Quantitative Inventory Uncertainty

It is a requirement in the *Product Standard* and a recommendation in the *Value Chain (Scope 3) Standard* that companies perform and report qualitative uncertainty. This document provides guidance for companies wishing to go beyond qualitative and quantify inventory uncertainty.

Introduction

Single parameter uncertainty arises from four types of parameters used in calculating product inventories: direct emissions data, activity data, emission factors, and global warming potential (GWP) factors. Any uncertainties from parameters used to quantify these should also be considered. An important exception to this classification is those cases where emissions are directly measured, in which case uncertainty in that measurement replaces the need to consider activity and emission factor uncertainty.

Parameter uncertainty can be represented by a probability distribution or as a range. Common distributions include, but are not limited to, the normal distribution, lognormal distribution, uniform distribution and triangular distribution[1]. For activity data and emission factor data, the log-normal distribution is often determined to be a reasonable fit. Guidance on quantifying parameter uncertainty from direct emissions data has been developed by ISO[2] and is available in the GHG Protocol's *Measurement and Estimation Uncertainty of GHG Emissions tool.* This guidance focuses on quantifying parameter uncertainty from activity data and emission factors; however, the pedigree matrix approach and many of the propagation techniques discussed below may also apply for direct emissions data.

Different approaches of quantifying single parameter uncertainty include:

- Measured uncertainty (represented by standard deviations);
- The pedigree matrix approach, based on data quality indicators (DQIs)[3];
- Default uncertainties for specific activities or sector data (reported in various literature[4]);
- Probability distributions from commercial databases;
- Uncertainty factors reported in literature; and
- Other approaches reported by literature.

Pedigree Matrix

If measured single parameter uncertainties are unknown, a pedigree matrix approach can be used to calculate uncertainties. Once the single parameter uncertainty values have been determined using this approach, the values can be propagated using techniques such as Monte Carlo simulation or Taylor Series expansion (discussed below).

In the pedigree matrix approach, the qualitative data quality assessment results (see section 9.2.8) are used to relate the data quality indicators to uncertainty ranges for individual parameters[5,6,7]. Data quality assessment results from activity data and emission factors should be translated separately; they are considered together in the propagating parameter uncertainty section.

In the pedigree matrix an uncertainty factor is assigned to each of the five data quality indicators and four data quality criteria (very good, good, fair, and poor). The uncertainty factors are used to compute the GSD^2 (the square of the geometric standard deviation). These uncertainty factors, shown in table 1, are ultimately based on expert judgment.

Table [1] Suggested pedigree matrix for determining uncertainty scaling factors based on data quality ratings

Indicator score	Very good	Good	Fair	Poor
Precision	1.00	1.10	1.20	1.50
Completeness	1.00	1.05	1.10	1.20
Temporal representativeness	1.00	1.10	1.20	1.50
Geographical representativeness	1.00	1.02	1.05	1.10
Technological representativeness	1.00	1.20	1.50	2.00

The total uncertainty, expressed as a 95% confidence interval, SD_{g95} (the square of the geometric standard deviation), is calculated using the formula shown below[8]:

$$SD_{g95} \cong \sigma^2{}_g = \exp^{\sqrt{[\ln(U_1)]^2+[\ln(U_2)]^2+[\ln(U_3)]^2+[\ln(U_4)]^2+[\ln(U_5)]^2+[\ln(U_b)]^2}}$$

where:

U_1= uncertainty factor of precision[9]
U_2= uncertainty factor of completeness
U_3= uncertainty factor of temporal representativeness
U_4= uncertainty factor of geographic representativeness
U_5= uncertainty factor of other technological representativeness
U_b= basic uncertainty factor

When not enough information is available for a particular data point to apply the data quality criteria, companies should assign a default low score (i.e., “poor”) in order to make a conservative estimate of uncertainty. Furthermore, all scores should be disclosed along with the results in order to promote transparency and ensure accountability of uncertainty analysis results. Single parameter uncertainties based on the pedigree matrix approach can be supplemented and used in combination with distributions determined through other methods.

