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6 **Ecoinvent 3: assessing water use in LCA and**

7 **facilitating water footprinting**

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25 **Abstract**

26 **Purpose** Water footprinting and the assessment of water use in life cycle assessment have become of
27 major interest in sustainability assessments. Various initiatives for combining water resource issues with
28 consumption of products and services have been initiated in the last decade. However, comprehensive
29 databases fulfilling the requirements for addressing these issues have been lacking and are necessary to
30 facilitate efficient and consistent assessments of products and services. To this purpose, ecoinvent focused
31 on integrating appropriate water use data into version 3, since previously water use data has been
32 inconsistently reported and some essential flows were missing. This paper describes the structure of the
33 water use data in ecoinvent, how the data has been compiled and the way it can be used for water
34 footprinting.

35 **Methods** The main changes required for proper assessment of water use are the addition of environmental
36 and product flows in order to allow a water balance over each process. This is in accordance with the
37 strict paradigm in ecoinvent 3 to focus on mass balances, which requires the inclusion of water contents
38 of all products (also for e.g. waste water flows), as well as emissions of water to soil, air and various
39 water bodies. Water inputs from air (e.g. rainwater harvesting) is introduced but is not yet used by any
40 activity.

41 **Results** Ecoinvent version 3.1 consistently includes the relevant flows to address water use in LCA and
42 calculate water footprints on the product level for most processes including uncertainty information.
43 Although some problems regarding data quality and spatial resolution remain, this is an important step
44 forward and can limit efforts for detailed data collection to the most sensitive processes in the product
45 system. With the combination of data on water use and emissions to water for each process, concentration
46 and corresponding water classes can also be calculated and assessed with existing impact assessment
47 methods.

48

49 **Keywords** water use • water footprint • inventory

50

51 **1. Introduction**

52 Water is vital for humans and the ecosystem, and it is under pressure although being a globally abundant,
53 renewable resource (Rockström et al. 2009). Distribution of water use and availability as well as the
54 enlarged future population is threatening life in many regions (Ridoutt and Pfister 2010a), and therefore
55 reducing water use and consumption is one of the most important actions for sustainable consumption. In
56 this context, several initiatives to create public awareness and to facilitate proper assessment and
57 communication of water problems and risks in products and services have been initiated, such as the
58 water working group of UNEP–SETAC Life Cycle Initiative (WULCA, Koehler 2008). The need for
59 good water use data has been raised in many conferences and publications in last few years, in particular
60 by the CEO Water Mandate (Morrison and Schulte 2010), the water footprint network (WFN; Hoekstra et
61 al. 2011) and UNEP (Mc Glade et al. 2012). Also within LCA the demand for assessing water use
62 properly has become more important as LCA per definition tries to address all relevant environmental
63 impacts (ISO 2006a,b). The structure required for properly assessing impacts of water use is based on the
64 distinction between consumptive water use (local loss of freshwater by evaporation, product integration
65 and release in a different watershed or to sea) and degradative water use (quality change only) as well as
66 between in-stream and off-stream use (Bayart et al. 2010, Pfister et al. 2009). Whileecoinvent data before
67 version 3 were mainly accounting for water withdrawal (combination of consumptive and degradative
68 off-stream use), freshwater consumption had not been represented in the database. In response, different
69 publications addressed these lacks of data for the agricultural and power production sectors (e.g. Scown et
70 al. 2011, Pfister et al. 2011a/b, Stoessel et al. 2012). However, no synchronized database has been created
71 that allows to consistently and transparently assess water use within the LCA framework (Kounina et al.
72 2013). The GaBi database (PE 2012) includes data for assessing water consumption consistently but
73 without required transparency on unit process level and uncertainty information. Furthermore, consistent
74 integration into a process-based LCA database enables advanced water footprint assessment including
75 water quality aspects, such as suggested in various papers (Bayart et al. 2010, Ridoutt and Pfister 2010b,
76 Berger and Finkbeiner 2010, Boulay et al. 2011, Ridoutt and Pfister 2013) in order to provide an LCA-
77 based alternative to the “grey water footprint” approach described by Hoekstra et al. (2011). The need to
78 have data for water footprinting is also influenced by the fact that the International Organization for
79 Standardization (ISO) developed a water footprint standard ISO 14046 (ISO 2014).

80 One main challenge is the need for regionalized inventory and impact assessment. While a high spatial
81 resolution is preferable from a scientific point of view (Pfister et al. 2011b), practitioners are often
82 satisfied with a country level resolution for background systems (Vionnet et al. 2012), since time
83 constraints might not allow for advanced regionalization. Proper integration of spatial information is an
84 additional demand, and use of a country level resolution seems to be the state-of-the-art practice for full
85 life cycle assessments (especially the background systems). An additional feature helping regionalization
86 of supply chains is the automatic geographic linking of inputs from technosphere through the market
87 activities in ecoinvent (Weidema et al. 2013). This means that if a process from China uses Chinese
88 electricity, the electricity input will be automatically adjusted to US electricity if the process location is
89 changed to US when creating a new dataset for updates of the ecoinvent database.

90 The ecoinvent database v3 structure serves the need for data that allows companies and public agencies to
91 better assess their businesses, products and activities (especially their supply chain) regarding impacts on
92 water resources for managing and eventually reducing them. The update of ecoinvent regarding the water
93 inventory is based on the Quantis Water Database (WDB) project that was launched in collaboration with
94 ecoinvent in end of 2010 together with eight private companies (Veolia Environnement, Natura,
95 Steelcase, Kraft, Danone, Molson Coors, Unilever, L'Oréal) and ended in early 2012. To quantify water
96 inputs and outputs, the WDB was built on the ecoinvent 2.2 water data and typical water consumption
97 rates for different industries based on literature data. Additionally, primary data was collected from
98 literature for several hundred processes. The details are described in Vionnet et al. (2012). The resulting
99 inventory database was used to update inventories that existed in ecoinvent v2.2 for ecoinvent v3.0.
100 Ecoinvent v3.1 updated all processes/activities of version 3.0 to the same standard based on the procedure
101 of the WDB.

