

Work Package 1 – Shared modelling framework and learnings

Task 1.4 – Framework for Interpreting uncertainty D1.2 – Description of scientific methods

Guide on the appraisal of uncertainty in the LCA of biobased products

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Acronyms and abbreviations

Executive summary

This guide presents practical approaches to handle uncertainty in the Life Cycle Assessment (LCA) of bio-based products within the ALIGNED project. The primary aim is to improve decision making in the bio-based industries and sectors – because such transition is heavily informed by and dependent on comparative assessment studies.

As in the case of all ALIGNED WP1 outputs on methodological framework, all guidance is here provided using a tiered approach, i.e. different options are provided to perform a specific task or apply a specific method, in order of increasing accuracy but also increasing complexity. This is reported in a specific action paragraph in each section.

The document is accompanied but other tools such as tutorials and calculators in excel and python that are made available in the T1.4 repository.

Introduction

Nowadays the number of environmental assessments and related modelling approaches and tools is booming. Besides LCA studies under the ISO framework (ISO, 2020), the Environmental Product Declaration system (EPD International, 2023) and now the Product Environmental Footprint (DG Environment, 2021) guidelines from the European Commission, but also studies under the framework of Greenhouse Gas Emission protocol (WRI & WBCSD, 2011) and the Science Based Targets and many others are all essentially based on quantitative models to calculate and return a numerical estimate of environmental footprint. All the results of these models are affected by uncertainty.

Uncertainty can be defined as unknowns about the reality. Since a model is a simplified representation of reality and our understanding of reality is always incomplete, then the lack of knowledge about how the model should be designed is transferred to the results of such model (Lo Piano & Benini, 2022).

In even simpler words the uncertainty of the result of a product footprint model can be intended as a range: every produced number should be intended as one in a distribution of possible outcomes.

Uncertainty is related to sensitivity. While uncertainty analysis is about the qualification and quantification of the uncertainty in the inputs and outputs of a model, sensitivity analysis focuses on understanding how the changes in the inputs of a model influence the model outputs. Sensitivity analysis helps shaping uncertainty analysis and vice-versa.

Recently several studies have argued for an increased focus on uncertainty and sensitivity analysis (Lo Piano & Benini, 2022; Saltelli, Bammer, et al., 2020) and on the limit of LCA models and in general of the limits of quantification in decision making for sustainability (Saltelli, Benini, et al., 2020).

1. Types of uncertainty: classification used in this document

There are different ways of defining uncertainty and for the LCA domain. Igos et al. (2019) suggest to classify uncertainty either according to its intrinsic nature - epistemic or aleatory, or according to its location in a LCA model. In the latter case one can distinguish between uncertainty regarding the structure of the model, the quantities used in the model, or the context in which the model is used.

From Igos et al. (2019): *"Regarding the nature of uncertainty, epistemic uncertainty is due to a lack of knowledge or representativeness and can be reduced with more research and efforts (e.g., more collected data, higher model complexity). Aleatory or ontic uncertainty is due to the inherent variability and the lack of determinability of the system (inherent randomness of nature, observer effect) and cannot be reduced. Both natures of uncertainty can be present for quantity uncertainty, model structure uncertainty, and context uncertainty"* (Igos et al., 2019).

In their report on the prospective assessment of bio-based technologies the JRC and European Commission (2022) also classify uncertainties depending on either their nature (epistemic and ontic) their location (data, model, context), and their scale (from moderate to deep uncertainty). We refer the reader to the original report (European Commission et al., 2022) for a more extensive description of each.

Not all these classifications are however equally useful for practical purposes. Since this is a guide addressing LCA practitioners in the bio-based industries, and users of the models provided by the project, the pragmatic choice done in the ALIGNED project was to simplify the classification to two types of uncertainty: data and model uncertainty – as this also allows to define appropriate handling strategies in terms of uncertainty and sensitivity analysis respectively.

Data uncertainty refers to the choice of the numerical values to be used in the LCA model.

Examples: lack of knowledge regarding….

