1 Documentation of the PB-LCIA method in OpenLCA

This documention of the integration of the PB-LCIA in OpenLCA has been written and developed by Manja Nørrekær Lund, Anna Kristina Schjerbeck and Simon Winther Schor. For further information, visit: https://github.com/SWintherS/PB-LCIA2.03_OpenLCA.

1.1 Introduction

The planetary boundaries was introduced by Rockström et al. (2009) and updated by Steffen et al. (2015). Traditional LCIA-methodologies, like EF3.0 or ReCiPe cannot directly be used to evaluate the planetary boundaries, thus a set of characterisation factors was developed by Ryberg et al. (2018), referred to as the PB-LCIA method. The PB-LCIA method is still novel and is not part of the LCIA-methods that can be added to SimaPro or OpenLCA automatically.

Morten Ryberg has produced a csv-file for implementation of PB-LCIA method in SimaPro. To make the method available to more LCA practitioners, we have created a migration of the SimaPro version to a version which conforms to the linking syntax needed for OpenLCA. The method is developed for use in OpenLCA 1.11, and is additionally tested on OpenLCA 2.0 beta and OpenLCA 2.0 with good results. See Table 2.

1.2 Method

The 85 characterisation factors (CF) derived by Ryberg et al. (2018) could manually have been added as an LCIA method in OpenLCA. Though, the CFs applies to multiple compartments and subcompartments, which implies that much more than the 85 elementary flows would need to be addressed. To avoid a tedious manual process OpenLCA 2.0 beta was used to convert the csv-file "PB-LCIA 2.03" meant for SimaPro and written by Morten Ryberg to a xml-files with a syntax that is compliant with OpenLCA. However, the syntax in the file generated with OpenLCA 2.0 beta was not totally compliant with the naming convention in OpenLCA 1.11 for categories and subcategories. As an example the xml-file generated with OpenLCA 2.0 beta used the name "Resources" for the category that contains all elementary flows concerning the use of resources, whereas the correct naming is "Resource".

The naming was corrected along with issues concerning specific CFs for *Freshwater use - Basin humid*, *Biogeochemcial flows - Regional P*. The latter issues are discussed in the Sections 1.2.1 and 1.2.2. Additionally, a section discussing issues related to the impact category *Land-system change* is discussed in Section 1.2.3.

Table 1 gives an overview of the naming in the csv-file written by Morten Ryberg alongside with the naming in the file generated by OpenLCA 2.0 beta and the naming in the final file that can be imported to OpenLCA 1.11 and OpenLCA 2.0.

Note that SimpaPro uses the terminology "compartments" and "subcompartments" whereas OpenLCA uses "category" and "subcategory".

Table 1: The naming in csv-file meant for SimaPro written by Morten Ryberg, the xml-file generated with OpenLCA 2.0 beta and the edited xml-file with syntax that is compliant with naming convention in OpenLCA 1.11.

PB-LCIA 2.03.csv (for SimaPro)		xml-file generated with OpenLCA 2.0 beta		xml-file with OpenLCA 1.11 syntax	
Comp.	Subcomp.	Cat.	Subcat.	Cat.	Subcat.
Air	low. pop.	Emissions to air	low. pop., long-term	Emission to air	low population density, long-term
	unspecified		indoor		indoor
	unspecified		stratosphere		stratosphere
	unspecified				unspecified
	unspecified		high. pop.		high population density
	unspecified		stratosphere + troposphere		lower stratosphere + upper troposphere
Raw	unspecified	Resources	biotic	Resource	biotic
	unspecified		in water		in water
	unspecified				unspecified
	unspecified		land		land
	unspecified		in air		in air
	unspecified		in ground		in ground
Water	unspecified	Emissions to water		Emission to water	unspecified
	unspecified		groundwater		ground water
	unspecified		groundwater, long-term		ground water, long-term
	unspecified		ocean		ocean
	unspecified		fossilwater		fossil-
	river		river		surface water
	river		lake		surface water
	river		river, long-term		surface water

1.2.1 Water use issue

According to Ryberg et al. (2018) the impact category *Freshwater use - Basin humid* describes the blue water withdrawal in humid areas. The CFs for this category subsequently addresses the use of the resource water. However, the CSV-file, meant for implementation of the PB-LCIA CFs in SimpaPro, contains a CF for the release of water to the water compartment in Switzerland under the impact category *Freshwater use - Basin humid*. This is not in accordance with the flows that the impact category should address. After correspondence with Morten Ryberg the CF addressing the release of water to the compartment "water" in Switzerland are removed from the XML-file used for implementation of PB-LCIA CFs in OpenLCA.

