

Titre: IMPACT World+: a globally regionalized life cycle impact assessment method. Supplément

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Supporting information section 1: List of equations, symbols and indices

Acronyms in text

AoP Area of Protection

AoC Area of Concern

Damage_{AOP} Impact category unit for corresponding AoP

CF Characterization factor

FF Fate factor

XF Exposure factor

ERF Exposure-response factor

SF Severity factor

CSI Competition scarcity index, that expresses the quantity of resource that is going to deprive competing users (current or future) sharing the same resource per quantity of resource used in a dissipative manner

Δ_x Difference in metric x described in subscript

t_1 lower time limit for time integration of impacts; $t_1 = 100$ yr for damage level long-term indicators, $t_1 = 0$ for all other indicators.

t_2 higher time limit for time integration of impacts; $t_2 = 100$ yr for shorter term indicators, $t_2 = 500$ yr for climate change, long-term indicators, $t_2 = \infty$ for other indicators

Indices - superscripts

s = elementary flow (or environmental intervention)

k = impact category (midpoint or damage level)

AOP = Area of Protection

AOC = Area of Concern

Indices – subscripts

i = emitting environmental compartment

j = receiving environmental compartment

a = emitting region (or spatial unit) (native or aggregated at country, continental or global level)

n = native emitting region (or spatial unit) for a considered impact category

b = receiving region (or spatial unit)

p = exposure pathway per unit of active substance

r = response due to a change in exposure of human population or ecosystems

u = user affected by the competition for the resource

midpoint = midpoint level

damage = damage level

Abbreviations and Symbols (units will usually depend on the considered impact category)

I^k Impact score at midpoint or damage levels for impact category k
 m_i^s Inventory elementary flow s emitted to or extracted from an emitting compartment i
 CF_i^{sk} Characterization factor for elementary flow s, impact category k and emitting compartment i
 I_a^k Impact score at midpoint or damage levels for impact category k and an emitting region a
 M_{ia}^s Inventory elementary flow s emitted to or extracted from an emitting compartment i and an emitting region a
 CF_{ai}^{sk} Characterization factor for elementary flow s, impact category k and emitting compartment i and an emitting region a

FF_{ji}^{sk} Fate factor for impact category k and for elementary flow s emitted into or extracted from emitting compartment i and transfer into receiving compartment j
 XF_{pj}^{sk} Exposure factor for impact category k and for elementary flow s in the receiving compartment j through the exposure pathway p
 ERF_{rp}^{sk} Exposure-response factor, for impact category k and elementary flow s, for the response r due to a change in exposure pathway p of human population or ecosystems
 SF_r^{sk} Severity factor, for impact category k and elementary flow s, for a response r due to a change in exposure of human population or ecosystems
 CSI_{ui}^{sk} Competition scarcity index factor for impact category k and elementary flow s, that expresses the quantity of resource in compartment i that is going to deprive competing user u (current or future) sharing the same resource per quantity of resource used in a dissipative manner
 XF_{pu}^{sk} Exposure factor, for impact category k and elementary flow s, for the user u affected by the competition for the resource through the exposure pathway p

CF_{ni}^{sk} Characterization factor for elementary flow s, impact category k and emitting compartment i and an emitting native region n
 FF_{jbni}^{sk} Fate factor for impact category k and for elementary flow s emitted into or extracted from emitting compartment i and emitting native region n and transfer into receiving compartment j and receiving region b
 XF_{pbj}^{sk} Exposure factor for impact category k and for elementary flow s in the receiving compartment j and receiving region b through the exposure pathway p
 ERF_{rbp}^{sk} Exposure-response factor, for impact category k and elementary flow s, for the response r in receiving region b due to a change in exposure pathway p of human population or ecosystems
 CSI_{ubni}^{sk} Competition scarcity index factor for impact category k and elementary flow s, that expresses the quantity of resource in compartment i and in receiving region b that is going to deprive competing user u (current or future) sharing the same resource per quantity of resource used in a dissipative manner
 XF_{pbu}^{sk} Exposure factor, for impact category k and elementary flow s, for the user u affected by the competition for the resource through the exposure pathway p in receiving region b

SPF_{ni}^{sk} Spatial proportionality factor used to aggregate CF_{ni}^{sk} into a coarser resolution a (for instance national, continental, or global).

F_{ni}^s overall annual environmental intervention for elementary flow s within the native spatial unit n for an emitting compartment i
 F_{ai}^s overall annual environmental intervention for elementary flow s within the region a for an emitting compartment i
 A_n surface area of the native spatial unit n
 A_a surface area of the emitting spatial unit a
 $A_{n \cap a}$ surface area intersecting of the native spatial unit n and the emitting spatial unit a
 S^{AOP} Aggregated impact score in AOP
 S^{AOC} Aggregated impact score in AOC
 NF^{AOP} Normalization factors of IMPACT World+ for AOP
 $I_{world\ annual}^k$ Impact score at damage levels for impact category k due to the total world emissions and extractions for one year
 $N_{world\ pop}$ Total world population count
 $S_{world\ annual}^{AOP}$ Aggregated impact score in AOP due to all the total world emissions and extractions for one year

1. The impact score at midpoint or damage level for an impact category

$$I^k = \sum_s \overrightarrow{CF^{sk}} \cdot \overrightarrow{m^s} \text{ (Eq. SI1)}$$

With:

- $Dim(x)$ is the number of elements along the x axis
- I^k a scalar
- $\overrightarrow{CF^{sk}}$ a vector with $(Dim(i))$ dimension and elements defined as CF_i^{sk}
- $\overrightarrow{m^s}$ a vector with $(Dim(i))$ dimension and elements defined as m_i^s
- The operator “.” is defined as the inner product (or dot product) between vector such as $V = \overrightarrow{T} \cdot \overrightarrow{U}$ is equivalent to $V = \sum_i T_i U_i$.

And elements given by:

$$I^k = \sum_s \sum_i CF_i^{sk} m_i^s \text{ (Eq. SI1.1)}$$

1.1. For regionalized impact calculation

$$I^k = \sum_s \overrightarrow{1} \cdot \overrightarrow{CF^{sk}} \circ \overrightarrow{M^s} \text{ (Eq. SI1_regio)}$$

With:

- $Dim(x)$ is the number of elements along the x axis
- I^k a vector with $(Dim(a))$ dimension and elements defined as I_a^k
- $\overrightarrow{CF^{sk}}$ a matrix with $(Dim(a) \times Dim(i))$ dimensions and elements defined as CF_{ai}^{sk}
- $\overrightarrow{M^s}$ a matrix with $(Dim(i) \times Dim(a))$ dimensions and elements defined as M_{ia}^s
- $\overrightarrow{1}$ a vector with $Dim(i)$ dimension and all elements equal to 1
- The operator “ \circ ” is defined as the Hadamard product such as $V = T \circ U$ with elements given by $V_{ij} = T_{ij} U_{ij}$.

- The operator “.” is defined as the inner product (or dot product) such as $V = T \cdot U$ elements given by $V_{ik} = \sum_j T_{ij} U_{jk}$.

And elements given by:

$$I_a^k = \sum_s \sum_i CF_{ai}^{sk} M_{ia}^s \text{ (Eq. SI1_regio.1)}$$

2. Damage CF for an impact category and for an elementary flow

2.1. Damage CF for emission related impact category

2.1.1. For non-regionalized impact category

$$\overrightarrow{CF}^{sk} = \overrightarrow{SF}^{sk} \cdot \mathbf{ERF}^{sk} \cdot \mathbf{XF}^{sk} \cdot \mathbf{FF}^{sk} \text{ (Eq. SI2)}$$

With:

- $Dim(x)$ is the number of elements along the x axis
- \overrightarrow{CF}^{sk} a vector with $(Dim(i))$ dimension and elements defined as CF_i^{sk}
- \mathbf{FF}^{sk} a matrix with $(Dim(j) \times Dim(i))$ dimensions and elements defined as FF_{ji}^{sk}
- \mathbf{XF}^{sk} a matrix with $(Dim(p) \times Dim(j))$ dimensions and elements defined as XF_{pj}^{sk}
- \mathbf{ERF}^{sk} a matrix with $(Dim(r) \times Dim(p))$ dimensions and elements defined as ERF_{rp}^{sk}
- \overrightarrow{SF}^{sk} a vector with $(Dim(r))$ dimension and elements defined as SF_r^{sk}
- The operator “.” is defined as the inner product (or dot product) such as $V = T \cdot U$ elements given by $V_{ik} = \sum_j T_{ij} U_{jk}$.

And elements given by:

$$CF_i^{sk} = \sum_r SF_r^{sk} \left(\sum_p ERF_{rp}^{sk} \left(\sum_j XF_{pj}^{sk} FF_{ji}^{sk} \right) \right) \text{ (Eq. SI2.1)}$$

Which is equivalent to the following equation:

$$CF_i^{sk} = \sum_r \sum_p \sum_j SF_r^{sk} ERF_{rp}^{sk} XF_{pj}^{sk} FF_{ji}^{sk} \text{ (Eq. SI2.2)}$$

2.1.2. For regionalized impact category

$$\mathbf{CF}^{sk} = \vec{1} \cdot \overrightarrow{SF}^{sk} \cdot \mathbf{ERF}^{sk} \cdot \mathbf{XF}^{sk} \cdot \mathbf{FF}^{sk} \text{ (Eq. SI2_regio)}$$

With:

- $Dim(x)$ is the number of elements along the x axis
- \mathbf{CF}^{sk} a matrix with $(Dim(a) \times Dim(i))$ dimensions and elements defined as CF_{ni}^{sk}
- \mathbf{FF}^{sk} a matrix (or tensor) with $(Dim(j) \times Dim(b) \times Dim(n) \times Dim(i))$ dimensions and elements defined as FF_{jbni}^{sk}
- \mathbf{XF}^{sk} a matrix (or tensor) with $(Dim(p) \times Dim(b) \times Dim(j))$ dimensions and elements defined as XF_{pbj}^{sk}

- \mathbf{ERF}^{sk} a matrix (or tensor) with $(\text{Dim}(r) \times \text{Dim}(b) \times \text{Dim}(p))$ dimensions and elements defined as ERF_{rbp}^{sk}
- $\overrightarrow{\mathbf{SF}}^{\text{sk}}$ a vector with $(\text{Dim}(r))$ dimension and elements defined as SF_r^{sk}
- $\vec{1}$ a vector with $\text{Dim}(b)$ dimension and all elements equal to 1
- The operator “.” is defined as the inner product (or dot product) between tensors, matrices and vectors such as $\mathbf{V} = \mathbf{T} \cdot \mathbf{U}$ elements given by $V_{ijk} = \sum_l T_{ijl} U_{lk}$.

