



# Evaluating toxicity impacts of local chemical emissions in Life Cycle Assessment

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## Abstract

**Purpose** The local dimension of toxicity effect on humans and ecosystem from chemical emissions into rural environments is currently not considered in impact characterization models underlying the Life Cycle Assessment (LCA) methodology. The aim of the present study was to understand the relevance of considering a local exposure environment for the magnitude of damage related to human toxicity and ecotoxicity impacts associated with chemical emissions into a local environment. **Method** Unit and realistic European emission scenarios were considered in a proposed multimedia nested box model, based on an existing framework modified with the inclusion of a local scale, and tested for ten chemicals in an illustrative case study. **Results** A substantial damage increase in terms of characterization factors in the proposed model was found for human health, mainly for local freshwater emissions (up to three orders of magnitude compared to emissions into continental freshwater for naphthalene) and soil emissions (up to two orders of magnitude, in particular for emissions into natural soil for 1,2-dichloroethane). **Conclusions** Based on our results, we suggest to use the proposed framework in LCA applications, when more specific information about the local emission environment is known. With respect to considering the local-scale, however, spatialized models might be preferable over nested box models to properly capture local phenomena in rather highly densely populated areas.

**Keywords** Life Cycle Impact Assessment · USEtox · Local scale · Multimedia · Chemical emissions · Human toxicity · Ecotoxicity

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## 1 Introduction

The Life Cycle Assessment (LCA) methodology (UNI EN ISO 2006a, b) provides a quantification framework to assess the environmental impact performance over the entire life cycle of a product or technology, accounting for various impacts related to inputs and outputs of the studied system in terms of resource use and environmental emissions of, e.g., greenhouse gases, air pollutants, and toxic chemicals. The latter are characterized considering chemical multimedia fate, human and ecological exposure, and toxicological effects (Fantke et al. 2018a, b; von Borries et al. 2023), and can also be linked to ecosystem quality or biodiversity damage (Oginah et al. 2023a, b). The broad variety of impact categories that could be encompassed besides toxicity make LCA the instrument of choice to support policy makers in avoiding the shifting of burdens across impact categories, in space, i.e., between world regions, and in time (Sala et al. 2016; Sanyé-Mengual and Sala 2022). However, the local scale is insufficiently considered in LCA toxicity characterization models and limited to certain environmental

compartments, namely, urban air (Rosenbaum et al. 2008; Fantke et al. 2021).

The main reason is that, usually in LCA, the location of the emission, and the surrounding population density, is not reported over the entire product or technology life cycle; therefore, emission locations are currently addressed at generic continental level. By contrast, risk assessment, based on a receptor-oriented perspective, is able, at the proper tier of application, to consider finer resolutions and provide local risk characterizations (De Luca Peña et al. 2022). However, since the location of emissions in LCA become more and more available, it is relevant to include a local scale also in LCA. This is to not only address questions of risk and safety (i.e., risk assessment) but also questions of overall environmental performance of entire product or technology life cycles (i.e., LCA) at a more local level, especially when both tools should be consistently integrated with their complementary questions (Hauschild et al. 2022).

Moreover, the limited number of people exposed in a local environment has led to the local scale being regarded as irrelevant in many toxicity assessments. Indeed, the scarce use of local environmental compartments in multimedia fate modeling practice has led to the removal of the local scale from the pollutant dispersion model SimpleBox v. 4.0 (Hollander et al. 2016).

Other authors (Loiseau et al. 2018) have considered the role of LCA methodology applied to the territory; in particular, the so-called territorial LCA has been analyzed by considering a precise activity in a defined local context and considering a local context as a whole, comprehensive of all the anthropogenic activities. In both cases, the goal and scope and inventory phases only have been adapted to the local context, while stating the relevance of site-specific LCIA methods.

The absence of the local rural outdoor dimension in damage assessments leads the LCA practitioner to an inability to understand local impacts near emission sources where such emission data are available. This includes, for example, data available to the Italian City Council of Coriano (RN) in the Emilia-Romagna region, who asked to investigate the potential impacts caused by the local incinerator of municipal waste via toxicity impacts (Municipality of Coriano and Riccione (RN), 2019) in the frame of performing an LCA of the regional and municipal waste management system. The concerns of the local communities surrounding such waste treatment plants with a greater or lesser range is related to exposure to chemicals emitted to local environmental compartments, including indirect exposure via ingestion of local food.

Currently, some calculation methods take into account potential effects on high population urban scale due to air emissions (Bare 2011; Fantke et al. 2018b; Fazio et al. 2018;

Joint Research Centre (JRC) European Commission 2019; Bulle et al. 2019; Verones et al. 2020). However, damage on human and ecosystem health near multimedia emission sources with current LCIA methods are not evaluated by default, mainly due to lack of local emission data.

Several studies have investigated local effects of specific chemicals applying different models, e.g., nested box models, based on homogeneous standard environments of the “Mackay type” (Parnis and Mackay 2020), like EUSES tool (Lijzen & Rikken 2004) and SimpleBox 3.0 (Den Hollander et al. 2004), and spatialized environments. Related case studies are often limited to air emissions (Brandt et al. 2001; Breivik et al. 2021; Dennis et al. 2010; Derognat et al. 2003; Giannouli et al. 2011; Hollander et al. 2007; Kawamoto et al. 2012; Seigneur et al. 2004; Van De Meent et al. 2010; Van Zelm et al. 2007; Wannaz et al. 2018). Less analyzed are water emissions (Jaworskal et al. 1999) and soil emissions (Cooter et al. 2012). Concentration analysis has covered a broader spectrum of compartments, sometimes analyzing all the major ones (air, water, and soil, e.g., Van De Meent et al. 2010; Wannaz et al. 2018) or two receiving compartments (Jaworskal et al. 1999). We also point out the ExternE (European Commission 2005) tool for assessing external costs due to energy sector emissions, in which a local scale is taken into account limitedly to air emissions and where the concentration distribution for a point source is calculated using the Gaussian plume model (Allen and Durrenberger 2003).

The relevance of rural emissions in local environment in terms of concentration magnitude has been assessed in several studies (Hollander et al. 2007; Van De Meent et al. 2010; Wannaz et al. 2018), with the application of different models.

Hollander et al. (2007) have performed a simulation of PCB-153 emissions in Europe from 1981 to 2000, comparing the concentration results in air and soil provided by LOTUS-EUROS, a dynamic spatially resolved model with 14,000 cells of  $25 \times 25 \text{ km}^2$ , with those resulting from SimpleBox 3.0 (type IV, i.e., dynamic, non-steady-state). SimpleBox 3.0 returns higher average concentrations across scales in both air and soil compartments, namely, twice and 1.5–3 times, in particular the lower range of concentrations (occurring on the regional-continental scale) is overestimated, due to the averaging of regional and continental emissions, whereas the peaks on the local scale are comparable and confirmed by measured values. Generally, local air concentrations have resulted to be 2 orders of magnitude higher than continental concentrations.

Van De Meent et al. (2010) have applied EUSES to evaluate concentrations of petroleum hydrocarbons for every compartment, assuming a daily steady-state emission ratios of 1:10:100 in air, respectively for local, regional, and continental scales, reporting that the first ones are higher

than those found at regional and continental scales, ranging, in terms of orders of magnitude, from +5 to +6 for air, from +4 to +6 for freshwater and from +1 to +3 for soils.

