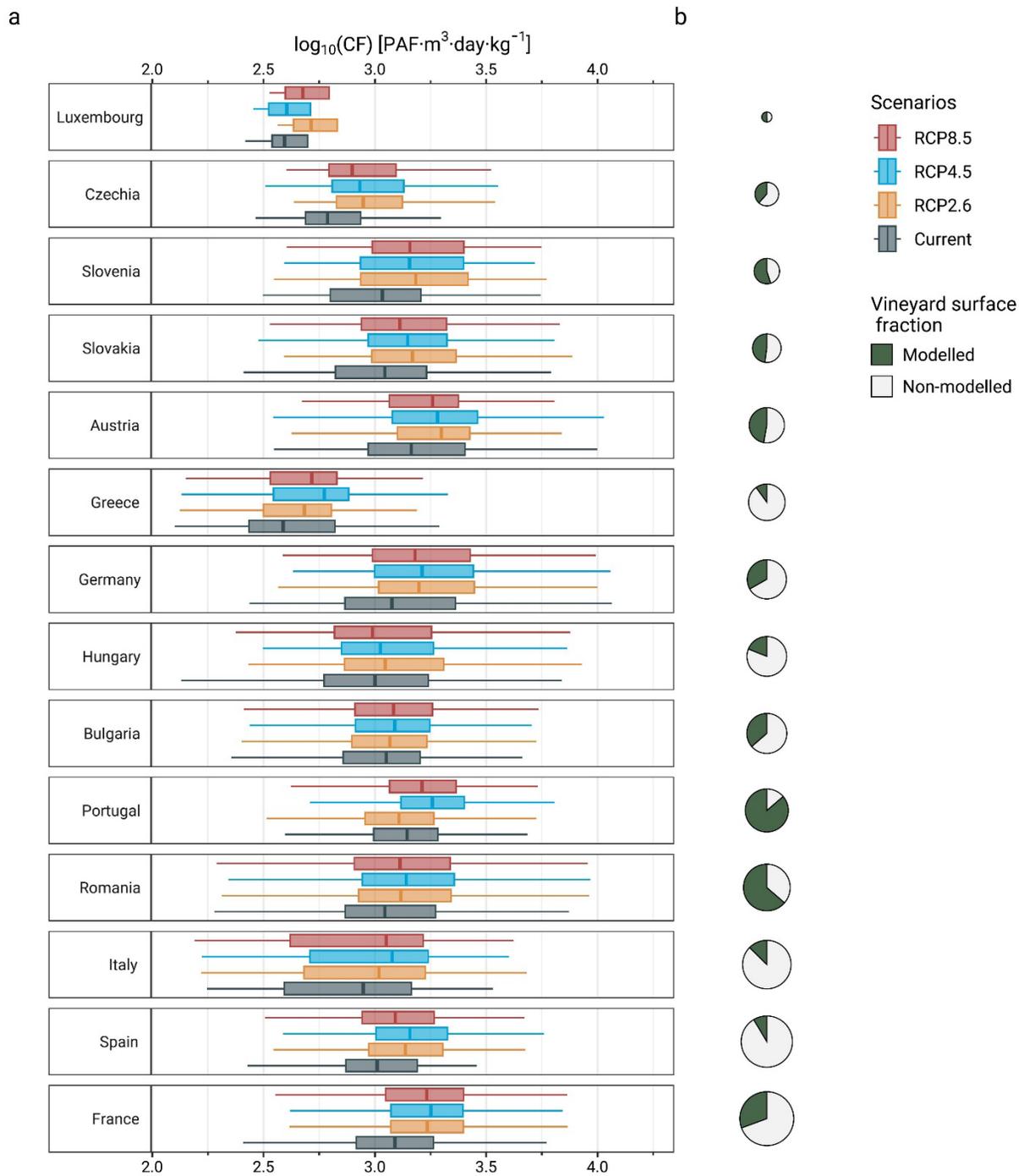


Fig. 1. Distribution of regionalized CFs ($\text{PAF}\cdot\text{m}^3\cdot\text{day}\cdot\text{kg}^{-1}$) for copper terrestrial ecotoxicity (a). The area of the pie charts is proportional to the surface of soils under vineyards for each country (logarithmic scale), and the green area indicates the vineyard surface fraction for which CFs were computed (non-calcareous soils) (b).

The largest spatial variability of CFs for non-calcareous European vineyard soils was found for Austria, expanding over 1.35 and 1.40 orders of magnitude under the current and future scenarios, respectively (Fig. 1 (a)). The spatial variability of CFs for Austria contrasts with its low share of the

European vineyard surface; however, the corresponding vineyard surface fraction modelled was relatively high (47%), which indicates high variability in soil properties. Comparably, the CFs for Italy exhibited a spatial variability of 1.23 and 1.31 orders of magnitude under the current and future scenarios, which is explained by its high share of the European vineyard surface (14%) and high variability in soil properties, even though its vineyard surface fraction modelled was low (12%).

Under the RCP4.5 scenario, the median CF values for all countries are projected to increase, compared to the corresponding ones under the current scenario, which indicates a general increase in CFs under the former scenario (Fig. 1 (a)). Under RCP2.6 and RCP8.5 scenarios, there are some exceptions to the trend of projected increases in median CFs across all countries. Regarding the RCP2.6 scenario, it is expected that the median CF for Portugal slightly decreases, compared to the median CF for the current scenario. This results from the projected increases in soil OM content (%) in a larger area of Portugal under RCP2.6 compared to other RCP scenarios (Fig. A4). Under the current scenario, CFs for Portugal within the range of 2.97 to 3.29 orders of magnitude extend over an area fraction of 70%, while it is projected to drop to 57% under the RCP2.6 scenario (Fig. 3). Similarly, under the RCP8.5 scenario, the median CF for Hungary is expected to slightly decline compared to the median CF under the current scenario. While the CFs for Hungary within the range of 3.08 to 4.25 orders of magnitude cover an area fraction of 40% under the current scenario, the RCP8.5 scenario projects a reduction of this area fraction to 35% because of expected increases in soil OM content (%) compared to other RCP scenarios (Fig. A4).