102 In this paper we describe the data structure and summarize data sources as well as procedures to define
103 water flows in ecoinvent v3.1. We also discuss the shortcomings and uncertainties related to the data, and
104 we illustrate the use of ecoinvent data for water footprinting and water use assessment in LCA.

105

106 **2. Method and data**

107 The structure of ecoinvent version 3 has been considerably changed since version 2 as described in
108 Weidema et al. (2013): Main changes are the consistent inclusion of mass balances and the avoidance of
109 allocation in multi-output processes on the unit process level. As water has not been integrated
110 consistently before version 3, changes are less relevant than the additions. While data required to assess
111 water withdrawal, such as in-stream use (turbined water), substance and heat emissions to water (water
112 pollution) and in-stream storage (“occupation of water bodies”; e.g. for power production) have been
113 partially present, the output flows (emission to water and air) to quantify water consumption and
114 degradative water use have been missing (Figure 1). Therefore, most water use impact assessment
115 methods could not connect to the inventory and so the approach taken in the WDB is used to update
116 existing ecoinvent v2.2 data, which allows for more detailed inventory and consequently impact
117 assessment of water consumption. Unfortunately, the thermal emissions to water are so far excluded in
118 version 3 of ecoinvent, but temperature can be added in the future as a property of the water flows to
119 calculate heat emissions to water. Substance emissions, which might be relevant in assessing a water
120 degradation footprint, are reported separately in ecoinvent.

121 ***[FIGURE 1]***

122 **2.1 Structure of water flows in ecoinvent.**

123 Water flows in ecoinvent are extended compared to the flows existing in version 2 in order to allow for a
124 complete water balance and therefore also the quantification of water consumption. The following flows
125 are captured in ecoinvent (environmental flows are summarized in Table 1 and conceptualized in Figure
126 2).

127

128 **Water Inputs:**

129 • Resource (inputs from environment)

130 ○ In air: This flow refers to precipitation collected from air. It is mainly associated with rainwater
131 harvesting and in most cases is not relevant. In agriculture, only the rainwater collected within
132 the technosphere (e.g. collected rainwater from roofs) is added as an input, while the natural
133 water supply used in agriculture (i.e. soil moisture and precipitation) is not accounted for in the
134 inventory, since these flows of water consumption and evapotranspiration are considered to
135 happen in the environment and not within the technosphere (compare figure 2). Currently no
136 activity is using this environmental exchange.

137 ○ In water: The most common exchange with the environment is input of water from natural
138 water bodies. These inputs are distinguished as fresh water and salt water. Fresh water has
139 origins within a lake, a river, the ground or is unspecified (if the origin is not defined). Salt
140 water flows can occur from a sea or brackish water. Furthermore, cooling water and turbinized
141 water are separated even though they are not actually different flows from the previously
142 mentioned ones (they are inherited from datasets of ecoinvent 2). They represent a description
143 of the process they are used in. Historically these water flows have been used since the process
144 level has not been detailed enough. New datasets should avoid cooling and turbinized water
145 flows.

146 ○ Land: Land use might be relevant in terms of water footprint as in-stream storage or use of
147 waterways might be part of water resource and water footprint assessments. The land use
148 category includes occupation and transformation effects, which might be included for impact
149 assessment methods related to water use in future.

150 ■ Products: This is the flow from another process in the system (technosphere flow). Each product has
151 water content (“water in wet mass”) and therefore can be used to balance the water flows for all inputs
152 and outputs. This is especially important for water transport and treatment processes (e.g. water

153 supply and waste water treatment). Please note that product water contents of biomass production are
154 generated without water consumption for non-irrigated crops (“biogenic” water consumption).

155 ▪ If the exact origin and/or destination of the freshwater exchanges are unknown, they are entered as
156 inputs from and/or outputs to the environmental sub-compartment ‘water, unspecified’.

157 **Water Outputs:**

158 • To air: Water evaporated or evapotranspired to air is generally the most relevant flow of water
159 consumption. The ecoinvent structure distinguishes between different locations of the emissions based
160 on population densities and has a separate flow for emissions in high altitudes (mainly for airplanes).
161 For emissions of water, this distinction does not matter as no impact of the emission as such is
162 modelled (no pollution).

163 • To water: Water releases are captured as flows to water bodies. If water is released to artificial ponds
164 or infiltrated, these processes should be modelled as separate activities, reporting flows to ground and
165 surface water as well as evaporation. Ecoinvent v3.1 contains water flows to surface water, sea,
166 groundwater and as unspecified (where no further information is available).

167 • Products: As for the inputs, the water in wet mass is quantified as a property of the product and can be
168 translated into a water flow going to another process in the system (technosphere flow). However, this
169 is not an environmental exchange.

170 Inputs and outputs are balanced in order to ensure mass conservation in each system process. Net
171 freshwater consumption of an activity can be derived by deducting water outputs to freshwater bodies
172 from freshwater inputs. The part of salt water evaporated can be balanced separately and deducted from
173 the total evaporation. For agricultural processes, irrigation is modelled as a separate process in order to
174 account for inputs of water sources, energy use and infrastructure. Depending on the level of detail of the
175 dataset, storage and distribution of water to fields should be separate processes also describing
176 evaporation seepage losses from different types of irrigation systems. This can be done manually and will
177 be addressed in future versions of ecoinvent. The product (reference flow) that the “irrigation” activity
178 delivers is a volume of irrigation water supplied to crops (and depending on the technology it has

179 different infrastructure and losses). In ecoinvent 3.0 this was dealt with depending on the data providers
180 of ecoinvent v3.0 datasets, however, for the processes of ecoinvent 2.2, water withdrawals in crop
181 production have been replaced by water from irrigation activities. For version 3.1, this has been
182 consistently adjusted. The same concept should be applied for cooling processes, which should exist as
183 separate processes if possible, but this is a future task of the ecoinvent database.

