INTERNSHIP REPORT

Report of a three month internship at the Centre for Design at the RMIT University in Melbourne, as part of the master program mechanical engineering *(15 EC)*

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PREFACE

An internship, which has to be carried out outside the university, is part of the master's curriculum of mechanical engineering. For me, this was a great opportunity to go abroad, apply my knowledge in a practical environment and to increase my competences. An important consideration for me, when I was looking for an internship, was an English speaking country outside Europe. I came in contact with the Centre for Design via ir. M.E. Toxopeus, assistant professor at the University of Twente. I was attracted by the work on sustainability from the Centre for Design and the Melbourne city life, so I was really glad they offered me an intern position.

At first, my assignment was to do development work on Greenfly, a new online tool that helps to design environmentally improved products. After two weeks it turned out that more development work had to be done by other people, before I could contribute to the development of Greenfly. Therefore, I was assigned to some small projects. One of them turned out to be quite interesting and therefore I put more effort in this project, so it became my major assignment during my internship. In the first few weeks it was not really clear in what direction we wanted to go and which results we wanted to obtain, but during the process this became clearer. Dr Enda Crossin, my supervisor at the Centre for Design, guided me very well in this, what contributed to results I have obtained. I would like to thank Enda Crossin very much for this. I would also like to thank Marten Toxopeus for getting in contact with the Centre for Design.

Looking back from my internship, I can say that it has been a valuable and truly amazing experience. The working environment and the people at the Centre for Design are really great, which makes all the difference. I learned al lot during my internship and also the experience of living abroad in a big city like Melbourne will remain forever.

Henk-Jan van den Hoorn
Enschede, Wednesday, 25 July 2012

SUMMARY

This report describes the work conducted during a three month internship at the Centre for Design at the RMIT University. This internship is part of the master's curriculum of mechanical engineering.

An Excel tool has been developed to modify the SimaPro database using the COM interface. Using this tool, it takes less than half an hour to substitute all electricity processes and associated uncertainty parameters in an ecoinvent 2.2 database containing about 4000 products.

A MATLAB LCA tool has been developed which can perform LCA analysis and Monte Carlo simulations. The tool is compatible with the ecoinvent 2.2 database and can import several impact assessment methods. Performance of the tool is more than 100 times faster than SimaPro. Because of its efficiency, the tool can quickly calculate the coefficient of variation per impact category for all the products in an ecoinvent 2.2 database. It would take about 2-3 days calculation time, whereas it would take about one year to calculate the same results in SimaPro. The coefficient of variation could be useful to incorporate uncertainty in streamlined life cycle assessment tools. How this could be useful presented to the user needs to be further investigated.

Using generic geographical processes in a LCI database affects the uncertainty and reliability of a life cycle assessment. The coefficient of variation for carbon dioxide emissions for a product can almost double when switching between geographical electricity grids.

Some minor projects conducted are also described in this report. This includes development work on Greenfly. This is an online streamlined life cycle assessment tool to design environmentally improved products. It needs to be further developed before it can be released as a final version

Land use change values for carbon stocks are calculated for the countries China, Europe, Japan, Mexico and New Zealand. The procedure for calculating these numbers has to be validated.

Another minor project was about exploring the capabilities and limitations of openLCA software. openLCA is compatible with the ecoinvent database and all features work well. The calculations are however quite time consuming compared to SimaPro and the software is not very responsive. openLCA is not compatible with the Australasian LCI database.

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CH. 1 - INTRODUCTION

This report gives an overview of the projects that I worked on during my internship, from 9 January 2012 to 5 April 2012, at the Centre for Design at the RMIT University in Melbourne, Australia. I worked on one major project and several smaller projects. This report focuses for the most part the major project and the smaller projects are more briefly described.

CH. 1.1 - PROJECTS

The major project I have been working on during my internship can be broken down into two topics, which are related to each other. The first topic was about a tool to automatically modify the SimaPro database. The second topic was about determining the data quality and uncertainty of this modified database.

