# Pre-calculated LCIs with uncertainties revisited

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We thank Reinout Heijungs, Patrik Henriksson, and Jeroen Guinée for their comments to our recent paper, *What distribution function do life cycle inventories follow?* (Qin and Suh 2016). Referring to their recent publication (Henriksson et al 2015), the authors rightly pointed out that dependent sampling is necessary when comparing two product systems in a Life Cycle Assessment (LCA) study (Heijungs et al 2017). We very much agree with the authors on this point. The authors further argued that using the pre-calculated geometric standard deviations (GSDs) that we derived for the Ecoinvent database "will lead to a large overestimation of the uncertainty of the results of comparative LCA". This statement was, however, unsubstantiated by the authors.

In this response, first, we discuss whether the use of pre-calculated GSDs in a comparative setting constitutes independent sampling that the authors criticized. Second, we show why the problem of independent sampling arises not only in comparative LCAs but also in a non-comparative context. Third, we empirically test whether the use of pre-calculated GSDs leads to a "large overestimation" of uncertainty in the results, and if so by how much. To our understanding, this issue has not been previously reported in the literature.

**Dependent sampling in Qin and Suh (2016)**

Would the use of pre-calculated GSDs for a comparative LCA constitute fully independent sampling? The GSDs were calculated in Qin and Suh (2016) using fully *dependent* sampling. For each perturbation, LCIs for all processes were obtained simultaneously, which was repeated for 1,000 times to estimate the distribution function of each elementary flow of each process for the entire Ecoinvent database (Qin and Suh 2016). Therefore, all LCIs obtained in each round of perturbation are all fully *dependently* sampled. The use of pre-calculated GSDs based on fully dependent sampling in Qin and Suh (2016), however, may constitute *partially* independent sampling, the extent of which depends on how the pre-calculated LCI data is used. Here we examine three use cases of pre-calculated LCI data.

**Use case 1.** Suppose that an LCA practitioner is using pre-calculated GSDs for a direct comparison between pre-calculated LCIs (Figure 1 (a)). The oval background shows the boundary within which all the parameters are fully dependently sampled when deriving pre-calculated GSDs. In this case, LCA practitioners can simply use the pre-calculated GSDs for analyzing uncertainties when comparing A and B (Figure 1 (b)), and there is no independent sampling problem.

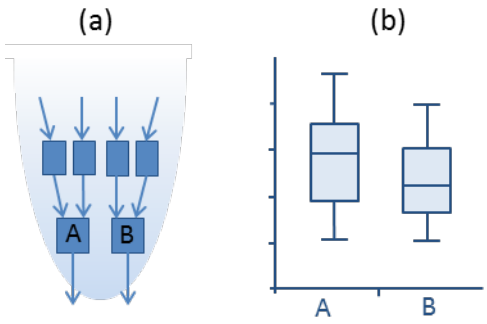


Figure 1. (a) A comparison between pre-calculated LCIs of A and B. Oval background indicates the boundary of fully dependent sampling. (b) Boxplot displaying the range of an elementary flow using pre-calculated GSDs.

However, Use case 1 is not the most typical application of pre-calculated LCI databases.

**Why dependence matters even in a non-comparative context**

**Use case 2.** A more common application of pre-calculated LCI databases is to use pre-calculated LCIs for the direct inputs to the foreground process of a product system under study. Figure 2 (a) illustrates this use case. Processes A and B are the unit processes in a pre-calculated LCI database, and one of the unit processes in the database, process C supplies its output to both A and B. Both A and B are used by the foreground process, P1. By using pre-calculated GSDs, the direct emission intensities (i.e., emission per unit output) and direct input intensities (i.e., direct input per unit output) of C are *independently* sampled *between* A and B, although they are fully *dependently* sampled *within* each (as indicated by the oval background) (Figure 2 (a)). But in reality, the same process C is used for both A and B, and therefore the parameters around it should be *dependently* sampled as shown in Figure 2 (b). Otherwise, the Monte Carlo simulation (MSC) results may misrepresent the uncertainty of the product system under study (Henriksson et al 2015). It is important to note that independent sampling problem is present in the case shown in Figure 2 (a), even if the study is not in a comparative context.