And elements given by:

$$CF_{ni}^{\text{sk}} = \sum_b \left(\sum_r SF_r^{\text{sk}} \left(\sum_p ERF_{rbp}^{\text{sk}} \left(\sum_j XF_{pbj}^{\text{sk}} FF_{jbni}^{\text{sk}} \right) \right) \right) \quad (\text{Eq. SI2_regio.1})$$

Which is equivalent to the following equation:

$$CF_{ni}^{\text{sk}} = \sum_b \sum_r \sum_p \sum_j SF_r^{\text{sk}} ERF_{rbp}^{\text{sk}} XF_{pbj}^{\text{sk}} FF_{jbni}^{\text{sk}} \quad (\text{Eq. SI2_regio.2})$$

2.2. Damage CF for resource related impact category

2.2.1. For non-regionalized impact category

$$\overrightarrow{\mathbf{CF}}^{\text{sk}} = \overrightarrow{\mathbf{SF}}^{\text{sk}} \cdot \mathbf{ERF}^{\text{sk}} \cdot \mathbf{XF}^{\text{sk}} \cdot \mathbf{CSI}^{\text{sk}} \quad (\text{Eq. SI2})$$

With:

- $\text{Dim}(x)$ is the number of elements along the x axis
- $\overrightarrow{\mathbf{CF}}^{\text{sk}}$ a vector with $(\text{Dim}(i))$ dimension and elements defined as CF_i^{sk}
- \mathbf{CSI}^{sk} a matrix with $(\text{Dim}(u) \times \text{Dim}(i))$ dimensions and elements defined as CSI_{ui}^{sk}
- \mathbf{XF}^{sk} a matrix with $(\text{Dim}(p) \times \text{Dim}(u))$ dimensions and elements defined as XF_{pu}^{sk}
- \mathbf{ERF}^{sk} a matrix with $(\text{Dim}(r) \times \text{Dim}(p))$ dimensions and elements defined as ERF_{rp}^{sk}
- $\overrightarrow{\mathbf{SF}}^{\text{sk}}$ a vector with $(\text{Dim}(r))$ dimension and elements defined as SF_r^{sk}
- The operator “.” is defined as the inner product (or dot product) such as $\mathbf{V} = \mathbf{T} \cdot \mathbf{U}$ elements given by $V_{ik} = \sum_j T_{ij} U_{jk}$.

And elements given by:

$$CF_i^{\text{sk}} = \sum_r SF_r^{\text{sk}} \left(\sum_p ERF_{rp}^{\text{sk}} \left(\sum_u XF_{pu}^{\text{sk}} CSI_{ui}^{\text{sk}} \right) \right) \quad (\text{Eq. SI2.1})$$

Which is equivalent to the following equation:

$$CF_i^{\text{sk}} = \sum_r \sum_p \sum_u SF_r^{\text{sk}} ERF_{rp}^{\text{sk}} XF_{pu}^{\text{sk}} CSI_{ui}^{\text{sk}} \quad (\text{Eq. SI2.2})$$

2.2.2. For regionalized impact category

$$\mathbf{CF}^{\text{sk}} = \vec{1} \cdot \overrightarrow{\mathbf{SF}}^{\text{sk}} \cdot \mathbf{ERF}^{\text{sk}} \cdot \mathbf{XF}^{\text{sk}} \cdot \mathbf{CSI}^{\text{sk}} \quad (\text{Eq. SI2_regio})$$

With:

- $\text{Dim}(x)$ is the number of elements along the x axis
- \mathbf{CF}^{sk} a matrix with $(\text{Dim}(n) \times \text{Dim}(i))$ dimensions and elements defined as CF_{ni}^{sk}

- **CSI^{sk}** a matrix (or tensor) with $(Dim(u) \times Dim(b) \times Dim(n) \times Dim(i))$ dimensions and elements defined as CSI_{ubni}^{sk}
- **XF^{sk}** a matrix (or tensor) with $(Dim(p) \times Dim(b) \times Dim(u))$ dimensions and elements defined as XF_{pbu}^{sk}
- **ERF^{sk}** a matrix (or tensor) with $(Dim(r) \times Dim(b) \times Dim(p))$ dimensions and elements defined as ERF_{rbp}^{sk}
- **SF^{sk}** a vector with $(Dim(r))$ dimension and elements defined as SF_r^{sk}
- **1** a vector with $Dim(b)$ dimension and all elements equal to 1
- The operator “.” is defined as the inner product (or dot product) between tensors, matrices and vectors such as $V = T \cdot U$ elements given by $V_{ijk} = \sum_l T_{ijl} U_{lk}$.

And elements given by:

$$CF_{ni}^{sk} = \sum_b (\sum_r SF_r^{sk} (\sum_p ERF_{rbp}^{sk} (\sum_u XF_{pbu}^{sk} CSI_{ubni}^{sk}))) \quad (\text{Eq. SI2_regio.1})$$

Which is equivalent to the following equation:

$$CF_{ni}^{sk} = \sum_b \sum_r \sum_p \sum_u SF_r^{sk} ERF_{rbp}^{sk} XF_{pbu}^{sk} CSI_{ubni}^{sk} \quad (\text{Eq. SI2_regio.2})$$

3. Spatial aggregation of CF for spatially differentiated impact categories

The aggregated CF for a given region a, for an elementary flow s, for an impact category k and for an emitting compartment I is given by:

$$CF_{ai}^{sk} = \sum_n CF_{ni}^{sk} \times SPF_{ni}^{sk} \quad (\text{Eq. SI3})$$

$$SPF_{ni}^{sk} = \frac{F_{ni}^s \times \frac{A_{n\cap a}}{A_a}}{\sum_n F_{ni}^s \times \frac{A_{n\cap a}}{A_a}} = \frac{F_{ni}^s \times \frac{A_{n\cap a}}{A_a}}{F_{ai}^s} \quad (\text{Eq. SI3.1})$$

$\frac{A_{n\cap a}}{A_a} = 1$ when the spatial unit n is totally included in the spatial unit a.

4. Midpoint level equations

Depending on the position of the midpoint indicator along the cause-effect chain, midpoint level characterization factors for emission-related impact categories follow Equation SI4.1 (freshwater eutrophication, water scarcity), SI4.2 (Climate change shorter term, climate change long term, terrestrial acidification, freshwater acidification, SI4.3 (marine eutrophication, freshwater ecotoxicity, human toxicity cancer, human toxicity non cancer, particulate matter formation, photochemical oxidant formation, ionising radiation HH, ionising radiation EQ) or SI4.4 (ozone layer depletion, water stream use and management, land transformation biodiversity, land occupation biodiversity) with

$SF_r^{sk}, ERF_{rbp}^{sk}, XF_{pbj}^{sk}, FF_{jbni}^{sk}$ defined as in damage level equations:

$$CF_{ni}^{sk} = \sum_b \sum_j FF_{jbni}^{sk} \quad (\text{Eq SI.4.1})$$

$$CF_{ni}^{sk} = \sum_b (\sum_j XF_{pbj}^{sk} FF_{jbni}^{sk}) \quad (\text{Eq SI.4.2})$$

$$CF_{ni}^{sk} = \sum_b (\sum_p ERF_{rbp}^{sk} (\sum_j XF_{pbj}^{sk} FF_{jbni}^{sk})) \quad (\text{Eq SI.4.3})$$

$$CF_{ni}^{sk} = \sum_b \left(\sum_r SF_r^{sk} \left(\sum_p ERF_{rbp}^{sk} \left(\sum_j XF_{pbj}^{sk} FF_{jbni}^{sk} \right) \right) \right) \quad (\text{Eq SI.4.4})$$

For both resource-related impact categories (mineral resources use, fossil energy use), midpoint level characterization factor follows Equation SI4.5 with XF_{pu}^{sk} , CSI_{ui}^{sk} defined as in damage level equations:

$$CF_i^{sk} = \sum_p \sum_u XF_{pu}^{sk} CSI_{ui}^{sk} \quad (\text{Eq SI4.5})$$

5. Overall damage on the AoPs considering all the different impact categories at damage level

$$S^{AOP} = \sum_{k \in AOP} I^k \quad (\text{Eq. SI5})$$

6. Overall damage contributing to the same AoC

$$S^{AOC} = \sum_{k \in AOC} I^k \quad (\text{Eq. SI6})$$

7. Normalization factors

$$NF^{AOP} = \frac{\sum_{k \in AOP} I_{world\ annual}^k}{N_{world\ pop}} = \frac{S_{world\ annual}^{AOP}}{N_{world\ pop}} \quad (\text{Eq. SI7})$$

Climate change

A greenhouse gas emission first leads to an increase in atmospheric concentration, which then leads to positive radiative forcing. This positive radiative forcing may cause different climate effects such as an increase in temperature or precipitation changes. IMPACT World+ focuses on the temperature increase pathway, not considering the other types of climate effects due to a lack of data and knowledge. An increase in the Earth average temperature leads to potential impacts on humans and ecosystems through several pathways.

The fate factor corresponds to the time-integrated mass of the greenhouse gas for a given mass emitted in the atmosphere. It is determined using the impulse response function proposed by Joos *et al.* (2013) and adopted by the IPCC (Myhre 2013). The exposure factor gives the time-integrated increase in temperature due to this time integrated mass in the atmosphere. This exposure factor can be decomposed in two sub-indicators: the time-integrated radiative forcing due to the time-integrated mass in the atmosphere, and the time-integrated increase in temperature due to the time-integrated radiative forcing.

The Global Warming Potential for a 100-year time horizon (GWP100) as adopted by the IPCC (Myhre 2013) is used as a midpoint indicator for shorter-term climate change, characterizing the cumulative radiative forcing per kg greenhouse gas emitted. The Global Temperature Potential for a 100-year time horizon (GTP100), as also proposed in the latest IPCC report (Myhre 2013), is our second midpoint indicator for long-term climate change impacts and represents a change in global mean surface temperature at a chosen point in time. It is therefore not a cumulative indicator, but it is consensually considered as an appropriate proxy to represent climate change long-term impacts (Levasseur *et al.* 2016). Those two indicators are needed because they express different impacts: GTP100 (climate change long-term) are impacts related to long-term cumulative warming (e.g. sea level rise), while GWP100 (climate change shorter-term) are impacts related to a rapid increase in temperature to which humans and species must adapt very quickly.

At the damage level, cumulative metrics need to be considered in LCIA to ensure additivity of impacts (Frischknecht *et al.* 2016). Hence the GTP100 cannot be used. To model the impact up to the damage, we therefore use the time-integrated temperature increase calculated from absolute GTP (aGTP) equations, as proposed by the IPCC (Myhre 2013). In compliance with what is proposed by the IPCC, the effect of CO₂ that is formed from the oxidation of CH₄ and CO is considered, but not the oxidation products of other VOCs (see supporting info, Section xxx for details). This time-integrated temperature increase is thus a combination of fate and exposure factors of humans and ecosystems to climate change. Human health effect factors are calculated based on the increase in risk of dying associated with a time-integrated temperature increase, as proposed by de Schryver *et al.* (2009), building on a study from the World Health Organization (2003). It provides the relative risk of dying from five different causes (cardiovascular diseases, malaria, diarrhoea, floods and malnutrition). This represents what is feasible today, and it is likely to represent only a fraction of the actual DALYs caused by climate change – the majority of which will likely results from conflicts in an unstable world (Barnett and Adger 2007). This is thus a proxy of

the lower bound of human health damage from climate change. The severity corresponding to each cause of risk (DALY/case) are taken from the Global Burden-of-Disease report (Mathers et al. 2008) for cardiovascular diseases, malaria, diarrhoea and malnutrition, while the International Disaster Database (2009) is used in combination with the Global Burden-of-Disease data for unintentional injuries to estimate DALY/case for floods. For ecosystem quality, as proposed by de Schryver *et al.* (2009), effect factors are calculated from a study compiling a number of regional studies that aim at predicting the extinction of species related to an increase in temperature (Thomas et al. 2004) considering a global surface of semi-natural terrestrial areas of the world of $2.29 \cdot 10^{13} \text{ m}^2$. Both damage level impact indicators on ecosystems and human health are temporally resolved: shorter-term cumulative impacts are calculated for a time horizon within 100 years from the emission, while long-term cumulative impacts are calculated between 100 years and 500 years.

IMPACT World+ also considers additional interim impact pathways related to climate change affecting the “resources and ecosystem services” AoP, as described the supporting information Section 4.

