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Allan Hayato Shimako, Ligia Tiruta-Barna, Ana Barbara Bisinella de Faria, Aras Ahmadi, Mathieu Spérandio

LISBP, Université de Toulouse, CNRS, INRA, INSA, Toulouse, France, 135 Avenue de Ranguetil, F-31077 Toulouse, France

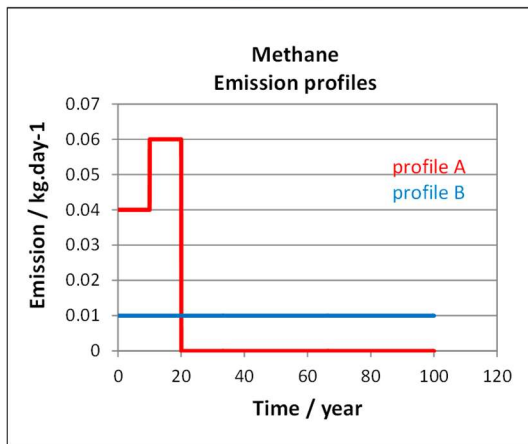
**Corresponding author:**

Ligia Tiruta-Barna  
INSA Toulouse  
LISBP  
135 Av de Ranguetil  
F-31077 Toulouse  
[ligia.barna@insa-toulouse.fr](mailto:ligia.barna@insa-toulouse.fr)  
+33 561559788

21 Graphical abstract

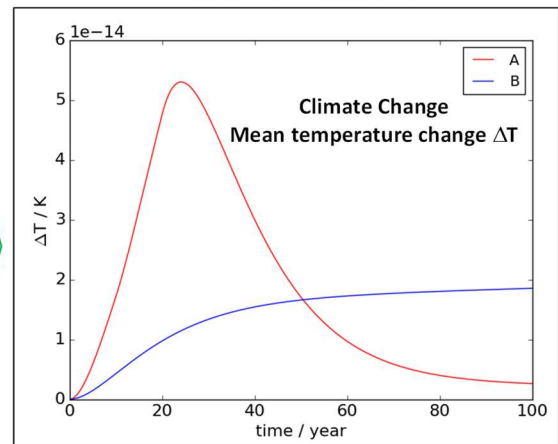
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Temporal LCI



Dynamic impact model

Temporal LCA results



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26

27 **Abstract**

28 Including the temporal dimension in the Life Cycle Assessment (LCA) method is a very recent research  
29 subject. A complete framework including dynamic Life Cycle Inventory (LCI) and dynamic Life Cycle  
30 Impact Assessment (LCIA) was proposed with the possibility to calculate temporal deployment of  
31 climate change and ecotoxicity/toxicity indicators. However, the influence of different temporal  
32 parameters involved in the new dynamic method was not still evaluated. In the new framework, LCI and  
33 LCIA results are obtained as discrete values in function of time (vectors and matrices). The objective of  
34 this study is to evaluate the influence of the temporal profile of the dynamic LCI and calculation time  
35 span (or time horizon in conventional LCA) on the final LCA results. Additionally, the influence of the  
36 time step used for the impact dynamic model resolution was analyzed. The range of variation of the  
37 different time steps was from 0.5 day to 1 year. The graphical representation of the dynamic LCA results  
38 shown important features such as the period in time and the intensity of the worst or relevant impact  
39 values. The use of a fixed time horizon as in conventional LCA does not allow the proper consideration  
40 of essential information especially for time periods encompassing the life time of the studied system.  
41 Regarding the different time step sizes used for the dynamic LCI definition, they did not have important  
42 influence on the dynamic climate change results. At the contrary, the dynamic ecotoxicity and human  
43 toxicity impacts were strongly affected by this parameter. Similarly, the time step for impact dynamic  
44 model resolution had no influence on climate change calculation (step size up to 1 year was supported),  
45 while the toxicity model resolution requires adaptive time step definition with maximum size of 0.5 day.

46

47 **Keywords:** Dynamic Life Cycle Assessment, Sensitivity Analysis, Toxicity, Climate Change

48 **Highlights:**

49 Dynamic LCA framework interconnects temporal inventory and dynamic impact models

50 Dynamic climate change is not sensitive to LCI time steps lower than 1 year

51 Dynamic (eco)toxicity indicators are very sensitive to LCI temporal definition

52 A predefined time horizon has no interest and relevance for dynamic LCA models

53

54

## 55 **1. Introduction**

56 Life Cycle Assessment (LCA) is a widely used methodology for evaluating products and processes.  
57 LCA methodology consists of four operational steps: the definition of the goal and scope, the  
58 construction of the Life Cycle Inventory (LCI) based on mass and energy balances over the whole life  
59 cycle of the system, the Life Cycle Impact Assessment (LCIA) based on various impact calculation  
60 models, and the interpretation step (ISO, 2006a; ISO, 2006b). One of the recognized limitations of the  
61 LCA method is the lack of a time dimension in the definition of both the LCI and LCIA steps (Finnveden  
62 et al., 2009). Such a time dimension has only recently been integrated into LCA and little research is  
63 currently in progress.

64 Beloin-Saint-Pierre et al. (2014) have developed an approach called Enhanced Structure Path Analysis  
65 for considering time in the LCI step. Cherubini et al. (2011) have performed a calculation considering  
66 dynamic carbon removal by the biomass, which is a step leading up to the calculation of the climate  
67 change impact, while Levasseur et al. (2010) and Kendall (2012) have studied the time dependency of  
68 climate change impact by calculating temporal characterization factors (CF) for substances and applying  
69 them to dynamic emissions. Huijbregts et al. (2000a, 2000b, 2001), Hellweg et al. (2003) and Lebailly  
70 et al. (2014) have also proposed adjustments of conventional methods to include temporal characteristics  
71 in the toxicity category. In a recent study, Beloin-Saint-Pierre et al. (2016) proposed a complete  
72 framework for the calculation of a dynamic LCA. Tiruta-Barna et al. (2016) provided a dynamic method  
73 for LCI in which they took the complex supply chain and processes present in the LCA system into  
74 account. Their method can be linked to a conventional LCA database, which facilitates its use by LCA  
75 practitioners. Shimako et al. (2016, 2017) applied this dynamic LCI method in two different case studies,  
76 combining it with a dynamic climate change model and a dynamic toxicity model.

77 Numerous parameters can influence the temporal profile of a dynamic LCA result. At LCI level, these  
78 are physical parameters describing the process and supply chain dynamics, the time scale and its  
79 granulometry, and also specific parameters of the numerical methods used for model resolution.  
80 Dynamic LCIA results are determined by the choice of the impact models/submodels (i.e. static or  
81 dynamic) and their physical parameters, along with numerical method parameters.

82 The processes and phenomena involved in all these models are characterized by very different dynamics  
83 and thus prioritization of the most influent parameters is a necessity in the development of a dynamic  
84 LCA method.

85 Dyckhoff and Kasah (2014) analysed the influence of a time horizon in the calculation of the dynamic  
86 global warming potential indicator. A comparison between the cumulative and instantaneous indicators  
87 demonstrated that contradictory conclusions could be drawn when different time horizons were used in  
88 calculations. The choice of a time horizon depends on the decision maker and is based more on policy  
89 than on scientific considerations. To the best of our knowledge, other important temporal parameters  
90 have not been analysed yet.

91 Sensitivity analysis is a valuable tool to evaluate the contribution of the temporal inputs to the dynamic  
92 results. There is general agreement that the input parameters of a model are sensitive in two distinct  
93 manners: (1) the uncertainty associated with an input parameter which is propagated in the model and  
94 contributes to the uncertainty of final results, or (2) the strong correlation between the inputs and outputs,  
95 such that a small change in the input leads to large changes in the output (Hamby, 1994). It is the second  
96 aspect that, at this stage of development of the dynamic approaches in LCA, allows the importance of  
97 the temporal parameters' influence on the LCA results to be identified, and will finally help further  
98 developments.

99 The objective of this work is to study the influence of temporal parameters involved in the dynamic  
100 LCA methodology we are currently developing. The global dynamic LCA framework was developed  
101 by using the dynamic inventory method proposed by Tiruta-Barna et al. (2016) and the dynamic impact  
102 assessment proposed by Shimako et al. (2016) and Shimako et al. (2017). One of the primary questions  
103 is how the dynamic LCI profile and the details of the inventory temporal definition will influence the  
104 final LCA results. In the aim of answering this question, a sensitivity analysis was conducted on a case  
105 study: a waste water treatment plant life cycle. The choice of the case was guided by the high temporal  
106 variability of the physical parameters involved in the process, leading to a complex LCI temporal profile.