By 2050, under the three RCP scenarios, the median CFs for copper terrestrial ecotoxicity are projected to increase, compared with that for the current scenario ($1.19 \times 10^3 \text{ PAF} \cdot \text{m}^3 \cdot \text{day} \cdot \text{kg}^{-1}$). The highest increase in the median CF is projected under RCP4.5, with a rise of 27%, which is explained by the fact that the RCP4.5 scenario projects the lowest decreases in soil OM content (%) in contrast to other RCP scenarios (Fig. A4). RCP2.6 and RCP8.5 scenarios project increases in median CFs of 14% and 19% in comparison with the current value, respectively. However, the highest spatial variability of CFs, calculated as the range between the lowest and the highest value, is expected under the RCP8.5 scenario (Fig. 1).

3.2. Contributions of changes in fate, accessibility, and bioavailability factors to characterization factors

In this study, changes in future CFs are related to variations in FFs (day), ACFs ($\text{kg}_{\text{reactive}} \cdot \text{kg}_{\text{total}}^{-1}$), and BF_s ($\text{kg}_{\text{free}} \cdot \text{kg}_{\text{reactive}}^{-1}$) (Equation 3), driven by changes in soil organic carbon, rainfall, and soil erosion (Table 1). Fig. 2 shows the major contributors to changes in CFs across non-calcareous European vineyard soils under three RCP scenarios. It was found that the changes in BF_s will be the principal contributors to the changes in CFs in around 89% of the modelled European vineyard surface. Particularly, the increases in CFs will be controlled by the increases in BF_s in roughly 87% of the total vineyard surface modelled, while the remaining 2% of the vineyard surface will exhibit decreases in CFs resulting from reductions in BF_s. The vineyard surface where increases in CFs will be dominated by rises in BF_s is the result of projected declines in organic matter under RCP scenarios compared to the current scenario (Fig. A4). This is explained by the operational definition of the BF, which corresponds to the free ion fraction of the reactive metal in soil (Equation A12). While lower matter content leads to decreases in reactive copper concentration, it causes increases in free copper concentration (Equation A8), leading to an overall increase in BF_s. Nonetheless, the characterization modelling of this study does not account for soil acidification that can be caused by episodes of extreme rainfall, which would result in a higher fraction of free copper concentration and consequently higher BF_s. Besides, soil erosion affects soil organic matter, but the employed characterization model only accounts for the direct impact of soil erosion on the fate of copper in soil and neglects its influence on metal speciation, induced by its impact on organic matter content. Among the RCP scenarios considered in this study, it was found that the major contributions of BF_s to increases in CFs are projected under the RCP4.5 scenario, with a 92% share of non-calcareous vineyard surface, whereas the lowest positive contribution will be expected under the RCP2.6 scenario in 81% of the non-calcareous vineyard area (Fig. 2).

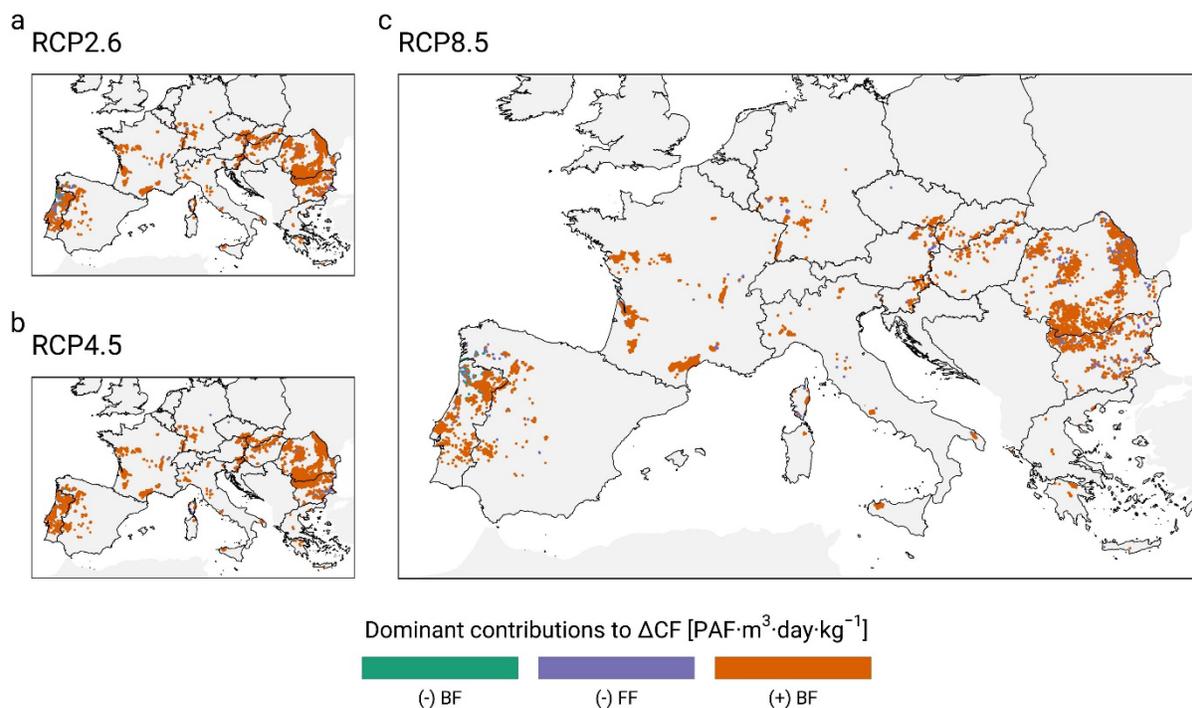


Fig. 2. Dominant contributions to changes in CFs ($\text{PAF}\cdot\text{m}^3\cdot\text{day}\cdot\text{kg}^{-1}$) under RCP2.6 (a), RCP4.5 (b), and RCP8.5 (c) scenarios across European vineyards. (-) and (+) indicate decreases and increases in BF ($\text{kg}_{\text{free}}\text{kg}_{\text{reactive}}^{-1}$) or FF (day), respectively.