Marine acidification

Carbon dioxide released into the atmosphere partly partitions into the oceans, and reacts with the water to form carbonic acid. Some of these carbonic acid molecules dissociate to give bicarbonate and hydronium ions, thus increasing the ocean's acidity (H^+ ion concentration). Other chemical reactions are also triggered (shift in the carbonate system toward lower pH), which results in an actual net decrease in the amount of carbonate ions available. In the oceans, this makes it more difficult for marine calcifying organisms, such as coral and some plankton, to form biogenic calcium carbonate, and such existing structures become vulnerable to dissolution.

To ensure consistency with climate change modelling, a) the fate model for CO_2 emissions is the same as for climate change (Myhre 2013); b) CH_4 and CO are also classified within this impact category to consider the effect of CO_2 that is formed from the oxidation of CH_4 and CO ; c) the model is temporally resolved, differentiating between impacts in the first 100 years and long-term impacts occurring between 100 and 500 years. The exposure factor considers the decrease in ocean pH due to an increase in CO_2 in the atmosphere (Azevedo et al. 2015). The effect factor is based on a species sensitivity distribution (SSD) curve using the $\text{HC50}_{\text{EC50}}$ (i.e. the H^+ concentration affecting 50% of the population of 50% of the considered species) due to pH modification on marine ecosystems (Azevedo et al. 2015). The effect model uses a linearity assumption of the SSD curve between 0 and the $\text{HC50}_{\text{EC50}}$. This is consistent with the way SSD curves are used in USEtox to generate effect factors for ecotoxicity.

Mineral and fossil resources use

For mineral resources use impact, IMPACT World+ uses the material competition scarcity index from de Bruille (2014) as a midpoint indicator. This factor represents the fraction of material needed by future users that are not able to adapt to a full dissipation of the easily available stock. It is expressed in terms of kg of deprived resource per kg of dissipated resource.

For fossil energy use impact, IMPACT World+ uses the primary energy content (Frischknecht 2003) as a midpoint indicator considering that it is a reasonable proxy to assess the MJ deprived per MJ consumed, under the assumption that fossil resources are mainly functional for energy purposes. A functionality specific effect factor from Fatemi (2012) for fossil energy use and from De Bruille (2014) for mineral resources use is then applied, giving the adaptation price to fulfil the need of non-adapted users using a backup technology (\$/kg deprived) to obtain the interim damage level CF.

These models are operational to assess mineral and fossil resources both at midpoint and damage levels, but have only yet been applied at damage level to coal and petroleum for fossil energy use and to aluminium, cadmium, cobalt, lithium, manganese, nickel and rare earths for mineral resources, assuming today's technology for backup. These damage level CFs are therefore considered as interim.

Acidification

When emitted to the atmosphere, acidifying substances will disperse, react with other substances in the atmosphere and travel potentially long distances before depositing on soil and/or water. These deposits may change the soil and water acidity levels. For every species, there is an optimum pH range, and a deviation from this optimum may be harmful for that specific species. Consequently, a change in pH may decrease the species distribution in an ecosystem.

The characterization factors presented by Roy *et al.* (Roy et al. 2014; Roy et al. 2012a; Roy et al. 2012b) are used for terrestrial and freshwater acidification respectively, both at midpoint and damage levels. The midpoint characterization factors express the change in pH in receiving environments (soil and freshwater, respectively) due to an emission of nitrogen oxides (NO_x), ammonia (NH₃) and sulphur dioxide (SO₂). It combines fate assessment addressing atmospheric source-deposition relationships using the GEOS Chem model and soil sensitivity assessment for terrestrial acidification. An additional soil fate assessment gives the transfer of H⁺ to freshwater ecosystems for freshwater acidification. Damages on ecosystem quality are expressed in terms of PDF·m²·yr per kg of substance emitted and computed combining the midpoint CF with an effect factor (Roy et al. 2014). For terrestrial acidification, the latter determines the change in vascular plant species per change in the soil pH. For freshwater acidification, it measures the change of potentially disappeared fraction of fish species per change in the water pH.

Eutrophication

Eutrophication is the result of increased nutrient loading to a surface water body, driving growth of primary producers, changing species abundance and diversity, ultimately leading to decreased levels of oxygen that affect freshwater or coastal ecosystems. As the underlying (simplifying) assumption, phosphorous is considered the only limiting nutrient causing freshwater eutrophication, whereas nitrogen is modelled as the limiting nutrient for marine coastal zones.

For freshwater eutrophication, the work of Helmes *et al.* (2012) is used to determine the fate factor of phosphorous in freshwater at a 0.5° x 0.5° resolution. This fate factor expresses the increase in phosphorus mass per kg_P discharged to freshwater and is used as the midpoint CF for freshwater eutrophication. A stoichiometric ratio between substances is used to generate CFs for other P containing substances (phosphate, phosphoric acid, phosphorus pentoxide) and an equivalency factor of 0.022 kg PO₄³⁻_{eq}/kg was considered for COD and BOD as recommended in CML (Guinée *et al.* 2002). The damage factor is obtained multiplying the midpoint CF by an effect factor of 11.4 PDF·m²·yr/kg PO₄³⁻_{eq} from Tirado-Seco (2005).

For marine eutrophication, the coastal zone considered is the zone where the ocean depth is less than 200 m, consistently with the (sub-)continental parameterisation of USEtox (Kounina *et al.* 2014). The same atmospheric fate model as used by Roy *et al.* (2012b) for acidification (GEOS Chem) is used to determine the source-to-deposition relationship of Ammonia (NH₃) and (NO_x) atmospheric emissions on coastal zones. For emissions to freshwater, 70% of the N containing substances discharged is assumed to reach the coastal zone as done in ReCiPe and EDIP (Goedkoop *et al.* 2013; Hauschild and Potting 2005; Hauschild and Wenzel 1998). This reflects the fact that elimination due to denitrification in anaerobic zones in freshwater is treated as a constant with a generic removal of 30 % in the CARMEN European model used in both LCIA methods. Hence, 70 % of the nitrogen input transports to sea. An empirically-based EF of 12.5 PDF·m²·yr/kg_{deposited} has been determined based on the ratio between observed eutrophied areas in highly eutrophied regions (Gulf of Mexico, Baltic sea, Chesapeake Bay) and nitrogen load. Eutrophication in the Gulf of Mexico, Baltic Sea and Chesapeake Bay are primarily caused by Nitrogen flux into the water system. To analyse this relationship and to get a correlation between the nutrient fluxes into the aquatic ecosystem in consideration and the extent of hypoxia, the metrics PDF m² year/kg N is used (see results in table S3.1). The average value of 12.5 PDF m² yr/ kgN is used as the marine eutrophication effect factor in IMPACT World+.

Table SI 5.1 : Hypoxic areas/kg nutrients for various affected water systems

Water Body	Analysis Years	Total Nitrogen/ Phosphorus (t/year)	Average Hypoxia Area (km ²)	Hypoxia Area/ kgN (PDF m ² year/ kg N)
Gulf of Mexico	1985-2010	1 419 760	13 810	9,7
Gulf of Mexico	2005-2010	1 368 200	17 300	12,6
Chesapeake Bay	1985-2011	91 330,45	1 183,20	13,0
Chesapeake Bay	1970-2011	94 823,95	1 105,40	11,7
Baltic Sea	1995-2009	3 729 000,00	48 000,00	12,9

An update of the Marine eutrophication indicator is to be expected in the near future to account for recent research developments done by Cosme (Cosme and Hauschild 2016).

Toxicity impacts

Outdoor and indoor emissions of chemical substances may cause toxic effects to human health and to ecosystems. Once emitted into air, freshwater or soil, the substances may

reach and affect freshwater, terrestrial and marine ecosystems. Humans may also be exposed to these substances through different pathways (e.g. inhalation of air, ingestion of food and water), which may cause multiple health outcomes and diseases in different human and/or ecosystem populations.

The UNEP/SETAC scientific consensus model USEtox for characterizing human toxicity and ecosystem toxicity impacts (Hauschild et al. 2008; Rosenbaum et al. 2008), that accounts for fate, exposure and effects of chemicals, is used and adapted to generate the IMPACT World+ (eco)toxicity CFs. Version 2.0 of USEtox is used to determine the global default CFs, including continental versions based on the work of Kounina et al. (2014). Characterization factors for human toxicity modeled with USEtox are expressed at the midpoint level in comparative toxic units (CTU_h) per unit mass of a chemical emitted, providing the estimated increase in morbidity in the global human population per unit mass of a chemical emitted into a specific environmental compartment (disease cases per kg emitted) both for cancer and non-cancer diseases. Since these two indicators should not be directly summed up without severity assessment (Rosenbaum et al. 2011), damage level CFs are calculated using severity factors of 11.5 and 2.7 DALY (Huijbregts et al. 2005) per disease case for cancer and non-cancer, respectively. Human toxicity CFs also include toxicity impacts from indoor emissions – using the USEtox indoor CFs for household and industrial indoor emissions – considering different archetypes for OECD countries and non OECD airtight and non airtight buildings (Hellweg et al. 2009; Rosenbaum et al. 2015; Wenger et al. 2012) and pesticide residues ingestion from crops (Fantke et al. 2011; Fantke and Jolliet 2016; Fantke et al. 2012) for both cancer and non-cancer effects.

Of special interest is the case of metals, which have typically contributed significantly to toxic impacts. There is a need to account for the essentiality of zinc, since most of the world population is reported to be deficient in Zn. We therefore only applied the toxicity non-cancer characterization factor of Zn to the small fraction of the population that may be exposed at potentially toxic levels – 2% according to expert judgement – (Nriagu 2014).

For freshwater ecotoxicity, USEtox midpoint level CFs are expressed as comparative toxic units (CTU_e) per per unit mass of a chemical emitted, providing an estimation of the potentially affected fraction (PAF) of the exposed ecosystem species integrated over time and water volume per unit mass of a chemical emitted ($PAF \cdot m^3 \cdot day/kg$). A generic severity factor of 0.5 is applied to convert PAF to PDF – the potentially disappeared fraction of species – based on the assumption that 50% of the affected species will disappear from the ecosystem after exposure (Jolliet et al. 2003a). An average surface water depth of 2.5 m is used to yield a damage expressed in $PDF \cdot m^2 \cdot day/kg$.

We acknowledge that the continental resolution with population density archetypes used to determine the fate in USEtox is meaningful for human toxicity, but not as relevant for ecotoxicity, because the target organisms are not distributed in the same way. Moreover, USEtox doesn't attempt to represent the spatial variability of (eco)toxicity. Further research is needed to adequately model the spatial variability of this impact category in a manageable way in an LCA context, knowing that thousands of substances have to be characterized for each native spatial unit.

USEtox CFs are differentiated between shorter-term impacts taking place over the first 100 years and long-term impacts from 100 years to infinity,, of which the latter are only substantial for very persistent substances, such as metals.

Interim CFs are also proposed for marine and terrestrial ecotoxicity impacts and are described in supporting information, Section 4.

Particulate matter formation

Inhalation of fine particulate matter (PM_{2.5}), i.e. particles with diameter less than 2.5 µm, is known to cause a number of health related issues and reduction in life expectancy, including chronic and acute respiratory and cardiovascular morbidity, chronic and acute mortality, lung cancer, diabetes, and adverse birth outcomes (Fantke et al. 2015). PM_{2.5} is composed of primary and secondary particles. The latter originates from the oxidation of primary gases such as sulfur oxides and nitrogen oxides into ammonium sulfates and ammonium nitrates PM_{2.5}.