Wannaz et al. (2018) have applied the Pangea modeling framework, a multimedia box model consisting of a set of compartments combined with multiscale varying grids, to finer resolution of  $7 \times 7 \text{ km}^2$  around the point of emission, for the evaluation of local up to global concentrations in the region of north-east of France in steady-state conditions for three chemicals (2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD), benzene and benzo[a]pyrene (B[a]P)). Air, water, and agricultural soil concentrations, due to emissions from 126 solid waste treatment plants, and consequent population intake fractions at local and global scale, have been estimated and compared, showing an extended area invested by high concentration of benzene in air (up to 9 orders of magnitude higher than global concentration). The major intake occurs via inhalation of benzene, with local peaks of intake up to 6 times higher than the continental one.

Compared to the mentioned studies, the scope of the present study is assessing the relevance of the local scale also for use in LCA, in terms of concentrations and corresponding damage on human and ecosystem health, made of 4 ground-level emission compartments (air, freshwater, natural soil and agricultural soil), nesting a local scale box within a continental scale environment of an existing framework. This framework is USEtox v. 2.1 (Rosenbaum et al. 2008),

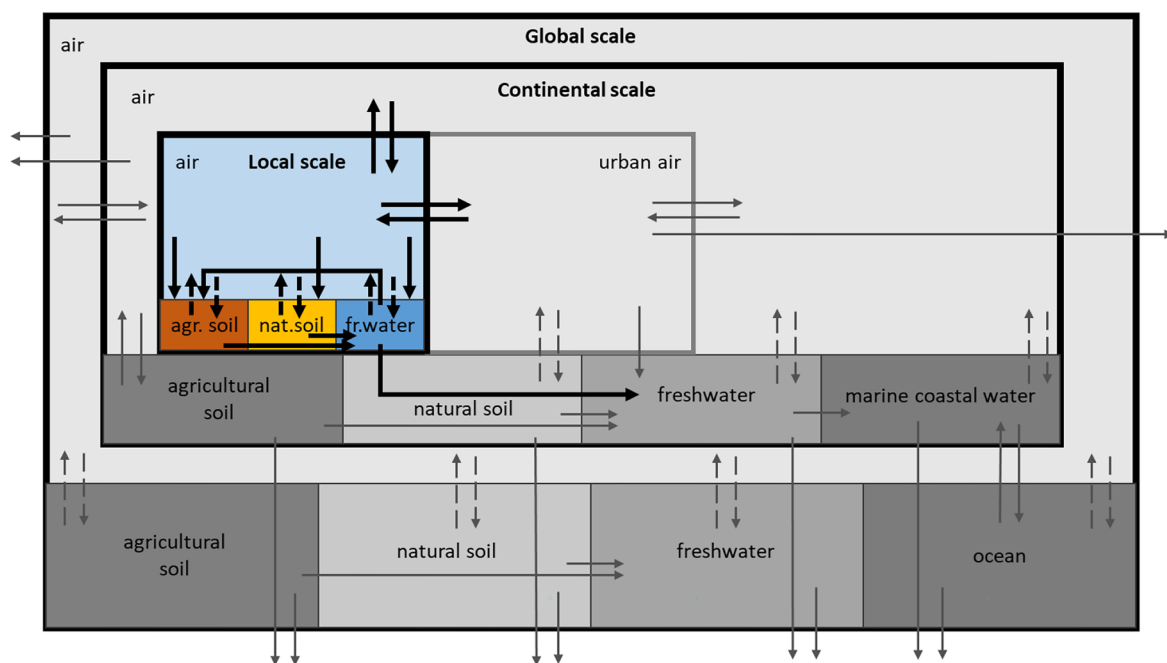
the global scientific consensus model for life cycle impact assessment, and widely used in LCA for human toxicity and ecotoxicity (Fantke et al. 2018a, b; Owsianiak et al. 2023; Westh et al. 2015).

Based on these considerations, the overall goal of the present study is to understand the role of the local rural scale on distribution and magnitude of emission-related human toxicity and ecotoxicity impacts in LCA. To achieve this goal, we focus on the following specific objectives: (a) to expand a current LCA toxicity characterization model by introducing a local scale environment, (b) to derive characterization factors for different scales and settings that incorporate the local scale as emission environment, and (c) to test the proposed approach in a case study on selected chemicals and reported emissions in Europe and derive recommendations of when the local impact is relevant in an LCA context.

## 2 Methods

### 2.1 Introduction of the local scale into a toxicity characterization model

USEtox v. 2.1 (Fantke et al. 2017, 2018b, 2021; Rosenbaum et al. 2008) was taken as reference method for the assessment of the relevance of the local scale since it is a model based on scientific consensus providing midpoint and endpoint



**Fig. 1** Introduction of the local scale in the compartment system based on USEtox, advective processes are represented with continuous arrows and diffusive processes with dotted arrows. Existing compartments are shown in gray. Black thick arrows denote only processes

related to the local scale, while processes in the original version of USEtox are clarified in Rosenbaum et al. (2008) and shown here as gray arrows. Degradation processes are also considered (not denoted by arrows)

characterization factors for human toxicological and freshwater ecotoxicological impacts of chemical emissions in LCA. Unlike the USEtox urban scale, that only connects to air and deposits onto freshwater, in the calculation method with the local dimension, the local scale, consisting of 4 ground-level emission and receiving compartments (rural air, freshwater, natural and agricultural soil), was introduced and nested in the continental box (Fig. 1). The local scale was linked with continental and urban scales via advective transport processes of air and freshwater compartments.

Intermedia partition processes between local compartments were included as well, respecting the structure of processes and rate constants described in USEtox.

The defined area of the local scale is  $1 \times 1 \text{ km}^2$ , and it was identified by means of Google Maps on the territory of the Emilia-Romagna region as reference, since it is one of the most industrialized regions in Italy. In this region, the distance between densely populated centers and production sites, e.g., from the ceramic sector typical of this region, can be as short as 400–500 m, as in the Sassuolo municipality area (measured with Google Maps). Due to this distance, the population density considered in the local scale is half of the population density in the urban scale. It includes the emission into air, water, and soil and the consequent intake by people through the exposure pathways already present in USEtox.

Since a well-mixed box model is not able to investigate very local phenomena, like distances between pollutant source and target populations and the evaluation of spatial distances would require appropriately spatialized models, the assumption of steady-state with instantaneous and homogeneous mixing in every compartment of a local scale was used to provide an estimate of the magnitude of local impacts compared to continental emitting scales, but it was not intended to provide realistic concentration distribution within the defined local scale.

The introduced scale added 4 new mass balance equations and related dimensions in the  $K$ -matrix, for consistency with USEtox approach, as reported in Supporting Information (SI) section S-1.

Compared to the original USEtox model (Rosenbaum et al. 2008), two differences are present (SI section S-2), in particular correcting the formula for the calculation of the chemical mass fraction associated to the gas phase of air compartment FRg, according to Holmquist et al. (2020) (SI, Eq. S1) that is proposed for inclusion into the formal USEtox model, and an extension of the existing formula for the calculation of the local irrigation velocity, where only the local agricultural soil area is considered (SI, Eq. S2).