The formula above includes a component of a “basic uncertainty factor.” This is a minimal uncertainty rating for specific process categories. It is important to note that this basic uncertainty factor may vary by process type or other factors. Table 2 suggests categories and factors for use as basic uncertainty factors, based on available information in literature sources.

Table [2] Suggested basic uncertainty factors[10]

Category of activity or emission	Suggested basic uncertainty factor
Thermal energy	1.05
Electricity	1.05
Semi-finished products	1.05
Raw materials	1.05
Transport services	2.00
Waste treatment services	1.05
Infrastructure	3.00
CO_2 emissions	1.05
Methane emissions from combustion	1.50
Methane emissions from agriculture	1.20
N_2O emissions from combustion	1.50
N_2O emissions from agriculture	1.40

Propagating parameter uncertainty

Various methods exist for propagating single parameter uncertainties in a product inventory to determine the overall parameter uncertainty, each with advantages and disadvantages. Some of these methods include Monte Carlo simulation[11,12,13], Bayesian statistics, analytical uncertainty propagation methods, calculation with intervals and fuzzy logic[14] , and Taylor series expansion. This guidance does not go into the details of these various methods but only provides a brief description of two popular methods: Taylor series expansion and Monte Carlo simulation.

Taylor series expansion

Taylor series expansion is an analytical method used to combine the uncertainty associated with individual parameters from a single scenario. The approximate squared geometric standard deviation (GSD^2) of the total product inventory result is determined as a function of the inventory result's sensitivity to each input parameter (i.e., each parameter's relative impact/influence on the total inventory result[15]) and the squared geometric standard deviation of each parameter. This Taylor series expansion method requires the assumption that the uncertainty distribution for each input parameter is log-normally distributed. Although there are limitations associated with using geometric standard deviation and assuming a lognormal distribution, its use prevents the occurrence of meaningless negative values for emission factors or characterization factors. It also accommodates factors that can vary over orders of magnitude and is more representative than a normal distribution.

The single parameter uncertainties can be used to determine the approximate uncertainty in the total inventory result based on the equation below.

$$(\ln GSD_y)^2 = S_1^2(\ln GSD_1)^2 + S_2^2(\ln GSD_2)^2 + \ldots + S_n^2(\ln GSD_n)^2$$

Where GSD_y is the geometric standard deviation of the total inventory result. GSD_1 is the geometric standard deviation of the first input (e.g., activity data or emission factor data) and S_1 is the sensitivity of the result to that factor. This equation applies when all input parameters are independent, otherwise covariance must also be considered. If this equation is applied to inputs that are correlated – even if they have independent activity values - then the uncertainty results will be overestimated. Most scenarios will have some degree of covariance and uncertainty will be overestimated, however, this is more favorable than underestimation.

Monte Carlo simulation

Monte Carlo simulation is a well-known form of random sampling used for uncertainty analysis and is a commonly used tool in commercial life cycle assessment software. In order to perform Monte Carlo simulation, input parameters (e.g., direct emissions data, activity data, or emission factors) must be specified as uncertainty distributions. The input parameters are varied at random, but restricted by the given uncertainty distributions. The randomly selected values from all the parameter uncertainty distributions are inserted into the emission calculations. Repeated calculations produce a distribution of the predicted result values, reflecting the combined uncertainty of the individual parameters.[16]

Box [1] Uncertainty and comparisons

The *Product Standard* does not support claims based on comparisons of products without additional specification such as product rules. Nevertheless, there may be valid instances where a comparison is made under the standard, such as in the case of evaluating the amount of improvement achieved by changes in a product or process for purposes of performance tracking. In cases where a comparative - rather than absolute - result is of interest, methods exist to evaluate the uncertainty of a comparative finding. For those applying a Taylor series approach, Hong et al. explain a method for making such an evaluation[18]. This method removes the uncertainty from parameters that are shared between the two scenarios. For those applying a Monte Carlo approach, most software can be configured to provide the uncertainty of a comparison.