Changes in FFs are the second principal contributors to projected changes in CFs. Nonetheless, in contrast to BFs, changes in FFs will solely lead to decreases in CFs for around 11% of the non-calcareous vineyard area (Fig. 2). In particular, the highest contribution of changes in FFs towards changes in CFs is expected under the RCP2.6 scenario for approximately 14% of the modelled vineyard surface, whereas the lower contribution of FFs towards decreases in CFs is projected under the RCP4.5 scenario with a vineyard area fraction of 8%. The declines in FFs are explained by the contribution of changes in K_d values, precipitation, and soil erosion projected under the RCP scenarios. Under future scenarios, on average, 63% of the surface where FFs control the changes in CFs, soil erosion is the main contributor to the declines in FFs due to an increase in the removal of copper by runoff (Equation A1). Whereas for roughly 23% of the same area, K_d values are expected to increase; however, their impact is counterbalanced by the projected increases in precipitation, leading to an increased influence of removal processes, namely runoff and leaching (Equations S1 and S2). For the remainder 14% of the area where changes in FFs control the

changes in CFs, even though precipitation is projected to decline, the decrease in K_d values is projected to entail lower residence time of copper in the soil, therefore decreasing the values in CFs.

3.3. Characterization factors at different spatial resolutions

Area-weighted averages of CFs for non-calcareous European vineyard soils were obtained for the current, RCP2.6, RCP4.5, and RCP8.5 scenarios at the spatial resolution of wine-growing regions, European regions, and European countries (Equation 4). Furthermore, in keeping with the IMPACT World+ methodology (Bulle et al., 2019), for each level of spatial aggregation, we report the spatial variability by providing the minimum, median, and maximum CFs values for each spatial unit. The datasets can be downloaded from a GitHub repository ([https://github.com/iviveros/viveros-santos et al 2023 jclp/tree/main/cf spatial res](https://github.com/iviveros/viveros-santos_et_al_2023_jclp/tree/main/cf_spatial_res)) and are complemented with a webpage ([https://iviveros.github.io/viveros-santos et al 2023 jclp/](https://iviveros.github.io/viveros-santos_et_al_2023_jclp/)) that presents interactive versions of Figs. 3, 4, 5, and 6 for interested readers.

3.3.1. Wine-growing regions

Future scenarios suggest that the changes in soil organic carbon, soil erosion, and rainfall may either increase or decrease CFs for copper terrestrial ecotoxicity by 2050 (Fig. 3). However, CFs under future scenarios will tend toward an overall increase (Fig. 3), which explains the increases in median CFs for most European countries across the RCP scenarios (Fig. 1 (a)).

The spatial patterns of CFs shown in Fig. 3 seem to vary slightly between the analyzed scenarios because the spatial variability of CFs is higher than the projected changes in CFs under future scenarios by 2050. Regarding the current scenario, CFs in the range of 2.82 to 2.97 orders of magnitude cover the largest area fraction for this scenario (29%). In contrast, under future scenarios, the highest area fraction corresponds to CFs in the range of 2.97 to 3.18 orders of magnitude, with 45% and 41% shares of the modelled vineyard surface for RCP2.6 and RCP4.5, respectively. Under the RCP4.5 scenario, the area fraction covered by CFs in the range of 2.09 to 3.29 orders of magnitude is close to that under RCP2.6, while the former scenario comprises a higher area fraction of CFs in the range of 3.29 to 4.25 orders of magnitude (28%) compared to 21% under RCP2.6 (Fig. 3). Under RCP8.5, the area fraction of CFs in the

range of 2.82 to 3.29 orders of magnitude is close to that under the current scenario. However, under the former scenario, the area fraction of CFs in the range of 3.29 to 4.25 orders of magnitude is 23%, while it amounts to 15% under the current scenario.