…the carbon content of a specific tree species.

- *…the amount of feedstock used to produce a biobased product in a year.*
- *…the amount of carbon emissions generated by composting a biobased product.*

Model uncertainty refers to all the possible way data are combined into a LCA model and the operations done with these data.

Examples: lack of knowledge regarding the choice of....

…characterisation factors for the global warming potential (GWP20 or GWP100).

- *…type of decay of biomass in the ground (linear versus nonlinear).*
- *…temporal range to calculate the yearly increment in biomass supply (5 years versus 20 years)*

…type of probability distribution selected for each parameter/input (uniform, triangular, etc.)

In Figure 1, a LCA model can be intended as a black box where input data points are transformed into output data points. When the specific value of the input is not precisely known ("cloud" of values rather than single value), we have uncertainty. The same applies when there are unknowns regarding how to structure the model ("shifting" shape of the box rather than single shape).

Sensitivity is instead the relation between input and output (arrows). While some techniques like stochastic error propagation allow to quantify the uncertainty associated with the output of a LCA model starting from the uncertainty in the inputs, techniques like local and global sensitivity analysis allow explain to what extent changes in model input or model structure, that are due to uncertainty, lead to variations in model results.

Figure 1 Uncertainty and sensitivity analysis for a generic model, for example a LCA model.

Uncertainty analysis quantifies the range of input and related outputs of a model, due to the unknowns (represented as blurred cloud instead of clear single data point, blurred structure of the model due to limited understanding of the phenomenon) in both data and model structure. Sensitivity analysis quantify the influence that a change in input has on the output (both represented as arrows), for different data and model structures.

2. General approaches to analysis of uncertainty and sensitivity

The toolbox that it is recommended for ALIGNED addresses the data and model uncertainties and uncertainty and sensitivity analysis respectively (Figure 2).

Figure 2 Practical toolbox for handling uncertainty and sensitivity of data and models in the ALIGNED framework (OAT: One At Time, GSA: Global Sensitivity Analysis).

3. Uncertainty analysis – focus on data

3.1. Defining uncertainty for input data, tiered approach

Rough estimate. The simplest but also least accurate approach is to define an arbitrary level of uncertainty for each exchange input data point (e.g., the kg of $CO₂$ emissions per kg output of an activity). For example, the uncertainty on each value can be assumed to be equal to 10% of the value. This percentage could be intended as a coefficient of variation (CV) in case of a normal distribution (ratio of the standard deviation (σ) to the mean (μ)). Or this can be the interval (+10%, -10%) in which the value is expected to be found with equal probability (uniform distribution). In situations of lack of reliable data or expert knowledge on uncertainty, this can be a starting point or screening method for estimating uncertainty that is easily applicable also a large scale (many datasets or a database) and is arguably better than assuming no uncertainty at all. The value can be chosen completely arbitrarily – and in that case this should be clearly communicated and sensitivity analysis using increasing estimates of uncertainties is recommended – or based on expert knowledge, information from literature, or other soundly motivated assumptions.

Pedigree matrix. A widely used approach is to use a semi-quantitative method to estimate uncertainty, i.e. the pedigree matrix. With this approach each exchange in a dataset is evaluated using a score from 1-5 by the LCA practitioner in five dimensions: *Pedigree Reliability, Pedigree Completeness, Pedigree Temporal correlation, Pedigree geographical correlation, Further technological correlation*. Each score is then converted in a measure of uncertainty using specific conversion tables and finally a overall measure of uncertainty is obtained, for example a coefficient of variation (Weidema & Wesnæs, 1996) or a "geometric mean" (Ciroth, 2013) for an assumed lognormal distribution¹ (Limpert et al., 2001) using a formula for analytical propagation of uncertainty. Detailed documentation on how to apply it available in published literature (Ciroth, 2013; Ciroth et al., 2016; Muller et al., 2016) and a simple calculator is also provided (*ALIGNED-T1.4-Pedigree-matrix-calculator-AAU.xlsx*). The approach is simple and easily applicable also at large scale (database). A disadvantage is that the approach has been criticised when used in combination with stochastic error propagation (Heijungs, 2019), the reason for this criticism is not entirely clear but supposedly because the pedigree method was originally not developed for the purpose of being used in stochastic simulations.

