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Citation

Núñez, M., Rosenbaum, R. K., Karimpour, S., Boulay, A. M., Lathuillière, M. J., Margni, M., … Pfister, S. (2018). A Multimedia Hydrological Fate Modeling Framework To Assess Water Consumption Impacts in Life Cycle Assessment. *Environmental Science & Technology*, *52*(8), 4658–4667. doi:10.1021/acs.est.7b05207

Author-produced version of the article published in Environmental Science & Technology, 2018, N°52(8), p. 4658-4667
The original publication is available at https://pubs.acs.org/doi/10.1021/acs.est.7b05207
Doi: 10.1021/acs.est.7b05207

A multimedia hydrological fate modelling framework to assess water consumption impacts in Life Cycle Assessment

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Abstract. Many new methods have recently been developed to address environmental consequences of water consumption in life cycle assessment (LCA). However, such methods can only partially be compared and combined, since their modelling structure and metrics are inconsistent. Moreover, they focus on specific water sources (e.g. river) and miss description of transport flows between water compartments (e.g. from river to atmosphere via evaporation) and regions (e.g. atmospheric advection). Consequently, they provide a partial regard of the local and global hydrological cycle and derived impacts on the environment. This paper proposes consensus-based guidelines for a harmonised development of the next generation of water consumption LCA indicators, with a focus on consequences of water consumption on ecosystem quality. To include the consideration of the multimedia water fate between compartments of the water cycle, we provide spatial regionalisation and temporal specification guidance. The principles and recommendations of the paper are applied to an illustrative case study. The guidelines set the basis of a more accurate, novel way of modelling water consumption impacts in LCA. Environmental relevance of this LCA impact category will improve. Yet, much research is needed to make the guidelines operational.

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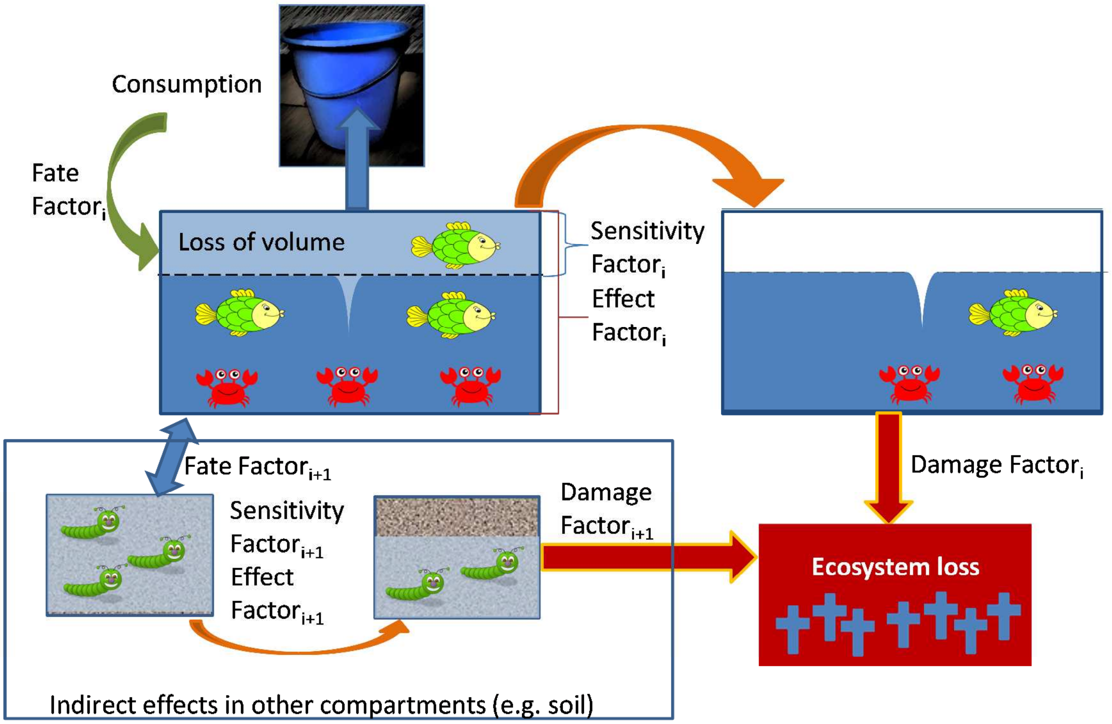
TOC



1. Introduction

The impact category describing impacts of (fresh-)water use and consumption in life cycle assessment (LCA) has been subject to large advancements in the last decade. The current water footprint principles, requirements and guidelines described in ISO 14046[1] build on the framework described by Bayart et al.,[2] and define freshwater consumption as any use of freshwater that changes water availability in a watershed through evapo(transpi)ration, product integration, direct release to the sea, and inter-basin transfers.

Available freshwater consumption-related indicators are based on either a volumetric approach of the water consumed[3] (what we call first generation of indicators) or on scarcity indices[4,5] (what we call second generation of indicators, see further details on both generations of indicators in section S1 of the Supporting Information, SI). The first generation of indicators

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only performs an inventory and thus not a footprint assessment according to ISO 14046[1], while the second generation of indicators shows limitations in describing the consequences of a lack of water on areas of protection (AoP), such as ecosystem quality. They assume that there are smaller or no impacts in areas of low water scarcity and greater impacts in areas of high water scarcity. However, it is possible that water rich areas may contain ecosystems that are accustomed to abundant water availability and may thus be more vulnerable than those in areas that are water stressed. To date, no LCA method comprehensively distinguishes water masses (e.g. surface water and ground water) and their transport flows (e.g. from river to atmosphere) within the boundaries of a watershed and beyond (e.g. air advection), thus overlooking details in hydrological processes that affect the environmental relevance of the assessment. In addition, a recent analysis[6] concluded that a structured life cycle impact assessment (LCIA) framework for assessing impacts of water consumption on ecosystems is currently lacking, as can be observed by the scattered and often incompatible developments of water impact assessment models published in recent years.[7–10] These models are all valuable contributions in themselves, but impossible to combine to an integrated, global characterisation model that makes such developments consistently operational in LCA.

