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Uncertainties in LCA (Subject editor: Andreas Ciroth)

Using Standard Statistics to Consider Uncertainty in Industry-Based Life Cycle Inventory Databases

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Abstract

Goal, Scope and Background. Decision-makers demand information about the range of possible outcomes of their actions. Therefore, for developing Life Cycle Assessment (LCA) as a decision-making tool, Life Cycle Inventory (LCI) databases should provide uncertainty information. Approaches for incorporating uncertainty should be selected properly contingent upon the characteristics of the LCI database. For example, in industry-based LCI databases where large amounts of up-to-date process data are collected, statistical methods might be useful for quantifying the uncertainties. However, in practice, there is still a lack of knowledge as to what statistical methods are most effective for obtaining the required parameters. Another concern from the industry's perspective is the confidentiality of the process data. The aim of this paper is to propose a procedure for incorporating uncertainty information with statistical methods in industry-based LCI databases, which at the same time preserves the confidentiality of individual data.

Methods. The proposed procedure for taking uncertainty in industry-based databases into account has two components: continuous probability distributions fitted to scattering unit process data, and rank order correlation coefficients between inventory flows. The type of probability distribution is selected using statistical methods such as goodness-of-fit statistics or experience based approaches. Parameters of probability distributions are estimated using maximum likelihood estimation. Rank order correlation coefficients are calculated for inventory items in order to preserve data interdependencies. Such probability distributions and rank order correlation coefficients may be used in Monte Carlo simulations in order to quantify uncertainties in LCA results as probability distribution.

Results and Discussion. A case study is performed on the technology selection of polyethylene terephthalate (PET) chemical recycling systems. Three processes are evaluated based on CO_2 reduction compared to the conventional incineration technology. To illustrate the application of the proposed procedure, assumptions were made about the uncertainty of LCI flows. The application of the probability distributions and the rank order correlation coefficient is shown, and a sensitivity analysis is performed. A potential use of the results of the hypothetical case study is discussed.

Conclusion and Outlook. The case study illustrates how the uncertainty information in LCI databases may be used in LCA. Since the actual scattering unit process data were not available for the case study, the uncertainty distribution of the LCA result is hypothetical. However, the merit of adopting the proposed procedure has been illustrated: more informed decision-making becomes possible, basing the decisions on the significance of the LCA results. With this illustration, the authors hope to encourage both database developers and data suppliers to incorporate uncertainty information in LCI databases.

Keywords: Decision making; Life Cycle Inventory (LCI) databases; Maximum Likelihood Estimation (MLE) method; Monte Carlo simulation; PET chemical recycling; rank order correlation coefficient; statistics; uncertainty analysis

Introduction

New Life Cycle Inventory (LCI) and Life Cycle Assessment (LCA) databases, such as the ecoinvent database [1,2] from Switzerland or JLCA-LCA database [3,4] from Japan, have recently been published. Covering a wide range of industry, representative unit process data on a national level (e.g. whole Japan) or regional level (e.g. Europe) have become available. In this paper, the term unit process data refers to the amount of input and output flow to produce a unit amount of product in an industrial process step. Concerning the uncertainty of unit process data, the ecoinvent database provides probability distributions of inventory data for most of the processes while the current version of the JLCA-LCA database does not include uncertainty information. Approaches for incorporating uncertainty should be selected appropriately because data development procedure is different from database to database. In ecoinvent database, for example, literature is the major basis. Therefore, the reliability of source data itself or inequality in scope between source data and the database (e.g. temporal or geographical gaps) is likely the major source of uncertainty. For this reason, in literature-based LCI databases, approaches that can quantify qualitative sources of uncertainty, such as the Pedigree Matrix approach [5], are important. Conversely, in industry-based LCI databases, up-to-date process data is often available and statistical methods might come into play. For the JLCA-LCA database, major industrial associations collect the most current gate-to-gate data from member companies and process their own data statistically with a critical review according to a guidance manual supplied by the database developer, JLCA. Each association reports unit process data,

averaged over factories, to the database developer. Individual unit process data and copyrights of the data remain with the corresponding industrial associations. Thus, statistical data treatment is left up to the individual association.