Empirical estimates. Empirical estimates are more reliable than assumptions because based on evidence, but obtaining these data might require more resources. A simple approach is to use a range to quantify exchange input data uncertainty. Estimates might be available for a max. and min. value of an exchange in a specific activity and then the assumptions can be limited to

¹ Using the notation of Limpert et al. (2001), for a variable X that is lognormally distributed, the «geometric mean » that is calculated with the pedigree formula in Ciroth et al. (2013) corresponds to $\sigma^* = \exp(\sigma)$ where σ is the standard deviation of the underlying normal distribution (logX)). This value represents a measure of scale and has to be coupled with the appropriate measure of location depending on the software (e.g., in the open source brightway the mean and standard deviation of the underlying distributions should be used: [https://stats](https://stats-arrays.readthedocs.io/en/latest/#id19)[arrays.readthedocs.io/en/latest/#id19\)](https://stats-arrays.readthedocs.io/en/latest/#id19)

the share of the distribution between these values, for example uniform or triangular. The most accurate approach to estimating uncertainty is to calculate descriptive statistics on a repeated sample of values for an exchange data input. An example is provided in Table 1 below where mean and standard deviations are calculated for the $CO₂$ emission per kg product from an unspecified activity (calculation in the file: *ALIGNED-T1.4-Uncertainty-from-measurementexample-AAU.xlsx*). A disadvantage of this method is that it is difficult to apply at scale as repeated measurements for each exchange of an activity are seldom available and even more seldom are available for multiple activities in the same system.

Table 1 Example of calculating uncertainty estimates for LCA model inputs from repeated measurements.

Action: *for each exchange in the inventory, provide a measure of uncertainty. The following methods should be applied in this order (increasing order of accuracy but also increasing complexity): rough estimate, empirical estimate using min and max values, pedigree matrix, empirical estimate using repeated measurements.*

3.2. Propagating uncertainty from input data to output, tiered approach

Analytical method. To quantify the uncertainty in model output that is due to uncertainties due to data, theory of uncertainty propagation can be applied to the LCA model in analytical way, i.e. using specific equations that are well established in literature and nowadays textbook material (Harvey, David, 2019) and have also been described for LCA (Imbeault-Tétreault et al., 2013).

The complexity of the calculation depends heavily on the structure of the model. An extremely simplified case could be the one of a product system that is the sum of three activities to provide a functional unit. For each of these a pre-calculated value of climate change impact (kg CO_2 -eq)

is calculated for the amount needed. A "rough estimate" (see above) of uncertainty is given using a coefficient of variation. The uncertainty of the results is calculating using the theory of error propagation of a sum (square root of the sum of the squares of each uncertainty). The outcome is an uncertainty of 3.5% on the model output. A calculator to reproduce this is provided as separate Excel file (*ALIGNED-T1.4-Analytical-error-propagation-calculator-AAU.xlsx*).

A more complex approach using multiple input data and the sensitivity indexes, based on the work of Imbeault-Tétreault et al. (2013) is provided as a separate file (*ALIGNED-T1.4-Analyticalerror-propagation-calculator-AAU.xlsx*). The file also includes a worked example for the case of comparative assessment where the ratio of the impact of the two alternatives should be used. The advantage of the method is its simplicity. The disadvantage is that is not easily applied to larger systems, so it works poorly at scale.

Table 2 Example of calculating uncertainty estimates for LCA model outputs with the analytical method.

Stochastic method. A very popular approach to error propagation in LCA is to use stochastic error propagation such as Monte Carlo simulation. This consists in randomly sampling inputs based on information about their uncertainty (for example, the assumed or measured shape, scale and location of their distribution), calculating model outputs, and iterating the process several times.