107

## 108 **2. Methods**

### 109 **2.1. Dynamic LCA framework**

110 *Global framework*

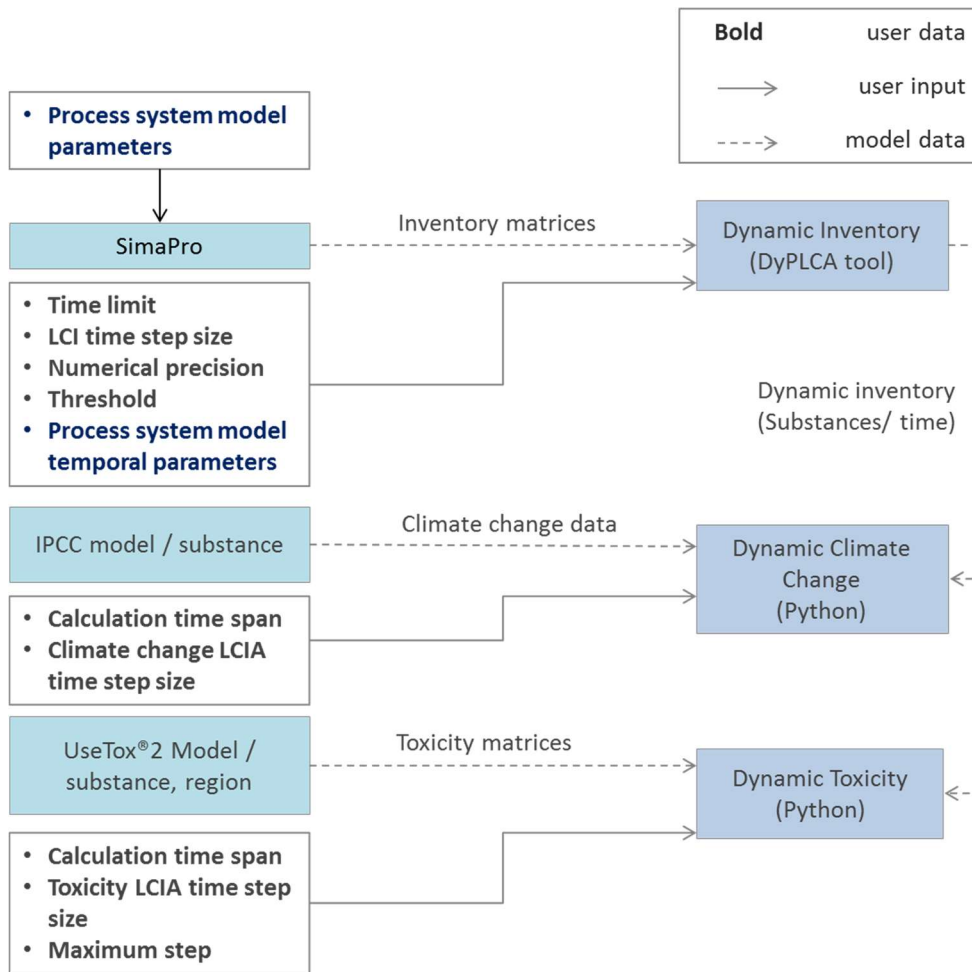
111 The global framework for dynamic LCA is presented in Figure 1.

112 First, SimaPro® LCA software was used for the traditional LCI resolution. This software delivers the  
113 LCI results in matrix form: a technological matrix and an environmental intervention matrix  
114 (interventions by compartments and processes). The dynamic inventory model and the DyPLCA  
115 software (web application <http://dyplca.univ-lehavre.fr/>) start from the conventional inventory matrix to  
116 create the process flow network as a graph structure and then adds temporal parameters related to  
117 processes and supply chains. After computation of the inventory model on the graph structure as a  
118 function of time, this tool delivers a time vector (days) and the associated environmental intervention  
119 vector (specific units.day<sup>-1</sup>, e.g. kg. day<sup>-1</sup>). Besides the temporal parameters specific to the processes and  
120 supply chains, the computation of a dynamic inventory requires specific parameters for the numerical  
121 methods (Figure 1): time step size of graph resolution and consequently the time step size with which  
122 the LCI is calculated (e.g. values of inventory at each 0.5 day), backward time limit (the algorithm will  
123 stop when reaching a specific value of time backwards), numerical precision of the results and threshold  
124 (lower limit of the mass flow value that the algorithm will consider).

125 The result of the dynamic inventory, i.e. environmental interventions distributed in time, is used for the  
126 calculation of dynamic climate change and toxicity impact categories. Homemade Python programs  
127 were developed with this aim. For the calculation of dynamic impacts, data and phenomenological  
128 dynamic models were implemented: (i) from IPCC (IPCC, 2013) for climate change, and (ii) from the  
129 USEtox® 2 model (Hauschild et al. 2008; Rosembaum et al. 2008) for toxicity categories.

130 The parameters required for both climate change and toxicity, in addition to specific phenomenological  
131 parameters, are the time span for the impacts calculation and the time step size for the numerical  
132 calculation and for results retrieval. The maximum step for the ordinary differential equations (ODE)  
133 solver used to find the mass balance in the toxicity dynamic model must also be specified.

134



135

136 Figure 1 – Parameters needed for the dynamic life cycle model in LCI and LCIA steps

137

138 The principles of the dynamic models for climate change and toxicity impacts are briefly described  
 139 below.

140

141 *Dynamic climate change model*

142 The dynamic climate change impact category was evaluated through two indicators: radiative forcing  
 143 and global mean temperature change. The atmospheric burden,  $B_s$ , is an important parameter in the  
 144 modelling of climate change potential. It can be calculated as the convolution product between the  
 145 dynamic emission of the substance  $s$ ,  $g_s$  ( $\text{kg}\cdot\text{day}^{-1}$ ) and the impulse response function of that substance,  
 146  $\text{IRF}_s$  (Olivie and Peters, 2013) :

147 
$$B_s(t) = \int_0^t g_s(t') \text{IRF}_s(t - t') dt' \quad (1)$$



148 where  $t$  and  $t'$  are time scales. Radiative forcing is described as the product between the radiative  
 149 efficiency,  $A_s$ , and the atmospheric burden,  $B_s$ . For sufficiently small emissions and approximately  
 150 constant background conditions, the radiative efficiency  $A_s$  ( $\text{W}\cdot\text{m}^{-2}\cdot\text{kg}^{-1}$ ) can be approximated as time-  
 151 invariant (Joos et al., 2013). For emissions starting at time  $t_0$  we have:

$$152 \quad n_{\text{radiative forcing},s}(t) = \int_{t_0}^t A_s(t)g_s(t')\text{IRF}_s(t-t')dt' \quad (2)$$

153 The dynamic global warming potential ( $n_{\text{radiative forcing}}(t)$  in  $\text{W}\cdot\text{m}^{-2}$ ) for all gases taken together is then:

$$154 \quad n_{\text{radiative forcing}}(t) = \sum_s n_{\text{radiative forcing},s}(t) \quad (3)$$

155 Then, the global warming potential for all gases ( $n_{\text{radiative forcing}}$  in  $\text{W}\cdot\text{m}^{-2}\cdot\text{day}$ ) over a given time span  $TH$   
 156 is:

$$157 \quad n_{\text{radiative forcing}} = \int_{t=t_0}^{TH} n_{\text{radiative forcing}}(t)dt \quad (4)$$

158 The second indicator, i.e. global temperature potential, is defined as the convolution product between  
 159 the radiative forcing and the temperature impulse response function (Olivié and Peters, 2013):

$$160 \quad n_{\text{temperature},s}(t) = \int_{t_0}^t \left( \int_{t_0}^{t'} A_s(t)g_s(t)\text{IRF}_s(t'-t)dt \right) \text{IRF}_T(t-t')dt' \quad (5)$$

161 where  $n_{\text{temperature},s}(t)$  is the global temperature potential for a substance  $s$  at time  $t$  and  $\text{IRF}_T$  is the  
 162 temperature impulse response function, which is independent of the type of GHG. The mean temperature  
 163 change at a given time  $t$ ,  $n_{\text{temperature}}(t)$  (K), is obtained by aggregating values for all the substances  
 164 concerned:

$$165 \quad n_{\text{temperature}}(t) = \sum_s n_{\text{temperature},s}(t) \quad (6)$$

166

### 167 *Dynamic toxicity model*

168 The dynamic toxicity approach was developed in Shimako et al. (2017) and only a brief background is  
 169 presented below. Traditionally, toxicity impact is calculated as the product of the substance mass and

170 its characterization factor (CF). CF is the result of combined models for substance fate in environment  
 171 (fate factor), exposure of organisms to the hazardous substance (exposure factor) and the negative effects  
 172 of the substance (effect factor). The dynamic approach replaces the fate factor by a dynamic model of  
 173 substance fate while keeping the exposure and effect factors from the conventional approach. The fate  
 174 model of a substance in the environment considers distinct mechanisms, such as the transport between  
 175 compartments, reaction processes (e.g. degradation), and removal (immobilization in different media).  
 176 The mass balance of a substance in the environment is described by a system of ODE (Mackay, 2002):

$$177 \quad \frac{dm_s}{dt} = K_s m_s + g_s \quad (7)$$

178 where K is the square matrix of rate constants (related to removal, degradation and transport processes)  
 179 in each compartment  $i$  ( $\text{day}^{-1}$ ),  $m$  is the mass vector of substance  $s$  in the respective environmental  
 180 compartments (kg),  $g$  is the vector of emission flows in each compartment ( $\text{kg day}^{-1}$ ), and  $t$  is time.

181 The generic dynamic fate model was adapted with the USEtox toxicity model (specific parameters per  
 182 substance and phenomenon, 13 environmental compartments; Jolliet et al., 2006; Ligthart et al., 2004;  
 183 McKone et al., 2006). By the end of the calculation, a mass vector (13 values corresponding to each  
 184 compartment) had been obtained for each discrete time value. For the toxicity results, following the  
 185 matrix approach proposed by Rosenbaum et al. (2007), each mass vector is multiplied by the exposure  
 186 matrix (XF) and effect matrix (EF):

$$187 \quad n_{human,s}(t) = m_s(t) \times XF_{human,s} \times EF_{human,s} \quad (8)$$

188  $n_{human,s}(t)$  is the vector that represents human toxicity (cancer and non-cancer,  $\text{cases.day}^{-1}$ ) for a certain  
 189 substance  $s$  in different compartments, at a given time  $t$ .

$$190 \quad n_{eco,s}(t) = m_s(t) \times XF_{eco,s} \times EF_{human,s} \quad (9)$$

191  $n_{eco,s}(t)$  represents the ecotoxicity expressed in  $(\text{PAF.m}^3.\text{day}).\text{day}^{-1}$ , due to an emission into a specific  
 192 compartment for a certain substance  $s$  at a given time  $t$ .

193 The result for the aggregation of all substances  $s$  and compartments  $i$ , for a given time  $t$ , is obtained by:

$$194 \quad n_{human}(t) = \sum_s \sum_i n_{human,s,i}(t) \quad (10)$$

195  $n_{eco}(t) = \sum_s \sum_i n_{eco,s,i}(t)$  (11)

196 The cumulated values,  $n_{human,cumul}$  (cases) and  $n_{eco,cumul}$  (PAF.m<sup>3</sup>.day) for human toxicity and ecotoxicity  
197 can then be calculated:

198  $n_{human,cumul}(TH) = \int_{t=t_0}^{TH} n_{human}(t)$  (12)

199  $n_{eco,cumul}(TH) = \int_{t=t_0}^{TH} n_{eco}(t)$  (13)

200 where  $t_0$  represents the time of the first emission into the environment and TH is the time span for which  
201 the cumulated impact is calculated.