Reporting quantitative uncertainty

Quantitative uncertainty can be reported in many ways, including qualitative descriptions of uncertainty source as well as quantitative depictions, such as error bars, histograms, etc. Although various methods and tools exist to address individual types of uncertainty, it is impossible to represent a true measure of total combined uncertainty in a single, consistent way. Nonetheless, it is useful to provide as complete a disclosure of uncertainty information as possible. Users of the information may then weigh the total set of information provided in judging their confidence in the information. The following provides a detailed example of calculating and reporting quantitative uncertainty.

[Example] Uncertainty assessment reporting

A product inventory has been created for a toner cartridge. The functional unit is the printing of 50,000 black-and-white pages, and the inventory result is 155 kg CO_2e per functional unit. The following sections describe an uncertainty assessment associated with this inventory.

Summary of sources of uncertainty

Table 3 lists (1) sources of uncertainty identified in compiling the product inventory and (2) a qualitative description of the anticipated importance of each area of uncertainty. Uncertainties chosen for scenario analysis (included below) are shown in italics.

Table [1] Sources and descriptions of uncertainty compiled throughout GHG inventory

Uncertainty type	Uncertainty source	Description	Importance
Parameter uncertainty	Toner cartridge resin production emission factor	Poor temporal and geographical representativeness	Moderate; cartridge resin is not a large emissions contributor
	Printer electricity activity data	Source: Electricity use is taken from an older model	Moderate; electricity use is important, but difference in models is expected to be small
Methodological uncertainty	*Choice of grid mix*	Choice has been made to use a the US national electricity grid mix	High; electricity use is important in the result and variation among and within countries is large
	Functional unit choice	Number of pages printed is chosen as the functional unit rather than area of ink printed	Low; within the assumption made for ink/page, little difference would be expected
Situational uncertainty	*User recycling behavior*	Some users may recycle more or less cartridges than the average	Moderate; influence of recycling is a small but not insignificant contributor
	Page yield variation[17]	Some users experience more or less pages printed per cartridge	Moderate; could affect electricity use or paper use, which are important factors
Model uncertainty	Electricity production	It is difficult or impossible to know the exact mix of production technologies supplying electricity to the printers	Moderate; electricity production is important, but the variation from the assumed production is expected to be relatively minor.

Summary of GHG inventory components and contributions

Table 4 summarizes the components of the GHG inventory, the activity and emission factor data used, and the percent of the total result contributed by each of the listed materials or processes.

Table [2] Summary of GHG inventory

Inventory category name	Emission factor geographic representativeness	Emission factor temporal representativeness	Unit	Technology type	Total GHG factor (kg CO_2e/unit)	Activity data	GHG total	Percent of total inventory
Electricity, manufacturing	US	Within 2 years	kWh	Electricity	0.84	30.0	25	16%
Electricity, assembly	US	Within 2 years	kWh	Electricity	0.84	10.0	8.4	5%
Electricity, use	US	Within 2 years	kWh	Electricity	0.84	63	53	34%
Heavy truck	RER	Within 2 years	tkm	Transport services	0.13	2.8	0.35	<1%
Aluminum	RER	Within 10 years	kg	Industrial products	12	0.077	0.94	1%
Copper	GLO	Within 10 years	kg	Industrial products	3.5	0.001	0.002	<1%
Steel	RER	Within 10 years	kg	Industrial products	5.2	0.39	2.0	1%
Polystyrene	RER	Within 10 years	kg	Industrial products	3.5	0.45	1.6	1%
Nylon	RER	Within 10 years	kg	Industrial products	9.2	0.028	0.26	<1%
PVC	RER	Within 10 years	kg	Industrial products	4.6	0.006	0.029	<1%
Polyurethane	RER	Within 10 years	kg	Industrial products	4.8	0.020	0.095	<1%
Corrugated board	RER	Within 10 years	kg	Agricultural products	1.4	0.48	0.66	<1%
Paper, packaging	RER	Within 10 years	kg	Agricultural products	1.3	0.024	0.031	<1%
LDPE	RER	Within 10 years	kg	Industrial products	2.1	0.026	0.055	<1%
Paper, use	RER	Within 10 years	kg	Agricultural products	1.3	50	63	41%
Total							**155**	

Data quality ratings and quantification of parameter uncertainty

The data sources listed in table 4 are assessed for their data quality based on the criteria recommended the GHG Protocol *Scope 3* and *Product Standards*. These data quality ratings are used to approximate an uncertainty range. The chosen data quality ratings and the resulting standard deviations are shown in table 5.[18] Uncertainty can be reported as GSD, minimum and maximum, confidence intervals, etc[20].