The approach has the drawback that it creates inconsistencies in life cycle inventories because mass balances are not conserved in the random sampling procedure. Sampling strategies should always be applied exclusively to independent variables of a model, but in LCA this is not possible. This is because LCA models are usually not parameterized: the value of an exchange in an inventory dataset is static and is not calculated from the value of another exchange, e.g. the output of $CO₂$ of an activity is not calculated automatically based on the value of the reference flow of the same activity. So when these are sampled independently an inconsistency or mismatch between the two is inevitably introduced. The extent of this imbalance and whether this is a pragmatically problem remains currently poorly understood in the scientific literature in LCA, to the best of our knowledge.

The method is sufficiently practically implementable in open and commercial LCA software. Particular attention should be paid when using the stochastic error propagation in comparative context (Pizzol, 2019) – in this case a paired sampling procedure must be used to avoid overestimating the uncertainty. Additionally, in comparative context excessive amount of iterations (over 10.000) might result in forced or "hacked" significant differences between

alternatives when the two distributions of results are compared using p values from a statistical test (Heijungs, 2019).

To avoid this problem it is recommended to calculate the difference (or ration) between iterations over the simulation and then define an arbitrary but strict threshold value for such difference, e.g. 95% of iterations should show a positive difference between the two alternatives for them to be significantly different when considering the alternatives. In this type of simulations p-values should only be compared in relative terms i.e. should be only compared across alternatives in the same simulation but not across studies or simulations. See separate notebook tutorial (*ALIGNED-T1.4-Comparative-MC-tutorial-AAU.ipynb*).

Action: *for the product system under analysis, perform a quantification of the uncertainty the following methods, listed in increasing order of accuracy but also increasing complexity: analytical method using simple model structure and terminated datasets; analytical method using sensitivity indexes, stochastic error propagation method. Note that the choice of method also depends on how the uncertainty has been quantified in the previous step (lognormal uncertainties are required to apply the analytical method with sensitivity indexes and the simple analytical method requires pre-calculated datasets).*

4. Sensitivity analysis – focus on data

The most practical approach is to use OAT (One At Time) sensitivity analysis. Once a set of specific data or parameters' values is chosen, these are varied one by one and the difference in output is then compared to the difference in input using sensitivity coefficients that can be calculated in different way (Bisinella et al., 2016).

Imbeault-Tétreault et al. (2013) defines a sensitivity index *Sx,h* as the relative variation in output *h* caused by a relative variation in input *x*. While this index should be calculated using the partial derivative of impact score h according to x, in practice the LCA practitioner usually calculated it based on discrete data, as the ration between the relative difference in output and input. This is defined as "sensitivity ration" by Bisinella et al. (2016) and approximated to the value obtained using the derivatives. See an example of calculation in a separate Excel file (*ALIGNED-T1.4- Sensitivity-Ration-example-AAU.xlsx*) and in a separate notebook tutorial (*ALIGNED-T1.4-OATtutorial-AAU.ipynb*). The result is a ranking of the most sensitive parameters based on their index value, where higher value indicates higher sensitivity of the results to changes in the value of the parameter.

The limitation is that a data point or parameter might have different sensitivity on the results under different modelling assumptions. For example, the sensitivity to energy use can depend on the carbon intensity of the energy mix assumed. The sensitivity might also change depending on the values taken by of the rest of the input parameters, this is the case when there are interactions between parameters and non-linear models.

Action: *for the product system under analysis, select a list of parameters for testing sensitivity. This selection can be informed by previous experience and familiarity with the model, results from a contribution analysis, special importance for the decision maker of the study, or because they are highly uncertain (lack of knowledge) or very variable (multitude of values can be expected). Test the sensitivity of the parameters by changing their value (e.g. by 10% as in the notebook), calculating new results, and then calculating sensitivity ratios. With more time and resources available, increase the number of parameters under analysis.*

5. Uncertainty analysis – focus on model

To understand the uncertainty in the results that is due to modelling choices, the suggested approach is to use scenarios. Scenarios are intended as plausible assumptions regarding a specific model structure, for example the assumption about a constrained flow or about what activity is substituted by a co-product, or model is used to calculate characterisation factors or emissions at the end of life, or the geographical location of a supplier, or the composition of the energy mix used.