Building on the recommendations by Núñez et al.[6] this paper aims to set a novel framework and methodological guidelines to support the consistent development of impact indicators for water consumption in LCA (third generation of indicators), with a focus on ecosystem quality, including comprehensive illustration of impact pathways that should be covered. The framework is applied to a hypothetical but realistic illustrative case study that represents water consumption in a generic coastal zone with a non-exhaustive number of phenomena represented.

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The study contributes to the current WULCA (Water Use in LCA, a global expert task force of the UN Environment Life Cycle Initiative) activity, whose overall objective is to develop consensus-based indicators for water use impact assessment as part of the global guidance LCIA project.[11] Consensus-based indicators for human health and for a generic scarcity-based indicator have already been developed and recommended.[12] This paper focuses on the third set of target indicators, namely ecosystem quality (or biodiversity), and does not consider aspects of water quality and consequences on ecosystems due to water quality degradation (see section S2 in SI).

2. Materials and methods

2.1. Methodological guidelines for water consumption impact assessment

Prior to introducing the guidelines, all the relevant environmental interventions and pathways, which may be associated with water consumption, are described (see section S2 in SI for further details). This step is necessary to identify to which causality chains the methodological guidelines of the article apply. We identified three types of environmental interventions that may lead to changes in water availability in one or more water compartments: consumptive use of water; land use and land use change; and water stream use and management. In addition, direct and indirect emissions to water, including degradative water use, are considered outside the scope of these guidelines since emissions do not lead to changes in purely physical water availability or water consumption. In the analysis, we introduced the consideration of hydrological stocks, which is going to redefine the environmental interventions and impact pathways that up to now have been associated with water consumption. Bayart et al.[2] describe the watershed as being the most relevant hydrological unit to consider for water consumption in LCA, as a first step on integrating regionalisation in LCIA. However, each watershed hosts a series of hydrological stocks (e.g. soil, aquifers) and flows (e.g. evaporation, percolation) that

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vary in space and time due to meteorological, environmental and biophysical conditions. We introduce the "water compartment" term defined as any water body where water is temporarily stored and between which water flows may take place, thereby affecting its water availability.

2.2. A mechanistic characterisation factor structure

Assessing the environmental impacts of water consumption on ecosystem quality implies the modelling of cause-effect pathways linking water consumption (i.e. life cycle inventory (LCI) data) to potential habitat modifications and biodiversity damages through characterisation models, as shown in Figure S1 to Figure S3. According to ISO 14040,[13] characterisation models "*should be based upon an identifiable environmental cause-effect mechanism and/or reproducible empirical observation*". Mechanistic characterisation factors (CFs) capture this recommendation well, since they translate the environmental intervention to its impact in the selected category indicator stepwise, based on a sequence of interconnected sub-factors, further described in Equation 1. Mechanistic models for use in LCA were first formally proposed by Udo de Haes et al.[14] and are today widely used to characterise the impact of emissions[15,16] in LCA. Mechanistic models for emissions link the pollutant emission (LCI) to the mass in different environmental compartments (fate factor, FF), to the intake by ecosystems or humans due to direct and indirect exposure through e.g. ingestion (exposure factor, XF), and to the potential effects on target organisms at the midpoint (effect factor, EF) or endpoint level (damage factor or severity factor, DF).[17,18] The CF is the product of these sub-factors. Some emission models (e.g. terrestrial acidification) use a sensitivity factor (SF) to distinguish between the buffering capacity of different regional receiving environments instead of the XF.[19] This terminology accommodates well to the nature of ecosystems impacts due to change in water

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availability. Therefore, the term SF is used in the article from here on. Equation 1 shows the generic formulation of a mechanistic CF.

$$\mathrm{CF} = \mathrm{FF} \times \mathrm{SF} \times \mathrm{EF} \times \mathrm{DF} \qquad \text{Equation 1}$$

In LCA, the use of matrix algebra to assess environmental loads in different media (freshwater, air, etc.) is common practice in the emission-related impact categories (e.g. by the toxicity models like USES-LCA,[20] IMPACT 2002+[21] and USEtox[22]). In contrast, impacts of water consumption are today typically calculated analytically, by multiplying in sequence the water consumption of every unit process with a CF that neither distinguishes different water compartments nor flows between them. Matrices are more intuitive, more flexible and more transparent to model water fate and transport between compartments and its related impacts. The benefits of adopting matrices to calculate mechanistic CFs for water consumption are further discussed in section S3 in the SI. Due to matrix algebra convention, the calculation of (CF) (i.e. CF matrix) is done by reversing the order of the sub-factors of the CF in Equation 1, as shown in Equation 2.

$$(\mathrm{CF}) = (\mathrm{DF}) \times (\mathrm{EF}) \times (\mathrm{SF}) \times (\mathrm{FF}) \qquad \text{Equation 2}$$

Although Equation 1 has already been applied in a few water consumption LCIA models,[8,10,23] there is no general recommendation for adopting such a modelling principle for water consumption impact assessment. We suggest here extending the recommendation of using mechanistic CFs, which so far has only been applied to emissions,[14] to model the impacts of resource consumption as well. Specifically, we propose adopting the mechanistic CF structure for assessing the impacts of freshwater consumption on ecosystems, based on the reasoning explained in section S4 in the SI.

We propose the below definitions of fate, sensitivity, effect and damage factors in a mechanistic CF representing freshwater consumption impacts on ecosystem quality.