The Centre for Design does a lot of development work on a streamlined Life Cycle Assessment (LCA) tool called PIQET. The background database of PIQET is a modified version of several databases combined. Modifying this database manually is a great deal of work. Therefore, there was a need for a tool to be able to quickly modify the database automatically. This was my first major project. When I completed this successfully, there arose a new topic to be addressed. The objective in this was determining the data quality of the modified database.

First I developed a tool to modify the SimaPro database, using the COM interface. I programmed this tool in Virtual Basic for Applications, a programming language within Excel. The main feature of this tool is to search for specific processes throughout the entire database -in all products- and substitute these processes for generic equivalents. In addition, it adjusts the uncertainty parameters that accompanies with the substitution of generic processes.

The second topic I worked on was about determining the data quality of this modified database. I ended up developing a MATLAB LCA tool, which can calculate the uncertainty of all the products in a database using Monte Carlo simulations. This uncertainty is then an indication of the data quality. SimaPro is also capable of performing Monte Carlo simulations, but the calculations are so time consuming that its use is practically impossible to calculate the uncertainty for an entire database.

One of the smaller projects I worked on was about Greenfly. Greenfly is a new online tool that helps to design environmentally improved products. It is a streamlined life cycle assessment tool, which incorporates EcoDesign strategies. It has been developed at the Centre for Design together with WSP Environmental, a consultants company, to a point where it has been released as a beta version. I did some testing and debugging on the tool and the website and was involved in the development process.

Another small project were I worked on was about the calculation of land use change values for carbon stocks. These values are calculated for several countries by Carbon Trust (BSI/Carbon Trust, 2011), but these values needed also to be calculated for other countries. I assisted in this project, worked out the calculations and ended up with the results. At the end of my internship it was still unclear whether we obtained the proper results, because Carbon Trust was not transparent in how they did their calculations.

I started my internship with a small project which was about exploring the features and capabilities of openLCA. openLCA is a freely available open source software for life cycle assessments. The purpose of exploring the software was to examine whether it could be used in student courses about life cycle assessment at the RMIT University. Now SimaPro software is used, but a major drawback of using this is that students are limited to use the software due to license restrictions. I have rewritten a tutorial about a comparison LCA study between a KeepCup and a typical disposal coffee cup over their entire life cycle, for modelling this in openLCA instead of SimaPro.

CH. 1.2 - WORK ENVIRONMENT

Established in 1988, the Centre for Design is recognised internationally for its sustainable systems research, innovative design and assessment tools and for research concerning the social and policy context of climate change. It is Australasia's key node of research activity in Life Cycle Assessment. The Centre for Design promotes sustainability through research, consulting, and capacity building through active dissemination and professional development.

The research at the Centre for Design is concentrated into four research clusters:

- Sustainable built environments
- Climate change and social context
- Sustainable products and packaging
- Life Cycle Assessment

I was working on the level where the Sustainable products and packaging and Life Cycle Assessment research teams are situated. Most of the projects I did were within the LCA group, only the work I did on Greenfly was within the Sustainable products and packaging group.

CH. 1.3 - STRUCTURE OF THE REPORT

Chapter two is about the tool I have developed to modify the SimaPro database. The background why this tool needed to be developed is explained. How uncertainty is incorporated in life cycle inventory databases is then described. This is important, because one of the modifications was about changing the uncertainty in the database. Then the process of writing the code is described, followed by a discussion.

The following chapter addresses the development of a MATLAB LCA tool, which can be used to calculate the uncertainty of a background database. The lognormal distribution is widely used to deal with the uncertainty in LCA and therefore the characteristics of this distribution are explained. The computational structure of LCA and how the tool is programmed follows. This chapter concludes with how the tool performs and a validation of the tool.

Chapter four shows an example of the uncertainty in a modified ecoinvent database with generic geographical processes. The substitution tool, as described in chapter two, is used to feed in generic electricity and natural gas processes in a standard ecoinvent 2.2 database. The uncertainty in this database with generic processes is then illustrated with an example.