The characteristics and dimensions of the local scale are reported in SI Table S2, and changes in dimensional parameters of the other scales are shown in SI Table S3, as

a consequence of the introduction of the local scale in the “Default USEtox” region.

## 2.2 Characterizing toxicity impacts for local and continental emissions

First of all, the  $K$ -matrix rate constants were derived for the local and continental compartments.

The calculation of the corresponding characterization factors (CFs) was performed adopting for the local scale the same factor structure used in USEtox (Eq. 1) (Rosenbaum et al. 2008), varying only the populations for the calculation of damage to human health according to the values reported in SI Tables S2 and S3.

$$CF = FF \times XF \times EF \quad (1)$$

where fate factor (FF) represents the dispersion of the contaminant in the environment, the exposure factor (XF) represents the chemical intake by humans and ecosystem exposure, and the effect factor (EF) represents the effects corresponding to the unit intake (kg) for humans or potentially affected fraction (PAF) of aquatic species integrated over the exposed water volume per kg bioavailable chemical in the aquatic environment.

The overall damage expressed by the CFs was broken down into the contributions on the different receiving scales by disaggregating the exposure matrix and the subsequent matrices, as reported in SI, section S-3. For the damage on the aquatic ecosystem, the disaggregation took place at the level of the effect factor matrix, since aquatic ecosystems models do not take into account species richness across regions.

In order to assess the relevance of the presence of local scale in the model with the local dimension, the latter was compared with a current LCA model, i.e., USEtox model, through the assessment of the impact score (IS) change for human health and freshwater toxicity, defined as Eq. 2:

$$\Delta\%IS_{x,i} = \frac{IS_{x,i(w/L)} - IS_{x,i(w/oL)}}{IS_{x,i(w/oL)}} \times 100 \quad (2)$$

where  $\Delta\%IS_{x,i}$  is the percentage damage change across the model versions for an emission of chemical  $x$  in compartment  $i$ ;  $IS_{x,i(w/L)}$  and  $IS_{x,i(w/oL)}$  are the impact scores for emissions of chemical  $x$  into local compartment  $i$  (model with local dimension, Eq. 3) or into continental compartment  $i$  (model without local dimension, Eq. 4), respectively.

$$IS_{x,i(w/L)} = CF_{x,i,L(w/L)} \times E_{x,i,L(w/L)} + CF_{x,i,C(w/L)} \times E_{x,i,C(w/L)} \quad (3)$$

$$IS_{x,i(w/oL)} = CF_{x,i,C(w/oL)} \times E_{x,i,Ctot(w/oL)} \quad (4)$$

where  $CF_{x,i,L(w/L)}$  and  $CF_{x,i,C(w/L)}$  are the characterization factors (DALY  $\text{kg}_{\text{em}}^{-1}$  or PDF  $\text{m}^3 \text{d kg}_{\text{em}}^{-1}$ ) for an emission of chemical  $x$  in respectively local and continental compartment  $i$ ,  $E_{x,i,L(w/L)}$  and  $E_{x,i,C(w/L)}$  are emissions (kg) of chemical  $x$  in respectively local and continental compartment  $i$ , all in the model with local dimension, and  $CF_{x,i,C(w/oL)}$  and  $E_{x,i,Ctot(w/oL)}$  are the characterization factor (DALY  $\text{kg}_{\text{em}}^{-1}$  or PDF  $\text{m}^3 \text{d kg}_{\text{em}}^{-1}$ ) and emission (kg) of chemical  $x$  in continental compartment  $i$  in the model without local dimension.

In order to obtain comparable results, the following correlation shall be respected (Eq. 5):

$$E_{x,i,Ctot(w/oL)} = E_{x,i,L(w/L)} + E_{x,i,C(w/L)} \quad (5)$$

Since damage variation is potentially driven by concentration variation, Eq. 6 was employed to show differences in fate between the two models:

$$\Delta C_{x,i} = \frac{C_{x,i,tot(w/L)} - C_{x,i,tot(w/oL)}}{C_{x,i,tot(w/oL)}} \quad (6)$$

where  $\Delta C_{x,i}$  is the concentration change across the models for an emission of a chemical  $x$  in a compartment  $i$ ,  $C_{x,i,tot(w/L)}$  is the sum of the concentrations in local and continental  $i$  compartments from the model with the local dimension for an emission of a chemical  $x$  in the same compartments, and  $C_{x,i,tot(w/oL)}$  is the concentration resulting from the model without the local dimension for an emission of chemical  $x$  in a continental compartment  $i$ , according to Eq. 5.

The purpose of summing up concentrations was to analyze the behavior of the two systems in terms of unit concentration (i.e., taking as reference  $1 \text{ m}^3$  for each scale). Thus, here we interpret the concentration as an average concentration across scales (local/continental or at continental scale for the two models).

In a first step, benzene was designated as an illustrative substance to explore the behavior of the newly introduced scale, since it is one of the most commonly studied organic chemicals.

In a second step, the proposed model was applied to 10 chemicals, chosen in order to consider different values of the main physico-chemical properties like degradation rates and partition coefficients and covered by both the USEtox and E-PRTR databases (EEA 2017), on which the simulation of local emissions  $E_{x,i,L(w/L)}$  defined according to real emission scenarios was based. In the present work, we are studying example chemicals—to generalize our results toward a wider chemical space, a broader set of chemicals with a diverse set of chemical properties and toxicity effects should be assessed in a future effort.

The main physical–chemical properties of the selected chemicals are reported in SI Table S6.

For IS calculation (Eqs. 3 and 4), unit emissions are considered for the selected chemicals to show damage

results on both local and continental scale of the model with the local dimension ( $E_{x,i,L(w/L)} = E_{x,i,C(w/L)} = 1 \text{ kg}$ ) and, consequently, 2 kg in the continental scale of the model without the local dimension, according to Eq. 5.

The mentioned quantities considered in this section are not intended to represent realistic emitting conditions, but only to assess at first glance the presence of a possible common trend to all selected chemicals in the comparison between one model and another.

### 2.3 Simulation of realistic emission scenarios for ten example chemicals in Europe

For impact score calculations (Eqs. 3 and 4), realistic emissions were considered for the selected chemicals from E-PRTR data for whole Europe. In particular, for each chemical, total yearly continental emissions were calculated by summing reported emissions in each emission compartment, from every facility or plant from every activity sector. The selected emission year was the most recent with the highest number of emitting point reported, taking care to avoid accidental releases as local emissions, identified as large amounts emitted that are not repeated in adjacent years to the one considered. Then, the total amount of the chemical  $x$  for the emission compartment  $i$  of the model without the local dimension was referred to daily emissions and called  $E_{x,i,Ctot(w/oL)}$ .