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Fate factor (FF). The FF models the propagation of water consumption between water compartments of the hydrological cycle, which results in a duration and magnitude of the effect in every affected compartment. It represents the mass balance in the system, which depends on momentum and energy, which accelerate mass transfer, as well as on environmental resistance, which are processes decelerating mass transfer between compartments. The sum of the factors representing these forces and processes (represented in rate constants (k values) in the article), regulates the exchange and movement of water between compartments and spatial units. Further details on k values and the k matrix are given in section S5 in SI. These calculations show how much and how long the withdrawal (and the release) of water from one storage compartment (e.g. groundwater withdrawal) affects water availability in other compartments (e.g. the withdrawal of groundwater reduces base flow towards rivers downstream and final discharge into the sea). The propagation effect can be measured at specific time steps (e.g. daily, monthly, and annually) or a time-independent, steady-state solution ($t \rightarrow \infty$) may be calculated (see below and S8 in SI). The result after applying the FF is interpreted as the change of mass or volume of water in each compartment (e.g. kg or m^3) as a function of the water withdrawal or release rate in this compartment or other connected compartments (e.g. kg/day or m^3/day). Alternatively, it can also be interpreted as residence time of water in a compartment for a water release and as duration of the absence of water in a compartment for a water withdrawal. The dimension of the FF is time (since the volumes stated above cancel out), with units of, for instance, days. FFs populate their respective cells of the fate matrix, where a column denotes the water withdrawal or release compartment i and a row denotes the affected compartment j to which a withdrawal or release of water is propagated. The size of the FF matrix is determined by the number of environmental compartments n_i considered and is always square ($n_i \times n_i$), since every affected

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compartment can also be a withdrawal/release compartment (see (FF) in the illustrative example).

Sensitivity factor (SF). SF models any ecosystem response as a result of a change in water quantity in a compartment in order to prevent the dependent ecosystem to be affected by the change in water availability. In other words, it reflects whether the change of available water in an affected compartment will be compensated for or will create a water deficit, similarly as defined in the adaptation capacity of the exposure factor by Boulay et al.[24] to model the human population affected by the change in water quantity. The result after applying the SF (i.e. FF×SF) can be interpreted as the time fraction of water availability change in a compartment affecting ecosystems. SFs can be defined at any ecosystem quality indicator level (e.g. species, guilds) and for any attribute of the ecosystem level selected (e.g. composition, function).[25] For instance, a SF based on functional properties of habitats can measure the physical stability of a habitat (e.g. river's resilience) against hydrological changes.[26] A SF based on species responses to habitat structure can assess the capacity of a species to access alternative freshwater resources.[23] In this latter case, the longer the distance to alternative freshwater resources, the lower the capacity of the species to compensate for the reduced water availability. The sensitivity of an ecosystem can also be considered as resilience and included in the effect factor, instead of in the sensitivity factor. To calculate SFs, the distinction between terrestrial, aerial and purely aquatic biodiversity can be important, since the capacity of each biodiversity type to withstand to changes in water availability varies. On the one hand, sessile organisms (e.g. terrestrial plants) and generally also aquatic species (e.g. fish) may often not be able to offset reduced water availability (except if water is added in the affected compartment, whose physical effects on the water balance are already accounted for in the FF). On the other hand, aerial and mobile terrestrial organisms may

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travel a certain distance in search of an alternative source of water to satisfy their vital needs. However, this can lead to additional competition between the native and the new species for the alternative resource, ultimately increasing water scarcity and leading to new impacts through a rebound phenomenon. To facilitate applicability, SFs calculated at detailed ecosystem levels (e.g. species) can be aggregated across taxonomic groups or ecosystem types (e.g. biodiversity of river ecosystems, biodiversity of lake ecosystems). A possible dimension for the SF is the distance that a species or community is able to travel to reach another waterbody in the region, which can be expressed with units of e.g. km or it can be dimensionless as the percentage in relation to a full compensation. Dispersal distances of taxa and species can be used for this purpose and are available in the literature.[27,28] The sensitivity factor matrix (SF) contains SF with a column denoting an affected compartment and a row denoting an ecosystem or one of its components. The size of (SF) is determined by the number of environmental compartments n_i considered and the number of ecosystems or ecosystem components considered and is thus ($n_{ecs} \times n_i$) (see (SF) of the illustrative example).

Effect factor (EF). The EF accounts for any kind of ecological changes in habitats and biodiversity that cannot offset changes in water availability in the compartment. For instance, an EF can measure a change in ecosystem productivity (e.g. in terms of net primary productivity) due to changes in water availability in the soil profile,[4] a change in a river habitat as a result of the habitat sensitivity to a change in river discharge,[26] and the species affected due to a change in habitat. The EF can also cover effects a species suffers when it cannot fully compensate for insufficient water availability and it needs to access other water resources. EFs should differentiate between aquatic, aerial and terrestrial ecosystems and between taxonomic groups, since water volume-to-effect response curves are very specific to each life form.[9] In nature, an

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environmental shift from baseline conditions can result in a community turnover determined by species-specific adaptation strategies (e.g. generalist, opportunistic, specialist taxa). Spatially-explicit curves and vulnerability statuses of the affected species can provide relevant information to capture regional biodiversity specificities and biodiversity damages.[23] For example, different species in terms of taxon, endemism, life traits and Red List status, dwelling in different habitats, will likely be affected differently by a change in water availability. The EF may be expressed in loss of habitat (e.g. in m^2 or m^3) or, when closer to the endpoint or damage, it can provide information on the effective influence of physical habitat change on target species, which results in an indicator expressed in terms of species affected (e.g. potentially affected fraction, PAF) per reduced water availability in each time. The effect factor matrix (EF) contains EF in its diagonal elements with each column and row denoting an ecosystem or ecosystem component and all off-diagonal elements being zero. The size of (EF) is determined by the number of ecosystem components n_{ecs} considered in all spatial units and thus it is always square ($n_{ecs} \times n_{ecs}$) (see (EF) of the illustrative example).