For the JLCA-LCA database, the developer has attempted to represent uncertainty by minimum and maximum values: the guidance manual asks each industry association to report minimum and maximum values of unit process data among comparable factories. However, this procedure has two major problems. One is that the deviation of the original distribution is not retrieved. For example, when very small or large values are minimum or maximum values, while most of the data points are centralized near mean value, such deviation cannot be reconstructed later. Another concern is that interdependencies of unit process data are not considered. Although industry associations have a large number of data points at their disposal, information such as deviation and interdependencies are lost in the current procedure. Another aspect in regard to industry data intensive databases is the confidentiality of the data. It is very important for industry that the bare industrial data is not published, but masked in the database. For example, experts in competing companies may detect which technology is involved in the other companies merely through anonymous data. As a result, in the case of the JLCA-LCA database, industrial associations have not, thus far, reported minimum and maximum values, since they are optional.

In order to palliate these shortcomings, we propose a data treatment procedure for industry-based LCI databases. The main aim of this article is to clarify (a) which statistical parameters should be obtained and (b) how classical statistics should be used to derive these parameters in industry-based LCI databases. This method also preserves the confidentiality of the individual data. Continuous probability distributions are fitted to the scattering individual unit process data. Correlation coefficients are used to represent interdependencies. The unit process data is described by probability distributions and correlation coefficients, which can be directly used in Monte Carlo simulations for overall LCI and LCA calculations. In a case study involving polyethylene terephthalate (PET) chemical recycling systems, we show how the presented uncertainty information can be used in LCA, thereby contributing to more informed decision-making.

1 Procedure for Considering Uncertainty in LCI Databases

1.1 Conventional method of reporting deterministic data in LCI databases

Fig. 1 illustrates a hypothetical situation in which an 'overall unit process model' is created. This model includes factories producing the same product in the scope or the corresponding region of the LCI database. This activity corresponds to the aggregating phase in the PHASETS (PHASES in the design of a model of a Technical System) procedure proposed by Carlson and Pålsson [6], where the same technical system is averaged. 'Individual factory data' is assumed to be obtained as raw material A_i [t/yr], utility input B_i [kWh/yr] and product output P_i [t/yr] for factory i. A linear relation is assumed between input and output flows (**Eq. 1**):

$$A_i = X_i P_i, \quad B_i = Y_i P_i \tag{1}$$

The value of the parameters X_i and Y_i can be scattering over factories. Hanssen and Asbjørnsen have shown such different unit process data from 26 pulp production sites in Sweden [7]. Huijbregts discussed and categorized sources of such uncertainty [8]. Ciroth et al. further discussed the relationship between geographical and technological differences in unit process data [9]. In this paper, the sources of the scattering are not discussed further. The focus lies in the data treatment after obtaining scattering industrial data.

One common way to determine X and Y, the parameters of the 'overall unit process model', is to use weighted averages based on the market share, as displayed in **Eq. 2**.

$$X = \mu_X = \sum_{i=1}^{n} w_i X_i, \quad Y = \mu_Y = \sum_{i=1}^{n} w_i Y_i, \quad w_i = \frac{P_i}{\sum_{i=1}^{n} P_i} \tag{2}$$

where w_i is the market share of factory i to the whole production amount, and n is the number of factories inside the database scope. This approach is often followed in conventional LCI databases. Information of scattering data is obviously lost. Ideally, the parameter X, for example, can be presented as a discrete function using the individual values