The quantities considered for the model with the local dimension were determined according to 3 emission scenarios as follows:

- The emissions of chemical  $x$  for local air and soils compartments  $E_{x,a/ns/as,L(w/L)}$  were defined in turn as the daily maximum/mean/minimum value among those reported for chemical industry sector. The mean value was calculated as the arithmetic mean of the admissible values.
- The emissions of chemical  $x$  for local water compartment  $E_{x,w,L(w/L)}$  were defined in turn as the daily maximum/mean/minimum value among those reported for urban wastewater treatment effluents. The mean value was calculated as the arithmetic mean of the admissible values.
- The emissions of chemical  $x$  for every  $i$  continental emission compartment  $E_{x,i,C(w/L)}$  were calculated according to Eq. 5.

Emissions in the local scale coincide with emissions from a facility or plant that had the above mentioned characteristics, as explained in SI section S-5. It is important to emphasize that the considerations reported above are intended only to identify the possible types of emitting sources near densely inhabited centers, since the simple box model is

not able to investigate very local phenomena, like distances between pollutant source and target populations.

Emissions in the local scale across Europe are reported in SI Table S7. Generally, for air compartment, the percentage on local scale ranges from 0.17 to 15.13% and for water compartment from 0.02 to 50.7% of total continental emissions.

For some chemical emission, not all the local compartments were considered due to the absence of the identified type of sources in E-PRTR database (EEA 2017).

### 3 Results

#### 3.1 Overview of the influence of the local scale for an illustrative substance

Considering an emission of  $1 \text{ kg day}^{-1}$  of benzene as an illustrative substance, the local and urban scales always have higher concentrations (Fig. 2) for an emission in the local scale compared to those found on the continental scale. This result is attributed to the greater volume of the continental scale, which lowers the concentration of the incoming mass. A detailed analysis of the fate results is reported in SI, section S-4.

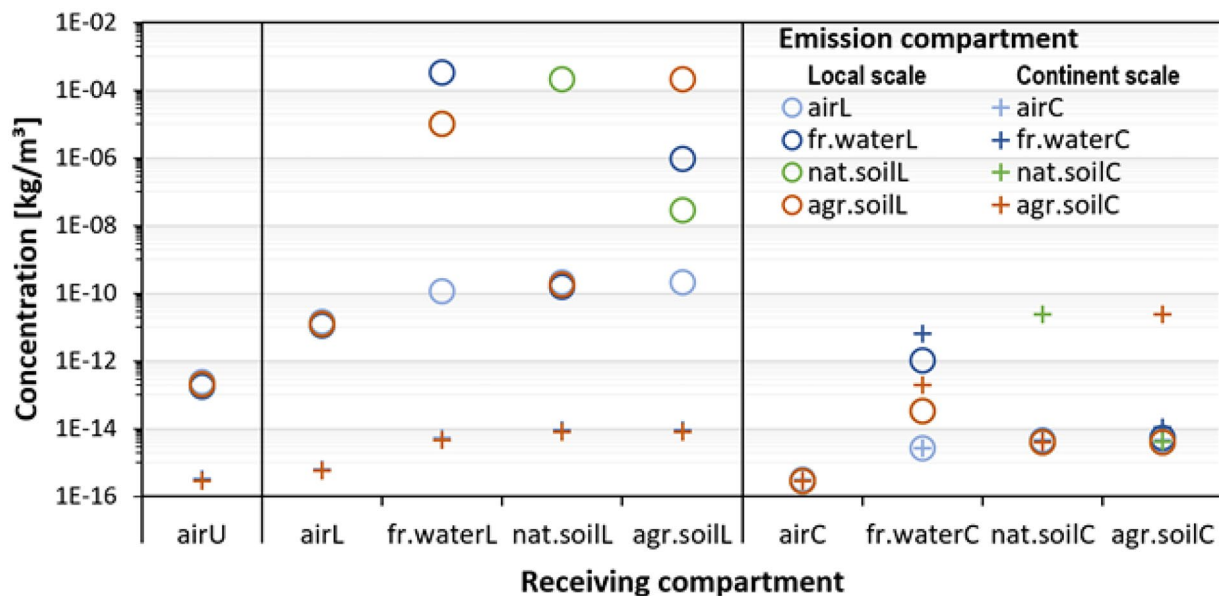
The associated damage calculated for unit emissions of benzene on both scales (Fig. 3) is always higher for local compartments, ranging from twice (air emission) to 2 orders of magnitude for human health, while the increase of the factors for the quality of the ecosystem remains more limited on the local scale (one order of magnitude is never reached).

A detailed analysis of the damage results for benzene, disaggregated per receiving scale, is reported in SI, section S-4.

#### 3.2 Analysis of the influence of physico-chemical properties on fate modelling results

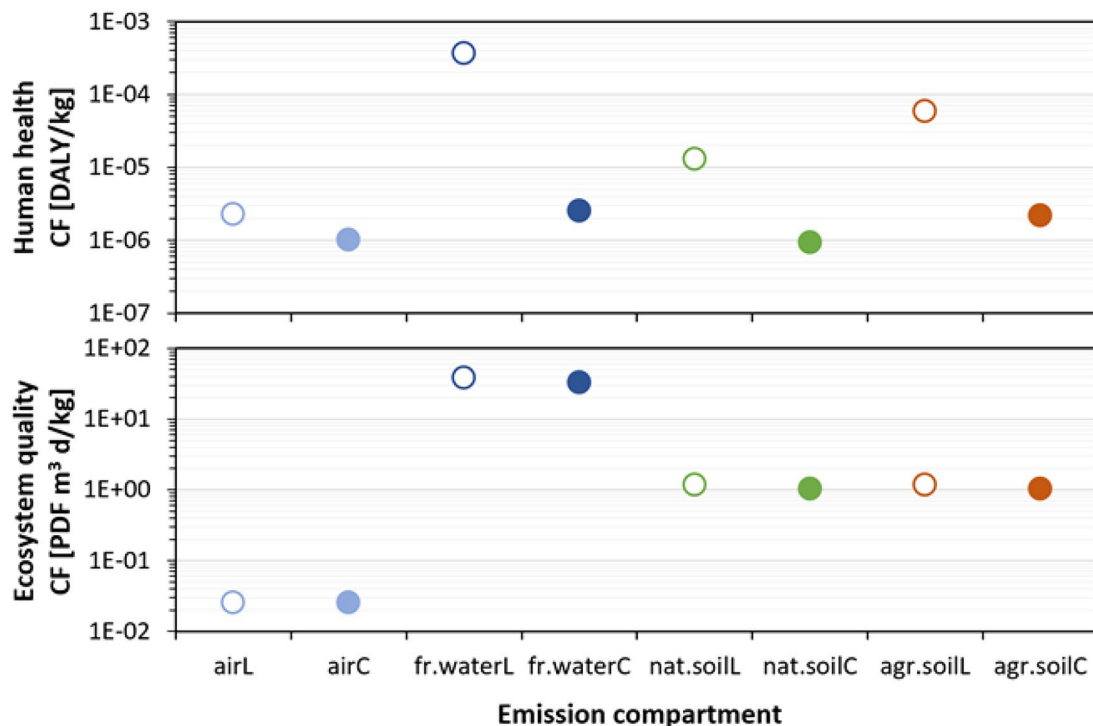
When expanding the analysis to 10 distinct example substances, the influence of the physico-chemical properties is analyzed with a twofold approach, namely, with respect to the fate results (masses and concentrations) deriving from emissions in local compartments of the USEtox model modified with the local scale as well as with respect to the concentration change results obtained from the comparison of the two models.