Characterization factors are modelled using epidemiologically derived factors from Humbert et al. (2011) and Gronlund et al. (2015). PM₁₀ is considered in those publications 1.67 times less toxic than PM_{2.5} and converted into PM_{2.5} equivalents via this factor. The midpoint CFs account for fate, exposure, and effect. Intake fractions for primary PM_{2.5} are defined as the fractions of the emission taken in (inhaled) by the overall population (Bennett et al. 2002; Hodas et al. 2015) and are consistent with USEtox fate factors using archetypes for remote, rural and urban outdoor environments. The intake fraction for secondary PM_{2.5} is the inhaled mass of PM_{2.5} attributable to (i.e. formed from) a specific precursor substance per mass emitted of this precursor. Midpoint CFs are expressed in PM_{2.5}-eq per kg, and correspond to the number of deaths per kilogram emitted normalised using PM_{2.5} as a reference substance. Damage level CFs are calculated assuming 0.0083 DALY/kg PM_{2.5}-eq, which corresponds to an average severity factor of 19 DALY per death for cardiopulmonary disease and lung cancer.

Water availability impact

IMPACT World+ uses the water scarcity AWARE model (Boulay et al. 2016) at the midpoint level as a proxy midpoint for all the water scarcity impacts. It is not directly on the cause effect chain leading to impacts on human health nor on the one leading to impacts on ecosystems, as no common midpoint exists between both cause effect chains, but it combines both users water needs (humans and ecosystems) to assess the water scarcity. This index is based on the remaining water available per area after human and aquatic ecosystem demand has been met, relative to the world average. It can be interpreted as the hypothetical surface-time equivalent necessary to generate an unused volume of water in a specific watershed, compared to the world average. AWARE is recommended by the UNEP/SETAC Life Cycle Initiative and the European Commission.

The approach of Boulay *et al.* (2011) is used to model the water availability impacts on human health. It includes a CSI (expressed in m³ deprived per m³ dissipated), an XF, which characterizes exposure of competing users to deprivation and accounts for adaptation capacity and water functionality (i.e. only competing users unable to adapt will suffer

human health impacts) and some function-specific EF. The latter are applied to obtain the impacts on human health per m³ deprived, focusing on the irrigation, domestic use and fisheries functions that are directly affecting human health. The model allows to account for the fact that consuming bad quality water affects less competing users (quality specific interim CFs are available) but the recommended default CFs do not account for water quality as LCA tools and databases are not mature enough to integrate water quality (see supporting information, Section 4 for details).

For damages on ecosystem quality, several methods are combined to model the cause-effect chain for water scarcity impacts, as recommended by Kounina *et al.* (2013). The work of Hanafiah *et al.* (2011) is used to model impacts of freshwater consumption on freshwater ecosystems and the model of van Zelm *et al.* (2011) is used to assess water scarcity impacts on terrestrial ecosystems from groundwater. A CF of 0 is considered for deep groundwater. Despite Kounina *et al.* (2013) suggestion to use it in combination with the other models assessing water scarcity impact on ecosystem quality, the model from Pfister *et al.* (2009) has not been integrated in IMPACT World+. This was done in order to keep the overall coherence of the method and to avoid double counting of the impact of groundwater consumption on terrestrial ecosystems (see supporting info, Section 4 for details). The model from Verones *et al.* (2010) is used to assess the impact of thermally polluted water, with the assumption that the “Water, cooling, unspecified natural origin” currently found in life cycle inventory databases with no further specification is released in a 3 m deep river with a 4 °C temperature increase.

IMPACT World+ also considers as interim indicators the impact of water availability on the resources & ecosystem services AoP, and water stream use and management impacts on ecosystem quality AoP, modelled using the Humbert & Maendly model (2009), both being described in supporting information, Section 4 and not yet being peer reviewed.

Land use

Human activities cause impacts to lands, which are either converted from natural state (land transformation) or occupied, i.e. maintained in a certain non-natural state (land occupation). Impacts on land have consequences in terms of terrestrial biodiversity but also in terms of fundamental ecosystem services for the human society such as biotic production, water regulation, freshwater recharge and filtration, climate regulation and erosion resistance.

Potential impacts of land occupation and land transformation on ecosystem quality are characterized using local empirical CFs at the biome level. Those CFs, from de Baan *et al.* (2013) were preferred over the regional and global CFs from Chaudhary *et al.* (2015) – despite the latter being preliminary recommended by the UNEP/SETAC Life Cycle Initiative. This choice was done to ensure coherence with the other impact categories on the physical meaning of impact scores at the damage level. *Regional and global impacts as modelled by Chaudhary et al. (2015) are meaningful as they give important complementary information on the (semi)-irreversible disappearance of species in a region or at the global scale. However, they are not consistent with the other ecosystem quality impact indicators of IMPACT World+ (acidification, eutrophication, ecotoxicity, water scarcity, etc.) or any other existing LCIA*

method, because their indicator has a different meaning. The regional PDF indicator from Chaudhary et al. (2015) quantifies the fraction of species disappeared forever from a region of the world, whereas the PDF.m2.yr indicators of the IMPACT World+ framework quantify the temporary disappearance of species (PDF) over a given surface (m2) during a certain time (yr). To our understanding, it is hardly possible to convert the regional PDF from Chaudhary et al. (2015) into PDF.m2.yr, because the former corresponds to a permanent disappearance and would therefore lead to an infinite impact. Using the Curran (2010) regeneration time to convert those PDFs in PDF.m2.yr – as proposed by Chaudhary et al. (2015) when calculating land transformation impact – seems inconsistent as this regeneration time is supposed to apply to an ecosystem and not to the irreversibly disappeared species. However, by doing so, the land use impact scores would be orders of magnitude lower than the local impacts of de Baan et al. (2013) as only a very small fraction of the species affected by land occupation or transformation will permanently disappear from the affected region. We therefore decided to use the de Baan et al. (2013) model, which quantifies damage indicators in PDF.m2.yr that are consistent with the damage indicators used in IMPACT World+. Nevertheless, we acknowledge the need to further develop regional CFs for the other impact categories in line with the approach proposed by Chaudhary et al. (2015) as complementary information to the assessment of local impacts as currently done in life cycle impact assessment.

For the case of land occupation impacts on terrestrial biodiversity, there is no need to consider fate and exposure since effects occur directly in the environmental compartment where the environmental intervention is reported. The characterization factor therefore directly relates the land occupation (in m²·yr) to the biodiversity loss (in PDF·m²·yr). Midpoint indicators are thus determined by dividing damage values by the global average CF for arable land, used as a reference, expressing these normalized damage values in m²·yr_{eq} of arable land. Land transformation impacts are considered as long-term impacts only, as they represent the remaining impacts once the occupation ends and the ecosystem recovers which, in most cases, will occur in the far future. They were calculated using the land occupation CFs and considering the recovery times from Curran (2010) as proposed by Chaudhary et al. (2015).

IMPACT World+ also considers, as interim indicators, the potential impact of land occupation and land transformation on the resources and ecosystem services AoP (including the following ecological soil functions: erosion resistance, freshwater recharge, physical and chemical filtration). Similarly, indirect land use impacts on human health due to the modification of freshwater recharge, or physical and chemical filtration are considered interim and computed consistently with the model used to assess water availability impacts on human health. Such indirect impacts from land transformation on the ecosystem quality AoP are not considered in IMPACT World+ as this may lead to double counting: the empirical CFs from de Baan et al. (2013) include all the impact pathways affecting local ecosystems, including the modification of its access to water. All those interim impact indicators are further described in supporting information, Section 4.

Photochemical oxidant formation, ionizing radiation, and ozone layer depletion

The ILCD handbook recommendations (European Commission 2011) were followed for these three impact categories. Model calculations were updated to account for the most up-

to-date World Meteorological Organization (WMO (World Meteorological Organization) 2014) values of ozone depletion potential.

Supporting information section 3: Interim impact categories

Climate change impacts on resources & ecosystem services

As proposed by Cao et al (2015) for land use impacts on carbon sequestration potential of soils, the social cost of carbon proposed by Ackerman and Stanton (2010) is used as an estimation of the cost due to the loss of service due to climate change. This effect factor is applied directly to the midpoint (and not to the temperature increase) as this value was initially determined based on GWP100.

Land use impacts on resources & ecosystem services

IMPACT World+ also consider as interim categories the impact of land transformation as well as the potential impact of land occupation on the following soil ecological functions: erosion prevention, groundwater recharge, physical and chemical filtration and are described in section xxx of the supporting information. The fate factors (Saad et al. 2011) describes the modification of biophysical indicators per quantity of land occupation (in m²-yr). Biophysical indicators are further modelled with respect to the loss of ecosystem services using the model of Cao et al. (2015). Damage oriented CFs express the social cost to compensate (or adapt) to the loss of ecosystem service related to the change of soil ecological function due to land use (\$_{Service lost}/m²-yr). These are calculated as the multiplication of a dimensionless exposure factor defining the loss of service per change of the biophysical indicator ($\text{Service}_{\text{lost}} / \Delta \text{Biophys. Indicator } i$) and an effect factor (\$/service lost) that monetizes the value of a given ecosystem service. The exposure factor accounts for the fraction of service loss that is affecting the population and for the adaptation capacity of the society.

Given the still exploratory state of these models, we consider the biophysical midpoints and damage CFs as interim. Thus, only land occupation impacts on biodiversity are considered in the recommended version of IMPACT World+.

Water availability impacts

Water availability impacts on Human health CFs are provided for the different level of water quality detailed in the table SI2 to complement the default water availability impact on human health CFs which are not accounting for the water quality.

Table SI 4.1: Description of the water quality classes

	Excellent	Good	Average	Average-Tox	Average-Bio	Poor	Very poor	Unusable
S Surface	1	2a	2b	2c	2d	3	4	5
G Groundwater								
Coliforms	low	low	medium	low	high	high	high	Unusable
Toxics	low	medium	medium	high	low	medium	high	

Those CFs are to be used with care, acknowledging a lack of coherence between human toxicity impacts modeled with USEtox and this water availability model, which may lead to an overlap and a potential double counting.

Those water quality classes were originally developed to acknowledge the fact that a bad quality water is not functional for as many users as a good quality water, hence using some non conventional sources of water (such as for example treated wastewater) would have less impact in term of users deprivation than using very high quality water.

However, this assumption lead to a bias in the operationalization of the model, as a water balance is made to account only for the quantity of water that is consumed by a process. The quantity of water withdrawn and the quantity of water released are quantified and characterized to obtain the net water availability impact. If the water is released with a lower quality than the water originally withdrawn, the model mathematically considers that some usages of the water are “lost” due to quality degradation, leading to water availability impacts.

1) This is debatable due to the fate in surface water of the released emission which may lead to acceptable level of contamination quickly after the release, hence not depriving any competing users;

2) This is not consistent with the assumptions done in USEtox, both in term of toxic contaminant fate when emitted to water and in term of human exposure to toxic emission through drinking water. The water availability model considers that domestic users will be deprived of good quality water and will turn toward other bad quality water sources or adopt bad hygiene habits leading to diseases, ie will not consumed the degraded water, whereas USEtox assumes that a fraction of the toxic emission to be consumed through drinking water. Both assumptions are inconsistent.