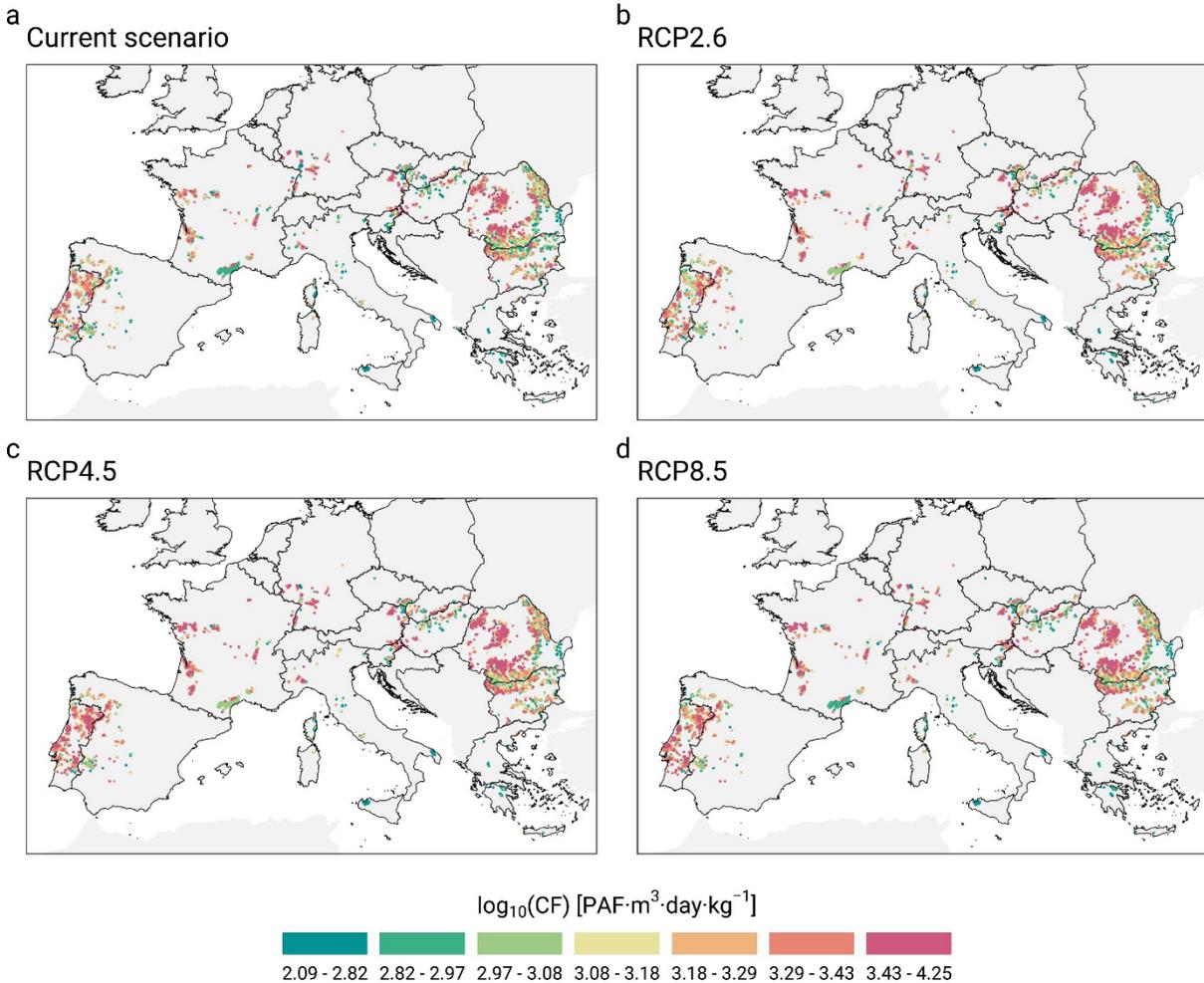


Fig. 3. CFs ($\text{PAF}\cdot\text{m}^3\cdot\text{day}\cdot\text{kg}^{-1}$) for copper terrestrial ecotoxicity aggregated at the level of European wine-growing regions under the current (a), RCP2.6 (b), RCP4.5 (c), and RCP8.5 (d) scenarios (coloured by quantiles). The reader is invited to consult the interactive version of this figure at: https://iviveros.github.io/iviveros-santos_et_al_2023_jclp/

Regarding the relative change (%) in CFs aggregated at the level of European wine-growing regions, the higher increases in CFs are projected under the RCP4.5 scenario with an area fraction of 82%, followed by the RCP8.5 (79.5%), and the RCP2.6 (74%). Under the RCP4.5 scenario, most of the projected increases in CFs will be in the range of 10% to 20%, encompassing a 29% area fraction of the non-calcareous soils, followed by increases in the range of 50%-100% representing 15% of the modelled vineyard surface (Fig.

4). In contrast, under the RCP2.6 scenario, the highest increases in CFs are expected in the range of 20%-30%, comprising an area fraction of approximately 26%, followed by increases in CFs by 0.5%-10%, covering 15% of the non-calcareous vineyard soils. The RCP8.5 scenario projects lower increases in future CFs, which will be mainly in the range of 0.5%-10%, with a 35% area fraction of non-calcareous vineyard soils. Still, the RCP8.5 scenario projects the highest area fraction (12%) with increases in CFs in the range of 30%-40%. The three RCP scenarios project increases in CFs higher than 100%; however, the area fraction of these increases is low (1.8% on average). Likewise, the area fraction where CFs will not change considerably (in the range of $\pm 0.5\%$) is around 0.5%.

Under future scenarios, the highest declines in CFs are in the range of -20% to -0.5%. More specifically, the RCP2.6 scenario projects the highest decrease in CFs within this range over an area fraction of 17.4%, followed by the RCP4.5 (14.6%) and the RCP8.5 (12.6%) scenarios. RCP2.6 and RCP8.5 scenarios forecast approximately the same area fraction (7%) for expected reductions in CFs by -40% to -20%. Finally, RCP4.5 and RCP8.5 scenarios project a 0.4% area fraction for decreases in CFs by -67% to -40%, while the RCP2.6 scenario forecast an area fraction of 1.2% for the same range in declines.

A possible use of the CFs aggregated at the level of European wine-growing regions is in the context of Territorial LCA (T-LCA). T-LCA is a variation of the conventional LCA that aims at evaluating the performance of a territory, in which agriculture is the principal economic activity, at a mesoscale and a related planning scenario (Rogy et al., 2022). Besides accounting for spatial differentiation at the inventory and characterization levels, T-LCA can be used to assess future scenarios (Loiseau et al., 2018; Rogy et al., 2022). In this context, aggregated CFs at the level of European wine-growing regions for future scenarios will have a potential application in prospective LCAs of viticulture that have addressed the impact of climate change at the inventory level (Viveros Santos et al., 2023).