In particular, the selected chemicals are used as example chemicals of classes defined according to the physico-chemical properties. To generalize results toward a wider chemical space, a broader set of chemicals with a diverse set of chemical properties and toxicity effects should be assessed.



**Fig. 2** Concentration in log scale results in the receiving compartments of the model with the local dimension for  $1 \text{ kg day}^{-1}$  of benzene for each emission compartment. airU is urban air compartment, airL is local rural air compartment, fr.waterL is local freshwater compartment, nat.soilL is local natural soil compartment, agr.soilL

is local agricultural soil compartment, airC is continental air compartment, fr.waterC is continental freshwater compartment, nat.soilC is continental natural soil compartment, and agr.soilC is continental agricultural soil compartment



**Fig. 3** Characterization factors (CFs) in log scale results for end point human health toxicity potential (DALY kg<sup>-1</sup>) and end point ecotoxicity potential (PDF m<sup>3</sup> day kg<sup>-1</sup>) for 1 kg day<sup>-1</sup> of benzene

For air emissions, both weakly volatile, high degrade chemicals (e.g., atrazine) and highly volatile, low degrade chemicals (e.g., 1,1,1-trichloroethane) show the highest masses in the continental air compartment ( $FF_{aC,aL} = 3.12E - 02$  and  $FF_{aC,aL} = 1.92E + 01$  kg<sub>comp</sub> per kg<sub>em</sub>/day, respectively) compared to the local masses ( $FF_{aL} = 2.73E - 03$  and  $FF_{aL} = 3.53E - 03$  kg<sub>comp</sub> per kg<sub>em</sub>/day, respectively), underlining the dominance of the advective process for local air compartment. On the other hand, concentration results show higher values in the local compartment ( $C_{aL} = 1.14E - 11$  and  $C_{aL} = 1.47E - 11$  kg m<sup>-3</sup> per kg<sub>em</sub>/day, respectively) compared to the continental one ( $C_{aC,aL} = 3.12E - 18$  and  $C_{aC,aL} = 1.92E - 15$  kg m<sup>-3</sup> per kg<sub>em</sub>/day, respectively), because of the difference in compartment volumes.

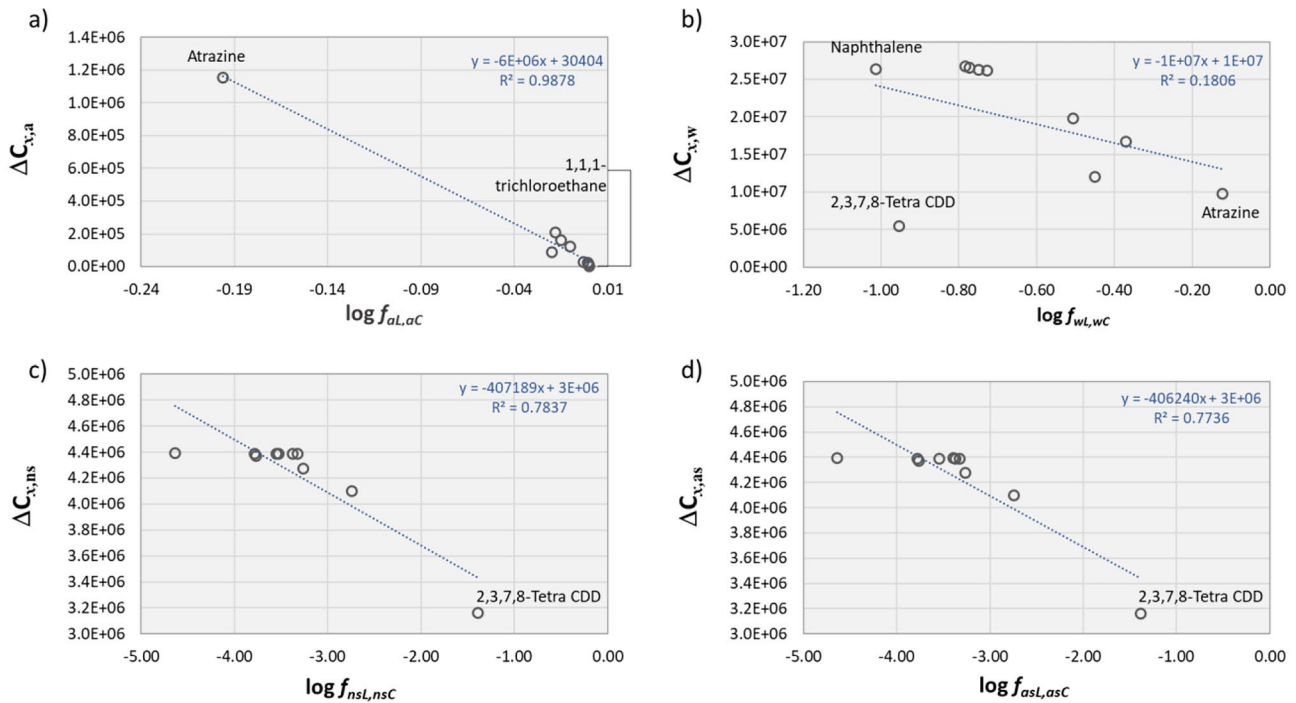
The influence of the physico-chemical properties of the selected chemicals on the fate results was analyzed by plotting the transfer coefficients (SI Table S8) that express the mass fraction of the emission in a local compartment transferred to the corresponding continental compartment, against the concentration change between the models (Fig. 4a–d).

Physico-chemical properties appear to primarily drive outcomes related to the air concentration change between the models (Fig. 4a). The chemical with the lowest  $f_{aL,aC}$  is atrazine, and it is the chemical with the highest concentra-

tion and damage increase between the models. Indeed, the low air–water partition coefficient leads to a reduction of the mass flux displaced via advection toward continental air due to the significant water absorption. On the other hand, low degradation rates (e.g., 1,1,1-trichloroethane) allow a high transport to the continental scale, resulting in the lowest concentration ( $\Delta C = 3.83E + 03$ ) and damage (Table S8 in SI) increase between the models.

For water emissions, weakly volatile chemicals (e.g., atrazine) show a higher mass in the continental freshwater compared to the local one ( $FF_{wC,wL} = 4.04E + 01$  kg<sub>comp</sub> per kg<sub>em</sub>/day and  $FF_{wL} = 1.94E + 01$  kg<sub>comp</sub> per kg<sub>em</sub>/day, respectively). Conversely, high degrade rate chemicals (e.g., naphthalene) show higher mass in the local freshwater compartment compared to the continental one ( $FF_{wL} = 2.49E + 00$  and  $FF_{wC,wL} = 2.48E - 01$  kg<sub>comp</sub> per kg<sub>em</sub>/day, respectively). Indeed, this property could determine a reduction of the mass transferred to the continental scale (i.e., the chemical does not have “time” to reach the continental scale). As for air emissions, concentration results show higher values in the local compartment ( $C_{wL} = 1.55E - 03$  and  $C_{wL} = 1.99E - 04$  kg m<sup>-3</sup> per kg<sub>em</sub>/day, respectively) compared to the continental ones ( $C_{wC,wL} = 5.98E - 11$  and  $C_{wC,wL} = 3.66E - 13$  kg m<sup>-3</sup> per kg<sub>em</sub>/day, respectively).