202

203 It is worth noting that both dynamic approaches, climate change and toxicity, provide impact results at  
204 any point in time and are independent of the notion of time horizon – a key and controversial concept in  
205 conventional LCA.

206

## 207 **2.2. Case study**

208 In this work, a conventional wastewater treatment plant, WWTP, was used for a case study. The reason  
209 for this choice was the high variability of treatment conditions, leading to variable environmental  
210 interventions in time. The case study allowed a detailed analysis of the influence of temporal parameters  
211 on the dynamic impact results.

### 212 Goal and scope definition

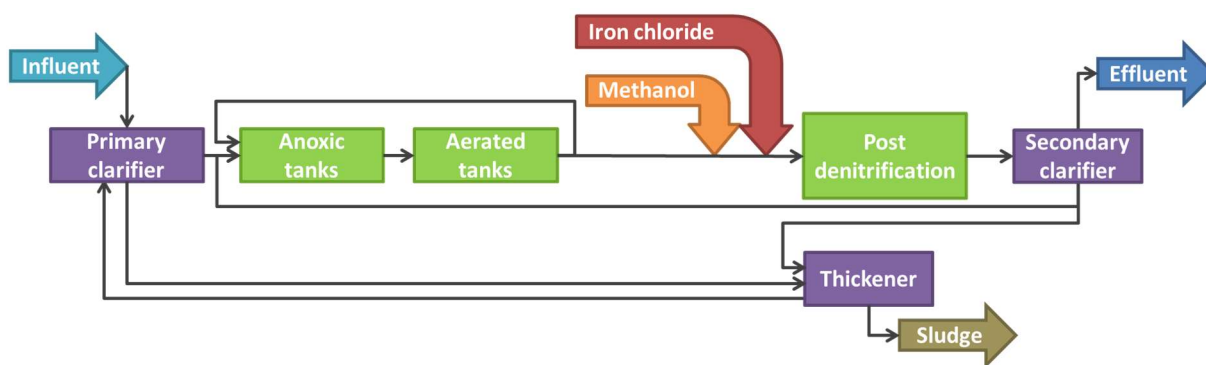
213 A conventional and a dynamic LCA were performed and the results were compared for the target impact  
214 categories: climate change, human toxicity and ecotoxicity. Determining the sensitivity of the LCA  
215 results to temporal parameters was the main objective of this work.

216 The unit function was 1 m<sup>3</sup> of waste water treated respecting the regulatory rejection limits for the outlet  
217 effluent (water discarded into the environment) and the plant lifetime was taken as 30 years.

### 218 LCI

219 Figure 2 shows the flowsheet of the WWTP studied. It comprised a primary clarification unit, 2 anoxic  
220 tanks and 3 aerobic tanks. A post denitrification zone was also added to achieve acceptable effluent  
221 quality. Nitrate was recycled from the aerobic to the anoxic zone. The sludge was separated in a  
222 secondary clarifier, which was also partly a wastage flow redirected to a thickener, and partly recycled  
223 in the anoxic zone. The resulting sludge was sent to incineration and the effluent discarded into the  
224 environment.

225



226

227 Figure 2 – Schema of the WWTP considered in the case study

228

229 WWTP unit processes involve a large number of biological and chemical reactions with various  
230 dynamics. Modelling all the processes would be extensive and time consuming. For this reason, the  
231 dynamic simulation of the WWTP (the foreground process in LCA) was performed in Sumo® software,  
232 a wastewater treatment process simulator that includes biological, chemical, and physical processes. The  
233 database ecoinvent 3.2 was used for the background processes such as the production of raw materials,  
234 energy and infrastructure.

235 External carbon (methanol) was required to complete the denitrification, and iron chloride ( $\text{FeCl}_3$ ) was  
236 added to chemically precipitate phosphorus in the sludge. Both additions were also necessary in order  
237 to satisfy legal discharge requirements for the effluent. The use of methanol releases carbon dioxide  
238 ( $\text{CO}_2$ ), a percentage of which originates from a fossil source and should be taken into account in the  
239 inventory. Emissions of  $\text{N}_2\text{O}$  from WWTPs are considered to be 0.5% of nitrified ammonia flows in  
240 dynamic conditions (Czepiel et al., 1995). The volume and composition of off-gas were calculated (in

241 Sumo<sup>®</sup> software) using gas/liquid transfer models. Calculations were based on transfer coefficients and  
242 concentration gradients with the atmosphere.

243 Heavy metal concentrations are not taken into account by Sumo<sup>®</sup> as these metals are considered to be  
244 inert for biological processes. Their input concentrations in WWTPs were therefore taken from Doka  
245 (2009) and Henze and Ledin (2001) and allocated to effluent and sludge in specific quantities, using the  
246 specific transfer coefficients proposed by the same authors.

247 The electricity consumption was calculated by taking the sum of all requirements: aeration of aerobic  
248 and nitrification tanks and thickener, mechanical mixing of anoxic tanks, pumping of main lines  
249 (influent input, dosing of chemicals, sludge output, recirculation lines, and effluent output), scraping  
250 and dewatering unit. Incineration of the sludge took account of gas-emissions in the form of CO<sub>2</sub>, and  
251 metals (copper, lead and zinc).

252 WWTP basic infrastructure was included using a class 2 capacity data set fromecoinvent (which  
253 includes dismantling) and an annual sewage volume of approximately 1.4E7 m<sup>3</sup> was considered.

254 All inventory results are presented in SI, along with theecoinvent reference for each flow.

### 255 Dynamic LCI

256 The flow rate and composition of the influent to a WWTP is commonly subject to time variations, i.e.  
257 low rate during the night and high rate during the day, weekend effect, influence of holidays, and  
258 seasonal effects (Gernaey et al., 2011) (flow variations presented in SI). In order to include these  
259 variations in the plant dynamic model, the influent generator of Gernaey et al. (2011) was used. Thus, it  
260 was considered that the operation of the plant and the influent it received had variable and cyclic  
261 behaviour with a period of 1 year. Consequently, the inventories of the foreground processes (direct  
262 emissions of CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O by the plant; CO<sub>2</sub>, N<sub>2</sub>O, heavy metals and organic substances from  
263 sludge treatment) and of the supply chain (iron chloride, methanol and electricity consumption) were  
264 also variable. The variations of emissions in the WWTP were calculated with Sumo<sup>®</sup> for the interval of  
265 one year and the results were replicated for every year of its life span.

266 Raw materials (methanol, iron chloride) were considered to be supplied every 2 months (delay of 60  
267 days and production period of 1 day). Electricity was considered to be supplied continuously during the  
268 life time of the WWTP. The time considered for the infrastructure construction of the WWTP was 3

269 years for the processes of building and 6 months' delay for the plant start up. The temporal parameters  
 270 used for the background processes are shown in SI. The temporal behaviour of the background  
 271 environmental interventions was calculated with the web-tool DyPLCA (Tiruta-Barna et al., 2016).  
 272 The inventory results obtained with Sumo and DyPLCA are in the form of discrete values in time for a  
 273 predefined time step of 0.5 days. This time step corresponds to the smallest duration for a significant  
 274 variation of physical parameters involved in the WWTP operation (variation of the influent flow rate  
 275 for instance). Coarser time granulometries can also be used, for capturing daily, monthly or seasonal  
 276 variations. Consequently, additional time step sizes were analysed: 1 day, 1 week, 1 month, 1 season  
 277 and 1 year. The discrete values of the initial dynamic inventory were thus recalculated for each time  
 278 granulometry:

$$279 \quad g_s(t)_{\Delta t_{high}} = \frac{1}{\Delta t_{high}} \sum_{t'=n}^{n+m-1} g_s(t')_{\Delta t_{lower}} \Delta t_{lower} \quad (14)$$

$$280 \quad \text{for } n = (t_0, t_0 + m, t_0 + 2m, \dots, t_{final}) \text{ and } m = \frac{\Delta t_{high}}{\Delta t_{lower}}$$

281 where  $t$  is the discrete time value for the new time scale granulometry;  $t'$  is the discrete time value in the  
 282 initial LCI time scale (step size of 0.5 days);  $s$  is the substance being analysed,  $t_{final}$  is the discrete time  
 283 at which the last emission of the dynamic inventory is released (day);  $g_s(t')$  is the mass flow value for  
 284 a specific substance and for a specific time  $t'$ , which is the result of the dynamic LCI ( $\text{kg}\cdot\text{day}^{-1}$ ),  $\Delta t_{lower}$   
 285 is the time step used for the calculation of the dynamic LCI (i.e. 0.5 days),  $\Delta t_{higher}$  is the new time step  
 286 required and  $t_0$  is the initial time in the dynamic LCI.

287 In this way, the same total quantity of a substance can be differently distributed in time (with different  
 288 granulometries), leading to different profiles of the dynamic LCI,  $g_s(t)$ .

289 Conventional LCI values,  $g_{s,total}$  (kg), can be retrieved by the time integration of the dynamic LCI:

$$290 \quad g_{s,total} = \int_{t=t_0}^{t_{final}} g_s(t) dt \quad (15)$$

291 LCIA

292 The impact categories chosen in this study are those for which a dynamic approach exists, as presented  
293 in section 2.1. The IPCC climate change and USEtox toxicity models are the basis of the dynamic impact  
294 models and were also used in conventional LCA applied to the case under study.

295 A calculation time span of 100 years was chosen for both dynamic impacts. In conventional LCA, a  
296 time horizon of 100 years is commonly used for climate change while, for toxicity categories steady  
297 state condition equivalent to an indefinite time horizon is considered.

298

### 299 **2.3. Sensitivity analysis**

300 Dynamic inventory results represent the emission variations due to the behaviour of the supply chain  
301 and processes. Moreover, dynamic impact assessment is based on environmental models that can be  
302 sensitive to different time scales (days, months, years, decades, etc.). One of the major questions  
303 subsequent to a time dependent approach of LCA concerns the extent to which the temporal parameters  
304 influence the LCA results and, in particular, how the time granulometry used in the definition of the  
305 dynamic flows will affect the temporal profile of the calculated impacts.