184 One limitation in the water balances is the potential chemical water formation (e.g. in a combustion
185 process) or chemical binding of water in a product (e.g. in concrete), but generally these volumes are not
186 very large. Another issue is that crop water content of non-irrigated crops or wood should be deducted
187 from the overall water balance of a product, since the input of such “green water” is not modelled. In
188 general these numbers are small compared to overall water consumption in crop production.

189 **[FIGURE 2]**

190

191 **[TABLE 1]**

192 **2.2 Database creation**

193 The main data source for water flows in ecoinvent 3 is the Quantis water database (WDB, Vionnet et al.
194 2012). The WDB updated and enhanced the water flows of existing ecoinvent 2.2 processes, and added
195 116 processes according to the described scheme, mainly in energy production. However, some
196 adjustments were required and are explained below. Only existing processes in ecoinvent 2.2 have a
197 consistent water inventory in ecoinvent 3.0, since additional processes have been inserted in parallel to
198 the new scheme and have only been adjusted in ecoinvent 3.1.

199

200 **2.2.1 Processing of WDB data into ecoinvent format**

201 The WDB is structured in two parts. The first part is the raw data (elementary exchanges, mainly based
202 on ecoinvent 2.2 data and data on consumptive use share of different industries), and the second part is
203 the modelling to produce a custom and highly detailed inventory for each process. This modelling allows
204 for the calculation, for example, of how much of the water is pumped in fossil, shallow or even depleted

205 aquifers. The latter is at the limit of the impact assessment and is not supported in the ecoinvent inventory
206 in order to keep the inventory as simple as possible and the impact assessment possibilities flexible. The
207 raw data of the first part of the Water Database is illustrated in Figure 2. This data is usually collected
208 from various sources ranging from national or international statistics to companies or industrial
209 association reports, and many sources are used by ecoinvent currently. The Water Database refined the
210 information already contained in ecoinvent 2 with an additional data collection effort as described in
211 detail in the WDB report (Vionnet et al. 2012) and summarized below.

212 A few main data sources are used for the three main categories by which we can classify the entirety of
213 ecoinvent activities: industrial, agricultural and electrical. For the industrial processes, a large portion of
214 data were derived based on Byers et al. (2002) that allowed for updating more than forty processes,
215 mostly chemicals and materials production. Most of the information found in addition to Byers et al.
216 (2002) did not clearly mention the consumption share of the water used. This consumption share is fairly
217 important in order to assess the output water as well as the amount of water resource that is no longer
218 available to other users (most impact assessment methods for water use require this information).
219 Therefore, this information has been collected when possible. However, for some processes, default
220 consumption rates are applied based on Schaffer et al. (2008) and Statistics Canada (2007). For
221 agricultural processes, most of the data available was in fact the consumed water as taken from Pfister et
222 al. (2011b) and processed according to Pfister and Bayer (2014) for crops and Siebert and Doell (2010)
223 for grass and pasture. To calculate the water input (irrigation amount), an irrigation efficiency value was
224 applied to the consumed water depending on country specific irrigation efficiencies (Siebert et al. 2010).
225 Lastly, water consumption in electricity production was refined based on Scown et al. (2011) for
226 thermoelectric power and is based on the hydroelectric processes in Pfister et al. (2011a). Further details
227 are presented in the SI and available in Vionnet et al. (2012).

228 Water supply processes are introduced for industry and domestic users (activities “tap water” and
229 “cooling water”) and for agriculture (activity “irrigation”). These flows are incorporated in ecoinvent as
230 technosphere flows as they represent a separate independent activity and, thus, can also be adjusted on a
231 case-by-case basis depending on the water supply system. A typical activity will have water supply
232 defined as a separate activity as well as a water discharge activity (a waste water treatment process most

233 of the time). A process can, however, have direct water flows to and from natural environment. For
234 instance the irrigation input is modelled as a technosphere input since this irrigation requires energy,
235 infrastructure, pipes, pumps, and implies losses of water during its transportation (Faist Emmenegger et
236 al. 2011). However its output water from the field is emitted directly to environment either to the
237 atmosphere (evaporated) or to the soil. Consequently, crop cultivation does not directly contain these
238 flows, but the irrigation process does. On the other hand, crop cultivation might cause changes in natural
239 water availability through change in soil moisture (green water), which should be determined by land use
240 impact assessment (Núñez et al. 2013) and not as an inventory flow.

241 **2.2.2 Consistency of water balance in ecoinvent v3.1 and known issues with v3.0**

242 Since new datasets were not updated for water flows in ecoinvent 3.0, many new electricity production
243 datasets for hydro power lacked an output of water, even though they did have an input for turbinated
244 water. In ecoinvent v3.1, the water balance is corrected by adding the water output to these datasets
245 (together with improvements in water balances for >2000 unit processes). In SimaPro 8.01
246 (PRéConsultants 2014) with ecoinvent v3.0, turbinated water inputs were not assessed in the water balance
247 while outputs were assessed as negative consumption. This led to the artefact that run-of-the-river
248 hydropower production that was updated in ecoinvent 3.0 caused significant negative impact, which is a
249 falsehood of the modelling and needed to be corrected manually. This is corrected in SimaPro 8.04 with
250 ecoinvent 3.1.