For the freshwater concentration change between the models (Fig. 4b), the most lipophilic chemical (i.e., 2,3,7,8-



**Fig. 4** Concentration change ( $\Delta C$ ) for every emission compartment—**a** rural air, **b** freshwater, **c** natural soil, and **d** agricultural soil—with respect to the log transfer coefficients

tetra CDD) ( $\Delta C = 5.42E + 06$ ,  $f_{wL,wC} = 1.11E - 01$ ) is not interpolated by the trend line. Indeed, the high  $K_{oc}$  (Table S3 in SI) determines the highest local removal for sedimentation process that lowers the mass in the local compartment compared to the continental one ( $FF_{wL} = 2.85$   $\text{kg}_{\text{comp}}$  per  $\text{kg}_{\text{em}}/\text{day}$ ,  $FF_{wC} = 1.42E + 01$   $\text{kg}_{\text{comp}}$  per  $\text{kg}_{\text{em}}/\text{day}$ ), producing a limited concentration increase compared to the other chemical classes.

The more rapidly degradable chemicals (e.g., naphthalene) show the highest  $\Delta C$ , as well as the highly volatile chemicals (e.g., benzene, dichloromethane, and 1,2-dichloroethane). Conversely, weakly volatile chemicals (e.g., atrazine) have a low concentration increase.

For soil emissions, both high degradation (e.g., naphthalene) and low degradation chemicals (e.g., 2,3,7,8-tetra CDD) show high masses in the local soil compartments ( $FF_{nsL} = 7.81E + 00$  and  $FF_{nsL} = 2.60E + 04$   $\text{kg}_{\text{comp}}$  per  $\text{kg}_{\text{em}}/\text{day}$ , respectively) compared to the continental masses ( $FF_{nsC,nsL} = 1.35E - 03$  and  $FF_{nsC,nsL} = 1.48E + 03$   $\text{kg}_{\text{comp}}$  per  $\text{kg}_{\text{em}}/\text{day}$ , respectively), due to the absence of the advective process for local soil compartments. As for the previous emission scenarios, concentration results show higher values in the local compartment ( $C_{nsL} = 1.57E - 04$  and  $C_{nsL} = 5.22E - 01$   $\text{kg m}^{-3}$  per  $\text{kg}_{\text{em}}/\text{day}$ , respectively) compared to the continental one ( $C_{nsC,nsL} = 3.08E - 15$  and  $C_{nsC,nsL} = 3.38E - 09$   $\text{kg m}^{-3}$  per  $\text{kg}_{\text{em}}/\text{day}$ , respectively).

Analyzing the concentration change between the models (Fig. 4c, d), there is a low variability of concentration with transfer coefficients change, with the exception of 2,3,7,8-tetra CDD, which combines the highest transfer coefficient with the lowest increase in concentration. This chemical is characterized by the lowest degradation rate in soil (Table S6 in SI) that allows a high transport to the continental scale.

Generally, all transfer coefficients of the soil compartments are much lower than the air and water compartments (up to 4 orders of magnitude, Table S8 in SI), mainly due to the absence of advective process linking the different scales. For this reason, no significant concentration increases are seen between the two models across chemicals.

In general, even if we do not see any clear relation between transferred fraction to continental scale for an emission in the local and concentration change between the models (expressed by Eq. 6), the overall tendency is that high transfer coefficients  $f_{iL,iC}$  for air lead to a lower mass stored in the local compartment and, consequently, a lower concentration increase  $\Delta C_{x,i}$ , defined according Eq. 6 in the hypothesis of a unit emission, between the two models compared to other emission compartments, as depicted in Fig. 4.

Even though soil transfer coefficients are lower compared to water compartment, the concentration increase is more significant for the latter for the smaller volume compared to soils.



### 3.3 Changes in impact scores for local and continental emissions

In Table S9 in SI, the percentage IS change  $\Delta\%IS$  for human health across the models is reported in the hypothesis of a unit emission for each scale of the model with the local dimension. The CFs used in Eq. 3 are reported in SI (Figs. S2 and S3).

For every chemical and every emission compartment, a damage increase is observed according to Eq. 2 for the model with the local scale compared to the original one (SI Table S9), in particular for rural air emissions, the range increase is more limited compared to the other compartments, due to the higher mass transferred from local scale to the continental one via advection, as shown by the transfer coefficients  $f_{iL,iC}$ , that express the mass fraction emitted in a  $i$  local compartment transferred to the corresponding  $i$  continental compartment (SI Table S8).

Since the IS is obtained by multiplication of three factors (FF, XF, and EF), the correlations shown above between  $\Delta C_{x,i}$  and  $f_{iL,iC}$  are less pronounced, or even not found, when  $\Delta\%IS_{x,i}$  is related to  $f_{iL,iC}$ , as reported in Fig. S4 in SI. Generally, a great variability in damage change across chemicals with similar transfer coefficients can be noticed for every emission compartment. This result can be attributed mainly to differences in toxicity effects of different chemicals. In a similar way, in Table S10 in SI, the percentage IS change  $\Delta\%IS$  for ecotoxicity across the models is reported in the hypothesis of a unit emission for each scale of the model with the local dimension.

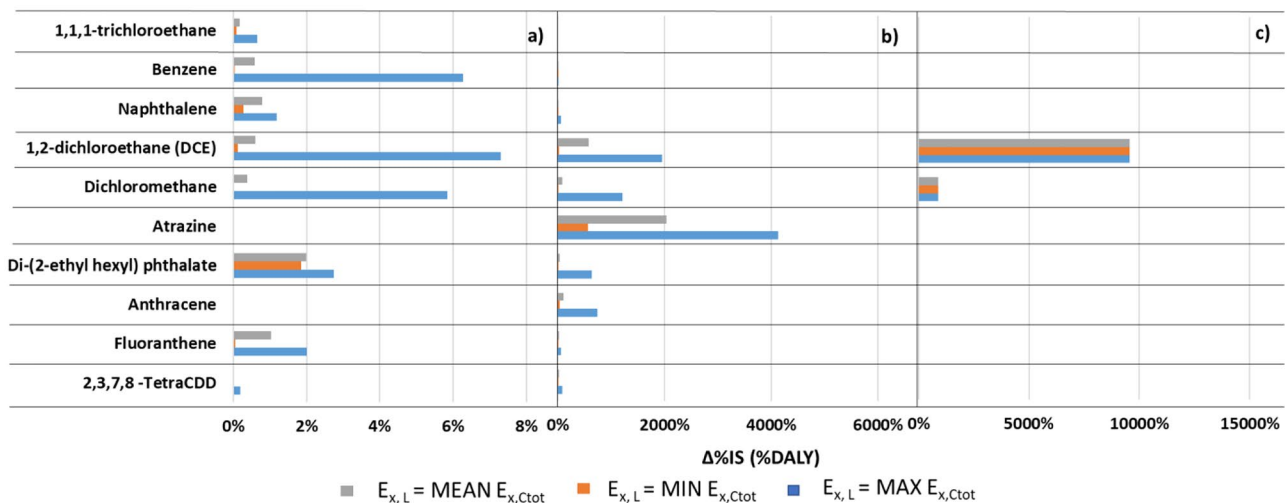
For the endpoint ecotoxicity potential, the IS increase is not always detectable, depending on the emission compartment and on the chemical. In particular, an IS decrease occurs for rural air emission of di-2-ethyl hexyl phthalate and for water and soils emissions of 2,3,7,8-tetra CDD and fluoranthene.