Damage factor (DF). The DF distinguishes the severity of effects. It converts the midpoint metric into an endpoint metric expressing an ecosystem quality loss, usually in terms of species disappearance (e.g. potentially disappeared fraction, PDF) per reduced water availability in each time, following the recommendation of the UN Environment Life Cycle Initiative.[29] As for the EF, it is important to distinguish between impacts taking place on a regional level (e.g. watershed level, representing a local loss of ecosystem functionality) or impacts happening at a global scale (global extinction of a species). This means specially that the vulnerability of species or ecosystems towards human interventions need to be taken into account. Although there are examples in the literature for aquatic ecosystems,[9,23] there is so far no consensus on the approach

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and no harmonisation across impact categories. This representation of vulnerability is currently investigated as part of phase 3 of the Global Guidance on LCIA Indicators project by the Life Cycle Initiative for ensuring a compatible approach among ecosystems (terrestrial, aquatic, and marine) and impact categories. Similar to the EF matrix (EF), the damage factor matrix (DF) contains DF in its diagonal elements with each column and row denoting an ecosystem or ecosystem component and all off-diagonal elements being zero. The size of (DF) is determined by the number of ecosystem components n_{ecs} considered in all spatial units and thus it is always square ($n_{ecs} \times n_{ecs}$).

A list and detailed analysis of the FF, SF, EF, and DF that have been used in the literature to model water use impacts on ecosystem quality up to the year 2014 is provided by Núñez et al.[6]

2.3. Fate factor

Spatial modelling aspects: multimedia water consumption setup. As shown in Figure 1, the FF multimedia model has two types of spatial components in a given spatial unit:

- Water compartments: individual building blocks of the hydrological cycle where water is temporally stored, for example the atmosphere
- Water flows: fluxes (displayed as arrows) into and out of every water compartment that together constitute the hydrological cycle, such as evaporation and precipitation

The water compartments and spatial units need to have variable sizes to account for local and global aspects to model the flows. Therefore, the model setup needs to apply techniques that simulate the flows across water compartments with optimal computational costs. Adaptive mesh refinement is a technique in high-performance scientific computing, which is applied in different contexts, such as hydrodynamic modelling and climate modelling,[30] with the purpose to adapt the mesh size to the resolution and detail required to represent the important features of the

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simulation in different scales and domains. We propose the same hierarchical structure used by many adaptive mesh refinement methods[31] to be used in the formulation of FFs, which can be stored both in raster and vector formats (see further information in section S6 in the SI).

The model setup extends over different nested spatial units (local, regional, and rest of the world, see below). There are different structural solutions in terms of number of spatial units and its resolution (see section S6 in SI). The three nested spatial scales of the model are the following:

- Local scale: any open water system nested in a region and in the world that can be considered a basic unit of the landscape and of the water cycle in the context of LCA. It is commonly a sub-watershed or a watershed, but depending on the modelling option applied, it may also be any other smaller (e.g. a farm or a grid cell with multiple layers) or bigger (e.g. a country) system. The local scale is the most refined spatial scale of the FF model. Within its boundaries, all existing (or at least relevant) water compartments and flows are differentiated (Figure 1) to the best possible extent.
- Regional scale: open water system nested in the globe, consisting of the connection of the local entity with its surrounding. The regional scale allows for the accounting of the effects that water consumption in the local scale has beyond its boundaries. For instance, it allows assessment of the cascade effect downstream the point of consumption in a watershed when associating sub-watersheds, and the assessment of the effects on a country's water availability when connecting evaporative recycling flows between watersheds. Some spatial configurations (e.g. Figure S7) do not need a regional scale. In terms of water compartments, the regional scale may be represented with different levels

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of detail from fully detailed to a simplified version depending on data availability, software capabilities, and the specific objectives of the LCIA model.

- Rest of the world (ROW) scale: closed water system within which the local and regional entities are nested. The sum of the water in the local, regional and ROW scales amount to the water in the globe. Since the objective of ROW is the conservation of a constant water mass balance on Earth, rather than the detail of its water stocks and flows, it can be represented by a single generic water compartment.

The proposed FF multimedia model follows the principle of parsimony (i.e. as simple as possible, as complex as necessary) successfully applied e.g. in USEtox.[22] Furthermore, it is based on the general architecture (compartments and flows) of global hydrological models and literature on land-surface-subsurface and climate interactions (see references in Table S1). The conceptual model is depicted in Figure 1, with what we consider to be the simplest, yet relevant, water cycle to model impacts of water consumption in a LCA context. This model is only a guideline for future method developers, who may add or remove components (i.e. compartments and flows) and adapt the configuration of the spatial scales depending on their model requirements (see further details in section S6 in SI). Definitions of the water compartments and water flows entering and leaving each compartment in Figure 1 are presented in Table S1.