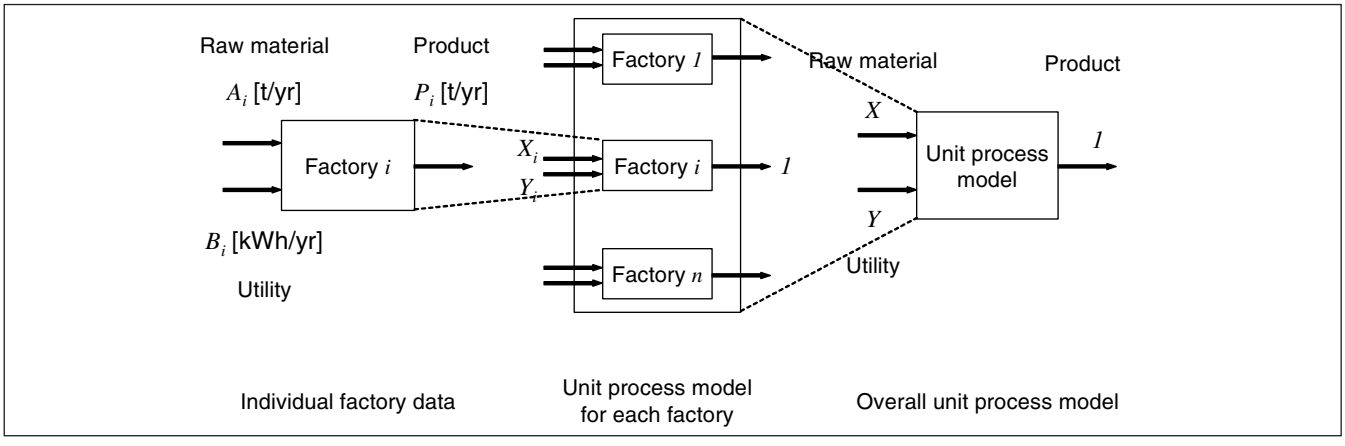

Fig. 1: Modeling a production process including several comparable factories. This example is used in section 1

of X_i and w_i. However, as mentioned before, it is often difficult to publish such individual data in LCI databases due to confidentiality reasons (see Fig. 1).

1.2 New procedure for including uncertainty information in industry-based LCI databases

The proposed procedure is comprised of two components: the first is fitting continuous probability distributions to X_i and Y_i (**Fig. 2**). Fitting continuous distributions is employed for the purpose of masking bare unit process data in each factory. After specifying the type of distribution, the characteristic parameters of the distribution (e.g. mean, standard deviation) are estimated using the Maximum Likelihood Estimation (MLE) method [10,11]. The second component is a correlation coefficient between X_i and Y_i. Such correlations are represented by the rank order correlation coefficient [11]. Derivation of these components is described in detail in the following sections.

The merits of this approach within LCA are the following: (a) It facilitates Monte Carlo simulations, which are simple, can manage every kind of distributions, and can be used with any kind of operation [12]. (b) Monte Carlo simulations are increasingly applied in LCA, e.g. [13–15]. (c) LCA software has started implementing this approach (e.g. GaBi 4 [16] or Sima Pro 6 [17]). A more detailed comparison of Monte Carlo simulations with other uncertainty propagation approaches is presented by Ciroth et al. [18].

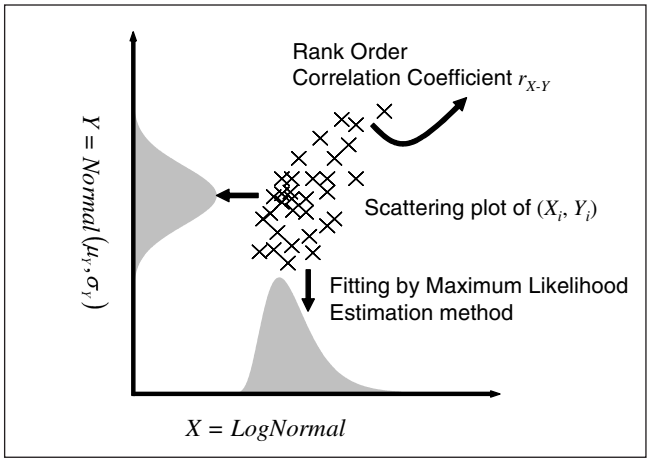

Fig. 2: Two components of the proposed procedure: probability distribution using the Maximum Likelihood Estimation (MLE) method and rank order correlation coefficient

1.2.1 Fitting probability distributions and estimating characteristic parameters by the Maximum Likelihood Estimation (MLE) method

There is no established rule for fitting probability distributions on scattering individual unit process data. However, several suggestions are found in literature. Hanssen and Asbjørnsen have analyzed unit process data from 26 production sites and found that binominal distributions can best estimate process emissions (e.g. SO_2 emission per product) [7]. If more than 30 data points are available, goodness-of-fit (GOF) statistics can assist in identifying the best-fit distribution among a set of candidates [11]. In cases where few data points are available, expert judgment may be needed. Maurice et al. have proposed the use of uniform, triangular and pert distributions (derived from beta distribution), which have a limited range [12]. Ecoinvent, in its current version, uses lognormal distributions for all unit process data [1,2].