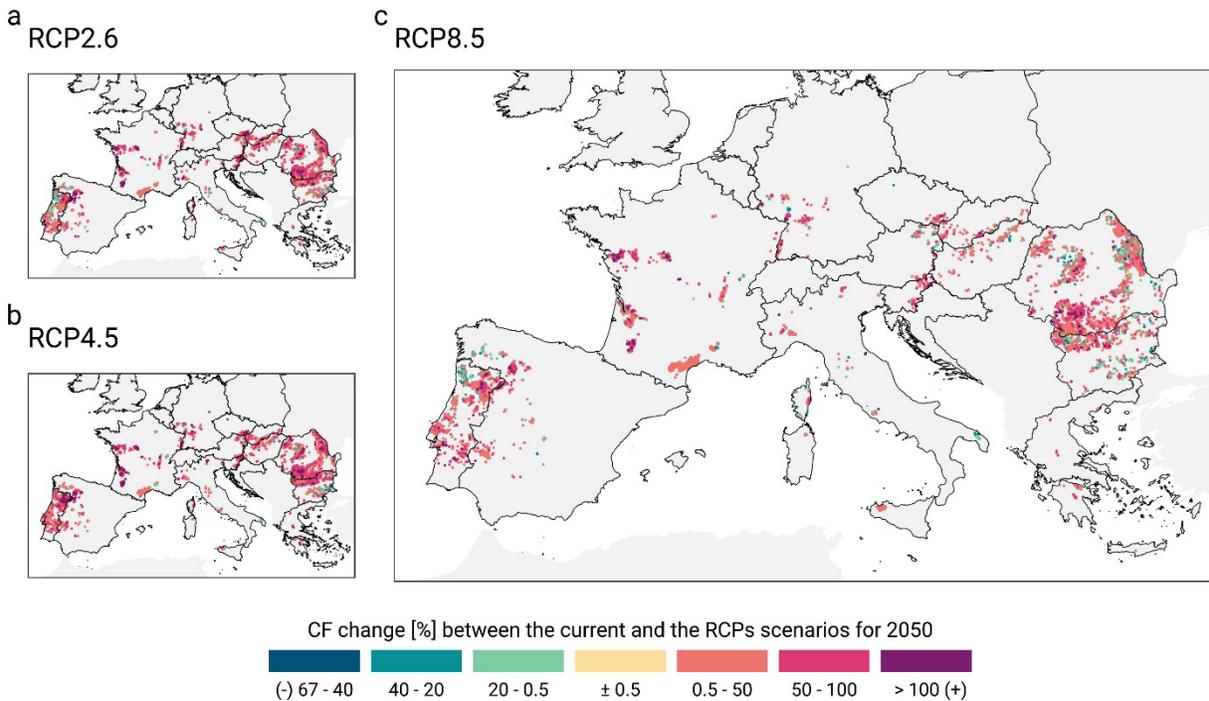


Fig. 4. Relative change (%) in CFs aggregated at the level of European wine-growing regions compared to the current scenario for RCP2.6 (a), RCP4.5 (b), and RCP8.5 (c) scenarios. The reader is invited to consult the interactive version of this figure at: https://iviveros.github.io/viveros-santos_et_al_2023_jclp/

3.3.2. European regions (NUTS2)

Fig. 5 depicts the spatial distribution of CFs aggregated at the level of European regions. Based on the performed spatial analysis, European vineyards extend across 124 European regions. However, CFs were derived for only 87 regions because of the range of applicability of the TBLMs employed for computing EFs and due to lack of data on soil OM content (%) (for Croatia and Cyprus). More specifically, CFs were not computed for one region from Cyprus, Czechia, Malta, and Portugal. Furthermore, CFs were not defined for two and three regions from Hungary and Croatia, respectively. In addition, CFs were not obtained for four regions from France and Greece. Finally, Italy and Spain are the countries with the largest number of regions for which CFs were not calculated, with 11 and 9 regions, respectively (Figure A13). In the case of Spain, the lack of CFs for 9 regions would be less problematic compared to Italy, since it has been reported that Spanish farmers do not employ copper-based fungicides extensively, compared to other countries such as France and Italy (Panagos et al., 2018).

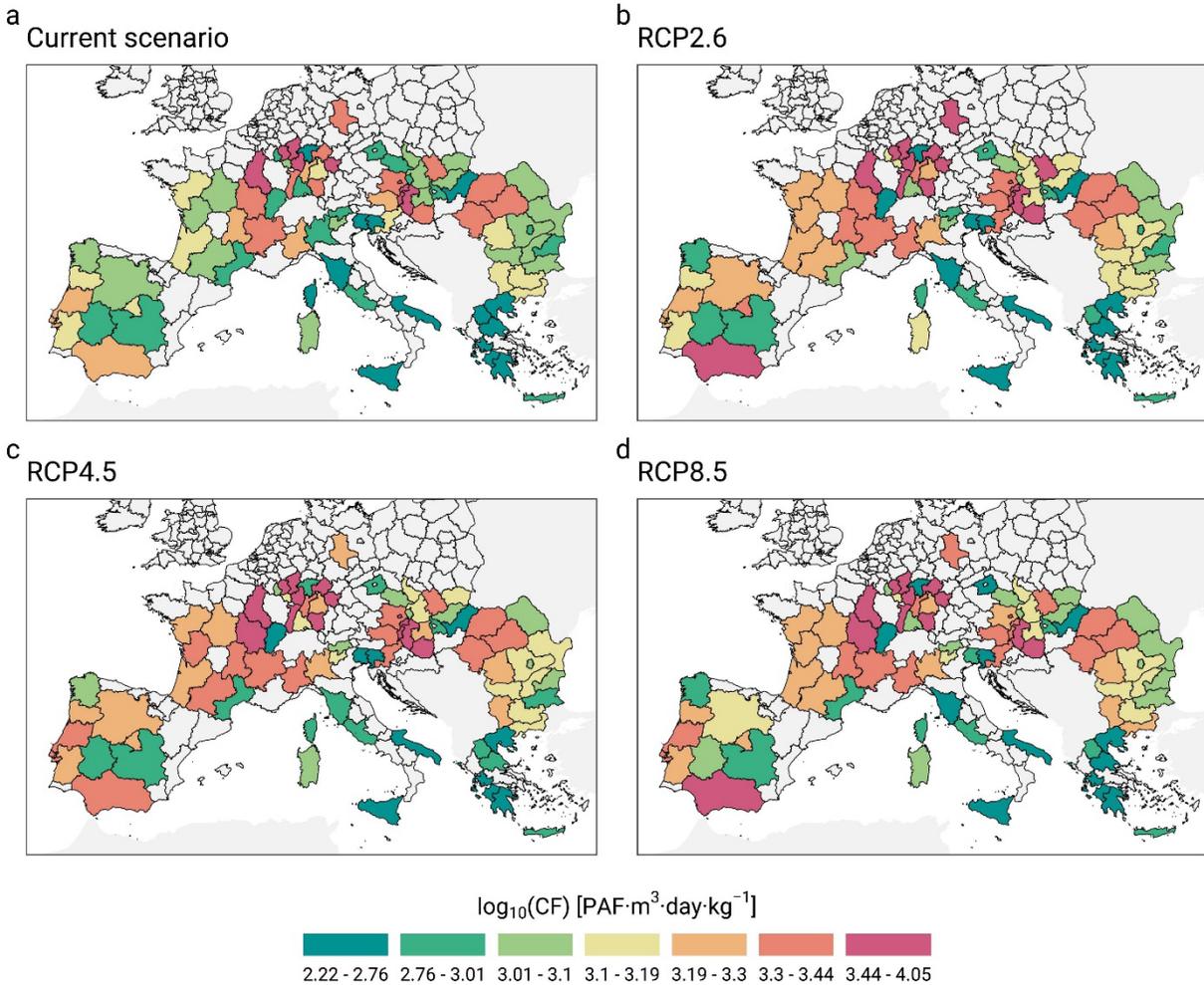


Fig. 5. CFs ($\text{PAF}\cdot\text{m}^3\cdot\text{day}\cdot\text{kg}^{-1}$) for copper terrestrial ecotoxicity aggregated at the level of European regions (NUTS2) under the current (a), RCP2.6 (b), RCP4.5 (c), and RCP 8.5 scenarios (coloured by quantiles). The reader is invited to consult the interactive version of this figure at: https://iviveros.github.io/viveros-santos_et_al_2023_jelp/