251

252 **2.3 Uncertainty information**

253 The uncertainties of the flows of an activity are determined using the pedigree matrix as described in
254 Weidema et al. (2013) and can be converted to k-values (based on Slob 1994): the expected value divided
255 and multiplied by k includes the 95% confidence interval and can be calculated as $k = e^{(1.96 * sd_ln)}$, where
256 sd_ln is the standard deviation of the ln-transformed values (assuming a log-normal distribution). For
257 water flows, the “basic uncertainty” is higher compared to the standard k-value, which is for most flows
258 $k=1.05$ and reflects the relatively high uncertainty of water flows in ecoinvent 3.1. Especially important
259 for the water use of agricultural processes is the spatial variability of climate and, consequently, irrigation
260 water flows. This uncertainty should be reported in the uncertainty value for the input of irrigation water

261 in new datasets (given that it is modelled as a separate process), because it is only partially accounted for
262 by the “basic uncertainty” value. The uncertainty parameters are summarized in Table 2.

263 [Table 2]

264

265 **2.4 Regionalization**

266 For water use, regional aspects are essential for impact assessment. Although ecoinvent 3 has the
267 structure to include any spatial detail (e.g. countries, watersheds, coordinates), the potential of this feature
268 is not fully used. The main reason for this is that ecoinvent only includes reviewed datasets with a full list
269 of environmental exchanges and, therefore, cannot include different levels of spatial details for different
270 emissions or resource consumptions. This means that especially for agriculture, a large gap exists
271 between existing water consumption data (Pfister et al. 2011b) that have been integrated in the WDB and
272 ecoinvent inventory coverage. In most cases, the activities represent a global average or are specified on a
273 country level. For such datasets, the variability is considered in the uncertainty assessment.

274 Of relevance for industrial processes is also water consumption in metal production, where ore production
275 is typically concentrated in a few places in the world and not generally found in the location of smelting.
276 This is accounted for on country level in the database based on ore origins. New activities can be included
277 e.g. by copying existing datasets and adjusting the water consumption and location, but this requires
278 manual effort.

279

280 **2.5 Application of data for LCA and water footprint**

281 Water issues in LCA and water footprinting can be separated in quantitative (water scarcity) and
282 degradative (pollution) concerns. Quantitative assessments are based on volumetric water flows, in most
283 cases using the net freshwater consumption, which can be calculated as described in section 2.1. Quality
284 issues to be considered in water footprinting (ISO 2014) are addressed by assessing emissions to water.

285 Assessing water use with ecoinvent v3.1 following a full LCA is possible, for instance, with SimaPro
286 8.04 (PRéConsultants 2014). The main lack of data is related to agricultural processes. If the focus is on a

287 water footprint or water consumption assessment, data sets can be copied for a new country (or region) by
288 adjusting the location of the irrigation activity and the irrigation water amount. As an example, we
289 analysed wheat in Egypt and copied the transformation activity “wheat grain, Spain, wheat production”
290 and the transformation activity “irrigation, Spain, processing” and saved it as “wheat grain, Egypt, wheat
291 production” and “irrigation, Egypt, processing”. SimaPro 8.04 assesses the impacts of water consumption
292 based on the country location by defining separate environmental exchanges for each country and type of
293 water resource (inputs from freshwater and outputs to freshwater) and nine integrated methods to assess
294 these flows on country level. We therefore adjusted the water input to the irrigation process in the
295 Egyptian production from Spanish groundwater and river water to Egyptian ones. In the wheat production
296 activity for Egypt, the respective irrigation process is used and the water volume for 1kg of wheat is
297 changed from 0.71 m³ in Spain to 1.02 m³ in Egypt based on the deficit irrigation number provided by
298 Pfister et al. (2011b). For impact assessment, we selected the method resulting in ReCiPe points (Pfister
299 et al. 2011a), which is among the integrated methods in SimaPro 8.04. This integration of LCIA methods
300 has not been provided by ecoinvent yet.

301 Since power production and tap water are important processes in many activities, we also show results for
302 four different options and most relevant flows and contributing activities in the supporting information.

303 Due to current limitations of available software to utilize the full set of features in the new ecoinvent
304 version, we used the WDB to illustrate the proper use of inventory analysis for a more complex system.
305 The results are largely consistent with ecoinvent v3.1, since the underlying data is the same. However,
306 some differences are expected to arise from the new allocation structure in ecoinvent that are not reflected
307 in the WDB, but the results are still helpful to demonstrate what is possible with ecoinvent v3.1 and
308 suitable software solutions.

309

310

311 **3. Results and Discussion**

312 **3.1 Ecoinvent version 3.1**

313 Although ecoinvent version 3.0 updated all processes of ecoinvent v2.2 consistently in terms of water
314 flows, some of the completely new processes in ecoinvent 3.0 did not properly report water flows.
315 Especially the newly introduced power production activities of v3.0 have incorrect water balances and
316 therefore should not be used. Out of the 4087 processes in ecoinvent v2.2, 1450 had a complete water
317 balance in v3.0. This is accounting for most activities since many processes in ecoinvent v2.2 were
318 market processes or transmission of electricity where water use is inexistent or marginal (further details in
319 SI).

320 Ecoinvent v3.1 consistently improved the water balance correcting 2468 unit processes. This includes
321 >1000 water flows to each air and water (since the main issue with ecoinvent 3.0 was the input of
322 turbined water without an output to the environment) and > 1400 “tap water” inputs. A summary of the
323 changes is shown in the SI. Version 3.1 now has an acceptable water balance for most of the 7155 unit
324 processes (UPR, including the product water property) as presented in Table 3. For the ~2000 activities
325 with water balances deviating by >15%, supply chain water consumption is typically more important,
326 since when analysing each activity “cradle-to-gate” with the supply chain, only ~2% of the inventory
327 results had more than 5% deviation (Figure S1). Most of these flows have a high product water content
328 that partially explains this difference (since only the environmental flows are balanced in this analysis). A
329 summary of the LCI results for the three different ecoinvent v3.1 models is presented in the SI (Figure
330 S1).