For air emission, some CFs for continental air of the model with the local dimension (Figs. S2 and S3 in SI) are lower than those resulting for the same emission compartment of the model without the local dimension. This result is always verified, for every chemical, emission compartment, and type of damage (i.e., DALYs and PDFs), and it is probably attributable to the introduction of a new receiving scale from the continental environment that reduces chemical mass stored there.

But, in particular for di-(2-ethyl hexyl) phthalate, a significant reduction is observed for  $CF_{aC}$  in the model with the local dimension compared to the original one, due to the update fate modeling according to Holmquist et al. (2020), as explained in section S-1 in SI.

The decrease in IS for 2,3,7,8-tetra CDD and fluoranthene for water and soil emissions is, instead, due to a reduced CF for the local scale compared to the continental scale of the model with the local dimension.

For the mentioned chemicals, the CF reduction on the local scale was proven to depend on a higher local removal rate for sedimentation that, for these chemicals, is the most relevant process in water compartments, compared to the continental scale, due to their high Koc.



**Fig. 5** Percentage IS ( $\Delta\%IS$ ) change for endpoint human health toxicity potential ( $\Delta\%DALYs$ ) for every inventoried chemical emitted in **a**) rural air, **b**) water, and **c**) natural soil according to the 3 emis-

sion scenarios (namely, local emission is mean, the minimum, and the maximum value of the continental emissions)

### 3.4 Sensitivity analysis using realistic European emission scenarios

The results reported in the following are highly dependent on the proportion between amounts at local and continental scale of chemical emitted.

In Fig. 5a, the results of human health toxicity change for rural air emissions are reported, in particular for each chemical, the damage increase is reported according to the 3 scenarios of local emission.

If the maximum local scenario is considered, the damage increase does not exceed 8% (1,2-dichloroethane, 7.31%); if the mean local scenario is considered, the damage increase does not exceed 2% (di-(2-ethyl hexyl) phthalate, 1.99%).

For water emissions (Fig. 5b), the highest IS increase is observed for atrazine (+4128.58%) in the maximum emission scenario, while the IS increase for the mean emission scenario ranges from +5.13 (naphthalene) to +2035.76% (atrazine).

For natural soil emissions (Fig. 5c), only two chemical emissions were available from E-PRTR database. Moreover, for dichloromethane and 1,2-dichloroethane, only one emission value from chemical industry source was reported; thus, the IS increase is the same for the 3 emission scenarios, ranging from 893.35 to 9573.52%.

The results reported in Fig. 6a show ecotoxicity change for each chemical emitted in rural air, where the highest damage increase is observed for fluoranthene in the maximum emission scenario (+0.42%), and the highest decrease occurs for di-(2-ethyl hexyl) phthalate (−31.78%) in the minimum emission scenario. Also, 2,3,7,8-tetra CDD shows a slight damage decrease (ranging from −0.31 to −0.26%, according to the emission scenario).

The results reported in Fig. 6b for water emission show a more varied situation than in the previous emission compartment, where chemicals with the highest damage increase (atrazine, dichloromethane, and 1,2-dichloroethane) and with the highest damage decrease (2,3,7,8-tetra CDD and fluoranthene) in the model with the local dimension compared to USEtox are emphasized by the considerable masses emitted in the maximum emission scenario.

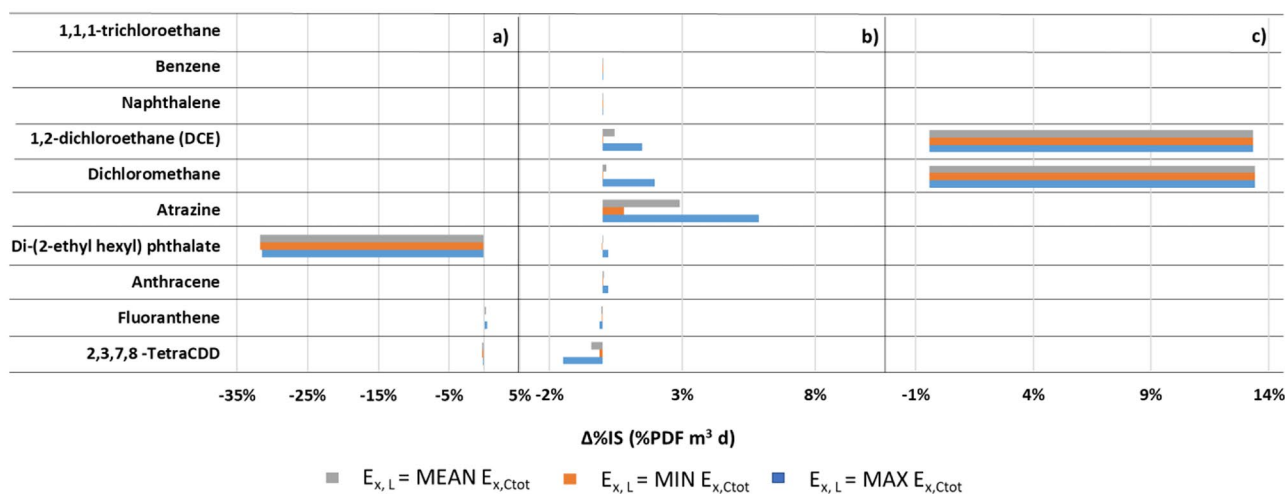
For the average emission scenario, the highest damage increase is observed for atrazine (+2.89%) and the highest damage decrease for 2,3,7,8-tetra CDD (−0.43%).

For natural soil emissions (Fig. 6c), the IS increase is the same for the 3 emission scenarios, ranging from 13.72 to 13.82%.

## 4 Discussion

The proposed model could be adapted with parameterized landscape and human exposure information typical of small scale environments. A limitation of this study is the absence of modeling of very local phenomena that could not be represented by the well-mixed box assumption. Very local phenomena and realistic concentration distribution within the so defined local scale would be better represented by properly spatialized or non-homogeneous mixing models. Such spatially resolved models that identify many neighboring “local” cells may provide a more realistic representation of actual emission-related distribution patterns of chemicals in the environment.

Furthermore, we note that overall human exposure associated with a product life cycle might be dominated by chemicals inside the product as compared to local or other chemical



**Fig. 6** Percentage IS ( $\Delta\%IS$ ) change for endpoint ecotoxicity potential ( $\Delta\%PDF\ m^3\ day$ ) for every inventoried chemical emitted in **a)** rural air, **b)** water, and **c)** natural soil according to the 3 emission scenarios (namely, local emission is mean, the minimum, and the maximum value of the continental emissions)

life cycle emissions. In such contexts, users should consider the inclusion of chemicals in products in addition to chemicals emitted along product life cycles (Fantke and Illner 2019; Joliet et al. 2021) as well as worker and bystander exposures during indoor/outdoor production stages (Hellweg et al. 2009; Ryberg et al. 2018). We propose to couple the assessment of both (local and continental) emissions and product-related exposures, while a suitable approach (e.g., input/output analysis) should be taken into account to include workers exposure (Kijko et al. 2016).