Chapter five contains the work conducted on some minor projects. These are the development work on Greenfly, the calculations of land use change values for carbon stocks for several countries and explorations on the capabilities and limitations of openLCA software.

Finally, the discussion, conclusions and recommendations can be found in the last three chapters.

CH. 2 - MODIFYING THE SIMAPRO DATABASE

In this chapter the development of a tool to automatically modify the SimaPro database is explained. First the background is explained; why there was a need for this tool. Then the SimaPro COM interface is explained and how it can be used to modify the SimaPro database. The pedigree matrix, which deals with the uncertainty in Life Cycle Inventory (LCI) databases, is explained. And finally the structure and working of the tool itself will be shown.

CH. 2.1 - BACKGROUND

The Sustainable Products and Packaging team in conjunction with the Life Cycle Assessment team at the Centre for Design have developed a web based business tool called PIQET (Verghese, Horne, & Carre, 2010). The Packaging Impact Quick Evaluation Tool (PIQET) is an online tool that identifies and reviews actions to reduce the environmental impact of packaging system formats, particularly at the design development stage. It is a streamlined tool for life cycle assessment. One of the features of the tool is that it uses generic geographic grids for electricity and natural gas in the background database. The benefit of these generic grids is that the user can easily specify a country for his assessment and this geographic information is then ‘fed into’ the background database through the generic grids. This allows users to customise and model different life cycle stages, from the cradle to the grave, occurring over different geographical regions.

An issue with the background database was that the generic process cards were only fed into the first and sometimes second linked unit-processes within the PIQET database and not into the entire database. The reason was that the substitution of the electricity and natural gas processes by generic equivalents was done manually and very time consuming. Therefore there was a need for a tool to do this automatically.

A tool has been programmed in Virtual Basics for Applications (VBA), a programming language within Excel. This tool communicates with SimaPro using a COM interface. The COM interface allows for communication between different software programs on Windows computers.

CH. 2.2 - THE SIMAPRO COM INTERFACE

There is a COM interface available in the SimaPro Developer version. This allows the user to control SimaPro from applications such as Excel, .NET applications, Delphi, PHP etc (Gelder & Moore, March 2010). Every caller (application) has its own workspace within SimaPro.

This workspace contains opened database, project and calculated results of the last calculation. The architecture is shown in

Figure 1. The ‘caller’ in this case is VBA within the Excel environment. Several methods are supported by SimaPro COM server, such as opening a database and analyse a process and most of the information in the SimaPro database can be accessed.

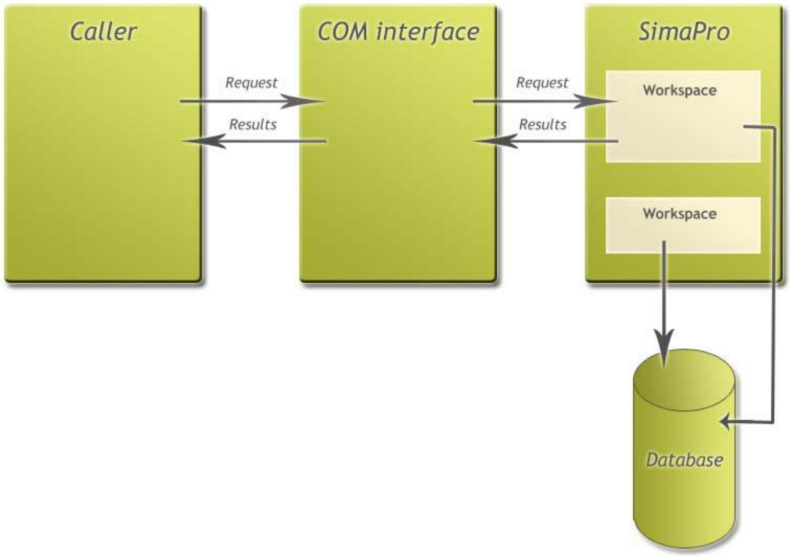

Figure 1 Architecture of the SimaPro COM interface

CH. 2.3 - GLOBAL STRUCTURE OF THE TOOL

What the tool basically does is searching within every product that is specified, whether it can find an electricity or natural gas process and if so, it substitutes that process with a generic equivalent. When generic processes are substituted in a product, the name of the product is changed to include a string ‘GENERAL’ and all the uncertainty parameters of all the processes and substances within that product are increased. This is done by changing the pedigree matrix of all the processes to account for the fact that it is now a general product with one or more generic processes. The following generic process cards are substituted in the database:

- Generic electricity grid, high voltage/PIQET
- Generic electricity grid, medium voltage/PIQET
- Generic electricity grid, low voltage/PIQET
- Generic natural gas/PIQET

The ‘Generic electricity grid, high voltage/PIQET’ process replaces all the high voltage electricity processes, the ‘Generic electricity grid, medium voltage/PIQET’ replaces all the medium voltage electricity processes and all the low voltage electricity processes are replaced by ‘Generic electricity grid, low voltage/PIQET’. Furthermore the natural gas processes within the category ‘Energy/ Heat’ are substituted with ‘Generic natural gas/PIQET’.

Inputs for the tool to work properly are database information such as location and name, a list of all products in which generic processes must be substituted and a list of processes that have to be replaced by their generic equivalents. The time for the tool to run is less than one hour with about 3600 products on a computer which is several years old. A guide to use the tool can be found in appendix II.

CH. 2.3.1 - PEDIGREE MATRIX FOR UNCERTAINTY ESTIMATION

In the ecoinvent database, most of the uncertainty information is based on a simplified standard procedure. The simplified approach includes a qualitative assessment of data quality indicators based on a pedigree matrix (Rolf Frischknecht; Jungbluth, Niels; Althaus, Hans-Jörg; Doka, Gabor; Dones, Roberto; Heck, Thomas et. al., December 2007). Data sources are then assessed according to the six characteristics ‘reliability’, ‘completeness’, ‘temporal correlation’, ‘geographic correlation’, ‘further technological correlation’ and ‘sample size’. An uncertainty factor (expressed as a contribution to the square of the geometric standard deviation) is attributed to each of the score of the six characteristics. These uncertainty factors are based on expert judgements and are shown in Table 1.

Table 1 Default uncertainty factors (contributing to the square of the geometric standard deviation) applied together

Indicator score	**1**	**2**	**3**	**4**	**5**
Reliability [U_1]	1.00	1.05	1.10	1.20	1.50
Completeness [U_2]	1.00	1.02	1.05	1.10	1.20
Temporal correlation [U_3]	1.00	1.03	1.10	1.20	1.50
Geographical correlation [U_4]	1.00	1.01	1.02	-	1.10
Further technological correlation [U_5]	1.00	-	1.20	1.50	2.00
Sample Size [U_6]	1.00	1.02	1.05	1.10	1.20

The square of the geometric standard deviation (95% interval – SD_{g95}) is then calculated with formula (1), where U_b is a basic uncertainty factor depending on the kind of input or output considered. It is assumed that for instance CO_2 emissions show in general a much lower uncertainty as compared to CO emissions.

$$SD^2{}_{g95} = \sigma_g^2 = e^{\sqrt{\ln^2(U_1)+\ln^2(U_2)+\ln^2(U_3)+\ln^2(U_4)+\ln^2(U_5)+\ln^2(U_6)+\ln^2(U_b)}} \qquad (1)$$

The set of six indicator scores is reported in the general comment field of each input and output, e.g. (5,4,1,1,1,5). The substitution tool can extract each of these indicator scores; change one of the indicators and save the modified comment to the database. For now, the tool only changes the indicator score for ‘Geographical correlation’ U_4. This is changed to the maximum value: ‘data from unknown or distinctly different area’. This accounts for the use of generic geographical grids. The new value for ${SD^2}_{g95}$ is then calculated by the tool and then written to the SimaPro database through the COM interface.