Table [3] Summary of data quality ratings and the resulting standard deviations

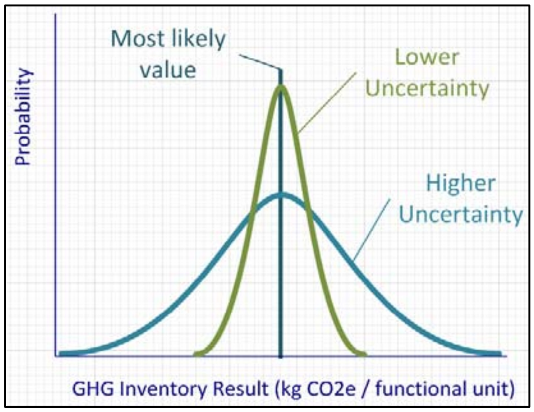
Inventory category name	Activity data precision	Activity data completeness	Activity data temporal representativeness	Activity data geographical representativeness	Activity data technological representativeness	Activity data GSD	Emission factor data precision	Emission factor data completeness	Emission factor data temporal representativeness	Emission factor data geographic Representativeness	Emission factor technological representativeness	Emission factor GSD	GWP GSD	Contribution to total uncertainty	Percent of total uncertainty contribution
Electricity, manufacturing	Fair	Poor	Good	Poor	Fair	1.28	Fair	Good	Poor	Fair	Fair	1.36	1.01	0.004	2.79%
Electricity, assembly	Poor	Poor	Good	Fair	Very good	1.26	Fair	Fair	Poor	Fair	Fair	1.36	1.01	0.0004	0.29%
Electricity, use	Fair	Very good	Fair	Poor	Poor	1.45	Poor	Poor	Poor	Poor	Poor	1.59	1.01	0.04	28.03%
Heavy truck	Fair	Poor	Good	Poor	Poor	1.67	Poor	Fair	Poor	Poor	Poor	1.77	1.16	3 E-06	0.00%
Aluminum	Poor	Poor	Good	Poor	Poor	1.52	Fair	Fair	Good	Poor	Good	1.17	1.16	8 E-06	0.01%
Copper	Good	Good	Good	Poor	Very good	1.09	Very good	Good	Good	Fair	Good	1.12	1.16	6 E-12	0.00%
Steel	Poor	Poor	Good	Fair	Fair	1.36	Very good	Good	Good	Fair	Good	1.12	1.16	2 E-05	0.01%
Polystyrene	Fair	Very good	Good	Poor	Poor	1.44	Poor	Poor	Fair	Poor	Poor	1.53	1.16	3 E-05	0.02%
Nylon	Poor	Poor	Good	Poor	Poor	1.52	Fair	Fair	Fair	Fair	Fair	1.28	1.16	7 E-07	0.00%
PVC	Fair	Good	Fair	Good	Very good	1.14	Poor	Good	Poor	Good	Very good	1.34	1.16	4 E-09	0.00%
Polyurethane	Poor	Poor	Fair	Fair	Fair	1.37	Fair	Poor	Poor	Poor	Fair	1.38	1.16	8 E-08	0.00%
Corrugated board	Fair	Poor	Fair	Good	Fair	1.54	Very good	Very good	Good	Very good	Good	1.44	1.16	6 E-06	0.00%
Paper, packaging	Poor	Poor	Fair	Fair	Fair	1.6	Fair	Poor	Very good	Poor	Good	1.47	1.16	1 E-08	0.00%
LDPE	Fair	Poor	Good	Poor	Poor	1.46	Good	Good	Good	Good	Good	1.13	1.16	2 E-08	0.00%
Paper, use	Fair	Good	Good	Fair	Poor	1.65	Poor	Fair	Poor	Poor	Poor	1.77	1.16	0.1	68.83%
												Total GSD^2		0.14	100 %

Using the calculated GSDs and the sensitivities/contributions of each inventory category to the total results, the Taylor series expansion method is applied to estimate the propagated parameter uncertainty of the product inventory result.