Based on our results, we suggest to use the proposed framework in LCA applications, when information about the local emission environment is known.

Despite the varied trend of mass stored (FFs) in local compartments compared to the continental scale for a unit emission in the local scale according to the physico-chemical properties, the analyzed chemicals show always higher concentrations in the local compartments compared to those found on the continental compartments per unit emission in the local scale.

The disaggregation of the CF for a unit emission of benzene in the various local compartments on the different receiving scales show that the greatest contribution to damage comes from the emission in the local scale for both human and ecosystem health, with the exception of local air, where, thanks to the high capacity of the air to be cleaned from pollutants by the wind, the greatest contribution to damage occurs on the urban scale for human toxicity and on the continental scale for ecotoxicity.

On the other hand, water advective process, depending on rain rate rather than water flow, is not as effective in transporting the mass of chemical to the continental scale.

The influence of the other processes was assessed, too: for example, 1,1,1-trichloroethane, which has a lower degradation rate in air than benzene ( $-2$  orders of magnitude), causes the greatest damage to human health on the global local scale ( $3.29\text{E}-08$  DALY  $\text{kg}^{-1}$  vs.  $1.81\text{E}-09$  DALY  $\text{kg}^{-1}$  on the urban scale and  $2.32\text{E}-10$  DALY  $\text{kg}^{-1}$  on the local scale), while anthracene (with a degradation rate  $+2$  orders of magnitude compared to benzene) affects the local scale more for a unit emission in air ( $4.48\text{E}-05$  DALY  $\text{kg}^{-1}$  on the urban scale,  $1.99\text{E}-04$  DALY  $\text{kg}^{-1}$  on the local scale).

For air emission, chemicals with lowest air–water partition coefficient (e.g., atrazine) produce the highest concentration increase ( $\Delta C_a > 10^6$ ), even if concentration increase could not be considered negligible for none of the selected chemicals. 1,1,1-trichloroethane experiences the lowest increase in concentration ( $\Delta C_a = 3.85\text{E}+03$ ) due to its high degradation rate.

For water emissions, we always observe significant concentration increase between the two models. Generally, chemicals with the highest degradation rate (naphthalene)

and highest air–water partition coefficients (benzene and dichloromethane) show the most significant concentration increase, up to  $\Delta C_w = 2.67\text{E}+07$  for benzene.

The influence of the mentioned properties on the concentration increase was assessed for the mentioned chemicals, that do not have “time” to reach the continental scale via advection, while the most transferred chemical, causing low concentration increase ( $\Delta C_w = 9.78\text{E}+06$ ), is atrazine, for its greater persistence in water determined by low air–water partition coefficient. The transfer coefficients for these chemicals are well fitted by the trend line with concentration change, unlike 2,3,7,8-tetra CDD that, due to its high  $K_{oc}$ , is characterized by the highest local removal for sedimentation process, producing the most limited concentration increase compared to the other chemicals ( $\Delta C_w = 5.42\text{E}+06$ ).

Soil compartments show significant concentration increase ( $3.16\text{E}+06 \leq \Delta C_{ns} \leq 4.39\text{E}+06$  across chemicals) and a low variability of concentration with transfer coefficients change, due to the small value of the fraction of the local mass transferred locally for soils, up to  $10^{-5}$ . The chemical with the lowest degradation rate in soil (2,3,7,8-tetra CDD) presents the lowest increase in concentration for both soils.

In the present work, we are studying example chemicals—to generalize our results toward a wider chemical space, a broader set of chemicals with a diverse set of chemical properties and toxicity effects should be assessed in a future effort.

The comparison between the model with the local dimension and the model without the local dimension shows mainly a significant relevance of the local scale for water and natural soil compartment for human health toxicity.

The consideration of average real amounts emitted in Europe shows that the neglecting local emissions leads to underestimating the damage for human health especially for water emissions of atrazine ( $\approx 2000\%$ ) and for soil emissions of 1,2-dichloroethane ( $\approx 9000\%$ ), while for air, damage increase does not exceed 2% (di-(2-ethyl hexyl) phthalate). Ecotoxicity shows a non-negligible damage significance only for the natural soil compartment, where the increase is around 14%.

Given that the EF is equal across scales, the ecotoxicity characterization results are driven by differences in FF and compartment volume that would yield a higher fraction of affected species (PAF) on the local scale. The PAF or PDF values alone can be used to express the magnitude of the impact generated on the total number of species present in each compartment. However, to derive the actual number of affected species at each scale, the CF would need to be combined with the actual number of species available at each scale, which is usually unknown for LCA contexts and requires further study.

As a future development, specific emission values from the study region or other local regions could be considered

in the simulation with average real amounts emitted in Europe for the 10 chemicals.

## 5 Conclusions

The aim of this study was to develop an assessment model applicable to LCA for damage on human and ecosystem health caused by known local rural environment emissions. This was achieved by introducing a local scale set of compartments into USEtox.

The relevance of the local scale was evaluated first by comparing the local impacts to larger emitting scales impacts provided by the proposed model with the local dimension, considering a unit emission for 10 chemicals.

Local scale results are relevant in terms of damage to human health by up to 3 orders of magnitude compared to emissions in the continental freshwater compartment (for naphthalene), mainly due to the high concentration to which the local population is exposed and up to 2 orders for emissions in natural soil of 1,2-dichloroethane. However, this is only relevant for selected chemicals and for scenarios, where locations with high industrial local emissions are also highly populated.

Unlike human health, ecotoxicity damages are marginally affected by the presence of the local scale. Given that the EF is equal across scales, the ecotoxicity characterization results are driven by differences in FF and compartment volume that would yield a higher fraction of affected species (PAF) on the local scale. The PAF or PDF values alone can be used to express the magnitude of the impact generated on the total number of species present in each compartment. However, to derive the actual number of affected species at each scale, the CF would need to be combined with the actual number of species available at each scale, which is usually unknown for LCA contexts and requires further study.

Furthermore, there is a reduction in damage compared to the continental scale for 2 chemicals (2,3,7,8-tetra CDD and fluoranthene) characterized by the highest local removal rates by sedimentation and Koc values.

Overall, the local environment is relevant for selected emission situations and chemicals, mostly for human health. For estimates of the magnitude of the local scale impacts in LCA compared to emissions in the continental scale, the proposed model is suggested, since it is based on the global consensus model for life cycle impact assessment, i.e., USEtox 2.12, widely used in LCA for human toxicity and eco-toxicity characterization. On the other hand, to properly capture very local phenomena in rather highly densely populated areas, we propose to apply spatialized models, while for unknown emission locations,

we propose to keep a more generic spatial setup as in the original USEtox model.

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**Data availability** All data generated or analyzed during this study are included in this published article (and its supplementary information files).

## Declarations

**Conflict of interest** The authors declare no conflict of interest.

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