After specifying the type of probability distribution, the characteristic parameters of the distribution should be estimated. We propose the use of the MLE method, which is the most common technique used to fit distributions to available data sets [11]. The maximum likelihood estimators of a distribution are the values of its parameters that produce the maximum joint probability density for the observed data. Consider a probability distribution type defined by a single parameter, α. The likelihood function $L(\alpha)$ is proportional to the probability that a set of n data points X_i could be generated from the distribution with probability density $f(X)$ and given by **Eq. 3**

$$X = \mu_X = \sum_{i=1}^{n} w_i X_i, \quad Y = \mu_Y = \sum_{i=1}^{n} w_i Y_i, \quad w_i = \frac{P_i}{\sum_{i=1}^{n} P_i} \tag{3}$$

For incorporating the market share w_i, the likelihood function is modified and redefined as (**Eq. 4**)

$$L(\alpha) = \prod_{i=1}^{n} \left(f(X_i, \alpha) \right)^{Nw_i} \tag{4}$$

where N is an arbitrary number such as 1000, which is large enough to make Nw_i an integer. Technically, X_i is treated as quasi Nw_i numbers of data points. For example, X_j, with 35.2% market share w_j, is treated as 352 data points of X_j when N is 1000. By having the power term Nw_i, values of X_i with a larger market share receive more weight and vice versa. The maximum likelihood estimator is then the value of α that maximizes $L(\alpha)$. It is determined by taking the partial differential of $L(\alpha)$ with respect to α and setting it to zero [11] (**Eq. 5**).

$$\frac{\delta L(\alpha)}{\delta \alpha} = 0 \tag{5}$$

Estimated parameters depend on the type of the distribution. For example, in the case of normal or lognormal distribution, both mean and standard deviation determine the property of the distribution and become maximum likelihood estimators. When normal distribution or lognormal distribution is fitted to X, Y in the example of Fig. 1, MLE provides the mean and standard deviation, which then define the distribution. For example, X can be expressed as (**Eq. 6**),

$$X = Lognormal\left(\mu_X, \sigma_X\right) \tag{6}$$

where the mean value μ_X is equivalent to the value in Eq. (2). The fittings based on MLE and GOF statistics are available in commercial software (e.g. BESTFIT [19]).

1.2.2 Preserving interdependency of inventory items by rank order correlation coefficient

In order to preserve interdependencies of inventory items, we propose the use of Spearman's rank order correlation coefficient (**Eq. 7**) [11].

$$r_{X-Y} = 1 - \frac{6}{N^3 - N} \sum_{i=1}^{N} \left(rank(X_i) - rank(Y_i) \right)^2 \quad (7)$$

Here again, it is assumed that a number of Nw_i data points have the value of X_i, and Y_i. $rank(X_i)$ is the rank among the N tuple data points. For example, X_1, the largest among all X, is treated as Nw_1 numbers of points with rank 1. X_2, the second largest, is treated as Nw_2 points with rank 1 + Nw_1. As seen in Eq. 7, if X_i and Y_i have the same rank for every i, the correlation coefficient becomes 1. The use of rank order correlation coefficient instead of regression correlation coefficient makes it possible to generate correlated variables from two probability distributions in the Monte Carlo simulation; numbers which were once generated independently are transformed to desired distributions preserving rank order correlation coefficient [20]. This algorithm is implemented in commercial software, e.g. @RISK® [19], which is an add-in software to MS-EXCEL®.

1.3 Unit process model to process chain model

The LCI can be calculated by creating process chain models. A simple example is shown in **Fig. 3**, where the product of process B is the raw material of the process A. The parameters of each unit process, normalized by its product amount, are described by probability distributions and correlation coefficients. Using the product amount of process A as a functional unit, the overall input (*SX*, *TX* and *Y*) can be calculated by using Monte Carlo simulation.

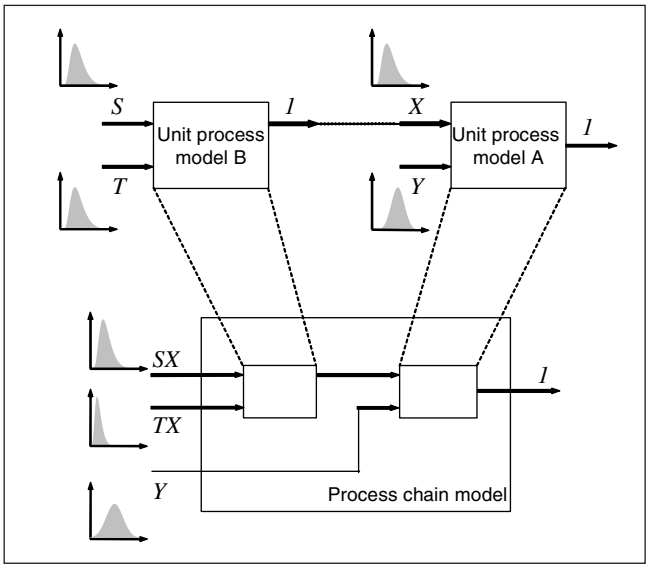

Fig. 3: Creation of the process chain model from two unit process models. The product of the process B is the raw material for the process A. The parameters for the whole process chain models are normalized by the unit production amount of process A