306 To investigate this, the influence of each of the following parameters was analysed: i) the detail of the  
307 temporal definition of the inventory (a process and supply chain characteristic), ii) the calculation time  
308 span (time horizon in conventional LCA) for the dynamic impact methods, iii) the time step size  
309 resolution of the dynamic impact models (including the ODE specifications).

310

311 For this study, several emissions from the system's life cycle were selected based on a significant  
312 variation in their temporal profile, and also based on their important contribution to the LCA results as  
313 pointed out by previous studies (Bisinella de Faria et al., 2015; Bisinella de Faria et al., 2016). In this  
314 sense, CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O were considered as they are direct emissions from the WWTP, from sludge  
315 incineration and from the infrastructure processes. Metals emitted by sludge incineration (copper, zinc,  
316 lead, chromium, mercury) and infrastructure processes (mercury) were analysed, all of them being  
317 included in the USEtox database. Phenomenological parameters inherent to the LCIA models had  
318 already been investigated for climate change and toxicity in other studies (IPCC, 2013; Henderson et al.  
319 2011; Rosebaum et al. 2011) and were not analysed in this work.

320 Several approaches exist for sensitivity analysis, such as variance decompositions, partial derivatives or  
321 elementary effects. A one-at-a-time sensitivity method was used, i.e. the effects of only one parameter  
322 were investigated at a time. The sensitivity indicator is the relative difference between the impact results  
323 of a given scenario (with a modified parameter) and the reference scenario (reference values for the  
324 temporal parameters), calculated by:

$$325 \text{ relative difference (t)} = \frac{n(t)_{step} - n(t)_{step}^{ref}}{n(t)_{step}^{ref}} \quad (16)$$

326 where  $n(t)_{step}$  is the impact value at time  $t$  for the calculation scenario with a variable temporal parameter  
327 'step' (e.g. LCI time step size), 'ref' indicates the reference calculation scenario with predefined values  
328 for the temporal parameters (e.g. LCI time step of 1 year).

329

### 330 **3. Results and discussion**

#### 331 **3.1. Influence of the dynamic LCI profile and the time span of the impact calculation**

332 LCI results for different time steps are available for all the substances selected in this work. The mass  
333 balance was verified by calculating the cumulated inventory  $g_{s,total}$  per substance. Table 1 shows that the  
334 values do not present any great variation when the step size is changed. The calculation of the relative  
335 difference between the cumulated values for different step sizes and the reference (time step size of 1  
336 year) did not exceed 1%. These results are in accordance with the mass balance, which does not change  
337 with the calculation time step.

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345 Table 1 - Cumulated LCI results for WWTP case study calculated with different time step sizes (0.5  
 346 day, 1 day, 1 week, 1 month, 1 season and 1 year).

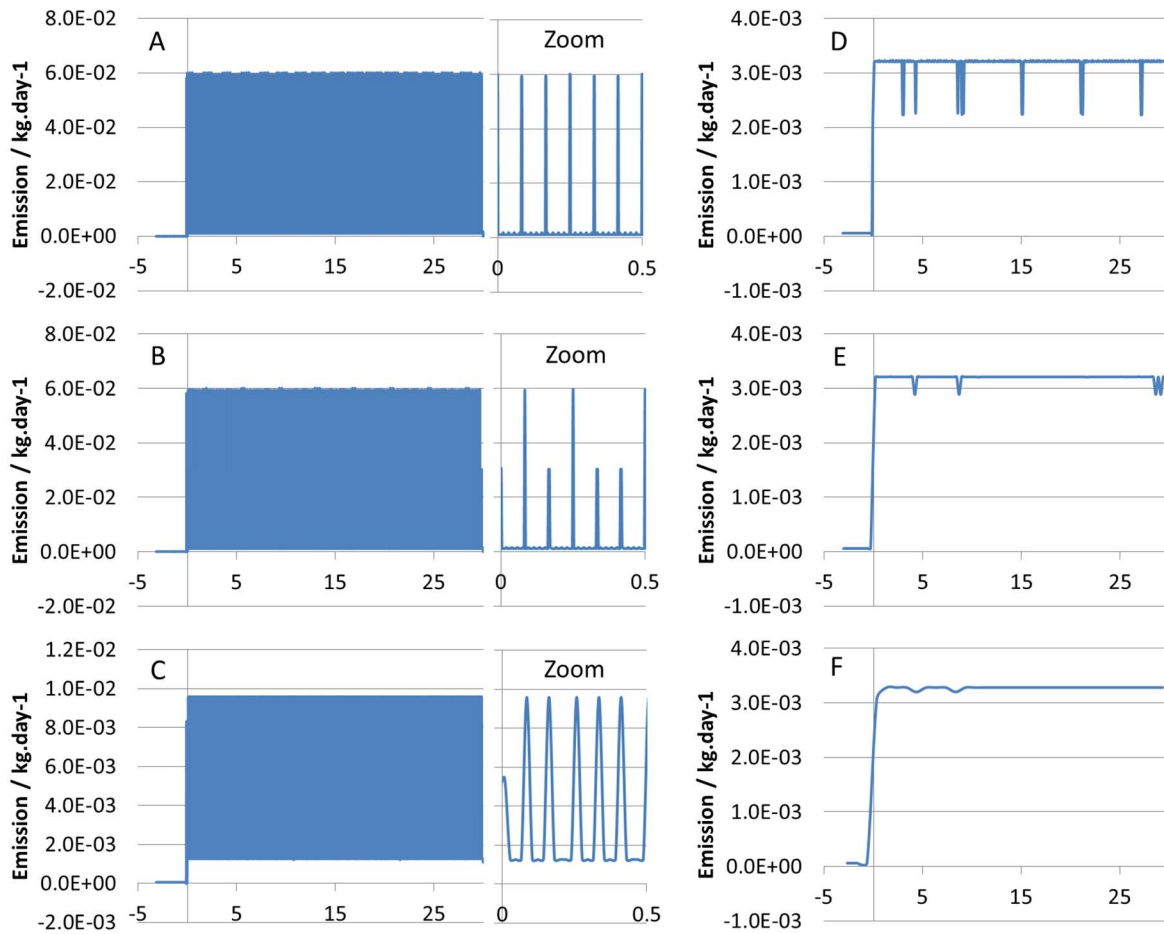
	Carbon dioxide	Methane	Dinitrogen monoxide	Copper	Lead	Zinc	Copper
0.5 day	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 day	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 week	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 month	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 season	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 year	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.0E-08
	Lead	Zinc	Methylene chloride	Chloroform	Chromium III	Mercury	
0.5 day	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 day	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 week	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 month	2.0E-08	1.1E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 season	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 year	2.0E-08	1.1E-07	7.8E-08	1.7E-07	3.3E-09	2.9E-11	

347

348

349 *Climate change results*

350 Figure 3 shows the dynamic LCI results for the emission of carbon dioxide in kg.day<sup>-1</sup> during the life  
 351 cycle of the WWTP studied. The different graphics of Figure 3 were obtained for LCI time step sizes of  
 352 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year.



353

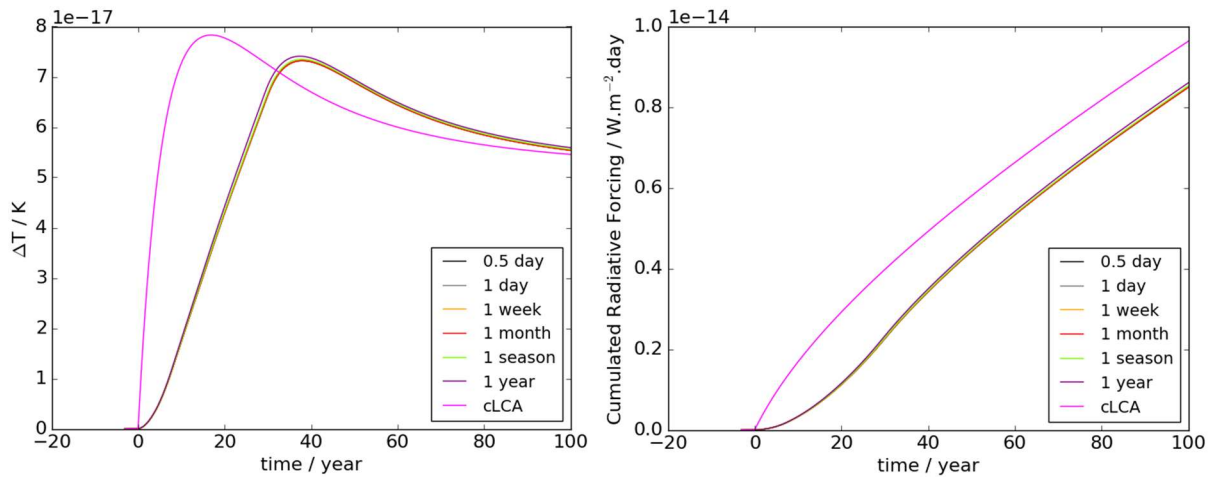
354 Figure 3 – CO<sub>2</sub> emission by the life cycle system of a WWTP. Dynamic inventory for different time  
 355 step sizes (A - 0.5 day, B - 1 day, C - 1 week, D- 1 month, E- 1 season and F- 1 year). Zoom on the year  
 356 between 0 and 0.5 for A, B and C.

357

358 Figures 3.A, B and C show the important influence of the variation of emissions due to the different  
 359 temporal characteristics of the process. On the other hand, the profile of emissions represented in the  
 360 graphics 3.D, E and F tend to a constant value around 3.3E-3 kg.day<sup>-1</sup>, representing almost steady state  
 361 conditions. For this reason, the calculation scenario with the time step of 1 year was chosen as the  
 362 reference calculation scenario (ref in formula 16). The maximum time step for which the inventory  
 363 variations can be clearly distinguished is a week for this case study. The amplitude of the emissions also  
 364 change: the values for the emissions in Figure 3.A range between 0 and 0.06 kg.day<sup>-1</sup> while they range  
 365 only between 0.001 and 0.01 kg.day<sup>-1</sup> in Figure 3.C.