The modelling choice might affect multiple activities simultaneously in a complex way, for example the choice of allocation key (economic vs mass) or the choice of modelling approach (attributional versus consequential) or even of background system model (cut-off versus APOS versus consequential for the same ecoinvent version) are all modelling choices that affect simultaneously several activities in the product system.

In practice the analysis is performed by changing the assumption and thus the model structure according to different scenarios, and then calculate new model outputs. This can be iterated for several options, see a simplified example in the notebook on changing electricity mix (*ALIGNED-T1.4-Model-Uncertainty-tutorial-AAU.ipynb*).

Note that the use of different scenarios here is practically similar but conceptually different from doing an OAT sensitivity analysis on the modelling choice. It is practically similar because in the way it is implemented because it consists in a calculating a series of results based on different model configurations. However, since each modelling choice is a discrete choice - because either one model structure or another structure can be considered each time - the "variable" that is modified is a categorical type of variable and not a continuous one as in the case of OAT. In other words, it is the *type* of exchanges that is modified whereas in OAT the numerical *value* of an exchange is modified. The presence of a categorical variable prevents to calculate sensitivity rations on the modelling choice as in the case of OAT (previous section). The scenario analysis approach is then conceptually different from sensitivity analysis because its objective is *quantification* of uncertainty. The objective of the uncertainty analysis is to obtain a range or distribution of output values due to different modelling choices, while the objective of OAT and GSA is to obtain a measure of sensitivity of results due to the change in model structure.

Action: *for the product system under analysis identify a set of discrete modelling choices that are expected to influence results. (cf. also tables 3-7). For these, perform calculations using different scenarios, i.e. model structures obtained from different assumptions, and present results together making clear what is the quantitative difference that is due to the assumption made. A common approach is to test the sensitivity to the choice of energy mix.*

6. Sensitivity analysis – focus on model

To overcome the limitation of OAT, the only approach that can allow to investigate sensitivity to model assumptions is Global Sensitivity Analysis (GSA) (Cucurachi et al., 2016; Saltelli, 2005).

GSA is a systematic perturbation of the model, in the sense that all parameter values are changed simultaneously using a predefined sampling strategy (e.g. Morris, Hypercube latin, etc.) and the influence of each parameter on the results under varying conditions is then determined using appropriate indices of sensitivity (Delta, Sobol). This approach allows to mitigate the limits of OAT previously mentioned.

For example, calculating the average and standard deviations of the sensitivity ratios for one parameter while all the others are being modified allows to derive sensitivity indices for the parameter that take into account possible changes in model structure (Morris method).

GSA is however more complex than OAT to implement in practice in LCA and it is not feasible with commercial LCA software and had larger computational requirements the higher the number of parameters are included in the analysis, because this results in a larger number of combinations between these parameters with the need to perform a larger number of simulations. In some situations GSA might also be not strictly necessary: Kim et al. (2022) show that since several LCA models are linear or close to linear (the output is directly proportional to a change in input over the entire input space, i.e. across all possible values of all inputs) a simpler approach can be applied, i.e. using a correlation analysis.

The tiered recommendation is to first investigate qualitatively if any model assumption might change the results of OAT, and if this is found to be the case perform a simplified version doing multiple OAT on a limited set of selected critical modelling assumptions and investigate the differences in results using sensitivity ratios.

A second step can be to perform a larger simulation considering several key parameters and calculating correlation coefficients for each of those (Kim et al., 2022). Guidance for carrying out this type of analysis is provided in a separate notebook tutorial (*ALIGNED-T1.4-GSA-tutorial-corr-AAU.ipynb*).

A third and more complex but also more informative approach is to apply GSA using a predefined sampling strategy and then analysing results using corresponding sensitivity indexes. Guidance is provided in separate notebook tutorial (*ALIGNED-T1.4-GSA-tutorial-FAST-AAU.ipynb*).

