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

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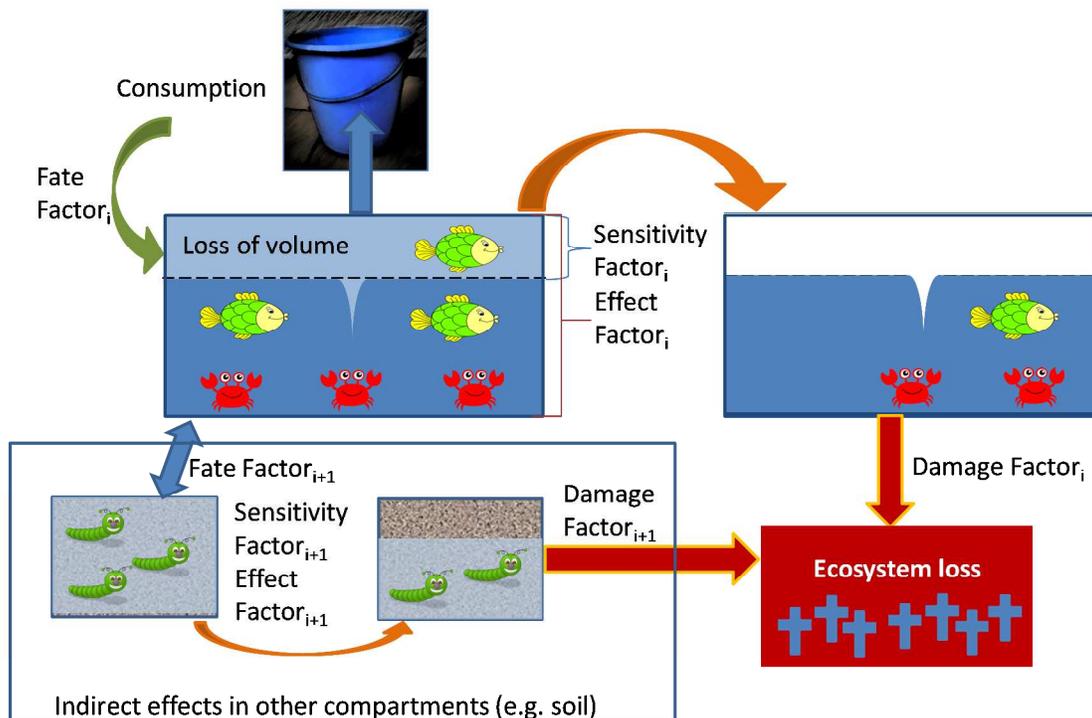
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19 **Abstract.** Many new methods have recently been developed to address environmental  
20 consequences of water consumption in life cycle assessment (LCA). However, such methods can  
21 only partially be compared and combined, since their modelling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