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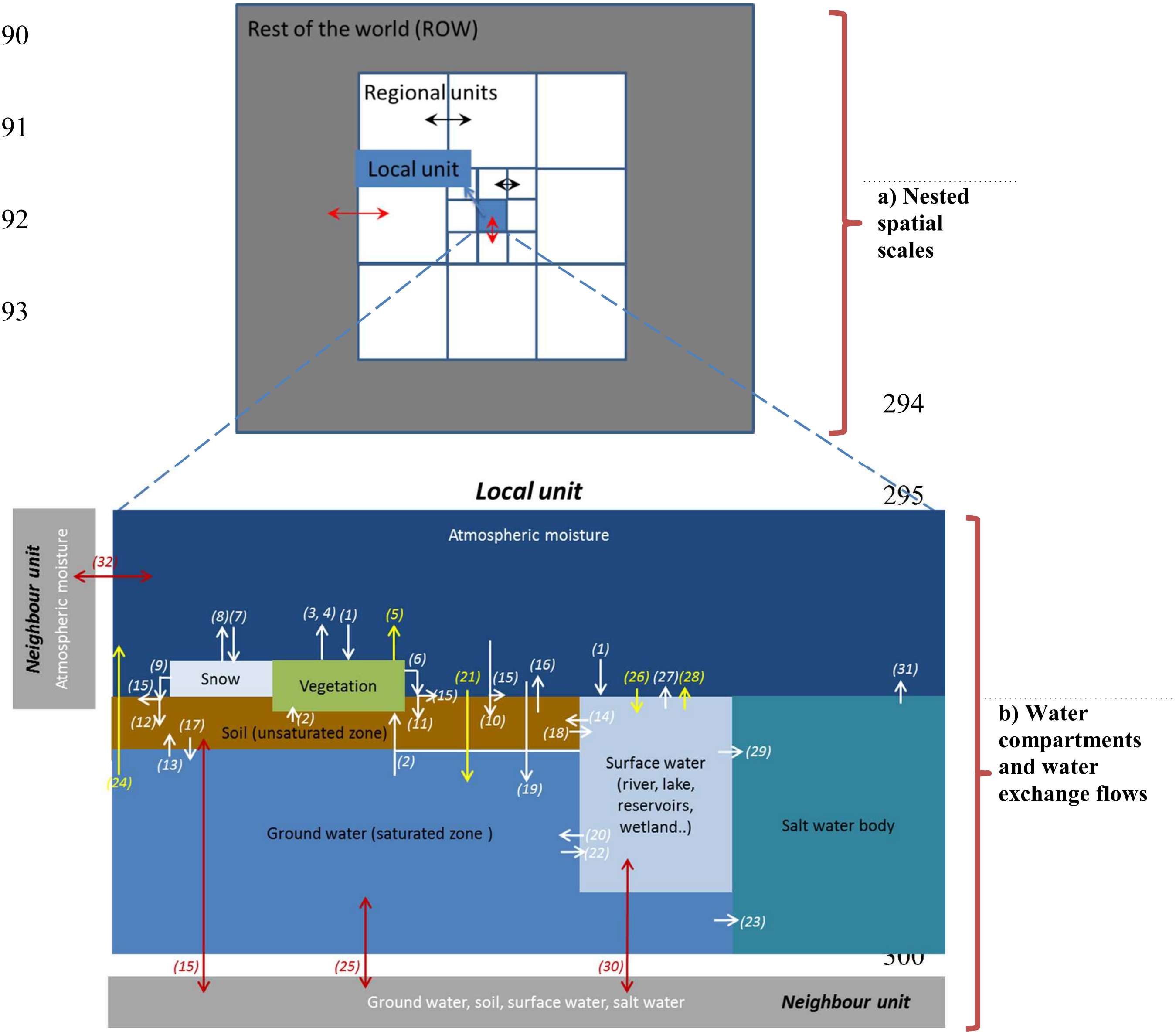

Figure 1. Multimedia hydrological fate model: a) the three nested spatial scales. Note that the use of squares is only a way of representing the spatial information, which can be encoded in the model both in raster and vector formats; b) the water compartments and flows in a local unit. White arrows represent natural flows, yellow arrows represent human interventions and red arrows are for exchanges between local and adjacent entities. Numbers in brackets identify the flows in and out displayed in Table S1.

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Since the aim of most LCA studies is the comparative assessment of marginal changes in the environment, the reference state of our FF model represents a contemporary water balance under anthropogenic influence. This representation explains why artificial water bodies such as reservoirs are included in the surface water compartment, and modelled as part of the environment. Further FF models representing alternative hydrological cycles for different LCA purposes can also be developed. For instance, a pristine water balance under pristine land use (without e.g. agriculture) or a contemporary water balance without human withdrawals may be modelled. These two options may be used as possible reference states (baseline scenarios) to assess current water consumption-related impacts against historical changes in the water cycle for non-marginal uses of LCA. For example, to assess non-marginal deforestation impacts on the water cycle in the Amazon, one could compare current versus past, less human-modified land-use scenarios. Such baselines are also needed for deriving average CFs or normalisation factors in LCIA.[32,33]

Temporal modelling aspects: steady-state and dynamic system solutions. For a FF, the magnitude of the effect that a volume of water withdrawal (or release) has on a water compartment depends on the time frame of the assessment, as shown in Equation 3:

$$\mathrm{FF_{r,s}} = \frac{\int_{\mathrm{t=0}}^{\theta} \mathrm{MPS_s\ dt}}{\Delta\ \mathrm{Environmental\ Intervention_r}} \qquad \text{Equation 3}$$

where *r* denotes the compartment where the environmental intervention (i.e. water withdrawal or release) occurs and *s* denotes the compartment where the midpoint stressor (MPS, i.e. change in mass, or volume, of water after the environmental intervention) is modelled.[6]

Hence, FFs can be estimated following two different temporal approaches: 1) Steady-state (i.e. time-independent solution predicting change in mass (or volume) of water per water

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compartment with the system at steady-state, $\theta = \infty$); and 2) dynamic (synonymous with transient, where *t* is set to specific time frames, $\theta = a$). An in-depth discussion of both options and their implications can be found in section S8 of SI.

3. Results

Illustrative example - system's description. In order to demonstrate the principles described in the article, we employed a hypothetical but realistic illustrative example that represents water consumption in a generic coastal zone (Figure S9) with a non-exhaustive number of phenomena represented. The zone consists of a local spatial unit with six compartments (atmospheric moisture or air (a), soil (s), ground water (gw), fossil ground water (fw), surface water (sw), and vegetation (v)), nested in two regional units (region 1 and region 2) with respectively five (air, soil, ground water, fossil ground water, and surface water) and four (air, soil, surface water, ground water) compartments, and the rest of the world unit aggregated into one single water mass (ROW) exchanging with the local and regional units. In the example, region 1 and region 2 are located downstream and upstream the local unit. The type of spatial setup represented in the example is a nested configuration of high spatial local detail, but other structural solutions could also have been applied, as explained in section S6. Every spatial unit has five ecosystem components: river (r-ecs), lake (l-ecs), aerial (a-ecs), sessile terrestrial (ster-ecs) and mobile terrestrial (mter-ecs) ecosystems. The environmental intervention assessed is the withdrawal of 2 m^3/functional unit (FU) of freshwater from ground water in the local unit. The release is of $1 m^3$/FU to the air in the local unit and of $1 m^3$/FU to surface water in region 1. Temporal dynamics of the hydrological flows are not considered (i.e. steady-state solution), which translates in only one set of FFs, instead of having different sets of FFs adapted to the granularity of every time step.