1.2.2 Biogeochemical flows - Regional P issue

For the impact category *Biogeochemical flows - Regional P*, we identified that CFs for phosphate and phosphorous were not defined for several subcompartments. Phosphate is solely defined for "river", leaving 11 possible subcompartments unaccounted for, while in Phosphorous' case, 6 subcompartments were unaccounted for. To investigate the importance of this matter, copies of the respective CFs were made, linking any potential

"missing" flows in ecoinvent.

The results showed major differences in the characterised results, indicating the possibility that several ecoinvent elementary flows are unaccounted for in the original PB-LCIA version. However, as further investigation is needed to truly confirm this, and to stay consistent to the original version, the described changes was not finally implemented in the migrated version of PB-LCIA.

1.2.3 Land-system change issue

For the impact category *Land-system change* Ryberg et al. (2018) has defined CFs at global scale and three biome area types; *tropical*, *temperate* and *boreal*. In our CSV-file applied to the OpenLCA modelling of the PB-LCIA method all CFs are defined. Though, it is noticed that flows belonging to the *boreal* and the *temperate* biome area types do not have matching flows in ecoinvent 3.7 due to ecoinvent's lack of detailing. This is however kept if a future updated version of ecoinvent should include this. For the global scale of *Land-system change* and the biome type *tropic* this is not a problem, since the level of detailing of the CFs match with defined flows in ecoinvent 3.7.

1.3 Validation

To validate the migration, two similar product systems where calculated with PB-LCIA 2.03 for Simapro 9.2.0.2, OpenLCA 1.11 and OpenLCA 2.0 beta, respectively. The calculation in SimPro 9.2.0.2 was done on the basis of the ecoinvent 3.7.1 database whereas ecoinvent 3.7 was used in the calculation done with OpenLCA 1.11 and 2.0 beta. Table 2 shows the characterised results for the three systems, as well as the ratios between the SimaPro results and the two OpenLCA results. Ratios exceeding 1‰ change is marked in red colour.

Table 2: Validation results

Impact category	Unit	SimaPro 9.4.0.2	Open LCA 1.11	Ratio	OpenLCA 2.0 beta	Ratio
Climate change - Energy imbalance	W/m^2	1.05E-04	1.05E-04	1.00001	1.05E-04	1.00001
Climate change - CO_2 concentration	ppm	7.78E-03	7.78E-03	1.00001	7.78E-03	1.00001
Ocean acidification	Omega Aragon	2.38E-05	2.38E-05	1.00001	2.38E-05	1.00001
Stratospheric ozone depletion	DU	1.96E-07	1.96E-07	1.00000	1.96E-07	1.00000
Land-system change - Global	%	-1.32E-08	-1.32E-08	1.00000	-1.32E-08	1.00000
Freshwater use - Basin semidry	-	2.60E-06	2.60E-06	1.00000	2.60E-06	1.00000
Freshwater use - Basin dry	-	3.02E-04	3.02E-04	1.00000	3.02E-04	1.00000
Freshwater use - Basin humid	-	1.26E-06	7.78E-07	1.61521	7.78E-07	1.61521
Atmospheric aerosol loading	AOD	2.26E-06	2.25E-06	1.00071	2.25E-06	1.00071
Biogeochemical flows - Regional P	Tg P	2.46E-05	2.46E-05	1.00000	2.46E-05	1.00000
Biogeochemical flows - N	Tg N	1.57E-03	1.57E-03	1.00000	1.57E-03	1.00000
Land-system change - Boreal	%	0.00E+00	0.00E+00	-	0.00E+00	-
Land-system change - Tropic	%	9.72E-07	9.72E-07	1.00000	9.72E-07	1.00000
Land-system change - Temperate	%	0.00E+00	0.00E+00	-	0.00E+00	-
Freshwater use - Global	km^3	1.81E-03	1.91E-03	0.94629	1.91E-03	0.94629