331 However, there are still many agricultural processes missing in ecoinvent 3.1 (e.g. olives, peanuts or
332 millet) and only a few countries have specific datasets, while agriculture is responsible for ~85% of
333 global water consumption (Shiklomanov 1999). Additional efforts are therefore required in the future for
334 proper assessment of agriculturally-based product water footprints.

335 [Table 3]

336 **3.2 Analysis of ecoinvent 3.1 in SimaPro 8.04**

337 The results for wheat grain production show that all relevant water consumption is caused by irrigation,
338 which is modelled as separate activities in ecoinvent v3.1 (Figure 3). The differences in water
339 consumption and related environmental impacts are substantial and reflect the high spatial variability of
340 water consumption in crop production. Water consumed for Spanish wheat production is ~70% of the
341 amount consumed for Egyptian production. When the water stress index (WSI, Pfister et al. 2009) is
342 applied for midpoint assessment, the resulting difference between Egypt and Spain is a factor of 2, while
343 the endpoint characterization factors (Pfister et al. 2009 and 2011a) reveal a factor of ~6 for human
344 health, ~10 for resources and ~50 for ecosystem quality (Figure 3). These results illustrate the need for a
345 combined assessment of regionalized inventories and impact, and they show how this can be analysed on
346 a country level in available, commercial LCA software.

347 When agricultural products are not important in the supply chain, results are often driven by power
348 production. Therefore, we present the results of four different processes for tap water and power
349 production in different countries in the SI (which can be directly assessed by ecoinvent processes and
350 methods provided in SimaPro 8.04). For power production, turbinized water use is the most important
351 water flow, but typically this flow is balanced with release of the water back into the river (relatively
352 small consumptive use). Therefore, decarbonized water consumed in cooling towers is as important as
353 water evaporation in dams. For the case of tap water production, turbinized water is equally important as
354 water supplied to the water works, but it is again mainly non-consumptive. Since tap water has its water
355 consumption primarily through incorporation into the product, the activities producing tap water are
356 mainly important in terms of water consumption in this cradle-to-gate assessment, but they will have a
357 lower impact in a cradle-to-grave assessment since most of the tap water is released back after treatment
358 into natural water bodies.

359

360 **[Figure 3]**

361

362 **3.3 Results of application of WDB (industrial case study)**

363 A bottle of water produced by Danone on the Evian production site is taken as an illustrative example.
364 The entire life cycle of the bottle is considered from raw material production (primary, secondary and
365 tertiary packaging), through the bottling plant, distribution, storage, use phase and end-of-life.

366 **[FIGURE 4]**

367 Figure 4 shows that most of the water entering the system of the bottled water is used for cooling
368 purposes, especially for energy use at the use stage, at the distribution/storage stage, for packaging
369 production and at the production site. The water that is being incorporated in the bottle of water is only
370 coming from groundwater (at the production site stage) and is included in the category “to products” as
371 well at the same life cycle stage. A consumer then drinks the water at the use stage, and it is thus
372 categorized as “from products”. This water is eventually also considered to be consumed (emitted to air).
373 This is a simplification as water might be released after wastewater treatment, depending on how much of
374 the water is transpired by the user.

375 The bottle of water is an industrial product and, thus, it does not consume a lot of biomass in its life cycle.
376 The delta soil moisture is by consequence small, which would not be the case for sugar containing
377 beverages for example.

378 This inventory allows us to have a precise idea of where and how much water is entering our system and
379 how it is emitted back to the environment or to the technosphere. This vision is really useful in water
380 footprinting in order to optimize a system and focus on the most important life cycle stages. In addition,
381 when dealing with regionalization, this disaggregation of data is, for example, mandatory to apply
382 regionalized characterization factors.

383

384 **3.4 Data gaps and uncertainties**

385 The massive extent of the ecoinvent database and limited data availability of water flows lead to many
386 uncertainties. Besides the data gaps of processes intrinsic to ecoinvent, data gaps are filled with estimates
387 and expert judgements. All this is reflected in the data sets but must be considered when carrying out
388 LCA or water footprints. Error propagation e.g. by Monte Carlo is still not applied as a standard
389 procedure in such studies. However, uncertainty assessment is especially relevant for water issues due to

390 the geographic variability and generally relatively rough data quality. In addition, using processes from
391 different locations as proxies is more delicate than for many other flows, particularly in the case of
392 agricultural products. This must be kept in mind when using data from ecoinvent in addition to the
393 general uncertainty reported for the processes.

394 A minor data gap issue is the missing flow of soil moisture change during the process (e.g. cultivation of
395 potatoes) compared to the reference situation. Generally, this value can be assumed to be zero in the
396 datasets since the difference of soil moisture of an activity's land use compared to the reference situation
397 is difficult to model and also since the reference state is not clearly defined and has been an issue for land
398 use in impact assessment (Mila i Canals et al. 2007). For rain-fed agriculture, it may be relevant, and the
399 environmental exchange should be considered in future versions of ecoinvent based on data availability.

400 Another flow that is relevant for the water footprint are the thermal emissions (Verones et al. 2010, Pfister
401 and Suh 2015) that have been removed in version 3 and should be reintroduced to future versions in order
402 to allow the impact assessment of heat releases to water. Water quality classes of water released to the
403 environment (outputs), as suggested by Boulay et al. (2011), can be calculated from the substance and
404 water emissions to water of each activity. For water inputs, quality classes depend on the natural
405 environment and can therefore be characterized by impact assessment methods.