## 34 TOC



35

36 **1. Introduction**

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

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

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

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

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

## 76 **2. Materials and methods**

### 77 **2.1. Methodological guidelines for water consumption impact assessment**

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

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

## 95 **2.2. A mechanistic characterisation factor structure**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

### 238 **2.3. Fate factor**

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

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

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

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

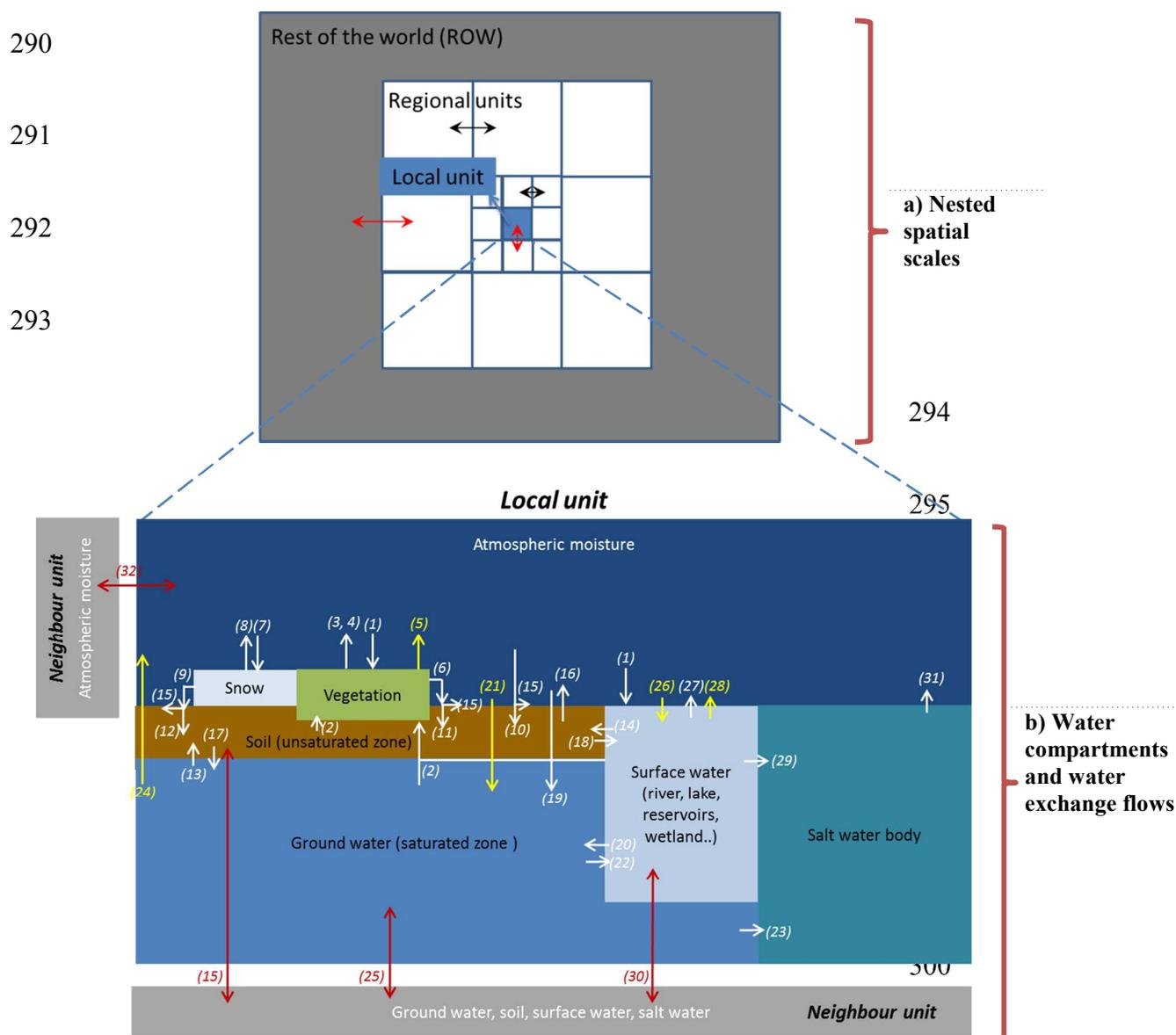
254 The model setup extends over different nested spatial units (local, regional, and rest of the  
255 world, see below). There are different structural solutions in terms of number of spatial units and  
256 its resolution (see section S6 in SI). The three nested spatial scales of the model are the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

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

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

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

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



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

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

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

$$FF_{r,s} = \frac{\int_{t=0}^{\theta} MPS_s dt}{\Delta \text{Environmental Intervention}_r} \quad \text{Equation 3}$$

323 where  $r$  denotes the compartment where the environmental intervention (i.e. water withdrawal  
324 or release) occurs and  $s$  denotes the compartment where the midpoint stressor (MPS, i.e. change  
325 in mass, or volume, of water after the environmental intervention) is modelled.<sup>6</sup>

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

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

### 331 3. Results

332 **Illustrative example - system's description.** In order to demonstrate the principles described  
333 in the article, we employed a hypothetical but realistic illustrative example that represents water  
334 consumption in a generic coastal zone (Figure S9) with a non-exhaustive number of phenomena  
335 represented. The zone consists of a local spatial unit with six compartments (atmospheric  
336 moisture or air (a), soil (s), ground water (gw), fossil ground water (fw), surface water (sw), and  
337 vegetation (v)), nested in two regional units (region 1 and region 2) with respectively five (air,  
338 soil, ground water, fossil ground water, and surface water) and four (air, soil, surface water,  
339 ground water) compartments, and the rest of the world unit aggregated into one single water  
340 mass (ROW) exchanging with the local and regional units. In the example, region 1 and region 2  
341 are located downstream and upstream the local unit. The type of spatial setup represented in the  
342 example is a nested configuration of high spatial local detail, but other structural solutions could  
343 also have been applied, as explained in section S6. Every spatial unit has five ecosystem  
344 components: river (r-ecs), lake (l-ecs), aerial (a-ecs), sessile terrestrial (ster-ecs) and mobile  
345 terrestrial (mter-ecs) ecosystems. The environmental intervention assessed is the withdrawal of 2  
346  $\text{m}^3/\text{functional unit (FU)}$  of freshwater from ground water in the local unit. The release is of  
347  $1\text{m}^3/\text{FU}$  to the air in the local unit and of  $1\text{ m}^3/\text{FU}$  to surface water in region 1. Temporal  
348 dynamics of the hydrological flows are not considered (i.e. steady-state solution), which  
349 translates in only one set of FFs, instead of having different sets of FFs adapted to the granularity  
350 of every time step.