Reporting parameter uncertainty

Parameter uncertainty can be presented as a probability density function, such as the familiar normal curve (or with one of many other distributions that might be chosen). The shape of the representation depends upon the distribution type used to represent it, and the width of the distribution reflects the relative magnitude of the uncertainty. A distribution example is shown below in figure 1.

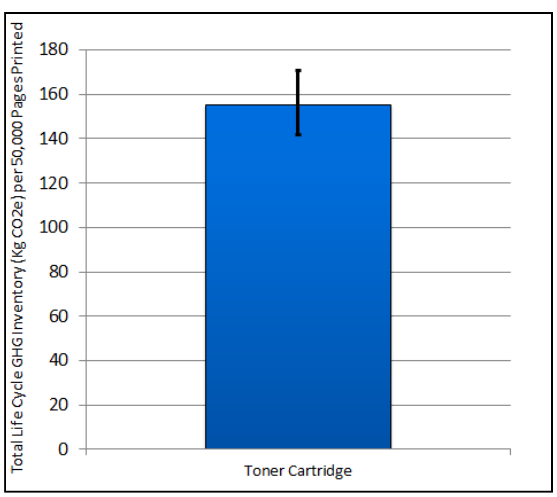
Figure [1] Example of parameter uncertainty distribution



Another convenient means of representing parameter uncertainty is with the use of "error bars," which can be used to depict, for example, the 95 percent confidence limit of the value in question. It is important when using error bars to identify the confidence interval that is represented.

Using the toner cartridge example, the inventory results are presented in Figure 2. The column (blue bar) is the inventory result of 155 kg CO_2e per functional unit, and the uncertainty is represented by the error bar (-15 and +15 kg CO_2e). Combined, these result in a range of inventory result values of 141 to 170 kg CO_2e.

Figure [2] Impact assessment results of toner cartridge GHG inventory study

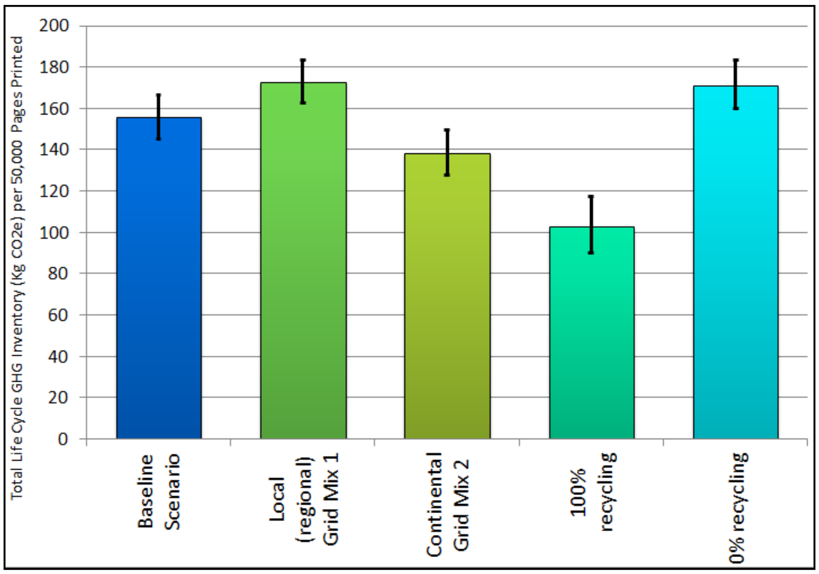


Scenario uncertainty assessment and reporting

In this example scenario assessment is performed on two of the areas identified as potentially important sources of scenario uncertainty. These include the choice of electrical grid mix (where both a more localized grid mix and a continental grid mix have been tested as replacements for the national grid mix assumed in the initial inventory) and the use of the national average of 40 percent plastic recycling (where both the case of no recycling and 100 percent recycling have been tested as the extreme cases of toner cartridge use by an individual).