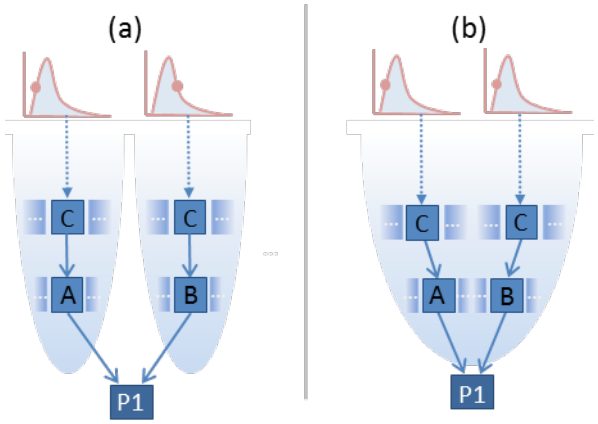

Figure 2. Non-comparative LCA involving two processes, A and B drawn from an LCI database. (a) partially independent sampling and (b) fully dependent sampling. Oval background indicates the boundary of fully dependent sampling.

**Difference between GSDs from partially independent and fully dependent sampling**

How large the magnitude of overestimation in the GSDs of resulting LCI would be when partially independent sampling (Figure 2 (a)) is used instead of fully dependent sampling (Figure 2 (b))? Given that the answer to this question would vary case by case, it can be best answered in statistical terms. We conducted an empirical test for a sample of about 186,900 data points—1,869 elementary flows by 100 randomly selected Ecoinvent unit processes—to answer this question. A fuller analysis involving 1,000 unit processes is underway and will be reported under a separate paper.

We compared (1) the GSDs in the LCI results using partially independent sampling (PIS) (Figure 2 (a)), where values are sampled fully dependently within each input to P1, but not between them, and (2) those using fully dependent sampling (FDS) for both inputs (Figure 2 (b)). In other words, under PIS the *k*th iteration of MCS for the LCI vector of product system *j* was calculated by:

$$LCI_j^{PIS,k} = \sum_i (LCI_{i,j} + \delta LCI_{i,j}^k) + (B_j + \delta B_j^k) \quad (1)$$

$LCI_{i,j}$ is the LCI vector of input *i* to *j*, and $\delta LCI_{i,j}^k$ is the *k*th perturbation to $LCI_{i,j}$ drawn from pre-calculated GSDs. Likewise, $B_j$ is the vector of direct elementary flow for a unit of output *j*, and $\delta B_j^k$ is its *k*th perturbation. In this case $\delta LCI_{i,j}^k$ is drawn independently over *i*.

Alternatively, *k*th iteration of the LCI vector is calculated under FDS by (see Qin and Suh 2016):

$$LCI_j^{FDS,k} = \left[ (B + \delta B^k)(A + \delta A^k)^{-1} \right]_j \quad (2)$$

Now, we can empirically test the argument by the authors that the use of the pre-calculated GSDs that we derived "will lead to a large overestimation of the uncertainty of the results of comparative LCA". Before discussing what is large or small, let's first test whether it leads to an overestimation. The hypothesis that the use of pre-calculated GSDs overestimates the uncertainty is accepted when $E\left(GSD^{FDS}/GSD^{PIS}\right) < 1$ is statistically significant.

Figure 3 shows the distribution of the 186,900 data points each showing the ratio, $GSD^{FDS}/GSD^{PIS}$ for all elements in the randomly selected 100 LCIs in Ecoinvent. The mean value of the ratios in our results was 1.069. To test whether the resulting ratios, $GSD^{FDS}/GSD^{PIS}$ are significantly above 1, we further conducted a t-test. The *p*-value of the t-test was below 2.2e-16, meaning that the sample values are significantly above 1 in a statistical term. The confidence interval of the ratios ranged from 1.0681 to

1.0696 at the 95% confidence level. Therefore, the hypothesis that there is an overestimation of uncertainty in PIS, not to mention "large" overestimation, is rejected. Instead, the result indicates that the use of pre-calculated GSDs leads to an underestimation of uncertainty.