366 Figure 4 shows the comparison between the results for dynamic mean temperature change and  
 367 cumulated radiative forcing, calculated with different inventory step sizes (0.5 day, 1 day, 1 week, 1  
 368 month, 1 season and 1 year) for a time span of 100 years. Carbon dioxide, methane and dinitrogen  
 369 monoxide were considered. The step size used for the calculation of the dynamic climate change impact  
 370 was 0.5 days.

371



372

373 Figure 4 – Mean temperature change and cumulated radiative forcing for the case study of the WWTP,  
 374 calculated for a time span of 100 years. Dynamic LCI inventory step sizes analysed: 0.5 day, 1 day, 1  
 375 week, 1 month, 1 season and 1 year. Results for conventional methods: cLCA curve.

376

377 No noteworthy difference could be seen between the curves corresponding to the dynamic method,  
 378 highlighting the low response of the climate change model (both indicators) to the temporal variations  
 379 of emissions at daily to monthly levels.

380 Table 2 details the relative difference between the values calculated with the dynamic model for different  
 381 LCI time step sizes and the case when step size was 1 year. The case of step size of 1 year is considered  
 382 as the reference since the plant behaves as steady state system with constant emissions. The values of  
 383 dynamic impact for both climate change indicators were calculated at year 100. At this time point, they  
 384 did show a marked difference when the LCI step size was modified.

385

386 Table 2 – Relative difference of mean temperature change and cumulated radiative forcing for a time  
 387 span of 100 years. The reference is the case of LCI time step size of 1 year. LCI time step sizes of 0.5  
 388 day, 1 day, 1 week, 1 month and 1 season were analysed.

Relative difference of $\Delta T$ results at year 100 (K)					
Substance	0.5 day	1 day	1 week	1 month	1 season
Carbon dioxide	-1.2%	-1.2%	-1.2%	-1.1%	-0.8%
Methane	-0.6%	-0.6%	-0.5%	-0.4%	-0.3%
Dinitrogen monoxide	-1.1%	-1.1%	-1.1%	-1.0%	-0.8%
All substances	-1.2%	-1.2%	-1.2%	-1.1%	-0.8%
Relative difference of cumulated radiative forcing results at 100 years ( $W.m^{-2}.day$ )					
Substance	0.5 day	1 day	1 week	1 month	1 season
Carbon dioxide	-1.6%	-1.6%	-1.5%	-1.4%	-1.1%
Methane	-1.2%	-1.2%	-1.1%	-1.0%	-0.8%
Dinitrogen monoxide	-1.5%	-1.6%	-1.5%	-1.5%	-1.1%
All substances	-1.3%	-1.3%	-1.3%	-1.3%	-0.9%

389  
 390  
 391 As expected, the lower the time step size, the higher the relative difference (with respect to the steady  
 392 state emission) in the climate change results. However, these results show that the dynamic model is not  
 393 significantly sensitive to the time step size of LCI (at least for the present case study and similar systems)  
 394 at any time. This allows a higher time step size to be used in the dynamic inventory calculation, which  
 395 is more practical and easier to obtain, and requires less computational work and time.

396  
 397 Regarding the conventional mean temperature change in Figure 4 (left side), this method considers that  
 398 all the emission occurs at time zero. The maximum value for mean temperature change is higher for the  
 399 conventional method than for the dynamic method. The conventional method gives a maximum value  
 400 of  $7.8E-17$  K and it is reached by year 16. For the dynamic method, the maximum value is  $7.4E-17$  K  
 401 by year 37. The result obtained at year 100 is similar for both methods, presenting a value of around  
 402  $5.5E-17$  K. The cumulated radiative forcing is the impact indicator in the conventional climate change  
 403 impact method. In Figure 4 (right), the values attained at year 100 are around  $8.5E-15$   $W.m^{-2}.day$  for

404 the dynamic method and  $9.6E-15 \text{ W.m}^{-2}\cdot\text{day}$  for the conventional method. The difference between  
405 dynamic and conventional results is almost constant during the whole calculation period, showing that  
406 the conventional calculation overestimates the impact from the beginning.

407 Table 3 shows the mean temperature change and cumulated radiative forcing values for the WWTP case  
408 study at a time span of 100 years. It also shows the relative difference between dynamic and conventional  
409 values in parentheses. Considering the mean temperature change for a time span (or time horizon) of  
410 100 years, methane presented a large difference, of about 20%, between the conventional and dynamic  
411 results. On the other hand, the relative difference between the conventional and dynamic mean  
412 temperature change values for carbon dioxide was quite small, about 3%.

413 Considering the comparison between the dynamic and conventional cumulative radiative forcing, there  
414 is almost no difference for the methane results. On the other hand, dinitrogen monoxide and carbon  
415 dioxide present large differences. The global cumulated radiative forcing is higher in conventional LCA  
416 than in the dynamic approach, which signifies that, for a time horizon of 100 years, conventional LCA  
417 overestimates the climate change impact.

418 Table 3 also points out that the values obtained for all substances taken together are very close to the  
419 values obtained for  $\text{CO}_2$ , which is explained by the fact that  $\text{CO}_2$  is the major GHG in this case study.

420 Obviously this behaviour cannot be generalized.

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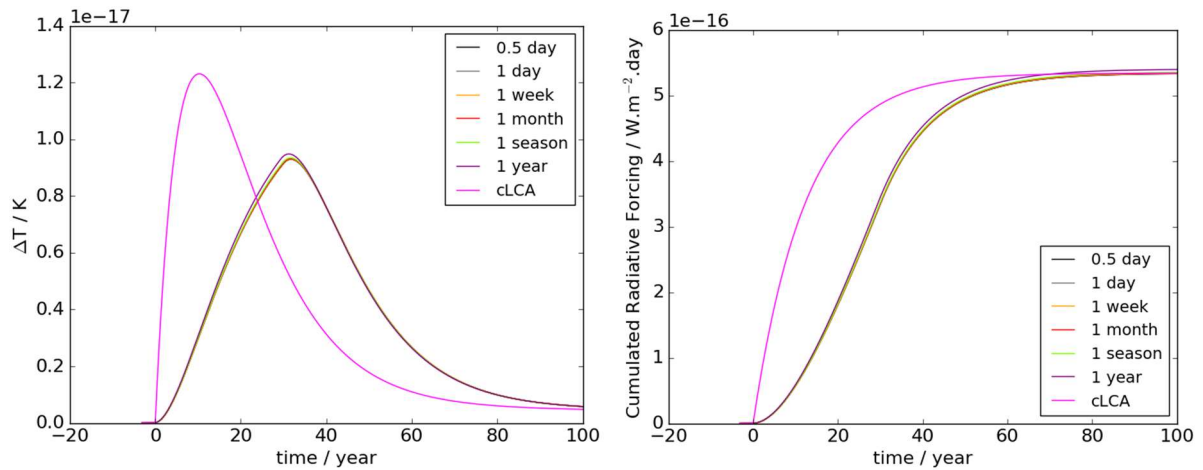
429

430 Table 3 –Dynamic and conventional climate change (cLCA) values (mean temperature change and  
 431 cumulated radiative forcing) for a time span of 100 years. In parentheses are the relative differences  
 432 between conventional and dynamic values.

Mean $\Delta T$ value at year 100 (K)							
Substance	Dynamic inventory step size						cLCA
	0.5 day	1 day	1 week	1 month	1 season	1 year	
Carbon dioxide	5.3E-17 (2.3%)	5.3E-17 (2.3%)	5.3E-17 (2.4%)	5.4E-17 (2.5%)	5.4E-17 (2.8%)	5.4E-17 (3.6%)	5.2E-17
Methane	5.7E-19 (19.3%)	5.7E-19 (19.3%)	5.7E-19 (19.4%)	5.7E-19 (19.6%)	5.7E-19 (19.6%)	5.8E-19 (20.0%)	4.8E-19
Dinitrogen monoxide	4.1E-19 (9.3%)	4.1E-19 (9.3%)	4.1E-19 (9.3%)	4.1E-19 (9.4%)	4.1E-19 (9.7%)	4.1E-19 (10.5%)	3.7E-19
All substances	5.4E-17 (2.5%)	5.4E-17 (2.5%)	5.4E-17 (2.6%)	5.4E-17 (2.7%)	5.5E-17 (3.0%)	5.5E-17 (3.8%)	5.3E-17
Cumulated radiative forcing at 100 years ( $W \cdot m^{-2} \cdot day$ )							
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Carbon dioxide	7.7E-15 (-12.0%)	7.7E-15 (-12.0%)	7.7E-15 (-12.0%)	7.7E-15 (-11.9%)	7.7E-15 (-11.6%)	7.8E-15 (-10.6%)	8.8E-15
Methane	5.3E-16 (-0.6%)	5.3E-16 (-0.6%)	5.3E-16 (-0.5%)	5.3E-16 (-0.4%)	5.3E-16 (-0.2%)	5.4E-16 (-0.6%)	5.4E-16
Dinitrogen monoxide	6.3E-17 (-10.8%)	6.3E-17 (-10.9%)	6.3E-17 (-10.8%)	6.4E-17 (-10.7%)	6.4E-17 (-10.5%)	6.4E-17 (-9.4%)	7.1E-17
All substances	8.5E-15 (-9.3%)	8.5E-15 (-9.3%)	8.5E-15 (-9.3%)	8.5E-15 (-9.3%)	8.5E-15 (-8.9%)	8.6E-15 (-8.1%)	9.4E-15

433  
 434  
 435 In order to flesh out the results observed above, Figure 5 shows the results obtained for methane with  
 436 the same calculation conditions as for Figure 4. Here too, no important difference can be seen between  
 437 the curves obtained for various inventory time step sizes. The maximum value for mean temperature  
 438 change is higher for the conventional method than for the dynamic method. It has a value of 1.2E-17 K,  
 439 which is reached by year 10. For the dynamic method, the maximum value is 9.5E-18 K by year 30.