The model from Pfister et al. (2009) has not been integrated in IMPACT World+ in order to keep the overall coherence and to avoid double counting the impact of groundwater consumption on terrestrial ecosystems. This model assesses the impact of water consumption (surface and groundwater) on plants, hence partly overlapping the impact pathway covered by the van Zelm *et al.* (2011) model which is focusing on the plant water deprivation due to water table lowering when pumping groundwater. We consider that van Zelm *et al.* (2011) has a more robust fate model based on hydrogeology to determine the fraction of water pumped which is going to deprive the plants from soil moisture. Pfister et al. (2009) considers this fraction as being 100%, which is very conservative . The other impact pathway covered by Pfister et al. (2009) is the water deprivation of terrestrial plants due to surface water consumption, which is not covered in IMPACT World+. Pfister et al. (2009) use again the very conservative assumption that 100% of the water pumped in surface water will deprive terrestrial plants in the watershed.

Water availability impacts on resources & ecosystem services

The same CSI scarcity index is used at midpoint for water use impacts on resources and ecosystem services. The exposure factor is complementary to the exposure factor considered for human health impacts: only competing users able to adapt will have to pay for this adaptation. The effect factor is the same as the one considered in land use impacts for groundwater recharge and filtration (in both cases, the same “service” is lost for the society and the adaptation costs to access to good quality water is the same)(Cao et al. 2015). At this stage, these unpublished characterization factors of water use impacts on resources and ecosystem services are considered interim.

Marine and terrestrial ecotoxicity

Interim CFs are also proposed for marine and terrestrial ecotoxicity based on the USEtox fate factors for the coastal zone and for the natural soil environmental compartments. The marine effect factors are considered equal as per freshwater ecotoxicity. As a side remark, no differentiation is currently done currently in the freshwater ecotox EFs determination in

USEtox between marine and freshwater species as both are mixed in the aquatic ecotox databases used to determine USEtox EFs, meaning that the assumption of similar ecosystem sensitivity is already implicitly done. The terrestrial ecosystem EF are extrapolated from the freshwater EF using the soil-water partition coefficient proposed by Hauschild and Wenzel (1998), as already done in IMPACT 2002+ (Jolliet et al. 2003b).

Photochemical oxidant formation

This category is related to the impacts of ozone and other reactive oxygen compounds formed as secondary contaminants in the troposphere (the region in the atmosphere closest to the surface) by the oxidation of the primary contaminants (Non Methane Volatile Organic Compounds, NMVOC, or carbon monoxide) in the presence of nitrogen oxides (NO_x) and under the influence of light. Ozone concentrations in the troposphere lead to increased frequency and severity of respiratory diseases, such as asthma and Chronic Obstructive Pulmonary Diseases. IMPACT World+ uses the method used in ReCiPe (Goedkoop et al. 2013) and recommended by the ILCD handbook (Margni et al. 2008) for both mid-points and end-points.

Ionizing radiation

The routine releases of radioactive material to the environment is responsible of both human health and ecosystem effects. Human health characterization factors are taken from Frischknecht et al. (Frischknecht et al. 2000) and characterization factors for ecosystems are based on the approach of Garnier-Laplace et al. (Garnier-Laplace et al. 2008), which is used consistently with the ecotoxicity assessment in USEtox as per the recommendations of the ILCD Handbook (Margni et al. 2008).

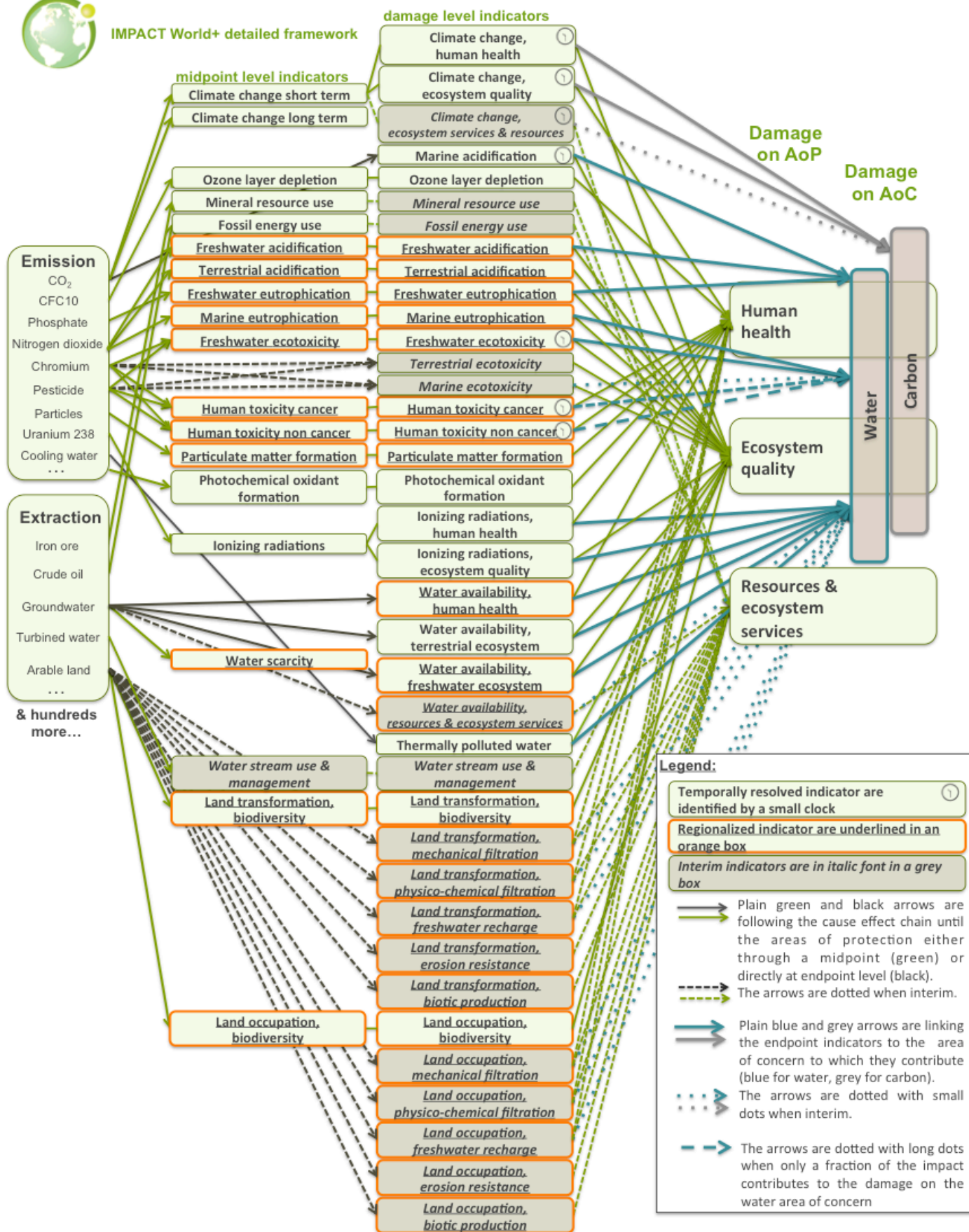
Ozone Layer depletion

Ozone depleting substances emitted by human activity destroy the ozone layer in the stratosphere, which blocks UVB, by breaking ozone molecules into molecular oxygen through heterogeneous catalysis. Exposure to UVB radiations increases the risk of skin cancer and cataract. It may also cause premature aging and suppression of the immune system. As recommended by the ILCD handbook, midpoint characterization factors are based on the ozone depletion potentials produced by the World and Global Meteorological Organisation (WMO (World Meteorological Organization) 2014) using the infinite time perspective and human health severity factors developed by Struijs et al. (Struijs et al. 2009). Model calculations were updated to account for the most up to date WMO2014 values of ozone depletion potential.

Supporting information section 4: Detailed IMPACT World+ framework



IMPACT World+ detailed framework



Supporting information section 5: Characterization factors database

The database joined as supporting information section 5 includes the characterization factors for all the recommended impact categories of IMPACT World+.

Alternatively, it can be found in the following dropbox file:

<https://www.dropbox.com/sh/2sdgbqf08yn91bc/AAA-mnN7YxkQxfyFx2LYK0PCa?dl=0>

For the regionalized impact categories, the characterization factors are available at four different resolution scales: at the native resolution scale and aggregated at the country, continent and global level. *Regionalized CFs are available for all 197 countries considered in the ISO 3166-2 norm (2013), which nomenclature is used to name the regionalized environmental intervention.* For the aggregated characterization factors, the uncertainty due to spatial variability within the geographical cell considered is also documented in the database with information on the minimum, the maximum, the 5th, 25th, 75th and 95th centiles, the mean and the weighted average using the probability of emission in each of the aggregated native resolution cells.

The compartments considered in the recommended impact categories are the following:

- *Air*
 - *With sub-compartments based on population density archetypes (high/low) for toxic and ecotoxic impacts as well as particulate matter formation and ionizing radiation*
 - *And an additional indoor sub-compartment for toxic impact*
- *Soil*
 - *With a sub compartment agricultural soil for human toxicological and ecotoxicological impacts as well as ionizing radiation*
- *Water*
 - *With sub compartments groundwater, lake, river, ocean for water use impacts*
 - *With sub compartment ocean for human toxicological, ecotoxicological, ionizing radiation impacts*
 - *With sub compartments groundwater and ocean for eutrophication impacts*
- *Raw material*
 - *With sub compartment land for land use impacts*
 - *With sub compartment water for water use impact*

Modelling assumptions coherence.

The same models are used to model similar environmental mechanisms for different impact categories:

- The same coherent framework was used across all the impact categories considering fate (or competition in the case of resources), exposure and effect
- Resources are all modelled using a functionality based approach, ie considering the loss of resources functional value for the humans (and not any intrinsic value loss)
- Water scarcity/availability and land use impact categories are strongly inter-related and modelled coherently: when land use is influencing the quality or the quantity of groundwater (through impacts on water recharge or water filtration), the water availability impacts are applied to complement the cause effect chain toward human health and resources & ecosystem services areas of protection.
- Climate change impacts and land use impacts on soil carbon sequestration are strongly inter-related and the loss of carbon sequestration potential is directly modelled under the climate change impact category.
- The method proposed by Cao et al to assess the impacts of land transformation on resources & ecosystem services area of protection has been coherently applied to other climate change contributing emission in the interim version of the methodology.
- The atmospheric fate of CO₂, CO and CH₄, contributing to both climate change and marine acidification impact categories, is computed with the same model from the IPCC.
- For both climate change and marine acidification, the CO₂ resulting from the quick oxidation of CO and CH₄ was considered in the model.
- The effect model for marine acidification uses a linearity proxy assumption of the SSD curve of H⁺ concentration between 0 and the HC50_{EC50}. This is consistent with the way SSD curves are used in USEtox to generate effect factors for ecotoxicity.
- Cancer, non cancer, marine, terrestrial and freshwater ecotoxicity models use the same fate factors, from USEtox
- The exposure and effect modelling assumptions across all those toxicity related impact categories are all coherent.
- The fate models for indoor exposure and pesticide residues that are integrated in the cancer and non-cancer impact categories are also coherent in term of fate, exposure and effect with the USEtox model.
- The atmospheric fate of NO_x and ammonia contributing to terrestrial acidification, aquatic acidification and marine eutrophication was computed with the same model (GEOS-Chem).
- The warming effect of CO₂ that is formed from the oxidation of methane is now included in the GWP value of methane published in the IPCC report (Myhre 2013). For consistency purposes, we decided to add a GWP value for CO to account for the warming effect of CO₂ that is formed from its oxidation. Since the lifetime of CO is very short (a few months), we consider that a molecule of CO instantly becomes a molecule of CO₂, leading to a GWP value equal to the ratio of their molar mass

($44/28 = 1.57$) since 1 kg of CO will oxidize into 1.57 kg CO₂. For consistency purpose, the formed CO₂ is also considered in marine acidification impact category.