406

407 **3.5 Impact assessment**

408 Most impact assessment methods require information about spatial detail below country level (at least on
409 the optimal scale) as further described in Kounina et al. (2013). As indicated in the case study, the flows
410 can be assessed on the country level if impact assessment methods provide such data. For most methods,
411 a combination of several environmental flows is required to properly address the respective water issue.
412 Some further distinction of flows such as differentiation of groundwater into shallow, deep and fossil, as
413 done in the WDB (Vionnet 2012), could be done on the impact assessment level: Based on most detailed
414 spatial information about foreground system processes or a detailed analysis of sensitive processes and
415 flows, inventory data should be assessed with respective best resolution characterization factors. This can
416 be done by using tools beyond the traditional LCA tools, e.g. with the concepts described in Mutel et al.
417 (2012) and summarized in the next section.

418

419 **3.6 ISO water footprint compatibility (ISO 14046)**

420 Ecoinvent data is so far not differentiated on the watershed level nor does it include temporal aspects,
421 which is, in principle, demanded by the ISO 14046 standard for a proper water footprint (ISO 2014) and
422 requested by some impact assessment methods (Hoekstra et al. 2011, Pfister and Bayer 2014). However,
423 currently this demand is not fulfilled, although it is technically possible. The amount of workload required
424 to update all datasets consistently in a background database is very high, while more detailed analysis can
425 be done already with existing tools for those processes that show a relevant contribution in a specific
426 analysis. Therefore it is expected that the technical report of "Illustrative examples on how to apply ISO
427 14046" (ISO 2015- TR 14073) will show some examples that explicitly aggregate data in supply chains in
428 order to make the ISO water footprint applicable in practice. This would make sense, since in most cases
429 the background system can be simplified without changing the overall results. By means of uncertainty
430 and sensitivity assessment, those activities within the system that require further attention can be adjusted
431 to the best level of temporal and spatial resolution. Typically, agriculture and power production processes
432 play a key role in production systems and therefore might require increased spatial and temporal detail.
433 For the foreground system and important processes in the supply chain, the spatial information can be
434 attached to any activity, and, therefore, watershed level data can be derived from country data by creating
435 child processes. The structure of ecoinvent 3 (based on unit processes) allows for any geographical unit to
436 be defined as an attribute (Weidema et al. 2013) and consequently for detecting water scarcity issues at
437 any spatial detail. The temporal dimension is even more challenging, since so far only total water
438 consumption over time is reported. As done for national average characterization factors (aggregated
439 based on watershed data), annual water scarcity factors can also be derived, reflecting typical water
440 consumption patterns, e.g. in agriculture, such as presented by Pfister and Bayer (2014) and therefore
441 allowing temporal aspects to be accounted for. For more detailed assessment in space and time, spatial
442 and temporal extension matrices can be applied to the water flows in order to differentiate aggregated LCI
443 flows into e.g. watersheds and monthly flows (Mutel et al. 2011, Pfister et al. 2013). In any case, the level
444 of detail needs to be defined in the goal and scope section of a water footprint study. Depending on the
445 outcome of the TR 14073, ecoinvent v3.1 might be directly applied for the background system in a water

446 footprint study complying with ISO 14046 or it needs to be enhanced by temporal and spatial extensions.
447 With such extensions, ecoinvent can also serve as basis for foreground system processes.

448

449 **4. Conclusions**

450 The presented data is a comprehensive collection of water use data on the process level and facilitates the
451 proper assessment of water use within an LCA and water footprints beyond agricultural production.
452 Especially in LCA, but also in tools for eco-design and specific water footprint, this data is essential and
453 leads to a cost-efficient way of assessing consumption choices and product design decisions with full
454 transparency. It further enhances the effectiveness of investing in data collection by performing
455 sensitivity analyses using ecoinvent data and only focus on the most relevant flows and processes –
456 generally location specific information for agricultural production.

457

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463

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568

569 **Table 1:** List of elementary flows relevant for water impact assessment and water footprint

Compartment	Sub-compartment	Flows	Units
INPUTS			
natural resource	in water	Water, cooling, unspecified natural origin	m3
natural resource	in water	Water, lake	m3
natural resource	in water	Water, river	m3
natural resource	in water	Water, salt, ocean	m3
natural resource	in water	Water, salt, sole	m3
natural resource	in water	Water, turbine use, unspecified natural origin*	m3
natural resource	in water	Water, unspecified natural origin	m3
natural resource	in water	Water, well, in ground	m3
natural resource	Land	Occupation, inland waterbody, unspecified	m2*year
natural resource	Land	Transformation, from inland waterbody, unspecified	m2
natural resource	Land	Transformation, to inland waterbody, unspecified*	m2
NEW natural resource	in air	Water, in air	m3
OUTPUTS			
air	urban air close to ground	Water	m3
air	non-urban air or from high stacks	Water	m3
air	low population density, long-term	Water	m3
air	lower stratosphere + upper troposphere	Water	m3
air	unspecified	Water	m3
NEW water	surface water	Water	m3
NEW water	ocean	Water	m3
NEW water	unspecified	Water	m3
NEW water	ground	Water	m3
NEW water	ground-, long-term	Water	m3

**In principal these flows can also be considered as outputs, but from the ecoinvent structure they are under resources and hence considered inputs*

570

571 **Table 2:** Default basic uncertainty information: dissipation factor k based on (Slob 1994) for the
572 water-related exchanges.

573

Basic uncertainty		combustion emissions	process emissions	agricultural emissions
		k	k	k
FromEnvironment	e.g. water, river	1.2	1.2	3.0
FromTechnosphere	e.g. irrigation or tap water	1.1	1.1	1.1
ToEnvironment	water emitted to air	1.5	1.5	3.0
ToEnvironment	water emitted (released) to water	1.5	1.5	3.0
ToTechnosphere	wastewater	1.1	1.1	1.1

574

575 **Table 3.** Overview of water balance in Version 3.1 unit processes (UPR). Summary of 3.0 data
576 and for the LCI results is available in the SI.