440 Both curves tend towards a low limit as methane has a limited lifetime in the atmosphere and is  
 441 transformed into CO<sub>2</sub>.  
 442



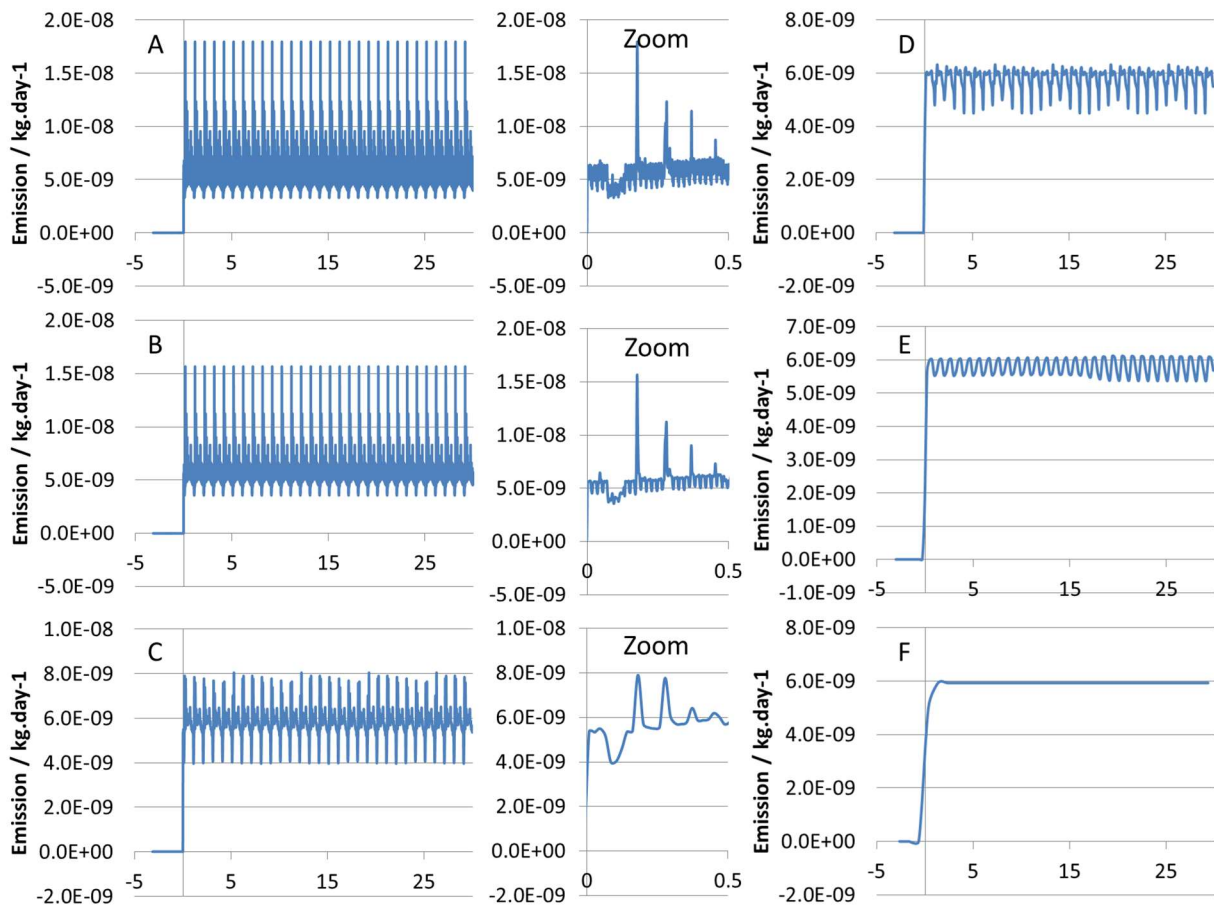
443  
 444 Figure 5 – Mean temperature change and cumulated radiative forcing for methane calculated for a time  
 445 span of 100 years. Dynamic LCI inventory step sizes analysed: 0.5 day, 1 day, 1 week, 1 month, 1 season  
 446 and 1 year. Results for conventional method: cLCA curve.

447  
 448 Figures 4 and 5 clearly show that the effects in terms of mean temperature change and cumulated  
 449 radiative forcing have amplitudes and positions on the time scale that depend on the GHG emission  
 450 duration and time position, and on the lifetime of each GHG. In conventional LCA, all information  
 451 related to the time occurrence of the (worst) effects, at the human time scale of about 100 years, is lost  
 452 by the zero time point emission on one hand, and by an arbitrarily chosen time horizon on the other. For  
 453 industrial processes with lifetimes of about 20 – 30 years, a time horizon of 100 years (or any other fixed  
 454 value) is not suitable. Instead, dynamic methods offer the possibility of monitoring the climate change  
 455 indicators over time.

456  
 457 *Toxicity results*

458 Figure 6 shows the dynamic LCI results for the emission of chloroform in  $kg.day^{-1}$  during the life cycle  
 459 of the WWTP studied. The different graphics of Figure 6 were obtained for step sizes of 0.5 day, 1 day,  
 460 1 week, 1 month, 1 season and 1 year.

461 Chloroform emission was directly linked to the effluent flow, which presents seasonal effects during the  
 462 year. Among the organic compound released, chloroform had the major influence on the toxicity. The  
 463 maximum amplitude of the emissions is observed for the smallest time step (0.5 days) in Figure 6.A. It  
 464 ranges between  $4\text{E-}9$  and  $1.8\text{E-}8$   $\text{kg}\cdot\text{day}^{-1}$ .  
 465



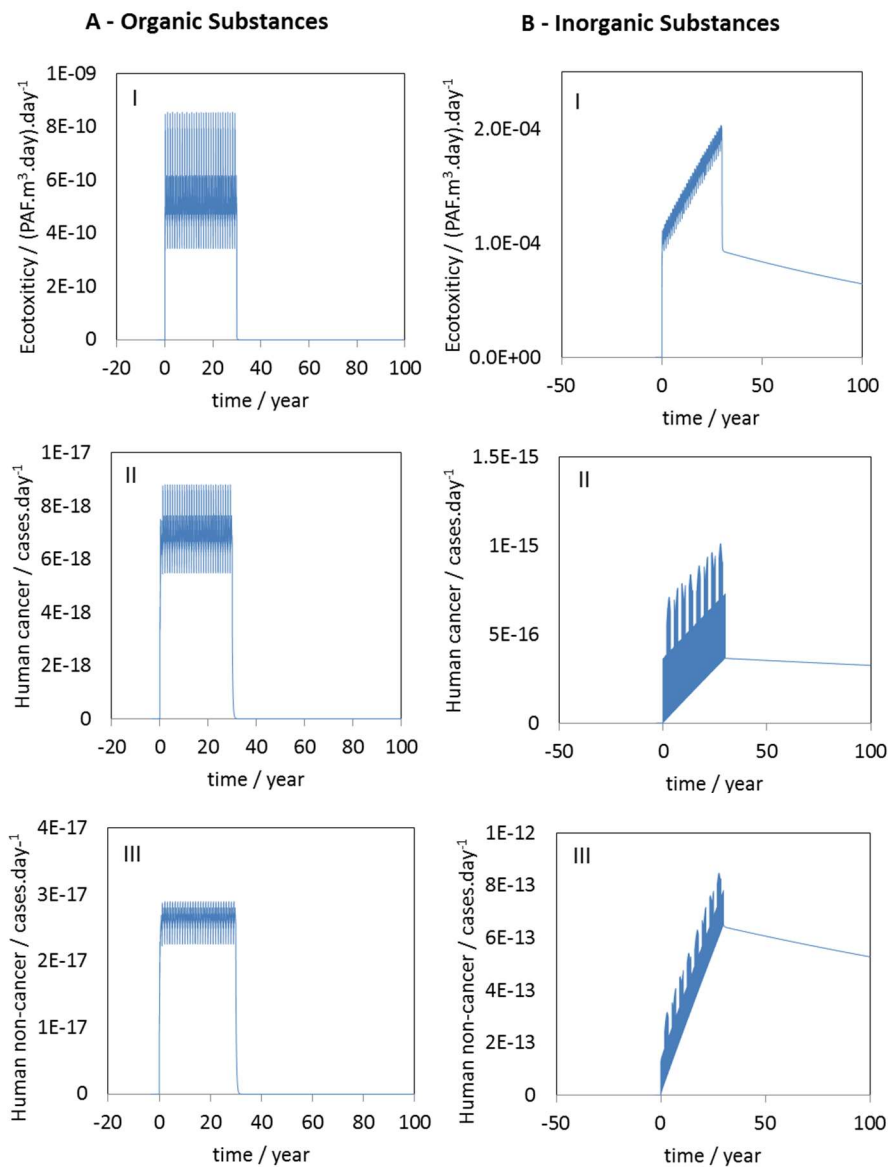
466  
 467 Figure 6 – Chloroform emission by the life cycle system of a WWTP. The dynamic inventory was  
 468 calculated for different time step sizes (A - 0.5 day, B - 1 day, C - 1 week, D- 1 month, E- 1 season and  
 469 F- 1 year) and zooms are presented for the time between 0 and 0.5 years in A, B and C.

470  
 471 Figures 7 and 8 show the results for the current ecotoxicity,  $n_{\text{eco}}(t)$ , and human toxicity,  $n_{\text{human}}(t)$ ,  
 472 calculated over 100 years with the dynamic approach.

473 In Figure 7 current human toxicity and ecotoxicity were calculated separately for organic (non  
 474 persistent) compounds and inorganic (persistent) substances. The origin of the different behaviours



475 observed for these two groups of substances was previously discussed (Shimako et al., 2017). Figure 7  
476 was obtained by simulations using a time step size of 1 day for the temporal LCI definition. As  
477 chloroform is the major contributor, the results in graphics A are dominated by chloroform's behaviour.  
478 The toxicity temporal profile follows the emission profile (Figure 6 – B: time step 1 day) in terms of  
479 periodicity and regularity of amplitudes. Overall, inorganic substances (Figure 7 – B) seemed to  
480 dominate the results, the toxicity values being of several orders of magnitude higher than those of  
481 organics.