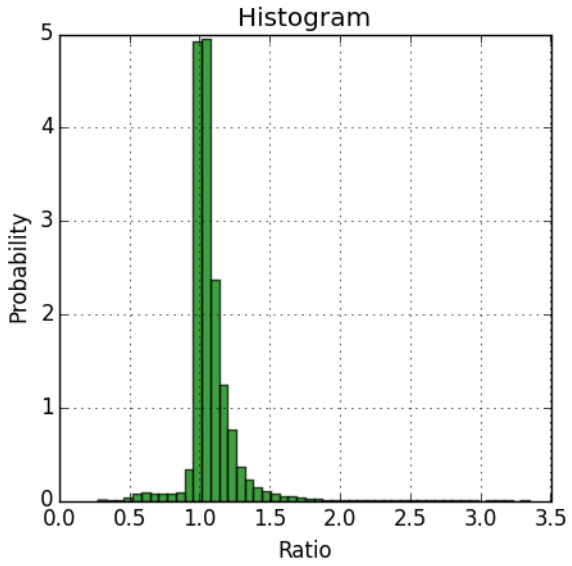


Figure 3: Histogram of the ratio, $GSD_{LCI_{i,j}^{FDS}} / GSD_{LCI_{i,j}^{PIS}}$.

Furthermore, our results show that GSDs in LCIs from partially independent sampling display meaningful but small difference as compared to those from fully dependent sampling: an average of 6.9% difference between $GSD^{FDS}$ and $GSD^{PIS}$. This also means that in the absence of any better data or the necessary resources to conduct a full MCS using FDS, 1.069 is a good rule-of-thumb scaling factor to convert $GSD^{PIS}$ to $GSD^{FDS}$, as discussed in the next section.

**Different level of dependency in comparative LCA**

**Use case 3**. Suppose that two product systems are being compared, where on-site data are collected for the foreground processes, and all the upstream data come from pre-calculated LCI databases.

In this case, we are comparing two product systems, P1 and P2. Figure 4 (a) shows the case of using pre-calculated GSDs for each input to each product system (inter-input independence + inter-product system independence, or III+IPI). In this case, the pre-calculated GSDs for an MCS will draw the direct input and output intensities of C independently between the inputs A and B *and* between the product systems P1 and P2. In other words, there will be four independent samplings performed in Figure 4 (a) as indicated by the four background ovals that show the boundary of fully dependent sampling. Note that the structure of dependency within each product system in Figure 4 (a) is the same as that in Figure 2 (a).

Figure 4 (b) shows the case of using FDS within each product system but *not* between them (inter-input dependence + inter-product system independence, or IID+IPI). Note also that each product system in Figure 4 (b) is structured in the same way as Figure 2 (b). This means that in the absence of any better

information, one can scale the GSDs calculated under III+IPI (Figure 4 (a)) to the GSDs under IID+IPI (Figure 4 (b)) by applying the scaling factor, 1.069 (see section 3). I.e.,

$$GSD^{IID+IPI} \approx 1.069 \times GSD^{III+IPI} \quad (3)$$

Finally, Figure 4 (c) shows the case of using FDS between the processes A and B *and* between the product systems P1 and P2 (inter-input dependence + inter-product system dependence, or IID+IPD). Basically all values in the two product systems are calculated using FDS. In the absence of any better information, again, the conversion of GSDs calculated based on the dependency structure shown in Figure 4 (b) ($GSD^{IID+IPI}$) to those based on fully dependent sampling shown in Figure 4 (c) ($GSD^{IID+IPD}$) can be done by applying the scaling factor, 1.069 to $GSD^{IID+IPI}$. In the same vein, in the absence of any better options available, $GSDs^{III+IPI}$ (Figure 4 (a)) can be converted into $GSDs^{IID+IPD}$ (Figure 4 (c)) such that:

$$GSD^{IID+IPD} \approx 1.069 \times GSD^{IID+IPI} \approx 1.069 \times 1.069 \times GSD^{III+IPI} = 1.14 \times GSD^{III+IPI} \quad (4)$$