The basic uncertainty factor U_b is 1.05 for most processes. When this factor is different, it is reported in the comment field as a seventh indicator. There is however not a table publicly available which relates this seventh indicator to a basic uncertainty factor. The basic uncertainty factor can still be determined by using formula (12).

$$U_b = e^{\sqrt{\ln^2({SD^2}_{g95}) - \ln^2(U_1) - \ln^2(U_2) - \ln^2(U_3) - \ln^2(U_4) - \ln^2(U_5) - \ln^2(U_6)}} \tag{2}$$

One issue arises here, namely that the value of U_b is highly sensitive to the number of decimal places of ${SD^2}_{g95}$. Several processes within the ecoinvent database have uncertainty numbers with only one or two decimal places, which is not enough to determine U_b properly. The difference can be up to twenty per cent. The ecoinvent Centre could fortunately provide the table which relates the indicator to a basic uncertainty factor. This table is shown in appendix I.

CH. 2.4 - CONCLUSION AND DISCUSSION

The developed tool is very useful to quickly ‘feed in’ generic processes throughout an entire LCI database. It used to take weeks for someone to substitute processes in a database and then it was not even fed into the entire database. Now it only takes half an hour.

Besides substituting processes, the tool is also capable of adjusting the uncertainty parameters that accompanies with feeding in generic processes. The limitation is that the tool can only handle lognormal distributions. For the ecoinvent database this is not a problem, because almost all uncertainty is defined with lognormal distributions. For other LCI databases, such as the Australasian LCI, this is a problem, because uniform and triangle distributions are used in this database.

The reason that the tool can only handle lognormal distributions is because the type of distribution specified cannot be read with the COM interface from VBA. A library must be added in VBA to be able to read this, but it is unclear what library this is. The documentation of the SimaPro COM interface is also very limited, which does not give must guidance.

To account for the substitution of generic processes, the uncertainty indicator for ‘geographical correlation’ is changed. Besides this, one could also think of changing the technological correlation indicator, because the technological correlation might change depending on the geographical area considered. How much this will change is however different for each product, i.e. the area considered. Thus each product has to be looked at individually, thus this has not been accounted for in the tool.

The supported COM interface in SimaPro is now only used to adjust the database. There are a lot more opportunities by utilising the COM interface. For example, running analyses and updating results in Excel working sheets. Or automatically updating graphs and tables containing analysis outcomes in Microsoft Word. Other opportunities are using SimaPro analyses and results in for example MATLAB.

CH. 3 - MATLAB LCA TOOL

In chapter two, the development of a tool to modify the SimaPro database is described. This chapter is about the development of a MATLAB LCA tool, which can be used to determine the data quality of a modified SimaPro database, or a SimaPro database in general.

First the background of developing a MATLAB LCA tool is described. Then the lognormal distribution will be introduced, because almost all input data in LCI databases is defined to be log normally distributed. The computational structure of LCA is then addressed and finally the performance and capabilities of the tool will be evaluated.

CH. 3.1 - BACKGROUND

PIQET, a streamlined life cycle assessment tool, uses generic geographic grids in the background database. This allows the user to quickly customise and model life cycle stages occurring over different geographic regions. Quality of the data, or in other words: how reliable are the results, is currently not available in PIQET. This would however be very useful information, especially when comparing product systems and making decisions about which product is better.

As an example see Figure 2. This figure shows a characterisation graph of a coffee cup LCA study performed in Greenfly, a streamlined LCA tool like PIQET. It shows two scenarios: using a disposable coffee cup (left) or using a reusable KeepCup (right). The graph clearly shows which scenario has a bigger environmental impact, but it does not show how reliable that results is. The outcome of scenario 1 might for example be so uncertain, that one cannot make a trustworthy decision about which scenario has a lower environmental impact.