Under future scenarios, apart from the RCP4.5 scenario, 16% of the European regions have CFs within the range of 2.22 to 2.76 orders of magnitude. Greece and Italy have the highest number of regions with CFs within the lower bound of CFs, with six and four regions, respectively (Fig. 5). Under the current scenario, CFs in the range of 2.76 to 3.19 orders of magnitude comprise 53% of the regions; however, this share is forecasted to decrease to around 40% by 2050. The largest numbers of regions with CFs falling within the latter range are projected for Italy (7), Romania (6), and Spain (5). While under the current scenario, CFs within the range of 3.19 to 4.05 orders of magnitude cover on average 31% of the European regions, this share is expected to increase to 47% under future scenarios (Fig. 5). The highest numbers of

regions with CFs within the latter range are forecasted for Germany (8), France (5), and Austria (4). In the case of France, RCP scenarios project an increase in the number of regions with CFs falling within the range of 3.19 to 4.05 orders of magnitude, moving from five to ten regions.

Regarding the number of regions for which their aggregated CF will not change ($\pm 2.5\%$ of variation), the RCP2.6 scenario projects this output for nine regions, while the RCP4.5 scenario forecasts this outcome for two regions. However, future scenarios suggest that aggregated CFs will increase by 2.5% to 85% for around 80% of the European regions (Fig. 6). More specifically, the RCP2.6 and RCP4.5 scenarios forecast increases in aggregated CFs by 2.5% to 50% for 56 out of 87 European regions, while the RCP8.5 scenario projects this outcome for 59 regions. The RCP4.5 scenario projects higher increases in aggregated CFs in the range of 20% to 30%. Furthermore, aggregated CFs are projected to increase by 50% to 85% for around 12% of European regions (Fig. 6).

RCP2.6 and RCP4.5 scenarios project that aggregated CFs will decrease by -38% to -20% for two regions. However, RCP4.5 scenario projects the same level of decrease for three regions. Decreases in aggregated CFs in the range of -20% to -10% will exhibit an uneven spatial distribution (Fig. 6). The RCP2.6 scenario projects this outcome for four regions; while the RCP4.5 and RCP8.5 scenarios project the same level of decrease for two and five regions, respectively. Furthermore, the spatial distribution of decreases in aggregated CFs by -10% to -2.5% is irregular. The RCP2.6 scenario projects decreases in aggregated CFs at this level for seven regions, and the RCP4.5 and RCP8.5 forecast this outcome for six and five regions, respectively.

Previous studies have shown the relevance of accounting for spatial differentiation at the inventory and impact assessment levels (Patouillard et al., 2020; Viveros Santos et al., 2018), and impact methodologies such as IMPACT World+ aim to improve the spatial differentiation of LCA results (Bulle et al., 2019). In the case of consequential LCA, it has been shown that a strategy to decrease the spatial uncertainty of the results is to employ regionalized CFs (Patouillard et al., 2020). In this context, we recommend using CFs aggregated at the wine-growing level (3.3.1). Nonetheless, a potential application of the CFs aggregated at the level of European regions (NUTS2) would be to support the decision-making

process by means of providing a better comprehension of the terrestrial ecotoxicity impact of copper depending on the average characteristics of the receiving soils and to consider potential changes in the level of impact under future scenarios in the definition of copper use regulations. In fact, in the European Union, policies are generally formulated at the level of regions (NUTS2) (European Commission, 2022; Panagos et al., 2021).

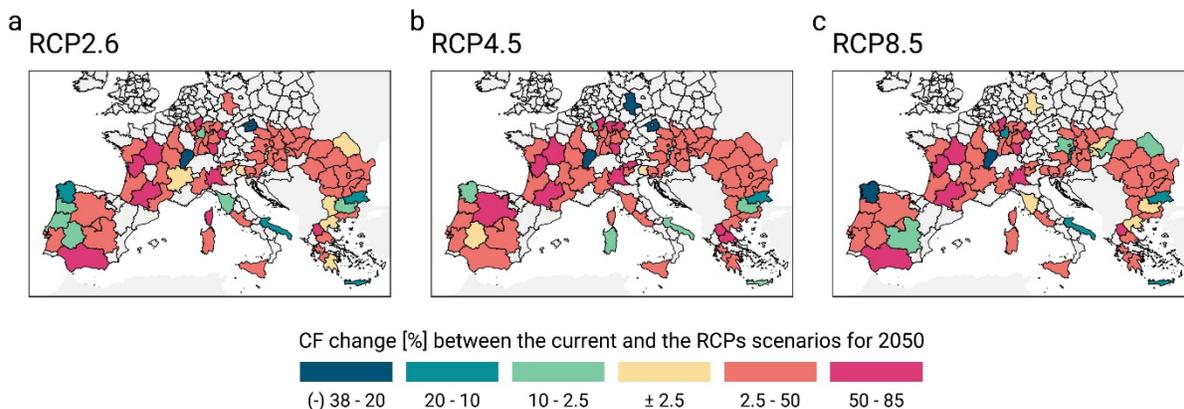


Fig. 6. Relative change (%) in CFs aggregated at the level of European regions compared to the current scenario for RCP2.6 (a), RCP4.5 (b), and RCP8.5 (c) scenarios. The reader is invited to consult the interactive version of this figure at: https://iviveros.github.io/viveros-santos_et_al_2023_jclp/