577

Description	Count	Share
UPR total	7155	100%
Number of UPR that have no water flows	2042	29%
Water balance with >15 % deviation	2057	29%
Water balance with 5.0 - 15 % deviation	487	7%
Water balance with 0.1 - 5.0 % deviation	686	10%
Water balance with <0.1 % deviation	1883	26%

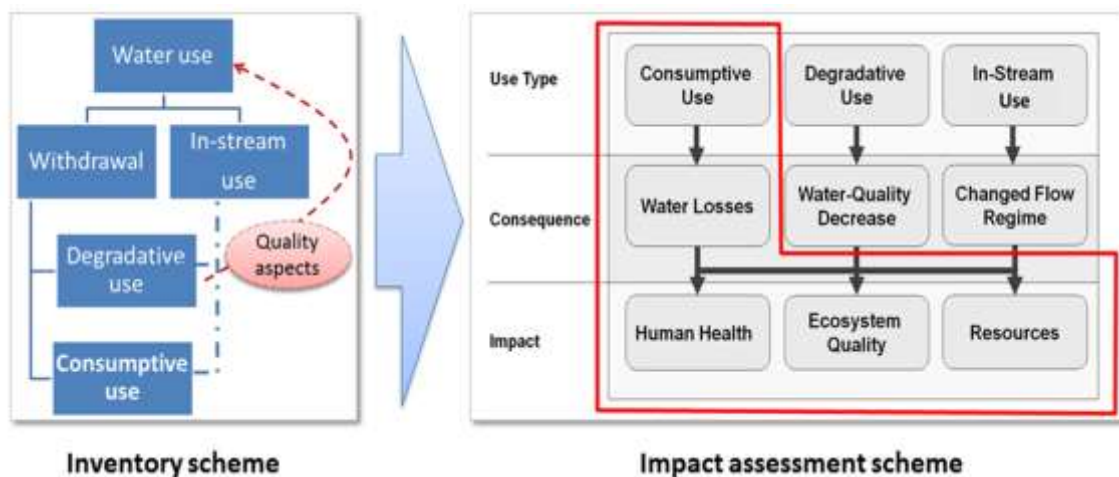
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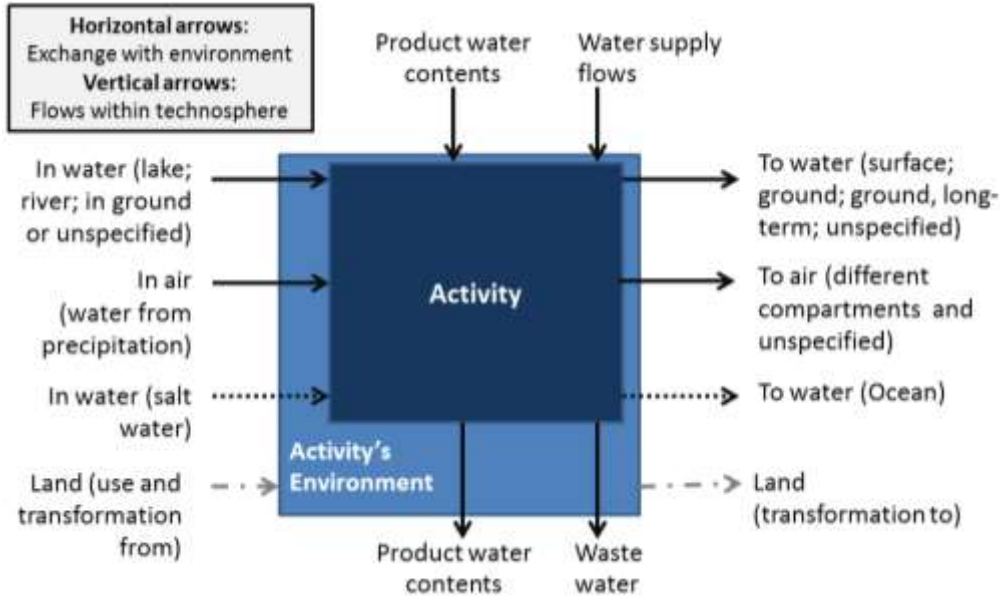
584 **Figure 1:** Concept for integrating water-use related environmental impacts in LCA (adopted from Pfister et al.,

585 2009): Life cycle inventory (LCI) data considers different types of water use: In-stream storage, consumptive use and

586 degradative use. Quality aspects, which are also important for water-reuse options, are covered by degradative use of

587 freshwater (left graph). Based on the inventory scheme, the proposed impact assessment framework illustrates the
588 damages to three areas of protection (right graph).