It should be noted that the GSA approach described in previous sections is in fact an approach to estimate the sensitivity to the choice of parameters values when also considering the structure of the model. However, the approach does not strictly assess sensitivity to the use of different model structures and consequently to different modelling choices, and neither does assess the or consider the combination of choices made on parameter values and modelling structure. GSA and scenario analysis can in principle be coupled to address this challenge (Blanco et al., 2020) but the theoretical approach is not yet practical operational in existing software tools to consider a large numbers of modelling choices and scenarios as in common LCA practice.

Action: *for the product system under analysis identify first qualitatively whether relations of interdependence between parameters require the need for a GSA. If this is the case, identify a set of parameters that must be included in the GSA. Define sampling strategies for these parameters and perform a simulation on the different models obtained from the combination of different values for different parameters. For simpler approach use uniform distributions to sample the parameters and use correlation indices to measure the sensitivity. With more resource and skills available use specific sampling strategies and specific sensitivity indexes.*

In the following, recommendations are provided for understanding the uncertainties in the models used in the ALIGNED framework for assessment of bio-based products. These are organized according to the tasks in the Work Package 1 of the project, that loosely follow the ISO phases of LCA. For each model in the framework, indications are provided regarding uncertainties of data and model type. Additional guidance is provided that illustrates practical tools to be used in the uncertainty and sensitivity analysis of the LCA of bio-based products.

Action: *when using the approaches, methods, and tools within the aligned modelling framework, read the indications provided in the tables below before performing uncertainty and sensitivity analysis. These can e.g. guide in the choice and selection of the parameters for a sensitivity analysis as well as in the understanding of the major sources of uncertainty and consequent strategies for reduction of uncertainty where possible (e.g., via additional collection of data and checking the soundness of assumptions with specific stakeholders) or for management of uncertainty where reduction is not possible (e.g. nuancing the presentation of results by reporting on the uncertainties).*

7.1. Uncertainty in background modelling (T1.1)

Table 3 Uncertainty and sensitivity of data in modelling of prospective scenarios using IAMs within the ALIGNED framework.

7.2. Uncertainty in foreground modelling (T1.2)

7.2.1. Dynamic carbon flux model

Table 4 Uncertainty and sensitivity in modelling dynamic carbon fluxes within the ALIGNED framework.

7.2.2. Constraints to biomass availability

Table 5 Uncertainty and sensitivity in modelling constraints to biomass availability within the ALIGNED framework.

7.3. Uncertainty in Life Cycle Impact Assessment (T1.3)

Table 6 Uncertainty and sensitivity in life cycle impact assessment within the ALIGNED framework.

7.4. Uncertainty in socio-economic assessment (T1.5)

Table 7 Uncertainty and sensitivity in socio-economic assessment within the ALIGNED framework.

8. Concluding remarks

This document has provided a selection of practical approaches to handle uncertainty in the environmental assessments of bio-based products within the ALIGNED project.

Guidance was provided using a tiered approach where the approaches are listed in order of increasing accuracy but also increasing complexity in a way that each LCA practitioner can find the approach that best fits to the level of expertise possessed, and accuracy needed.

Separate tutorials and calculators in excel and python where the approached proposed are applied in practice are available in the T1.4 repository and accompany this guide.

Additionally, a qualitative assessment of the main sources of data and model uncertainty and sensitivity respectively was provided for the models and approaches within the harmonized ALIGNED framework for assessing the environmental performance of bio-based products – which is intended to ease the application of the approaches, methods, and tools in this framework as well as the understanding of the uncertainties associated with the results of these models.

The primary audience for this guide is LCA practitioners in bio-based industries and sectors – but also beyond as the techniques here illustrated can be used for LCAs in other contexts.

The final remark is that given the importance of uncertainty and sensitivity analysis for the interpretation and communication of LCA results, it is important that these analyses are performed in all LCA studies, even if not all LCA studies would require uncertainty and sensitivity analysis at the highest level of complexity.

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