3.3.3. European countries

As shown in Fig. 7 (a), 5 out of 14 European countries have an aggregated CF higher than the mean area-weighted CF computed for the current scenario ($1.30 \times 10^3 \text{ PAF} \cdot \text{m}^3 \cdot \text{day} \cdot \text{kg}^{-1}$). More specifically, Germany and Austria have the highest aggregated CFs, which is explained by their high share (around 20%) of CFs within the range of 3.43 to 4.25 orders of magnitude (Fig. 1 and Fig. 3 (a)). Similarly, Portugal, Slovenia, and Romania have aggregated CFs 25% on average higher than the mean area-weighted CF. This is explained by the fact that most of the CFs for Portugal, Slovenia, and Romania fall in the range of 2.97 to 3.29 orders of magnitude, with shares of vineyard surface of 70%, 43%, and 42%, respectively (Fig. 3). In contrast, Italy, Greece, and Czechia have the lowest aggregated CFs with a mean value of $8.26 \times 10^2 \text{ PAF} \cdot \text{m}^3 \cdot \text{day} \cdot \text{kg}^{-1}$. This is related to the high share of CFs (around 60%) within the range of 2.09 to 2.82 orders of magnitude for these countries (Fig. 3). Aggregated CFs for Hungary, Bulgaria, Slovakia, France,

Spain, and Luxembourg are below the mean area-weighted CF and in the range of 3 orders of magnitude (Fig. 7 (a)).

Under future scenarios, the highest increase in aggregated CFs at the country level is projected under the RCP4.5 scenario with a mean increase of 21% compared to the current scenario (Fig. 7 (b)). The RCP2.6 scenario forecast an average increase of 19%, while the RCP8.5 scenario forecasts a mean increase of 16% in aggregated CFs at the country level (Fig. 7 (b)). Under the RCP4.5 scenario, the higher increases in aggregated CFs are projected for Czechia, Portugal, Slovenia, Slovakia, and Italy, with a mean increase of 33%, while the lowest increases are projected for Hungary, Greece, Bulgaria, Luxembourg, and Austria with an average increase of 11%. One exception to the increases in aggregated CFs at the country level is expected for Portugal under the RCP2.6 scenario, with a decline of 3% compared to the current scenario (Fig. 7 (b)). The reason is that the RCP2.6 scenario projects an increase in OM in a greater surface over Portugal in comparison to other scenarios, which leads to lower partitioning coefficients (K_d), and consequently to lower FFs and CFs (Fig. 3 and Fig. A4). The RCP8.5 scenario also forecast a reduction in the aggregated CF for Austria of 8% compared to the one calculated for the current scenario.

A potential application of the aggregated CFs at the level of countries for non-calcareous European vineyards soils is in cases where there is no site-dependent CF (Section 3.3.1), which is equivalent to using a generic CF, a current practice in LCA (Patouillard et al., 2020). In fact, most life cycle inventory consider a spatial differentiation at the country level, which would allow using the aggregated CFs presented in this section. Finally, in terms of policy definition on the use of copper, most countries will need to be more strict, given the potential increases in the level of impact of copper terrestrial ecotoxicity due to its interaction with climate change (Fig. 7 (b)), even if the projections indicate a relative low increase (19% on average) compared to the spatial variability of the CFs (1.96 orders of magnitude) for the current scenario (Section 3.1).

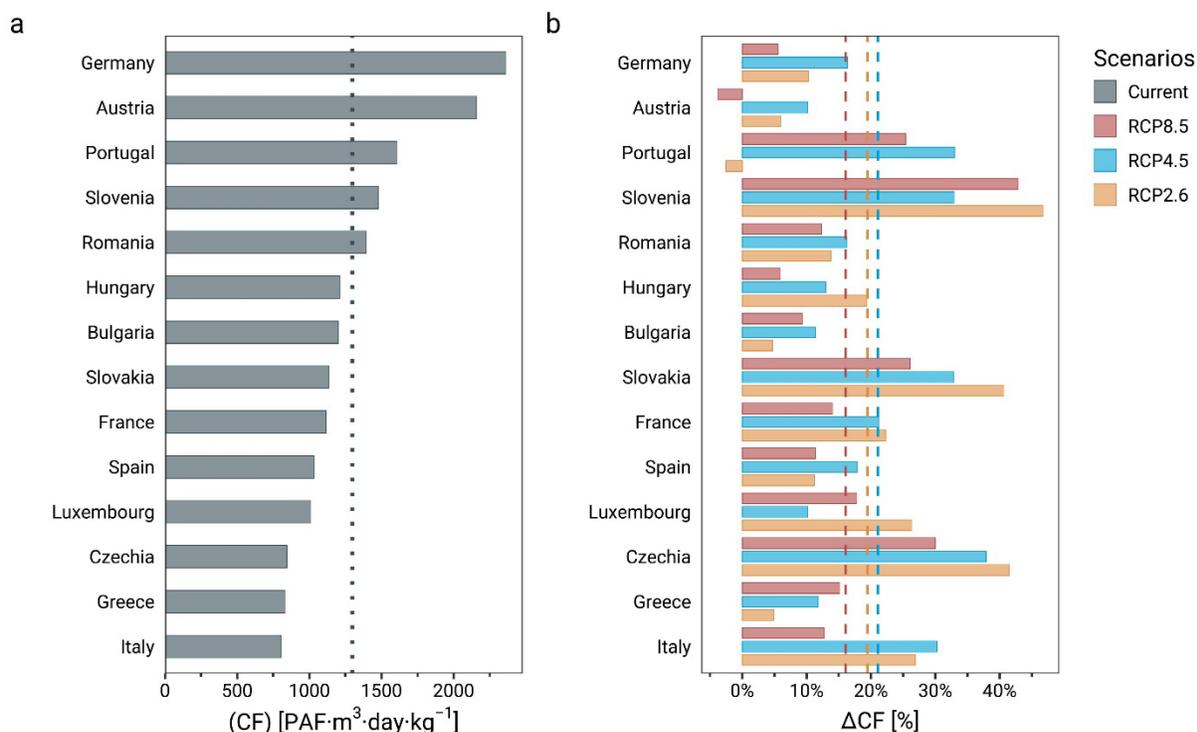


Fig. 7. Area-weighted average of CFs ($\text{PAF}\cdot\text{m}^3\cdot\text{day}\cdot\text{kg}^{-1}$) at the country level for the current scenario (a), and mean change in CFs for each European country by 2050 compared to the current scenario. The dotted vertical line in (a) indicates the mean area-weighted CF at the country level, whereas the dashed vertical lines in (b) represent the mean change (%) in CFs under RCP scenarios.