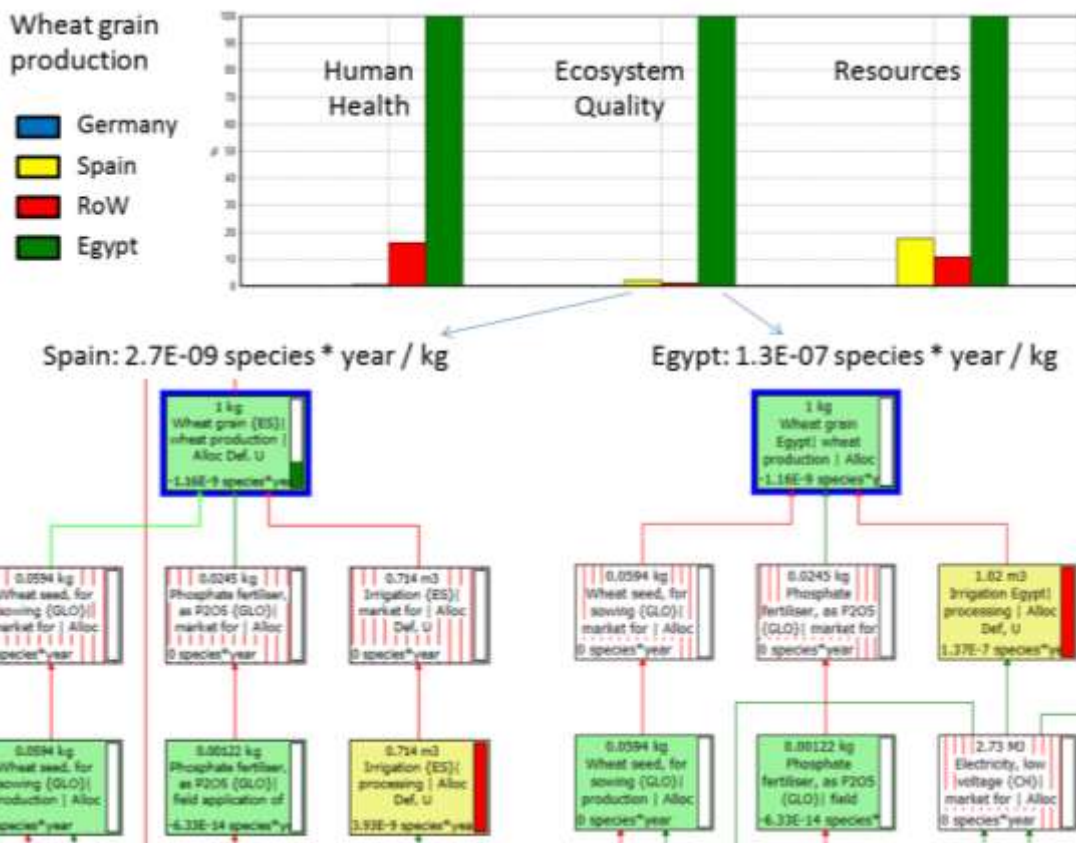
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591 **Figure 2:** The horizontal flows are exchanges with the environment and the vertical flows are technosphere flows.
592 The activity box shows the system boundaries for the activity considered. For agricultural processes the activity's
593 environment is usually included in water management (i.e. the water flows of natural water supply from soil and
594 precipitation; also called "green water"). In ecoinvent, these flows are considered to happen outside the product
595 system. Adapted from Pfister (2015).

596



597

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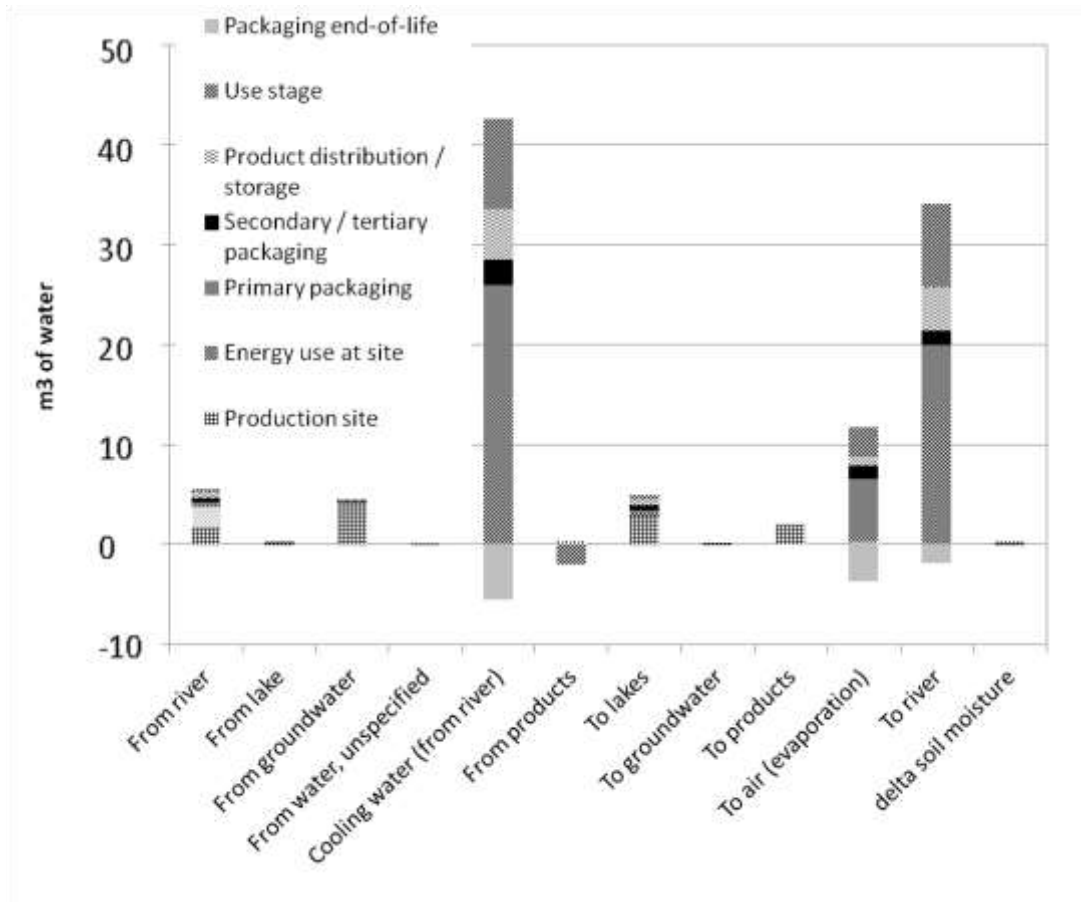
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Figure 3: Comparison of LCIA results of water consumption in ReCiPe units (Goedkoop et al. 2009, Pfister et al. 2011a) based on irrigation data from Pfister et al. (2011b) for wheat grain production: Spain, Germany and Rest of the World (RoW) have respective activities present in ecoinvent v3.1, and for Egypt it has been created in SimaPro 8.04 as a copy of Spanish activity.



603

604 **Figure 4:** Inventory analysis in the assessment of a litre of bottled water in France. The flows are attributed to life

605 cycle stages in order to provide more information on where to focus detailed assessments in the supply chain.

606