2 Case Study

2.1 Definition of the goal and scope

The goal of the case study is to illustrate the application of our procedure in the previous section. Emphasis is placed on highlighting the benefits of our procedure, rather than on the numerical facts. The intended decision-maker is, for example, a (local) government that wants to reduce CO_2 emissions by introducing a PET chemical recycling process with 1,000 t/yr capacity. Recycling options in the PET product life cycle are shown in **Fig. 4**. The functional unit of the study is 1,000 t/yr of used PET bottles. In this hypothetical case, we assume that the significance level is desired as 90% by the (local) government. The life cycle CO_2 emissions are compared before and after the installation of the recycling plant; i.e. the base case is the current condition, in which used bottles are incinerated with electricity generation at 10% thermal efficiency. Among emissions through the life cycle of PET bottles, CO_2, NO_X, SO_X are major contributing emissions within the Eco Indicator 99 method [21], using the LCI dataset 'PET, bottle grade, at plant (RER)' of the ecoinvent database [22]. In this work, CO_2 is taken as a reduced environmental metric because CO_2, NO_X and SO_X are emitted in conjunction (e.g. in fuel consumption). For the purposes of this study, namely the illustration of the method presented in Section 2, the assessment of CO_2 is sufficient, as other environmental metrics could be calculated in a similar way. In each option, 1,000 t/yr of used PET are supplied to recycling processes after pre-treatment in conventional flaking processes.

For the inventory analysis, existing unit processes are modeled using previous studies for PET products [23–25]. Unit processes inside the single dotted line in Fig. 4 are modeled with input and output flows, while the ones outside the line are modeled using cumulative CO_2 emission factors; i.e. total CO_2 amount emitted for providing the product up to the dotted line. Chemical recycling processes are modeled using the chemical process simulator HYSYS® [26] with information from literature [27–29] or corresponding industry. CO_2 emissions in each option or the base case are calculated using **Eq. 8**, and changes of CO_2 emissions from the base case are calculated with **Eq. 9**.

$$\Omega_i(CO_2, \boldsymbol{p}_i) = Out(CO_2, \boldsymbol{p}_i) + \sum_a In(a, \boldsymbol{p}_i) \cdot \varphi(CO_2, a) - \sum_b Out(b, \boldsymbol{p}_i) \cdot \varphi(CO_2, b) \quad (8)$$

$$\Delta\Omega_{i,\,BaseCase}(CO_2) = \Omega_i(CO_2, \boldsymbol{p}_i) - \Omega_{BaseCase}(CO_2, \boldsymbol{p}_{BaseCase}) \quad (9)$$

$\Omega(CO_2)$ are the CO_2 emissions from the life cycle systems (the whole system in Fig. 4) for i: option 1–3 or the base case. $Out(CO_2)$ are the CO_2 emissions occurring directly from the system (single dotted line). a and b refer to material or energy. *In* and *Out* are inputs and outputs to and from the boundary, and φ is the cumulative CO_2 emission