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The definition and interpretation of each sub-factor of the CF are provided above. The matrices described below are collated in the excel file of the SI, and a hypothetical CF solution and LCA score have been calculated for the purpose of showing the type of results obtained and their interpretation.

The k and the FF matrices. Environmental compartments in the illustrative example are exchanging water flows within a single spatial unit, but also beyond it (e.g. surface water of the local unit receives water from surface water from region 2 via river flow). All these exchange flows are quantified in the k values (see section S5). The off-diagonal elements of (k) represent transport of water between compartments within a spatial unit or beyond, going from compartment *i* (column) to compartment *j* (row). The diagonal elements reflect the difference between water gain (i.e. water generation) and water loss (i.e. sum of the off-diagonal elements in column *i*) in a specific compartment. Water generation refers to water that has been confined in the distant past in a compartment which today is disconnected to the rest of the water cycle (i.e. fossil water).

The fate matrix (FF) is a function of the inverse of the k matrix (k) for systems in steady-state conditions, which is the case in the example. (FF) for the local unit and the complete (FF) representing exchanges between compartments and units are collated in section S9. Matrix algebra determines that even though direct exchanges between two compartments are 0 (i.e. k-value = 0), FFs are positive, since they account for all direct and indirect (i.e. via third compartments) water exchanges.

The SF matrix. The SF can be quantified either for each spatial unit specifically (e.g. if the capacity of ecosystems to offset a change in water availability varies spatially, which is the case in the illustrative example, see Equation S3) or it can be one value per ecosystem component and

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Doi: 10.1021/acs.est.7b05207

affected compartment, which is the same for all spatial units. If the SF varies spatially, its matrix (SF) is populated similarly to (FF) in Equation S2, with the respective matrices for each spatial unit on the diagonal positions and in the same order as in (FF). The elements in the off-diagonal matrices in (SF) are then all zero. The size of (SF) in the example is (20 × 18).

The EF and the DF matrices. As in the SF, the ecosystem component may also be spatially variable and respond differently to a change in water availability. In the illustrative example, however, we assume that every ecosystem component reacts always similarly, hence (EF) has the same value per ecosystem component for all spatial units. The damage matrix is similar to (EF) but contains DF instead. In the illustrative example both matrices ((EF) and (DF)) are of (20 × 20) (see the matrices in S9 and in the SI excel file).

The CF matrix. The CF matrix contains the characterisation factors for each spatial unit (see section S9). Due to the propagation of water movement between compartments and spatial units, CFs vary spatially. Units of the CF in the illustrative example are in PDFm^3day/m^3 water consumption.

The LCI vector and the LCA score. The LCI vector of water consumption ($\overrightarrow{WC}$) contains the information on the water elementary flows per FU of the processes under study. Water withdrawals are identified with a positive sign [+m^3] and water releases are identified with a negative sign [-m^3]. The size of the LCI vector is determined by the total amount of water compartments in all spatial units (18 in the example, see the excel file).

The LCI vector times the regionalised CF matrix results in the LCA matrix with units of PDFm^3day, which estimates the environmental consequences on ecosystems due to the water consumption of the LCI. Since the LCI vector contains negative and positive flows, LCA scores

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Doi: 10.1021/acs.est.7b05207

are also negative (associated with potential environmental benefits) and positive (associated with potential environmental impacts). Intermediate results can also be calculated by multiplying the LCI vector to the FF matrix (meaning absence of water in each compartment due to the consumption of the LCI), and by multiplying the LCI vector to the FF×SF matrix (meaning the time effectively affecting each component of the ecosystem).

Comparison with the former generations of indicators. Figure 2 shows the application of the guidelines to the illustrative example and how the assessment compares to the use of the previous generations of indicators. The third generation (Figure 2 C) performs a characterisation of the environmental consequences of each LCI inflow (2 m^3/FU from GW, local) and outflow (-1 m^3/FU to air, local; -1 m^3/FU to surface water, region1) on the water compartments of the local unit and beyond. The second generation of indicators (Figure 2 B) characterises only the impacts (in terms of intensity of competition to access total available water resources) after water consumption in the whole watershed (i.e. 1 m^3/FU, which is the difference between the inflows and the outflows in the local unit of the LCI in the example). Whereas, the first generation (Figure 2 A) would just inform of the consumption of 1m^3/FU within the local unit, with no further characterisation of impacts. The figure highlights the significant differences in scope of the environmental processes described by each generation of indicators.