3.4. Limitations and future perspectives

One main limitation of this study is the restricted application of the developed CFs to non-calcareous vineyard soils, while an important area of European vineyards is established on calcareous soils. This limitation resulted from the use of TBLMs for computing EFs. While these models facilitated accounting for metal speciation and bioavailability, they are only valid for non-calcareous soils (Thakali et al., 2006). Besides, further research is needed to account for projected changes in temperature in the computation of EFs. Currently, studies suggest that changing environmental conditions affect the performance of terrestrial organisms, but it is not straightforward to isolate their impact on metal speciation from the impact on species sensitivity. Thus, the reported level of effect on organisms performance results from the combination of several stress factors, namely increasing temperature and changes in moisture content (Fu et al., 2018; González-Alcaraz and van Gestel, 2016). Accordingly, in this study, the EFs were assumed constant, to avoid a potential double counting of the interaction with climate change. Still, the influence of changing

parameters on the extent of copper effects was introduced via the BF since this factor depends on soil organic carbon content. Future research may consider a multifactorial approach to account for the combined effect of multiple stressors on soil organisms (Zandalinas et al., 2021).

There are also some uncertainties related to the parameters assumed constant under future scenarios. For instance, under episodes of heavy rainfall, pH may be reduced because of the leaching of basic cations. However, it is not feasible to account for those extreme events in the computation of FFs with USEtox. Still, the rate of changes in pH is slower in comparison to other environmental compartments, namely freshwater and the ocean, owing to the buffer effect of soil minerals (Biswas et al., 2018), which partially justifies the assumption of constant pH for future scenarios. A second effect not accounted for in the characterization modelling is the influence of precipitation on DOC, which may decrease after episodes of increased rainfall due to the increases in its leaching rate. Land-use changes were not integrated into the computation of copper fate in soils, but its influence on copper mobility has been reported and identified as research need to avoid problems related to the mobilization of copper in cases of reconversion of soil use that leads to more acid soils, such as the conversion of vineyards to forests (Villanueva-Rey et al., 2019). The mobilization of copper driven by the acidification of soils would increase the lixiviation of metal, thus potentially decreasing the associated terrestrial ecotoxicity impacts, but resulting in potential increases in aquatic ecotoxicity impacts.

Lastly, the applicability of the derived CFs of this study is limited to the characterization of direct emissions of copper to non-calcareous soils, which resulted from the choice of the fate factor. The assumption behind choosing a fate factor for a direct emission to soil is that a high fraction of the copper-based fungicide will remain within the parcel after pesticide application due to the influence of processes such as dry deposition and rain. Furthermore, the computed CFs of this study are compatible with LCI databases such as the World Food Life Cycle Database (Nemecek et al., 2019) andecoinvent (Nemecek and Kägi, 2007) that characterize pesticide emissions as direct emissions to agricultural soil, thus neglecting the primary distribution of pesticides. However, recently, the OLCA-Pest Project (Operationalising Life Cycle Assessment for Pesticides) recommended employing default emission fractions for estimating the

primary distribution of inorganic compounds, namely metal-based fungicides and sulphur (Nemecek et al, 2022). In this context, additional CFs for a direct emission to air and water will be required to characterize the impact of copper-based fungicides considering the influence of primary distribution. Furthermore, because under future scenarios, removal processes such as leaching and runoff are projected to have a stronger influence on the transfer of copper from soil to water compartment, future research may address the computation of characterization factors accounting for the interaction of climate change and aquatic ecotoxicity.

4. Conclusions

The objective of this work was to compute CFs for copper terrestrial ecotoxicity, including metal speciation and bioavailability as influenced by soil properties, for a current scenario and three future scenarios by 2050, for non-calcareous European vineyard soils. Furthermore, this exploratory study constitutes a first effort to account for projected changes in soil organic carbon, soil erosion, and rainfall, which are parameters relevant to the terrestrial ecotoxicity impact pathway.

Despite the inherent uncertainties of future projections, future changes in soil organic carbon, soil erosion, and rainfall are expected to lead to either increases or decreases in future CFs. Nevertheless, increases in CFs are projected over a larger share of the non-calcareous European vineyards, which will lead to rises in the median CFs in the order of 27% under RCP4.5 compared to the median for the current scenario. These results highlight the relevance of accounting for the interaction of climate change with the terrestrial ecotoxicity impact pathway. Because of the scope of this study, CFs for aquatic ecotoxicity were not derived; however, future research may address the interaction of climate change with this impact category since climate change is projected to influence the transfer from soil to freshwater ecosystems by leaching and runoff.

The CFs derived in this study are solely valid for non-calcareous soils, resulting from the scope of application of the TBLMs used to derive EFs. Therefore, future research may address extending the range of applicability of the characterization modelling to calcareous soils, since an important fraction of

vineyards is established in this type of soil. Furthermore, more research is needed on how to account for projected changes in temperature on species sensitivity to integrate it into the computation of EFs.

Finally, this study may contribute to the growing interest in performing prospective LCAs of product systems, which so far have focused mainly on projections at the life cycle inventory level. However, due to the projected changes in environmental conditions driven by climate change, the validity of applying current CFs decreases when using them in the assessment of prospective scenarios. Accordingly, the development of future CFs for other impact categories will allow the performing of future-oriented LCA studies that integrate the prospective dimension at both the inventory and the characterization levels, thus promoting its admissible use for decision-making in prospective analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Please consider the attached file JCLP_Appendix_A_Article_Viveros-Santos_et_al.pdf containing the supplementary data to this manuscript.

The shapefiles of CFs and the data files of the figures presented in this study can be found in the following repository:

[https://github.com/iviveros/viveros-santos et al 2023 jclp](https://github.com/iviveros/viveros-santos_et_al_2023_jclp)

The interactive maps that accompany this publication are found here:

[https://iviveros.github.io/viveros-santos et al 2023 jcjp/](https://iviveros.github.io/viveros-santos_et_al_2023_jcjp/)

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