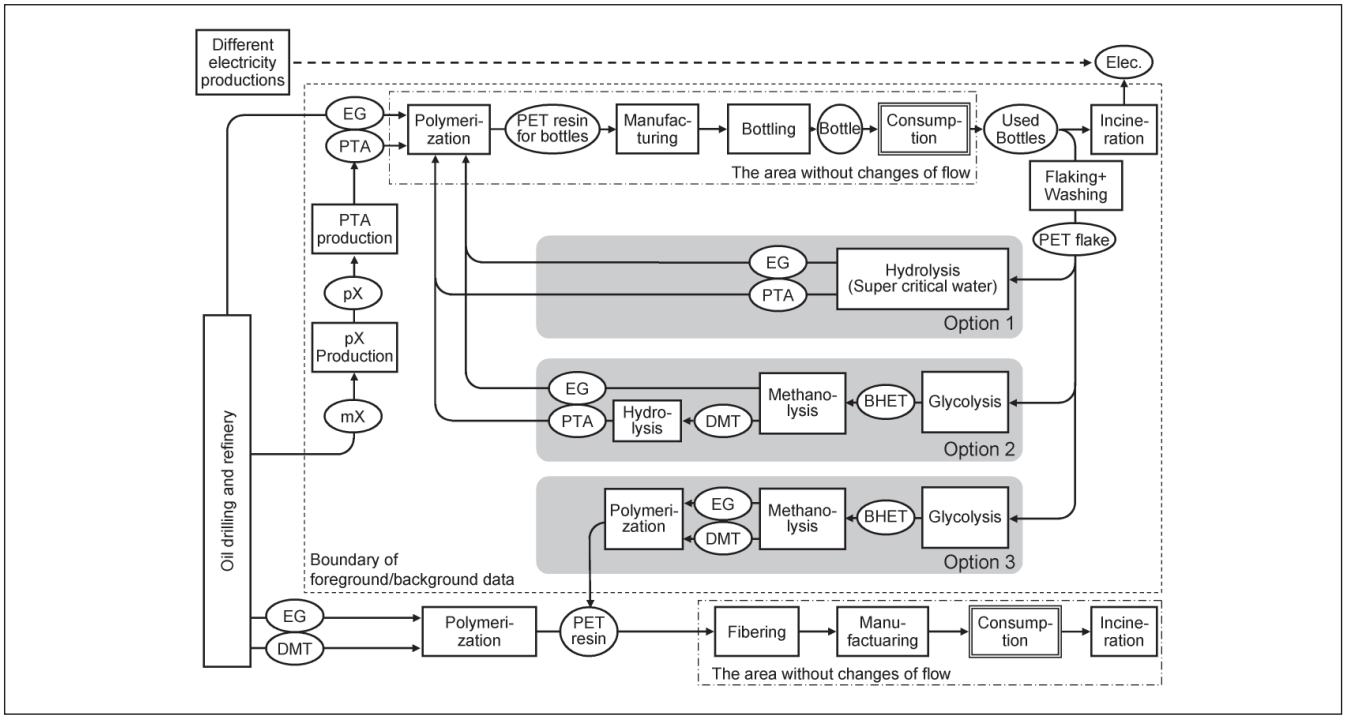

Fig. 4: Life cycle systems of PET products considering different options for chemical recycling processes. Abbreviation: pX refers to para xylene, mX to mixed xylene, BHET to bis(hydroxyethyl) terephthalate, DMT to dimethyl terephthalate and PTA to purified terephthalic acid

factor for the corresponding material or energy. $\boldsymbol{p}$ is a set of parameters representing the uncertainty of unit processes data consisting of the type of probability distribution, parameters for the distribution and correlation coefficients.

2.2 Uncertainty input information

In each of the foreground and existing processes (i.e. pX production, PTA production, incineration and flaking and washing processes), the amounts of utility consumption (e.g. electricity, steam and cooling water) were assumed to be log normally distributed. Reported data were used as mean values. The coefficient of variation, i.e. the ratio of standard deviation to the mean value, was set to 0.5 for electricity, 0.3 for steam and 0.1 for cooling water. Within one unit process, rank order coefficients between utility consumptions were assumed to be 0.8. It is reasonable to assume a positive correlation, because processes with better thermal efficiency tend to use less steam and cooling water. As an example, probability distributions in the primary PTA production are shown in **Table 1**. Additionally, transport distances are assumed to be triangle distributions, ranging ±50% around the mean values [23,25]. For the cumulative CO_2 emission factor of electricity, a discrete distribution is created based on the share of different production technologies [24]. No probability distribution is assumed on other cumulative CO_2 emission factors.

Table 1: Utility consumption in primary PTA production (excerpt from [23] normalized by 1 kg of PTA as a product)

Utility demand	Mean value	unit	Probability distribution
Electricity from grid	0.651	kWh	Lognormal, CV=0.5
Middle pressure steam from utility plant	0.848	kg	Lognormal, CV=0.3
Low pressure steam from utility plant	0.848	kg	Lognormal, CV=0.3
cooling water	193	kg	Lognormal, CV=0.1

2.3 LCA results and interpretation

Fig. 5 shows the deterministic values of $\Delta\Omega_{i,BaseCase}(CO_2)$ for option i (i = 1–3). On the one hand, CO_2 is emitted from the recycling processes. On the other hand, however, the substitution of virgin material for bottles and fibers leads to a saving of CO_2 emissions. CO_2 emissions also decrease in the incineration process of PET bottles, because stopping incin-