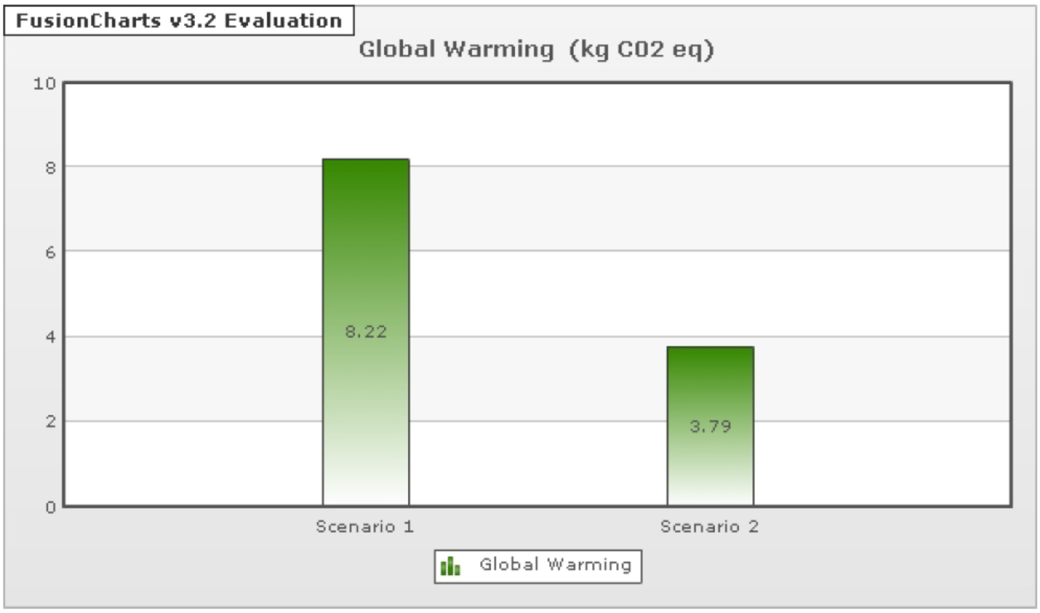

Figure 2 characterisation graph of coffee cup LCA study in greenfly. Impact of a disposable coffee cup (left) vs KeepCup (right)

SimaPro is able to perform Monte Carlo simulations to calculate uncertainty. A big drawback of SimaPro is that it takes a few hours to calculate the uncertainty for one product system. Therefore, other methods and tools have been discussed, in order to evaluate uncertainty and error propagation in LCI databases. As a pilot, a simple LCA tool has been programmed in MATLAB. This proved to be so quick and efficient that it is has been further developed and enhanced with features as Monte Carlo simulation.

CH. 3.2 - INTRODUCTION TO THE LOGNORMAL DISTRIBUTION

The lognormal distribution is most often used to deal with uncertainty in LCA. The lognormal distribution might be a bit confusing, especially with its relation to the normal distribution. The normal distribution is most often assumed to describe the random variation that occurs in the data from many scientific disciplines. However, many measurements show a more or less skewed distribution (Limpert, Stahel, & Abbt, 2001). Skewed distributions are particularly common when mean values are low, variances large, and values cannot be negative, as is the case for life cycle inventory data. According to (Hofstetter, 1998), lognormal distribution seems to be a more realistic approximation for the variability in fate and effect factors of LCI data than the normal distribution and for that reason it is applied in the ecoinvent database.

A random variable X is said to be lognormally distributed if $\log(X)$ is normally distributed. The lognormal distribution arises if it is multiplicative product of many independent and positive random variables and is described by the parameters mu μ and sigma σ. A clear distinction has to be made between the mean $\bar{x}$, and variance var of the lognormal distribution and their corresponding parameters μ and σ. Their relation is

$$\mu = \ln\left(\frac{\bar{x}^2}{\sqrt{var+\bar{x}^2}}\right) \tag{3}$$

$$\sigma = \sqrt{\ln\left(\frac{var}{\bar{x}^2+1}\right)} \tag{4}$$

The maximum likelihood estimators of the lognormal distribution parameters μ and σ can be calculated. Given a sample $(x_1, \ldots, x_n)$, it holds that