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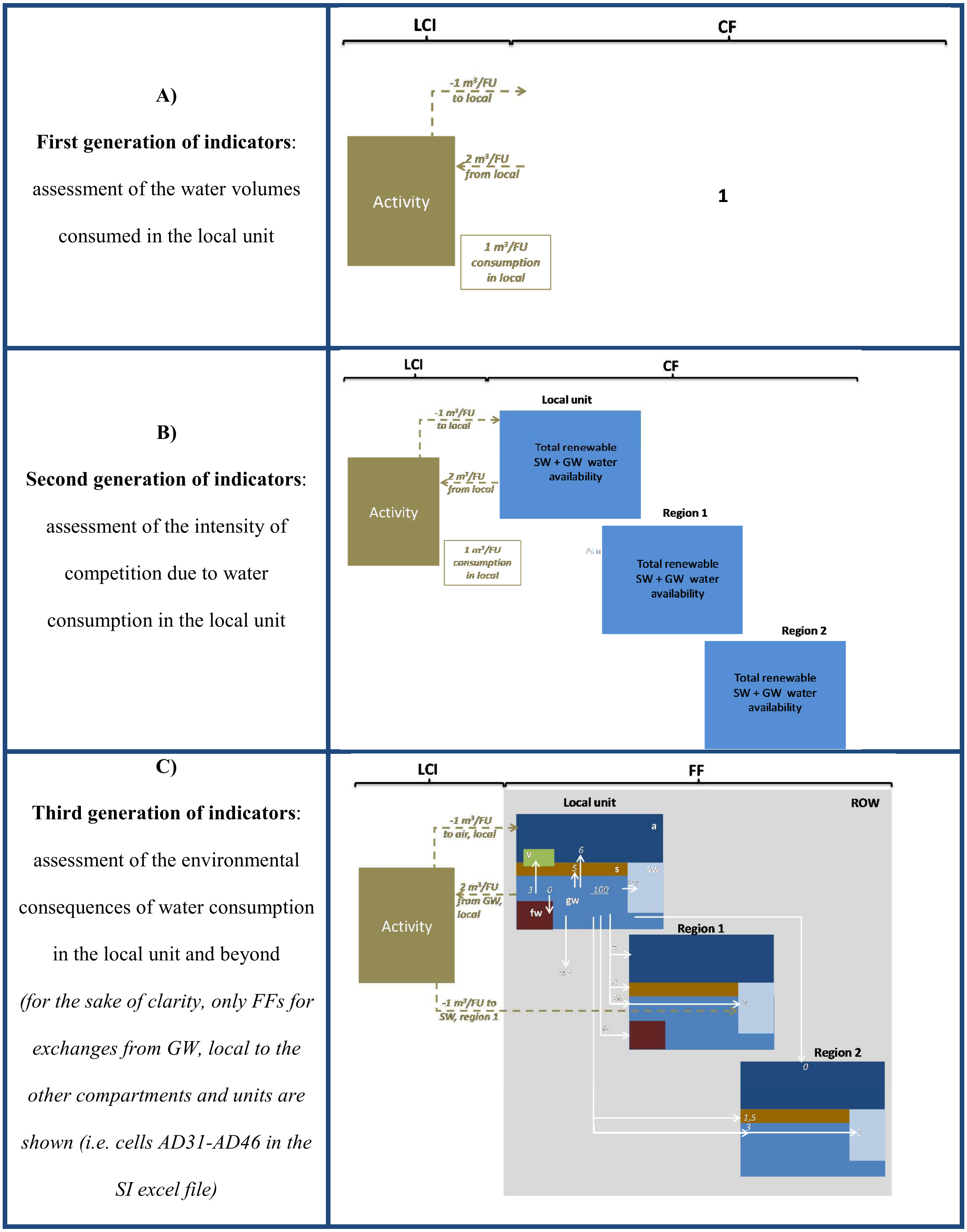
Doi: 10.1021/acs.est.7b05207



A)

First generation of indicators: assessment of the water volumes consumed in the local unit

B)

Second generation of indicators: assessment of the intensity of competition due to water consumption in the local unit

C)

Third generation of indicators: assessment of the environmental consequences of water consumption in the local unit and beyond

(for the sake of clarity, only FFs for exchanges from GW, local to the other compartments and units are shown (i.e. cells AD31-AD46 in the SI excel file)

413 **Figure 2**. Assessment of the illustrative example with the A) first generation of indicators; B)
414 second generation of indicators; and C) third generation of indicators.

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4. Discussion

Environmental relevance. The above set of guidelines serves to support the development of a third generation of impact indicators for water consumption in LCA. Its operationalisation will bring multiple benefits. First, it will allow for harmonisation and, to the possible extent, combination of existing water consumption impact assessment methods under a unique framework, including soil moisture consumption and effects of land use and land use change on the hydrological cycle. Second, it will ensure consistency of future methodological developments. Third, it will improve the relevance of the impact characterisation with respect to the local/regional and global hydrological cycles. All in all, the operationalisation of the guidelines will bring the characterisation of water consumption impacts to the same level of environmental relevance as the characterisation of emissions in LCA, thus increasing overall consistency and coherence between LCA impact categories. The latter effect is particularly important when indicator results are aggregated or compared to each other across impact categories, which is common and frequent practice.

The regionalised FF multimedia model allows for differentiation of impacts from consuming water from different sources in different environments. Moreover, since it captures the interrelation between water compartments, the distinction between impacts due to soil moisture consumption (also called green water in the literature[3]) and consumption from surface and ground water bodies (called blue water[3]) is no longer needed. This solves the debate about the consideration of green water in LCA.[34,35] Fossil water is also regarded in the FF model and, although its consumption does not lead to ecosystem quality damage, stress inflicted on available resources can already be measured in terms of renewal time. From this point in the causality chain, an indicator that links to the resources AoP could be developed. Overall, since fate factors

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Doi: 10.1021/acs.est.7b05207

only model the physical movement of water on Earth, they can also be used in the human health causality chain, which would then bring harmonisation of whole water consumption impact indicators. The type of midpoint indicator that we would obtain by applying the guidelines of this article is on the impact pathway for ecosystem quality, which the UN Environment Life Cycle Initiative encourages above the use of proxy midpoint indicators (e.g. water scarcity indicators) which are not defined along the cause-effect chain.[29] Furthermore, the guidelines could also be useful in other impact categories, both emission-based (e.g. toxicity models would benefit from modelling regionalised interactions of water flows) and resource-based (e.g. applying similar principles to the fate of soil loss due to erosion).