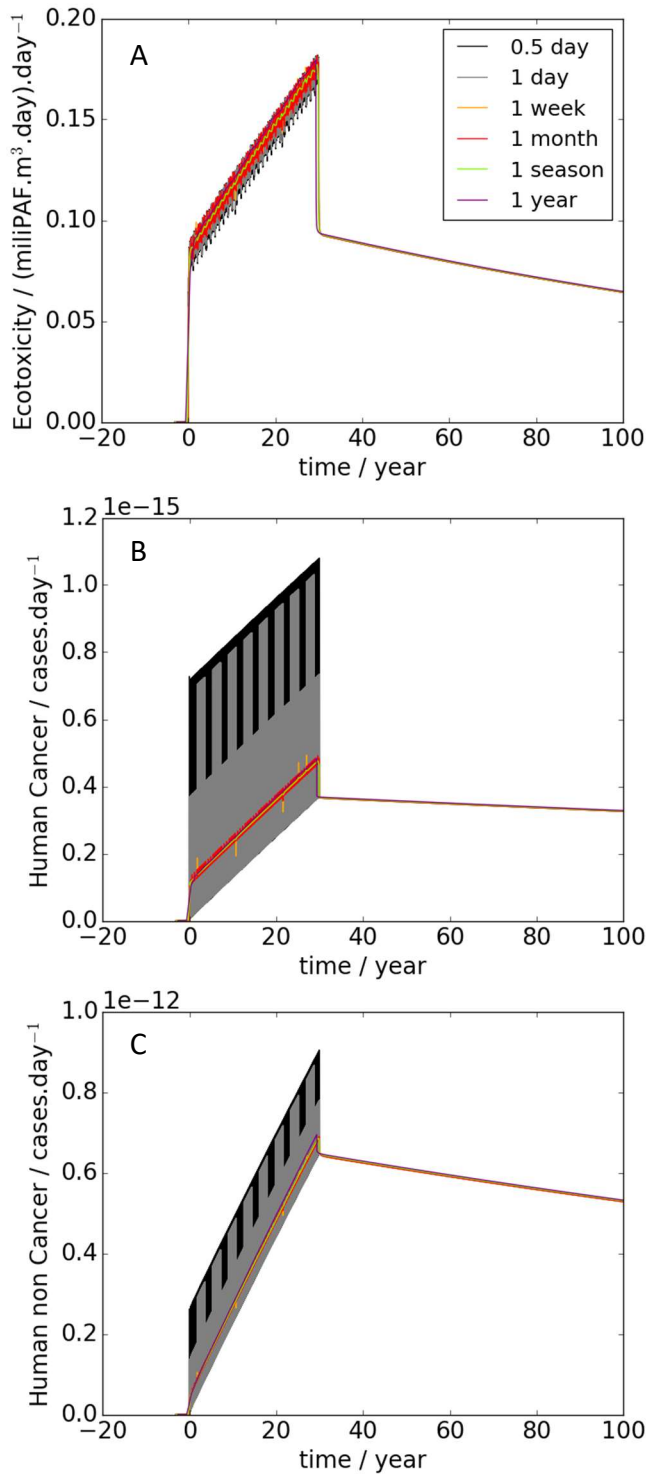
482

483 Figure 7 – Current toxicity (cancer: graphics II, non-cancer: graphics III) and ecotoxicity (graphics I).  
484 Calculation for all organic substances: graphics A (left side of the figure), and for all inorganic  
485 substances: graphics B (right side of the figure).

486

487

488 A more detailed analysis was performed on the global results obtained for all substances selected for the  
489 case study. In Figure 8 different time step sizes (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year)  
490 were used in the calculation of the dynamic inventory, which was the input to the dynamic toxicity  
491 model. The time step size used to retrieve toxicity results (from the toxicity model calculation) was the  
492 lowest one investigated, i.e. 0.5 day.



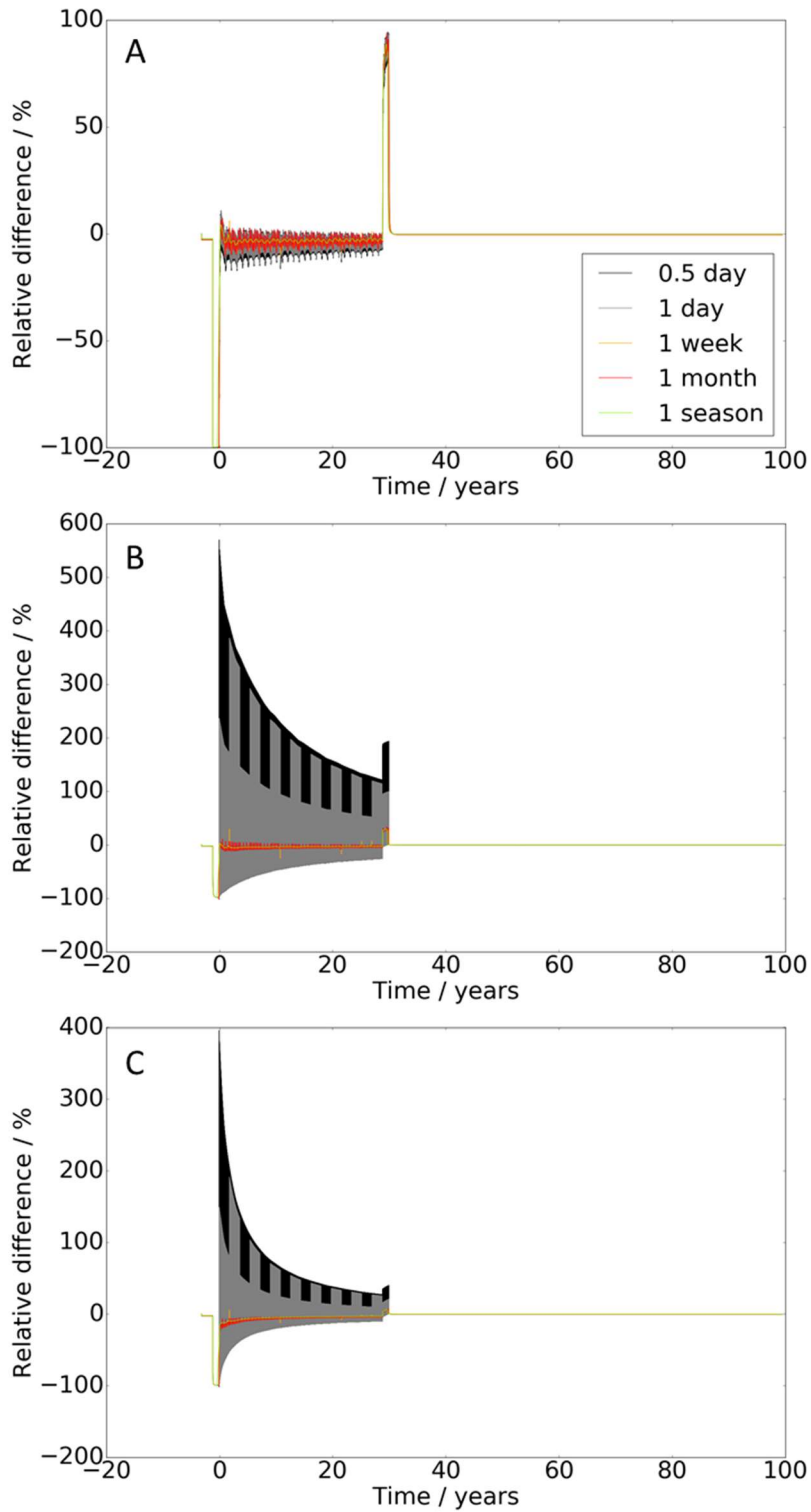
493

494 Figure 8 - Ecotoxicity (A), human cancer toxicity (B) and human non-cancer toxicity (C) for the case  
 495 study (all substances) calculated over 100 years, for different time step sizes in the LCI.

496

497

498 Ecotoxicity results present slight differences between the amplitudes and temporal profile of the impacts  
499 calculated with different step sizes. The difference of amplitudes is much greater for both cancer and  
500 non-cancer human toxicity results. The observed differences of amplitudes and temporal profiles in the  
501 dynamic toxicity results are the direct reflection of the substance emission behaviour of the life cycle  
502 system and thus of the dynamic LCI. This aspect has already been pointed out by Shimako et al. (2017).  
503 Figure 9 shows the relative difference between the results for dynamic toxicity (all substances)  
504 calculated with different step sizes compared with the reference result (step size of 1 year). The most  
505 spectacular differences are observed for human toxicity. The profiles calculated for 0.5 and 1 day present  
506 significantly higher amplitudes than those obtained with other time step sizes. The relative difference  
507 for ecotoxicity is much smaller. Two distinct high amplitudes were obtained, one by year 0 and the other  
508 by year 30 but this is, in fact, an artefact attributable to the numerical integration method (equation 14).  
509  
510



511

512 Figure 9 - Relative difference for current ecotoxicity (A), human cancer toxicity (B) and human non-  
 513 cancer toxicity (C), calculated with the dynamic approach for a time span of 100 years. Reference step  
 514 size = 1 year. Step sizes analysed: 0.5 day, 1 day, 1 week, 1 month and 1 season.

515

516 Table 4 shows the results of dynamic cumulated toxicity at 100 years, and the relative difference with  
517 respect to the conventional LCA results. In a previous study (Shimako et al., 2017), it was demonstrated  
518 that toxicity impacts due to non-persistent (organic) and persistent (mostly inorganic) substances had  
519 very different temporal profiles. For that reason, in the present work, calculations were performed  
520 considering all substances, or only organic substances, or only inorganic substances.

521 Differences between the dynamic approach and conventional LCA are very significant for “all  
522 substances” and “inorganic substances”, reaching 85% in the human cancer toxicity category. In  
523 contrast, relative differences are insignificant for “organic substances” at the chosen time span of 100  
524 years. The concentration of non-persistent organic substances in all environmental media tends to zero  
525 by year 100, while inorganics persist and generate more and more cumulated impact. As conventional  
526 LCA considers steady state conditions (theoretically reached for constant emissions over very long time  
527 frames), i.e. an infinite time horizon, the conventional toxicity method overestimates the effect of  
528 inorganic substances. The dynamic approach provides much more realistic results at a given moment on  
529 the time scale. Indeed, the contribution of sink reservoirs in the Simplebox model (substance degradation  
530 and removal) is much more influential in real systems and dynamic conditions (emissions taking place  
531 over a limited duration) as in the theoretical “ideal” condition of continuous constant emission over  
532 infinity.