Remark : Should this be extended to other non-GHG substances containing carbon and nitrogen that could ultimately be degraded into CO₂, CH₄ and N₂O, depending on the aerobic or anaerobic conditions in which they are degraded? This is less straight forward as on the one hand the degradation products depend on the degradation conditions, and on the other hand, some chemicals can take years to achieve full degradation, leading to delayed GHG emissions. The half-life of a chemical in a given environmental compartment should be put into perspective with the 100 years time frame of the mid-point characterization factors to keep consistency. In the case of methane and CO, oxidation is occurring quite rapidly. An attempt was made by (Muñoz et al. 2013) to calculate the potential GHG emissions (CO₂, CH₄ and N₂O) from the degradation of a few organic chemicals, showing that it may not be negligible. However, the climate change effect of GHGs formed from the mineralization of organic compounds was considered not mature enough to be integrated in the present version of IMPACT World+ and should be studied further.

Temporal coherence

Temporal coherence is respected across impact categories:

- For all long term the impact categories, a “shorter term” time horizon has been set coherently at 100 yrs after the emission occurs. This allows to express separately
- Long-term impacts are the remaining impacts after 100 yrs.
- Long-term impacts are integrated to the infinite when there is a full recovery.
- When some permanent remaining impacts occur, a 500 yrs time horizon has been chosen consistently across impact categories (this is the case for marine acidification and climate change) as an infinite time horizon would lead in that case to an almost infinite impact.
- Remark: to ensure temporal coherence between inventory and impact assessment, long-term emissions in the inventory (i.e. emitted in more than 100 yrs) should be considered to only have long-term impact.

Spatial coherence

Spatial coherence is also respected across impact categories:

- The same geographical parameterisation was used across all the regionalized impact categories. For example the coastal zone considered for impacts on marine ecosystems is the same for marine acidification, marine ecotoxicity and marine eutrophication and is defined as the zone where the depth of water is less than 200 meters.
- The same maps and projections are used to define countries and continents, the same geographical data (population density, etc) are used to model native resolution CFs and to aggregate them at the country / continental / global level.
- The same approach has been used across all the regionalized impact categories to generate CFs at the country / continent / global level based on the probability of emission (or resource consumption) in each of the native resolution scale geographical cell.

- For all the regionalized impact categories, when no CF is available for a specific region of the world, the global default CF is used and should be considered with the corresponding spatial variability.
- The modelling assumptions used for respiratory inorganic are coherent with the USEtox modelling assumption in term of definition of the urban archetype (population density)

Supporting information section 7: Residence time in air influence on the intake fractions of a substance

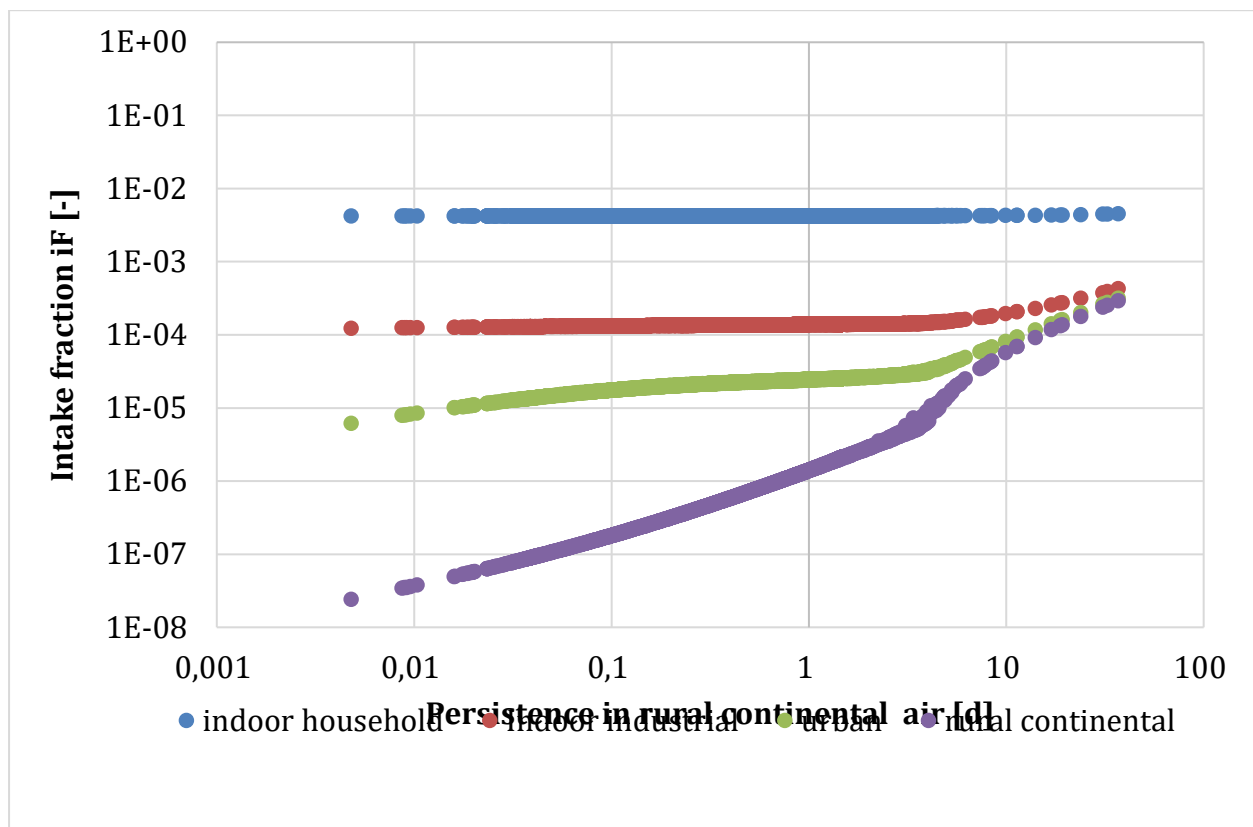
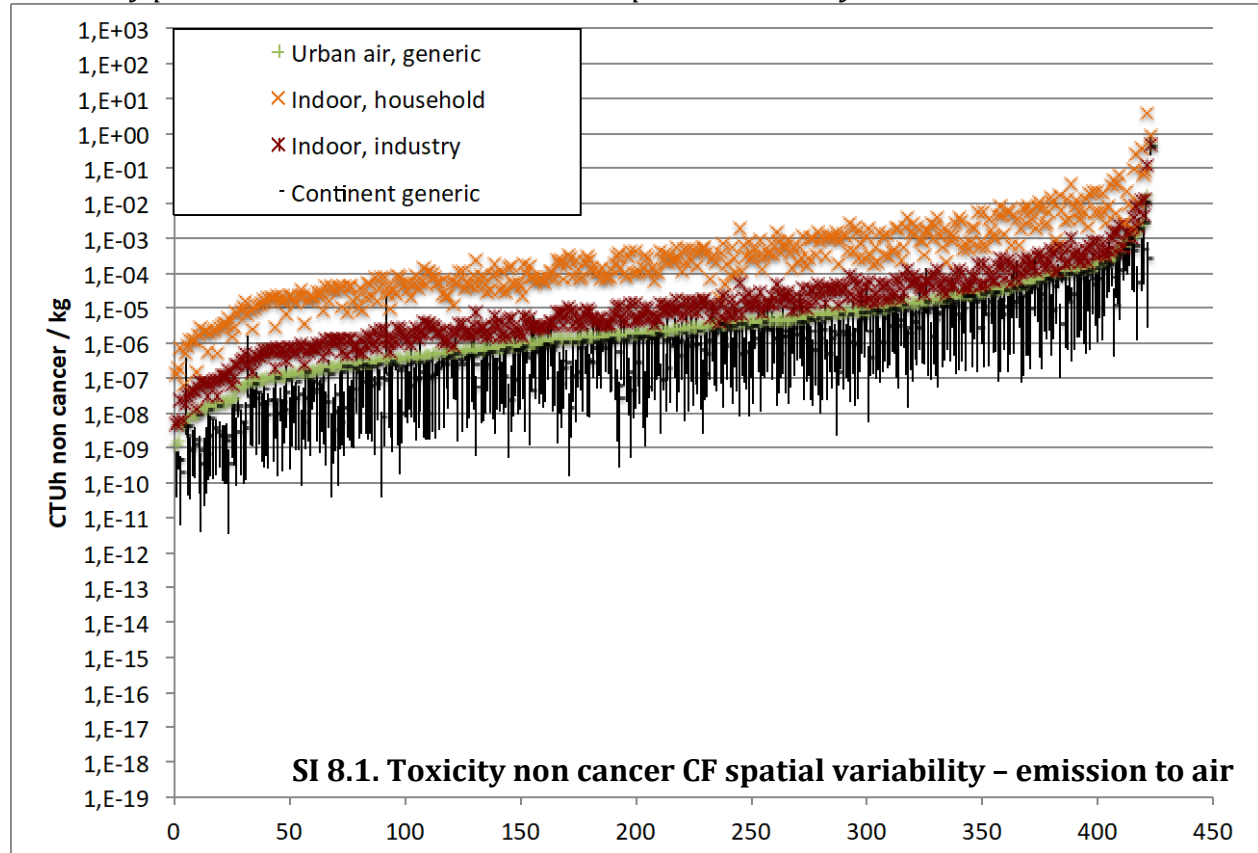