LCA scores obtained are both positive (associated with potential environmental impacts due to water withdrawal) and negative (associated with potential benefits due to water release) (see the illustrative example in SI). Negative scores are debatable, since they assume that when an ecosystem benefits from additional water, it responds by comparable proportion as it responds when facing a water drop. While this may be true for the FF since it is no more than a water balance, it is less certain for the sub-factors that reflect ecosystems' behaviour to water availability change. For the sake of transparency of LCA results and following ISO 14040,[1] we recommend reporting and interpretation of positive and negative scores separately instead of aggregating them assuming compensation.

LCI data requirements. To carry out an LCA study following the guidelines, the LCI shall record the following information: (a) freshwater balance of inflows (water withdrawal from the ecosphere) and outflows (water release to the ecosphere) expressed in mass or volume of water per functional unit (i.e. m^3/FU or kg/FU), and not as a continuous flow (i.e. m^3/y or kg/y), since the inventory flows must be scaled to the FU, (b) the geographical location of each exchange (c)

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Doi: 10.1021/acs.est.7b05207

the water compartment of each exchange, (d) temporal specification of each exchange if the FF (or any other CF sub-factor) reflects time dependency. For unit processes where the source compartment is unknown, the water supply mix[36] with regionalized statistics about the use of water sources per sector of activity can be used. Return flows to the technosphere may be considered sector-dependent, with for instance agricultural uses contributing to replenishing soil and groundwater, whereas domestic and industry users may most likely release to surface water.[37]

Uncertainty. The main objective of having a detailed spatial model is to (a) reduce uncertainty of the model and due to spatial variability and to (b) better reflect mechanistic relations in the cause-effect chain/impact pathway. Recent research resulted in more detailed datasets useful to improve the characterisation modelling at high spatial detail. Remote sensing products are increasingly allowing models to work with distributed data as inputs and not just interpolated parameters. Thus, parameter uncertainty can be considered and eventually reduced, which was highly limiting detailed modelling in the past. This means that the optima between parameter and model uncertainty[38] can be shifted towards more complex models. However, in order to find such optima for specific applications, uncertainty information of underlying models (e.g. hydrological models) needs to be assessed and propagated through the whole impact assessment model. The following uncertainty aspects should be differentiated and quantified:[12] (1) variability induced uncertainty; (2) Parameter uncertainty; (3) Model uncertainty; (4) Value choices; and (5) Scenario uncertainty.

Furthermore, all uncertainty results should be documented (including a description of the uncertainty method) and made publicly available for further research. Provision and analysis of uncertainty information is a key element of developing the models and allows prioritizing future

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Doi: 10.1021/acs.est.7b05207

research needs. Finally, these results facilitate proper uncertainty assessment in LCA, including impact assessment.

Towards practical implementation. The guidelines set the basis of a more accurate, novel way of modelling water consumption impacts in LCA. Operationalisation will therefore need much research, both in LCA and also for the development of hydrological models and datasets that LCA relies on. To start with, efforts may be directed towards:

- Performing simple, but real case studies similar to the illustrative example to serve as proofs of concept, like Verones et al.,[7] who modelled effects on wetland biodiversity in a coastal area in Peru prior to developing global CFs.[23,39] The case studies should ideally be located in contrasted local climatic conditions. A sensitivity analysis to figure out the appropriate temporal detail of the FFs should be conducted. The simulation may be performed in a system comprised of a few water compartments, where the comparison should focus on detecting the details of the system’s dynamic that steady-state solutions or large time steps would miss. Usually, steady-state solutions and large time steps bring along larger computational error.
- Adapting water flow exchanges between compartments and regions modelled in existing methods[39–41] to the harmonised framework.
- Developing new, coarse FFs at the global scale following both the spatial and temporal recommendations of the paper and considering lessons learned from the two points above, with the aim of identifying major modelling challenges and data gaps to overcome for further refinement. This base of FFs may also serve as starting point for further development, enhancing their quality and robustness. To help with operationalisation, Table S1 in the SI collects guidance on specific attributes to consider and bibliographic

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Doi: 10.1021/acs.est.7b05207

references per water compartment of the FF model. Some of the tools and strategies that are listed in Table S1 include hydrological models,[42,43] flow equations,[44] numerical and modelling techniques,[45] geographic information systems data,[46,47] and sensitivity analysis platforms.[48] Depending on the complexity and numbers of compartments and spatial units, few or all of these tools might be used.

- Analysing temporal dynamics of the sensitivity of ecosystems to water consumption and availability, since environmental water requirements vary a lot throughout the year. For that, and as done similarly with the FF, a sensitivity analysis comparing monthly or seasonal SFs to annual average SFs can be performed.

Associated content

Supporting information. The following files are available free of charge: i) further details on the scope of the guidelines, spatial and temporal FF modelling aspects, and a representation of matrices of the illustrative example (pdf file); ii) detailed matrices of the illustrative example (excel file).

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The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript.

Acknowledgements

Author-produced version of the article published in Environmental Science & Technology, 2018, N°52(8), p. 4658-4667
The original publication is available at https://pubs.acs.org/doi/10.1021/acs.est.7b05207
Doi: 10.1021/acs.est.7b05207

The authors are grateful for the contributions of other members of the Ecosystem Quality sub-group of WULCA (Jane Bare, Cécile Bulle, Mattia Damiani, Paula Quinteiro and Philippe Roux) and for the individual contributions of Christian Bouchard, Peter Fantke and Inga Klemmayer. M. Núñez and R.K. Rosenbaum acknowledge ANR, the Occitanie Region, ONEMA and the industrial partners (BRL, SCP, SUEZ, VINADEIS, Compagnie Fruitière) for the financial support of the Industrial Chair for Environmental and Social Sustainability Assessment "ELSA-PACT" (grant no. 13-CHIN-0005-01). The Sponsors of WULCA for the 2016-2018 period are also acknowledged for their financial contribution: Hydro-Quebec, Cotton inc, Veolia environment, L'Oréal, Danone, Engie.

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