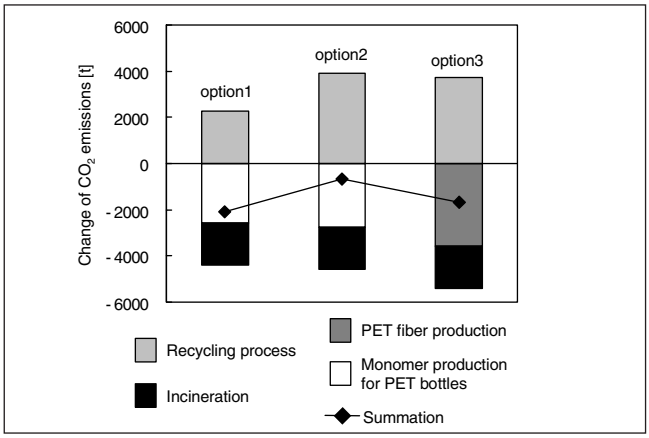

Fig. 5: Changes of CO_2 emission after installing recycling processes. The functional unit is the treatment of 1,000 t/yr of used beverage PET bottles

eration of PET directly reduces the CO_2 emissions. The substitution of conventional electricity production through PET incineration is included in the graph. However, this increase is very small due to the low net calorific value of PET and the low energy recovery efficiency (10% in [23,25]). The summation indicates that all three recycling options reduce CO_2 emissions. Option 1 is the most promising option; however, it is very close to option 3. In such cases, uncertainty analysis becomes instrumental in evaluating the significance of the difference between the two alternatives.

Relative indicators help us to judge the significance of such differences [30]. This can be calculated as follows (**Eq. 10**);

$$\Delta\Omega_{i,j}(CO_2) = \Omega_i(CO_2, \boldsymbol{p}_i) - \Omega_j(CO_2, \boldsymbol{p}_j) \quad (10)$$

In **Fig. 6**, the results of $\Delta\Omega_{i,\,option\,1}(CO_2)$ (i = option 2, 3) are shown. The probability that option 1 becomes superior to option 3 can be calculated from the integration of the probability distribution $\Delta\Omega_{option3,option1}(CO_2)$ above 0, which is 61%. Option 2 can be regarded as inferior to option 1 by 99%. If the decision-maker sets the significance level to 90%, option 2 can be rejected as promising for implementation. Option 3 may remain in the scope of comparison to be analyzed further. This illustrates that the deterministic analysis alone might have led to conclusions which are not statistically relevant. Conversely, after considering uncertainty, differences between options become more evident, enabling a more informed decision-making process. One prerequisite of such uncertainty analysis is an LCI database containing uncertainty information. Industry-based LCI databases can provide uncertainty information with the parameters and procedures proposed in this paper.

The contribution of each input uncertainty distribution to the cumulative uncertainty can be quantified by correlation coefficients between the values of each input distribution and the values of the output distribution. Because a linear model is used in this case study, multivariate stepwise regression method is used and normalized regression coefficients [20] are calculated. If the model is not linear, use of the rank order correlation coefficients is recommended [19]. Huijbregts et al. presented this correlation analysis as a sensitivity analysis, where input parameters are prioritized for further analysis [13]. **Fig. 7** shows the five highest contributing

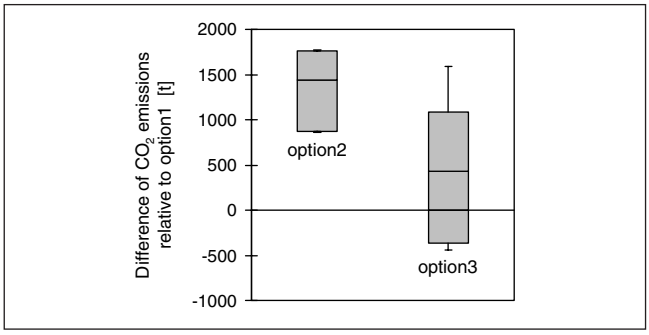

Fig. 6: Difference between options 2 and 3 and option 1($\Delta\Omega_{i,option1}(CO_2)$, *i=option 2, 3*) with indicators of 1%, 5%, mean, 95% and 99% points. Option 1 can be regarded as superior to option 3 at 61% probability by the integration of $\Delta\Omega_{option3,option1}(CO_2)$ above 1