As visible in Table 2, all impact categories except *Freshwater use - Basin humid* and *Freshwater use - Global* show less than 1‰ change. For the impact category *Freshwater use - Basin humid* the reason behind the deviation is described in Section 1.2.1. The reason for the deviation in the impact category *Freshwater use - Global* is both due to a deviation in the elementary flows which are characterised and to differences in inventories in SimaPro and OpenLCA. Three flows associated with use of water resources; "Water, well, Europe without Switzerland", "Water, well, CN" and "Water, lake, CA-QC" were not characterised in the calculation done with SimaPro, but is characterised in the calculation done with OpenLCA 1.11 and 2.0 beta. Additionally, it is found that one specific flow "Water, river, CA" has a different inventory contribution between the two LCA softwares. Further, no impact scores are calculated for the categories *Land-system change - Boreal* and *Land-system change - Temperate*. The cause behind this is described in Section 1.2.3.

1.3.1 Truncation error

For multiple impact categories, the calculations showed minor errors in spite of no apparent issues were identified. In an online discussion forum hosted by GreenDelta, Founder and CEO Andreas Ciroths states the following as a reply to a posted question:

"Hi, this is an often-discussed topic, with the same model, and the same flows, SimaPro and openLCA provide almost the same results, and not exactly the same, for several reasons:

- *SimaPro calculates (or calculated, in verison 9.1x I think when I last checked) with single precision but with a smart, commercial library that switches the decimal based on the size of the quantitative number, openLCA calculates with double precision (see e.g. https://web.archive.org/web/20120325162206/http://www.psc.edu/general/software/packages/ieee/ieee.php). The difference is larger for numerically less stable calculations, such as substracting to large amounts.*
- *Both softwares use a different algorithm, a simplified / approximated matrix inversion calculation with each will have different result.*

More severly, though, the export could be affected, by

- *truncation of SimaPro names in the SimaPro csv*
- *possibly different units that are not mapped*
- *maybe formulas that are ill-specified or also processes that are ill-specified in the csv export due to special characters in the SimaPro csv"*

(Ciroth, 2023)

While these points are important to keep in mind, several measures towards limiting the described sources of error has been made (as described in **??**), and no further corrections were made.

1.3.2 Ecoinvent version issue

As ecoinvent 3.7.1 was not available to us in OpenLCA at the time of the analysis. The comparison was done on the basis of two different version of ecoinvent database (3.7 and 3.7.1).

On their website, ecoinvent makes the following statement:

"An issue has been identified in version 3.7 of the ecoinvent database. Specifically, the iron sinter production dataset includes an error in the order of magnitude of the estimated emissions for dioxins and particulate matter (PM). This error distorts the results of the database calculated using human health and ecotoxicity indicators from most methods.
All other impact categories, including climate change, water depletion, cumulative energy demand, land use and land use change, fossil depletion, acidification, eutrophication, ionising radiation, renewable resources, stratospheric ozone depletion, photochemical oxidant formation, radioactive substances and ozone layer depletion, are not impacted by this issue.
To correct the issue, ecoinvent v3.7.1 was published in December 2020.
We strongly recommend that all ecoinvent users work with ecoinvent v3.7.1 from its release onwards. However, for ecoinvent users working with impact categories that are not affected by the changes, ecoinvent v3.7 will remain available."

(ecoinvent Association, 2020) (login is required).

As the validation result for *Atmospheric aerosol Loading* (AOD) showed little change to the investigated system, no further correction was made. Although only a validation using the entire array of ecoinvent processes can truly validate AOD, we have no reason to suspect any crucial errors.

References

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