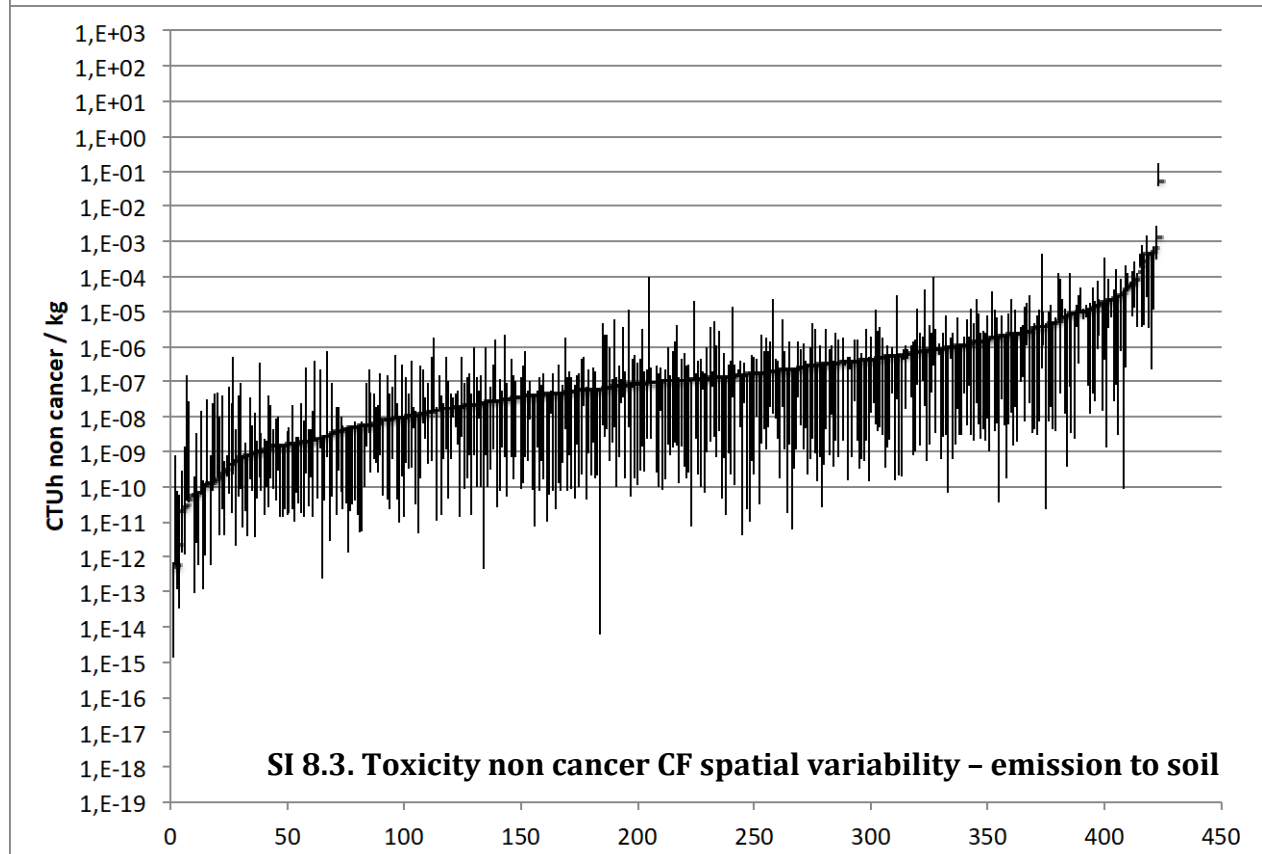
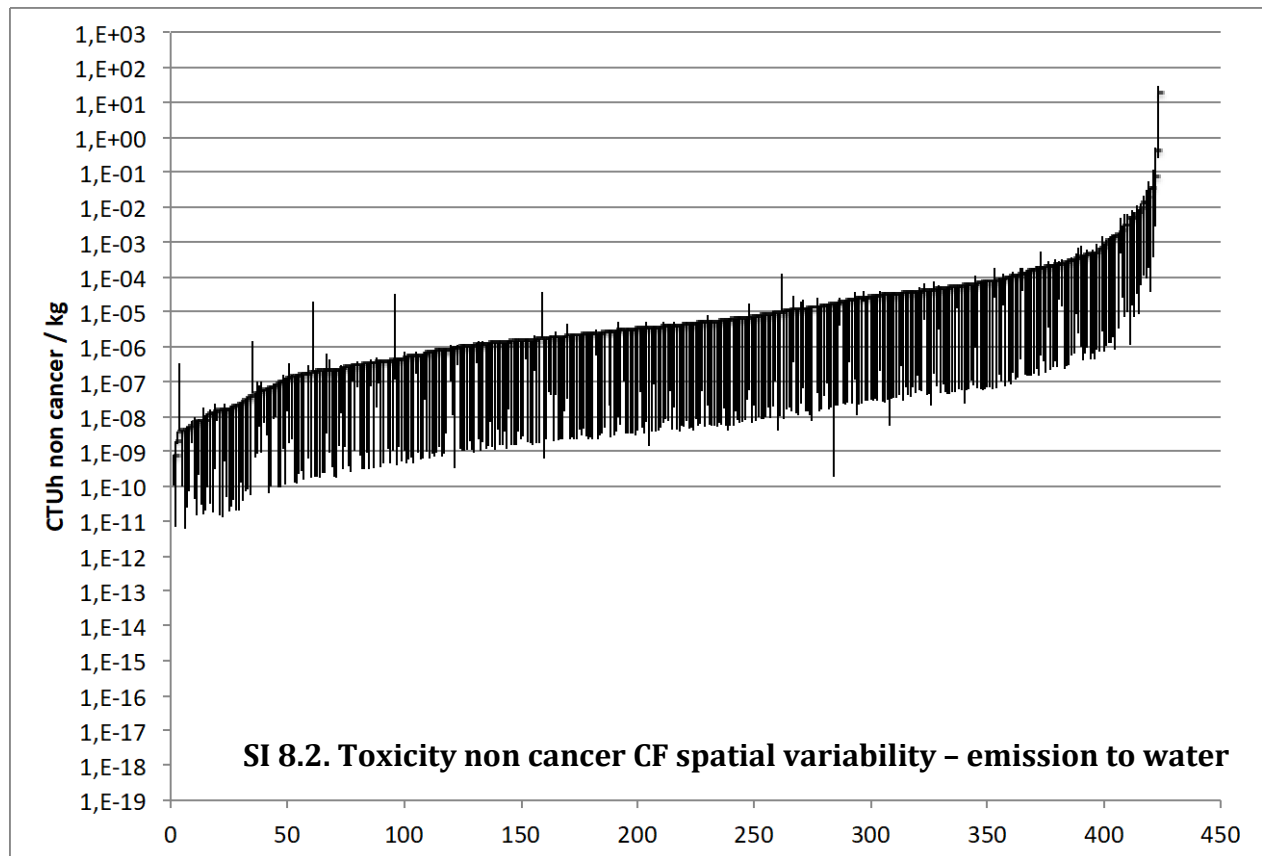
Figure SI 7.1: Indoor (OECD country average archetype), urban and rural intake fraction as a function of the fate factor (persistence) in rural continental air

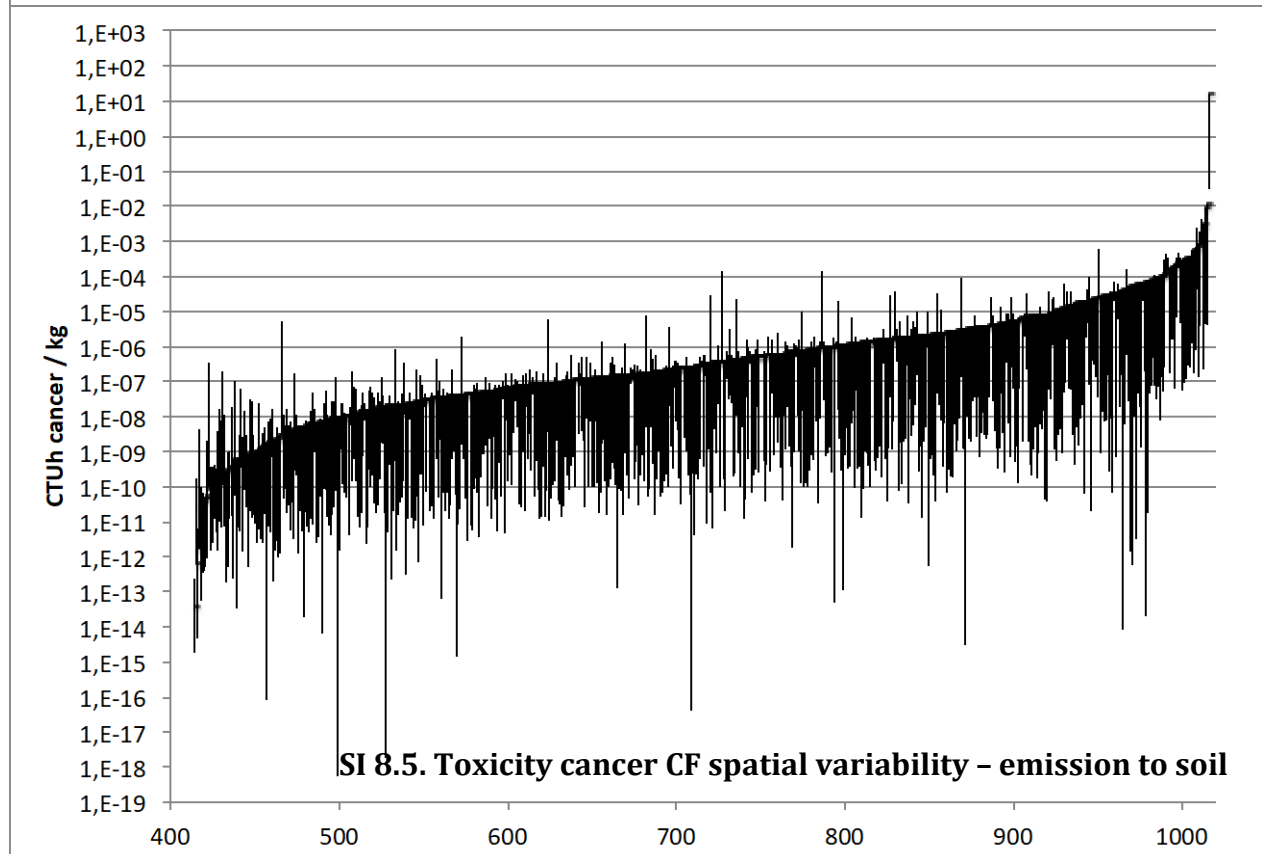
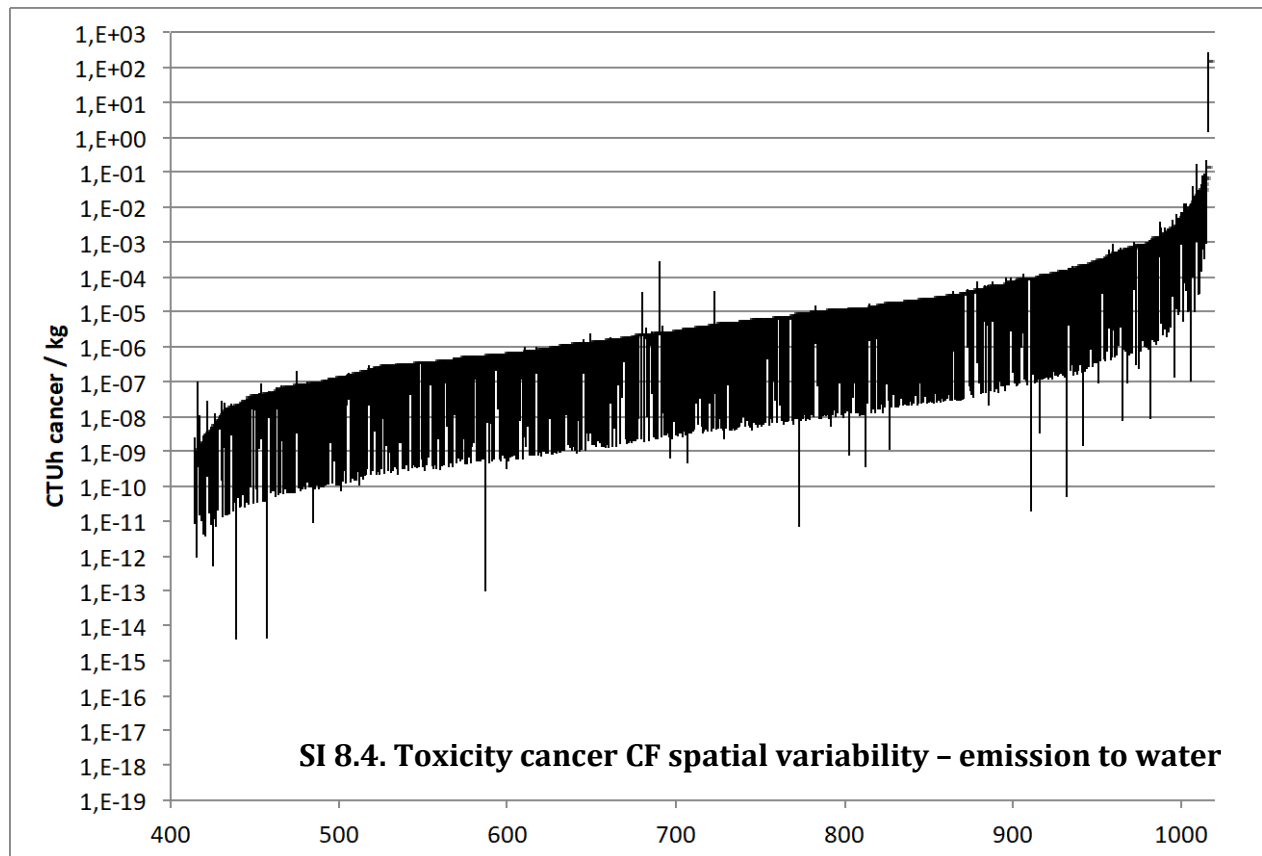
Supporting information section 8: Spatial variability of toxic impacts