533 Moreover, the LCI time step size is not a sensitive parameter when the dynamic and conventional results  
534 are compared since the observed gap is dominated by the predefined time horizon of infinity.

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542 Table 4 – Cumulated values for dynamic toxicity impact calculated over 100 years and values for  
 543 conventional LCA (cLCA). Relative difference between dynamic and conventional results is given in  
 544 parentheses.

All substances							
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF.m <sup>3</sup> .day)	3.1E+00 (56.5%)	3.1E+00 (56.5%)	3.1E+00 (56.4%)	3.1E+00 (56.4%)	3.1E+00 (56.2%)	3.1E+00 (55.8%)	7.1E+00
Human cancer (cases)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.5%)	1.2E-11 (85.3%)	7.8E-11
human non – cancer (cases)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.8%)	1.7E-08 (80.6%)	8.9E-08
Organic substances							
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF.m <sup>3</sup> .day)	2.8E-06 (-0.3%)	2.8E-06 (-0.3%)	2.8E-06 (-0.3%)	2.8E-06 (-0.3%)	2.8E-06 (-0.6%)	2.8E-06 (-1.1%)	2.7E-06
Human cancer (cases)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.1%)	3.8E-14 (-0.6%)	3.7E-14
human non – cancer (cases)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.4%)	1.4E-13 (0.8%)	1.4E-13
Inorganic substances							
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF.m <sup>3</sup> .day)	3.1E+00 (56.5%)	3.1E+00 (56.5%)	3.1E+00 (56.4%)	3.1E+00 (56.4%)	3.1E+00 (56.2%)	3.1E+00 (55.8%)	7.1E+00
Human cancer (cases)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.5%)	1.1E-11 (85.4%)	7.8E-11
human non – cancer (cases)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.8%)	1.7E-08 (80.8%)	1.7E-08 (80.6%)	8.9E-08

545

546

547 It can be concluded that current dynamic toxicity exhibits a temporal profile with marked variations and  
548 large amplitude differences when distinct LCI time step sizes are used. For all toxicity categories, the  
549 relative difference (between curves with different time step sizes) vanishes after the life time of the  
550 system, i.e. 30 years. At 100 years, the values of cumulated dynamic toxicities, calculated with different  
551 LCI time step sizes, are much the same (the relative differences between the reference case and the  
552 others do not exceed 1.7% - see SI). The temporal variation of the potential toxicity impact (cases.day<sup>-1</sup>)  
553 and thus the most relevant point in time for the assessment is information that is inaccessible in the  
554 conventional method.

555

### 556 **3.2. Influence of the time step of the dynamic impact model resolution**

#### 557 *Climate change*

558 The variation on the dynamic LCI step size (section 3.1) showed that there was no significant difference  
559 in the climate change results, for the mean temperature change, when calculations were performed with  
560 time steps from 0.5 day to 1 year. Using a 1 year step size for the inventory allows different step sizes  
561 (less than 1 year) to be used for the calculation of the dynamic climate change impact. The calculation  
562 was done for the dynamic LCIA step size of 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year.

563 The three main GHG were considered in this analysis (carbon dioxide, methane and dinitrogen  
564 monoxide). A time step greater than 1 year was not envisaged in the present case study as it would have  
565 neglected some discrete mass values from the dynamic inventory.

566 Table 5 shows the relative difference between the results obtained for the mean temperature change with  
567 different time step sizes. The relative difference is not significant for step sizes in the interval of 0.5 day  
568 to 1 season. However, the result obtained with a step size of 1 year shows differences of about 5%.  
569 Considering that the smallest time step size gives the most precise results, this means that any step  
570 between 0.5 days and 1 season can be used, given the insignificant difference between the results.

571

572

573



574 Table 5 – Relative difference for mean temperature change, obtained for different time step sizes in the  
 575 climate change model resolution.

Relative difference for $\Delta T$	0.5 day	1 day	1 week	1 month	1 season	1 year
0.5 day	0.0%	0.0%	0.0%	-0.1%	-0.4%	-5.2%
1 day	-	0.0%	0.0%	-0.1%	-0.4%	-5.2%
1 week	-	-	0.0%	-0.1%	-0.4%	-5.1%
1 month	-	-	-	0.0%	-0.3%	-5.0%
1 season	-	-	-	-	0.0%	-4.8%
1 year	-	-	-	-	-	0.0%
Calculation time	9h 34m 30s	2h 23m 20s	3m	15s	6s	8s

576

577

578 In this work, a personal computer with an Intel Core i5-2540M processor at 2.60 GHz and 4 GB of RAM  
 579 was used. Even though the computer can support multithread, only a single core was used for the  
 580 computation. The calculation time decreased substantially when the step size for the convolution  
 581 calculation was increased, because of the number of iterations required by a convolution product (Garge  
 582 and Shirali, 2012):

$$583 \text{ iterations} = \frac{\text{number of discretizations}(\text{number of discretizati})}{2} \quad (17)$$

584 As the difference between the results is not substantial, a time step size of 1 month or 1 season could be  
 585 envisaged for the calculation and would provide a good compromise between accuracy of results and  
 586 computational efficiency.

587

### 588 *Toxicity*

589 A similar comparison between different step sizes was not possible in the dynamic toxicity model  
 590 because the dynamic toxicity results are, first of all, very sensitive to the time step size of the inventory.

591 Calculation of dynamic toxicity using a 1 year step size for the dynamic inventory is not suitable as it  
592 does not consider all the potential variations and amplitudes of the toxicity impact. Moreover, it has  
593 been shown (Shimako et al., 2017) that the resolution of the dynamic toxicity model depends on the  
594 resolution of an ODE, which requires an adaptive integration time step. Thus, the lower the time step is,  
595 the more reliable is the dynamic impact profile and the more accurate is the numerical resolution. It is,  
596 however, possible to set the maximum step for the ODE solver in the toxicity model at the LCI step size,  
597 e.g. 0.5 days.

598

#### 599 **4. Conclusion**

600 The dynamic LCA framework presented here combined the DyPLCA inventory model with dynamic  
601 climate change and dynamic toxicity impact assessment models. Sensitivity analysis was conducted on  
602 a case study in order to identify the influence of the temporal profile of the dynamic LCI and of the time  
603 horizon on the final LCA results. Additionally, parameters of numerical methods used for the resolution  
604 of the impact models were investigated.

605

606 As a general remark, both impact categories exhibit high variation over the calculation period (100 years  
607 in this study), which cannot be captured in a single impact value at a given time (or a fixed time horizon),  
608 e.g. 100 years. Instead, a detailed analysis is necessary during the first few decades. In this case, a  
609 graphical representation of the LCA results is of great interest for the identification of the general  
610 temporal profile. The subsequent conclusion is that a fixed time horizon, as implemented in conventional  
611 LCA, deprives us of essential information, especially for short and medium time periods corresponding  
612 to the lifetime of the studied system and about the following twenty years.

613

614 For climate change impact, two dynamic indicators were analysed: the global mean temperature change  
615 and the cumulated radiative forcing. The temporal profile of both indicators depends on the target  
616 substance and the global positioning of the GHG emissions on the time scale, i.e. emission beginning  
617 and duration. In consequence, a fixed time horizon as in conventional LCA is highly arbitrary and does

618 not correspond to any point of interest on the time scale of the processes, i.e. temporal LCI and dynamic  
619 phenomena involved in impact deployment.

620 In this work it is shown that neither dynamic indicator is sensitive to the level of detail of the temporal  
621 LCI definition. Simulations performed for the same process system, but varying the granulometry of the  
622 LCI from 0.5 day to 1 year, led to similar results.

623 The dynamic climate change model is not sensitive to the change of time step size for numerical  
624 resolution, on condition that it lies below the LCI time step size (otherwise inventory information can  
625 be lost). For the case study, a time step of 1 month satisfied the resolution accuracy condition, for a very  
626 reasonable computational effort.

627

628 The dynamic toxicity model was based on USEtox model parameters. As in the case of climate change,  
629 the toxicity temporal profile depends on the target substance and temporal definition of LCI. However,  
630 unlike for climate change, in the case of toxicity, the level of detail of the LCI definition (time  
631 granulometry) has a major influence on the results: toxicity results are highly sensitive to the LCI time  
632 step. The time step size of the temporal LCI definition is intrinsically linked to the behaviour of the  
633 studied system and should not be chosen by the LCA practitioner. However, if a choice is possible, the  
634 smallest time step for toxicity assessment is advised.

635 Concerning the time span of calculation, as in the case of climate change, there is no justification for  
636 fixing a predefined value. In conventional LCA, the fate of substances in the environment is considered  
637 to be at steady state, i.e. the time horizon is undefined and sink processes are compensated by the  
638 continuous infinite emission. However, it is shown here that the most interesting period is the lifetime  
639 of the studied system, i.e. the emission duration, and several decades afterwards.

640 In the toxicity dynamic model, a finer time grid is necessary in order to capture the inventory information  
641 and for the resolution of the ODE system. The maximum time step could be set at the lowest LCI time  
642 step (e.g. 0.5 days).

643 Finally, the comparison with conventional LCA results shows that the dynamic toxicity results are very  
644 different in many aspects: (i) quantitatively, only the cumulated toxicity could be compared with  
645 conventional one; (ii) dynamic approach is more close to the risk assessment methods where the real

646 state of the substance in environment is identified and, from this point of view, the relevance of LCA  
647 result is improved; (iii) cumulated toxicity results can be very different from the conventional ones (e.g.  
648 10 times, 100 times), depending on the case study and on the point in time analysed; (iv) the position in  
649 time of the toxicity potential can be obtained only with a dynamic approach (e.g. for peoples living after  
650 the end of emissions there is no/less toxic potential from organics but still a toxic potential from  
651 inorganics).

652

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657

### 658 **Supplementary Information**

659 A Supplementary Information document is available containing calculation details, data and detailed  
660 results.

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