Scenario uncertainty is most appropriate to show as separate values on a chart. A variety of chart types could be used for such a purpose; one example, a histogram, is shown in figure 3.

Figure [3] Scenario uncertainty assessment shown with parameter uncertainty



Conclusion

The uncertainty assessment provides a perspective on the relative confidence report readers can have in the inventory results. In this example, parameter uncertainties combine to provide an interval of approximately +/- 15 CO_2e surrounding the inventory results value of 155 $kgCO_2e$ per functional unit. The impact of the user's recycling behavior is shown to be important for the toner cartridge, with users who do recycle most or all materials (cartridge and paper) having a substantially lesser impact than those that recycle very little. Due to these variations, individual users of the cartridge may produce very different emission totals than that shown in the inventory results. This example shows the importance of providing uncertainty information with the product inventory results to inform report readers of how to interpret the results.

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[1] For further discussion or the use of these distributions in LCA, see Heijungs, 2004, *A Review of Approaches to Treat Uncertainty in LCA* and for detail of additional distributions, see Lloyd, SM, 2007, *Characterizing, Propagating, and Analyzing Uncertainty in Life-Cycle Assessment*

[2] Guide to the Expression of Uncertainty in Measurement

[3] See data collection and quality chapter in the *Product Standard*

[4] Shannon M. Lloyd and Robert Ries, 2007.Characterizing, propagating, and analyzing uncertainty in Life-Cycle Assessment: a survey of quantitative approaches. Journal of Industrial Ecology 11 (1) :161-179

[5] Bo Pedersen Weidema, B.P. and Wesnaes, M.S., 1996. Data quality management of life cycle inventories-an example of using data quality indicators. J. Cleaner Prod. Vol. 4, No. 3-1, pp. 167-174
[6] Weidema, B.P., 1998. Multi-user test of the data quality matrix for product life cycle inventory data. Int. J. LCA3 (5) 259-265
[7] Data quality guidelines for the ecoinvent database version 3.0
[8] Overview and Methodology for Ecoinvent data v2.0 (2007)
[9] These terms are defined in the data quality section above.
[10] Adapted from Ecoinvent report No.1 Overview And Methodology (Data v2.0, 2007)
[11] Ibid.
[12] Lo, S.-C.; Ma, H.-W.; Lo, S.-L., (2005) Quantifying and reducing uncertainty in life cycle assessment using the Bayesian Monte Carlo method, Science of Total Environment 340 (1-3) 23-33
[13] Sonneman, G.W., M. Schuhmacher, and F. Castells. Uncertainty assessment by a Monte Carlo simulation in a life cycle inventory of electricity produced by a waste incinerator. *Journal of Cleaner Production* 11 (2003), 279-292.
[14] Tan, R.R., 2008. Using fuzzy numbers to propagate uncertainty in matrix-based LCI. Int. J Life Cycle Assess (2008) 13:585–592
[15] Sensitivity is defined as the percent response of the output to input modifications. This is the same as a percent contribution. When the parameter considered is a process, the sensitivity is simply the percentage of total impact contributed by that particular process, which can easily be calculated. For example, if a given process is responsible for 7% of the total GWP of the product system, its sensitivity (S) is 0.07.
[16] Huijbregts, M.A.J. (1998), Application of uncertainty and variability in LCA. Part 1: a general framework for the analysis of uncertainty and variability in life cycle assessment. Int. J. LCA 3(5):273-280
[18] Hong, et al., 2010. Analytical uncertainty propogation in life cycle inventory and impact assessment: application to an automobile front panel. Int. J. LCA (15) 499-510
[19] This falls under situational uncertainty because the page yield may vary depending on the usage variations of the printer. For example, User A may use the printer to print pictures, and User B may use it for reports. The page yield for these different functions can vary significantly.
[20] Note that the uncertainty of the global warming potential (GWP) for the six GHG Protocol gasses is assumed to be ± 35% for the 90% confidence interval (see Section 7.2).
[21] To calculate an approximate geometric 95% confidence interval, the minimum (or 2.5th percentile) is calculated as the mean (total impact) divided by the GSD^2, and the maximum (or 97.5th percentile) is calculated as the mean multiplied by the GSD^2.