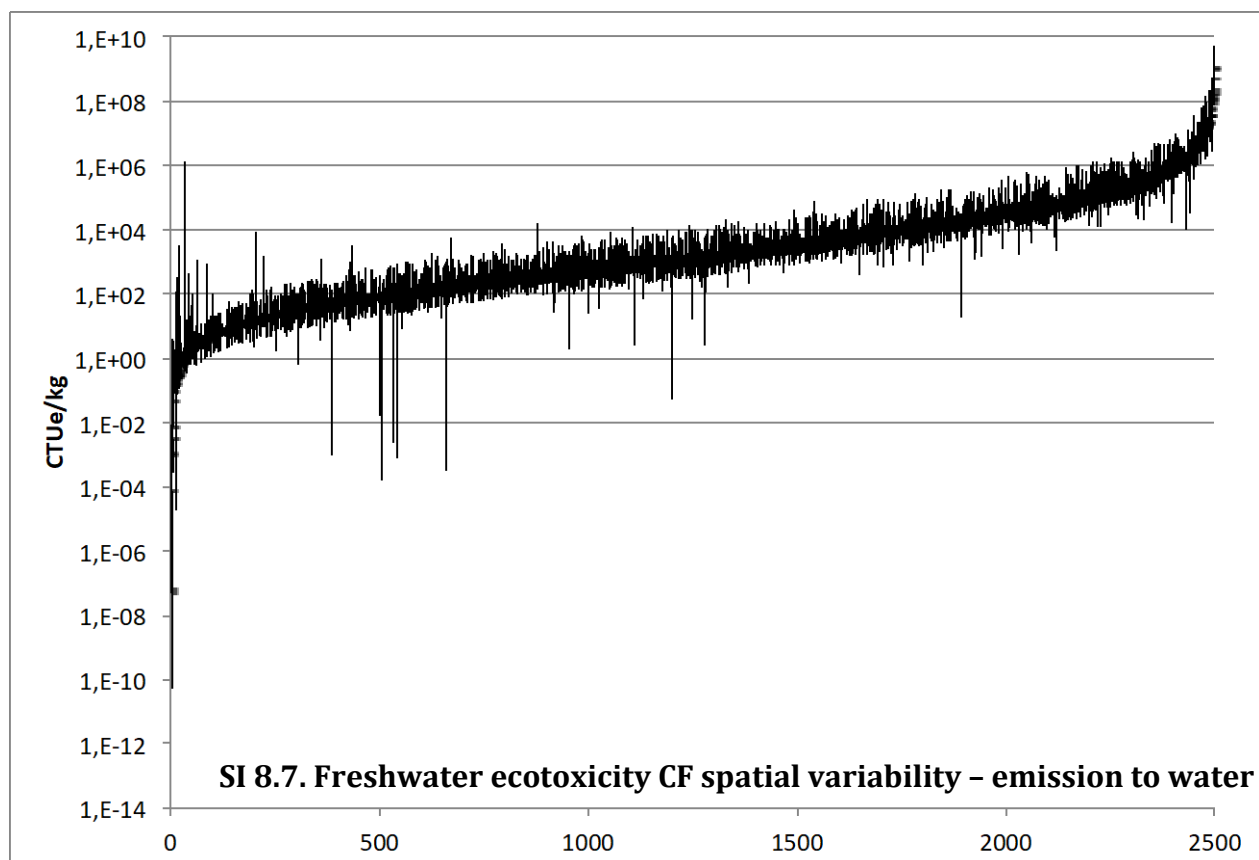
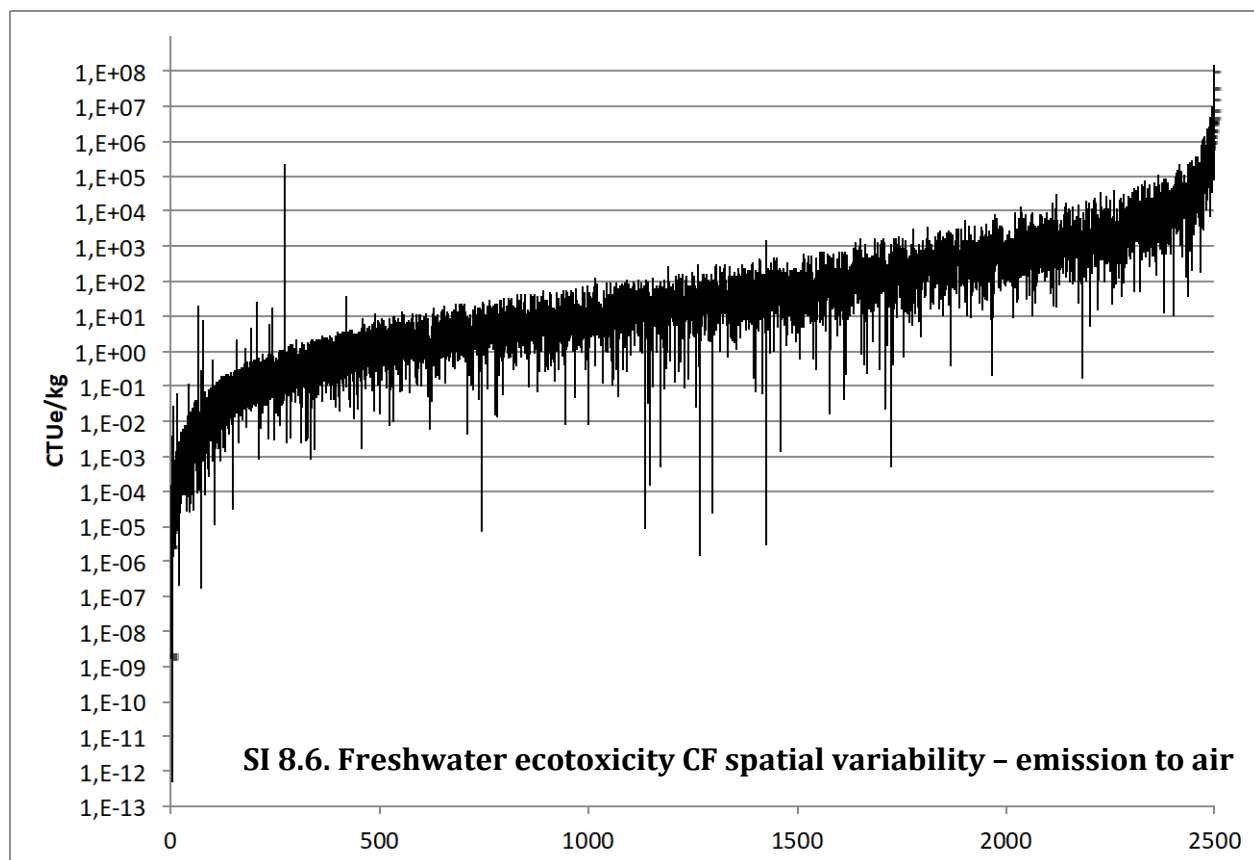
Carcinogen characterization factors for an emission to soil and water, non-carcinogen characterization factors for an emission to air, soil and water and freshwater ecotoxicological characterization factors for an emission to soil, air and water are shown in log₁₀ scale in Figures SI 8.1 to SI 8.8, differentiating min, max and generic values across continents and archetypes for air emissions.

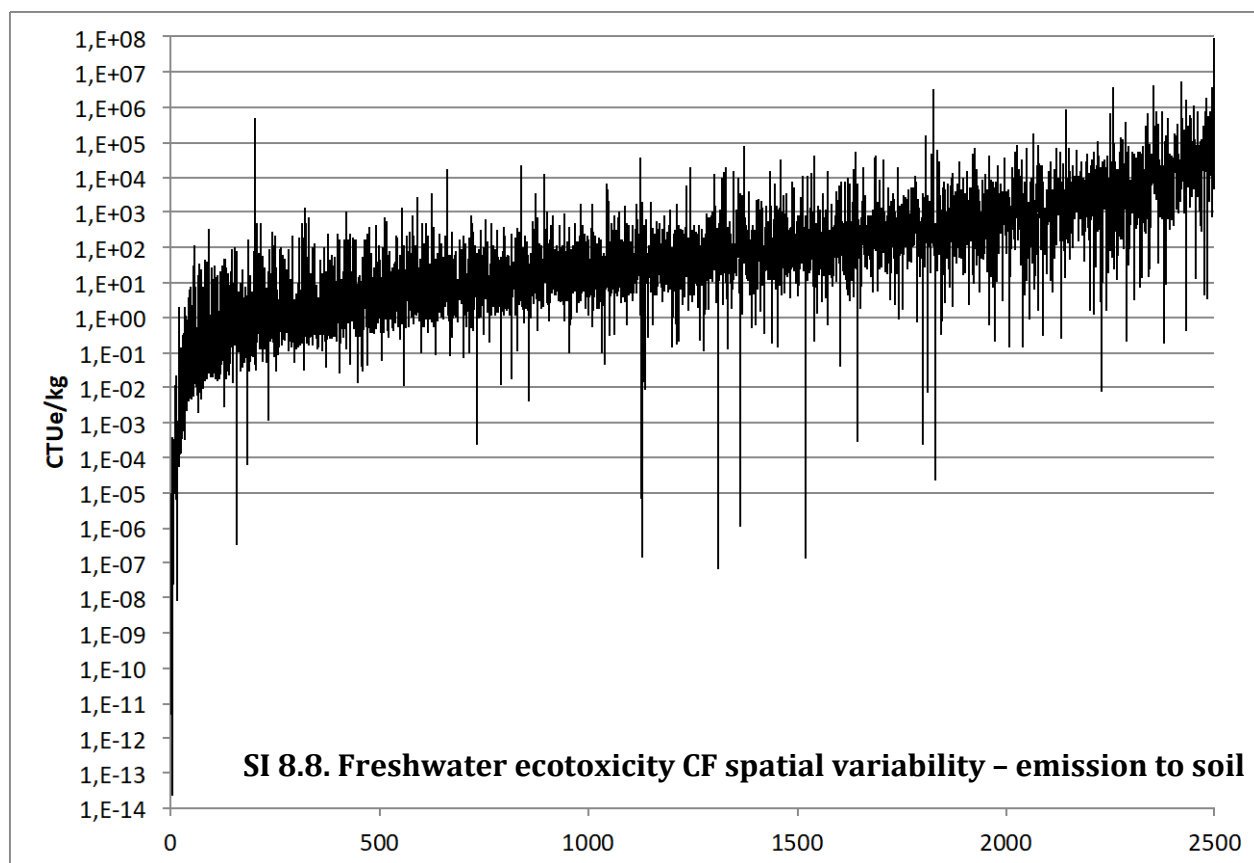
Those figures have to be interpreted with care: the population density archetype is meaningful to assess toxic impacts of airborne emissions, but are less relevant for emissions into water or soil and in general for ecotoxicity impact category. It is likely that intercontinental spatial variability presented here underestimates the spatial variability within each continent.











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