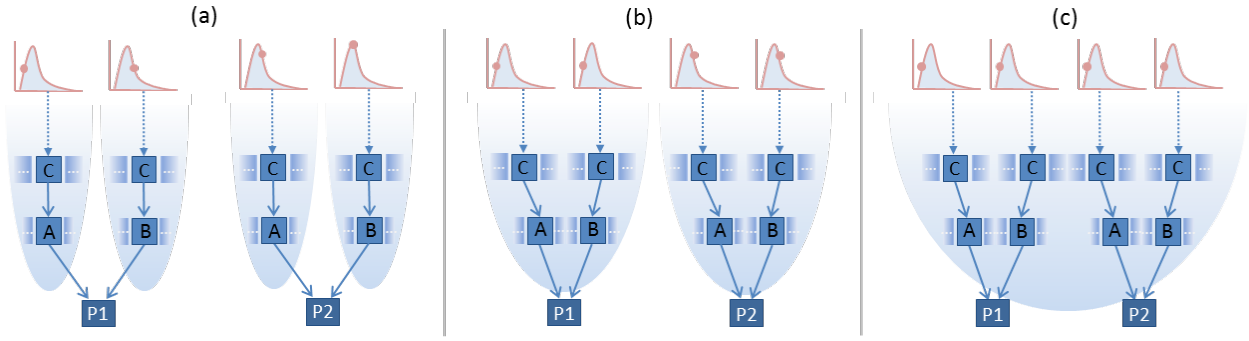


Figure 4. Comparative LCA involving two processes, A and B, which are drawn from an LCI database. (a) Partially independent sampling (III+IPI), (b) dependent sampling within each product system, independent sampling between product systems (IID+IPI), and (c) fully dependent sampling (IID+IPD). Oval background indicates the boundary of fully dependent sampling.

**Discussion**

Heijungs and colleagues' commentary, *Pre-calculated LCI systems with uncertainties cannot be used in comparative LCA* to our previous paper (Qin and Suh, 2016) argued that the use of pre-calculated LCIs raises the problem of independent sampling and overestimates the uncertainty. In this response, we show that the problem of independent sampling arises even in a non-comparative setting. We also clarify that the use of pre-calculated LCIs and corresponding GSDs constitutes a partially independent sampling not fully independent sampling. We further tested the difference in uncertainty estimates between fully dependent sampling and partially independent sampling, and our preliminary results indicate that GSDs from partially independent sampling (the use of pre-calculated LCIs) are pretty close to those from fully dependent sampling (6.9% difference in GSDs on average), although the difference was statistically significant. Furthermore, our preliminary results show that the use of pre-calculated LCIs and associated GSDs leads to a slight underestimation, not overestimation, of GSDs. Given that the distribution of the

ratios between the GSDs from fully dependent sampling and those from partially independent sampling are very dense with confidence interval of the ratio between them range from 1.0681 to 1.0696 at the 95% confidence level, we suggest that the GSDs from pre-calculated LCIs can be scaled up by multiplying 1.069 to gauge the magnitude of GSDs under fully dependent sampling in the absence of any better information or resources to conduct a full MCS.

The reason why fully dependent sampling returns higher uncertainty than partially independent sampling is not yet fully understood, but we speculate that it could be due to the cancelation effect of the changes in simulated direct input and output intensities when they are sampled independently. In PIS, as illustrated in Figure 2 (a), the randomly simulated values of unit process C used by processes A and B may move in the opposite directions often canceling their effects and keeping the results in a closer proximity to the average. In other words, partially independent sampling often counteracts the changes to each other and brings the results closer to the center of the distribution.

The current result is limited by the sample size, and therefore we call for a caution in using the results for decision support. We are currently conducting the same test for a larger sample, and the results will be reported separately.

Uncertainty characterization is an important issue in LCA, while due to the growing size of LCA databases, fully dependent sampling for MCS, despite its theoretical favorability, is often a challenge to lay users. In the absence of necessary computational resources, we believe that pre-calculated LCIs and associated GSDs can be used as a proxy in understanding the uncertainty and variability in the results as described in the previous section of this response. Otherwise, the alternative is no uncertainty analysis for those who have no access to necessary computational resources, which is certainly not preferable.

It is also important to note that under the current practice, uncertainty analysis itself is a highly uncertain process. Derivation of GSDs for unit process data is subject to a large uncertainty to begin with. The results of uncertainty analysis, therefore, should be interpreted cautiously taking the underlying uncertainties in GSDs and other systemic uncertainties that are not captured in GSDs into account. Given the situation, the magnitude of differences between GSDs from pre-calculated values and full-scale MCS should not prevent LCA practitioners from using pre-calculated GSDs when no better option is reasonably practicable.

Again, we appreciate Heijungs and colleagues for their comments. We hope that the uncertainty characterization could become easier and faster with the pre-calculated GSDs, so that uncertainty analysis becomes a standard in LCA studies in the future.

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**Reference**

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