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

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

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

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

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

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

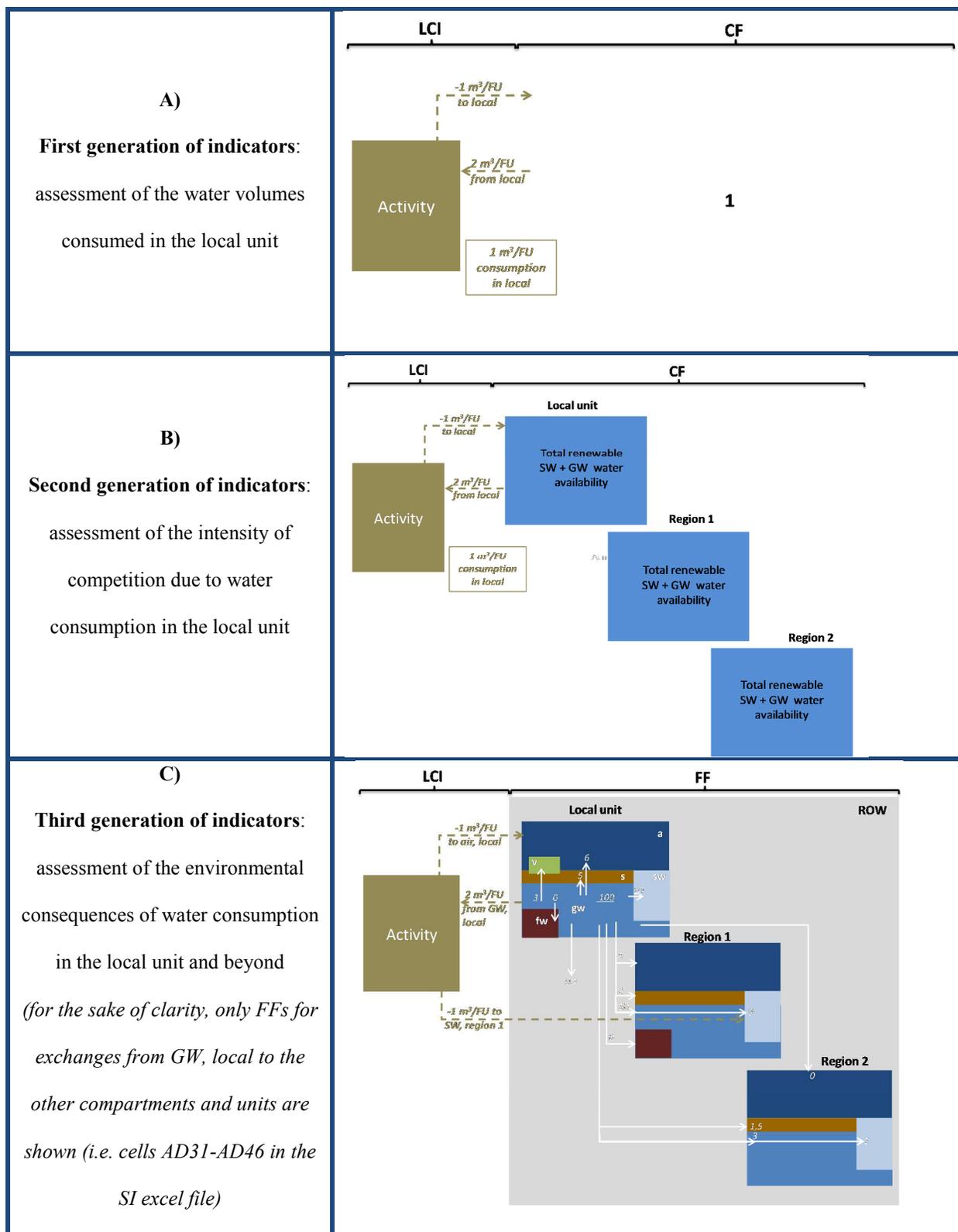
384 **The CF matrix.** The CF matrix contains the characterisation factors for each spatial unit (see  
385 section S9). Due to the propagation of water movement between compartments and spatial units,  
386 CFs vary spatially. Units of the CF in the illustrative example are in  $\text{PDFm}^3\text{day}/\text{m}^3$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

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

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

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

401 **Comparison with the former generations of indicators.** Figure 2 shows the application of  
402 the guidelines to the illustrative example and how the assessment compares to the use of the  
403 previous generations of indicators. The third generation (Figure 2 C) performs a characterisation  
404 of the environmental consequences of each LCI inflow ( $2 \text{ m}^3/\text{FU}$  from GW, local) and outflow (-  
405  $1 \text{ m}^3/\text{FU}$  to air, local;  $-1 \text{ m}^3/\text{FU}$  to surface water, region1) on the water compartments of the local  
406 unit and beyond. The second generation of indicators (Figure 2 B) characterises only the impacts  
407 (in terms of intensity of competition to access total available water resources) after water  
408 consumption in the whole watershed (i.e.  $1 \text{ m}^3/\text{FU}$ , which is the difference between the inflows  
409 and the outflows in the local unit of the LCI in the example). Whereas, the first generation  
410 (Figure 2 A) would just inform of the consumption of  $1 \text{ m}^3/\text{FU}$  within the local unit, with no  
411 further characterisation of impacts. The figure highlights the significant differences in scope of  
412 the environmental processes described by each generation of indicators.



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.

#### 415 4. Discussion

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

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

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

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

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

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

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

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

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

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

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

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

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

#### 516 **Associated content**

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

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