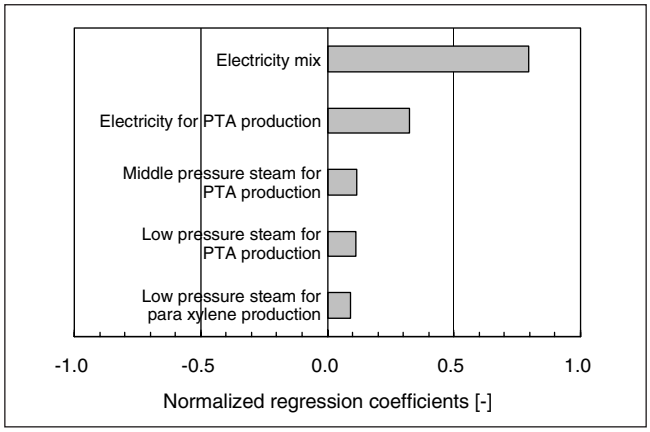

Fig. 7: Sensitivity analysis to $\Delta\Omega_{option3,option1}(CO_2)$ showing the normalized regression coefficients between input probability distributions to the probability distribution of $\Delta\Omega_{option3,option1}(CO_2)$

parameters for $\Delta\Omega_{option3,option1}(CO_2)$. The results show that the discrete distribution of the CO_2 emission factor dependent on the electricity mix contributes most to $\Delta\Omega_{option3,option1}(CO_2)$. The coefficient value 0.8 of electricity mix means that a one standard deviation increase in the electricity mix increases $\Delta\Omega_{option3,option1}(CO_2)$ by 0.8 standard deviations. Thus, the electricity mix should be given priority in further analysis. A possible refinement would be to check the latest emission factor, as the technology mix of electricity production changes from year to year. Another possibility would be to examine whether some processes use specific electricity sources. For example, less expensive nighttime electricity is usually dominated by nuclear electricity generation in Japan. The second contribution comes from electricity consumption in the primary PTA process, followed by other process data. Through these means of analysis, potential areas of improvement in the LCI model and data can be identified. This can be considered a further benefit of introducing uncertainty parameters in LCI databases. Parameters with larger absolute coefficient values should get priorities for further analysis. In Fig. 7, we only show the parameters with coefficients larger than 0.08, because the contribution of all other parameters to the cumulative uncertainty is less than 10% of the contribution of the most influential parameter (electricity mix).

3 Conclusions

Drawing on the problems of the JLCA-LCA database, we have proposed a procedure for incorporating uncertainty information in industry-based LCI databases, using standard statistical methods. The goal of our procedure is to support industry-based LCI databases to incorporate scattering unit process data while retaining confidentiality in order to achieve more informed decision-makings in LCA. This procedure has two components: fitting probability distributions to scattering data, and rank order correlation coefficients between interdependent LCI flows. This data can be directly applied in LCA using the Monte Carlo simulation. It is quite probable that problems similar to those in the JLCA-LCA database occur in other industry-based LCI databases (e.g. GaBi [16]). Therefore, the use of the proposed procedure is not limited to the JLCA-LCA database.

Consistency of raw data points is important in our approach. In general, statistical methods require a homogeny of individual data (e.g. data measured with the same experimental apparatus). Furthermore, in LCI study, as pointed out by Weidema et al. [31], individual models should have sufficient coherency when aggregated, which is the same process we are illustrating here. For industry-based LCI databases, the same periodical data from the desired scope (e.g. country-wide) are typically available as is in practice in the JLCA-LCA database. However, before the application of this approach, a check has to be made on the consistency of raw data points. Concerning data consistency, the application of our approach may be limited, where literature-based LCA databases which refer to various sources of literature are concerned.

In the case study presented here, we have illustrated the application of uncertainty information in LCI databases which may be presented by following our procedure, and the accompanying benefits. Since the actual scattering unit process data were not available for the case study, the uncertainty distribution of the LCA result is hypothetical. However, the merit of adopting the proposed procedure has been illustrated: more informed decision-making becomes possible, basing the decisions on the significance of the LCA results. This is a great benefit for LCA users, such as companies who do not want to run the risk of making uninformed decisions. It should be noted that additional costs for LCI data suppliers arise: when the procedure is applied in the JLCA-LCA database, the industry associations will have to check the temporal and geographical consistency of the reported data from the member companies and execute the statistical analysis presented in Section 2. The database developer will need to publish the uncertainty information in a usable way. If crucial data is missing, some of the companies might have to report the process data again. However, terms such as probability distributions and correlation coefficients are not new to LCI database developers (e.g. [32,33]). Moreover, our proposed method has the advantage of protecting member companies from revealing bare process data. In our opinion, it is worth making the additional effort.

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