$$\hat{\mu} = \frac{\sum_n \ln x_n}{N} \tag{5}$$

$$\hat{\sigma} = \sqrt{\frac{\sum_n (\ln x_n - \hat{\mu})^2}{N}} \tag{6}$$

Within the ecoinvent database, the uncertainty is provided as the square of the geometric standard deviation SD_g^2. This yields for a mean value of one. To transform this SD_g^2 to a distribution with a different mean value $\bar{x}$ and variance var, the following formula is applied

$$var = \left[\bar{x} \cdot \ln\sqrt{SD_g^2}\right]^2 \tag{7}$$

In formula (12), the square of the geometric standard deviation is first transformed to a normal distribution. Then a linear transformation is applied with factor $\bar{x}$. This value is then squared to obtain the variance for the lognormal distribution with mean $\bar{x}$. Now these values can be substituted in formulas (3) and (4) to obtain the parameters μ and σ for the lognormal distribution. Given these parameters, the 95% confidence interval for the lognormal distribution with parameters μ and σ is

$$x_{2.5\%}, x_{97.5\%} = e^{\mu \pm 1.96 \cdot \sigma} \tag{8}$$

CH. 3.3 - THE COMPUTATIONAL STRUCTURE OF LIFE CYCLE ASSESSMENT

The computational aspects of LCA are very clearly presented in (Heijungs & Suh, 2002). This is used as a basis for developing the LCA tool in MATLAB. The matrix approach is used to solve the inventory problem. In the following, a concise overview of the computational structure is given.

The inventory problem can be seen as the task of scaling all unit processes in the system in such a way that they exactly produce the reference flow (or functional unit). In mathematical form this can be written as

$$\boldsymbol{As} = \boldsymbol{f} \tag{9}$$

where $\boldsymbol{A}$ is the technology matrix, which represents the flows within the economic system, $\boldsymbol{f}$ is the final demand vector, which represents the set of economic flows that corresponds to the reference flow and $\boldsymbol{s}$ is the scaling vector between them. Both $\boldsymbol{A}$ and $\boldsymbol{f}$ are known and a unique solution for $\boldsymbol{s}$ can be found, provided that $\boldsymbol{A}$ is square and non-singular. The system of equations in formula (12) can be solved using matrix inversion; however this is quite computational intensive. MATLAB provides a much more efficient function for solving this system of equations namely using the 'matrix division operator', i.e. $\boldsymbol{s} = \boldsymbol{A} \backslash \boldsymbol{f}$. This produces the solution using several algorithms under which Gaussian elimination. The matrix division operator in MATLAB also allows for multi-thread calculation, which significantly increases the speed. The vector with environmental interventions $\boldsymbol{g}$ can be calculated when the scaling vector is known

$$\boldsymbol{g} = \boldsymbol{Bs} \tag{10}$$

where $\boldsymbol{B}$ is the intervention matrix. Characterisation into various impact categories is done by multiplying the vector with interventions with the characterisation matrix $\boldsymbol{Q}$.

$$\boldsymbol{h} = \boldsymbol{Qg} \tag{11}$$

where $\boldsymbol{h}$ is a vector containing the characterised results per impact category.

CH. 3.4 - PROGRAMMING THE MATLAB LCA TOOL

In this section it is explained how the MATLAB LCA tool is developed. It started quite basic in the early stage of the development to evaluate its potential and is thereafter further developed with features as Monte Carlo simulation and CSV import of LCI databases and Impact Assessment Methods (IAM). This paragraph includes some technical programming issues that have been solved.

CH. 3.4.1 - IMPORTING LCI DATABASE AND IAM

Within SimaPro, it is possible to export the process matrix of a database, which includes both the technology matrix $\boldsymbol{A}$ and the intervention matrix $\boldsymbol{B}$. This process matrix was first imported in MATLAB to build the LCA tool, but it had some limitations. One of them was that the process matrix has no sign difference between input flows and avoided products. Also, this matrix does not include uncertainty information. The latter has first been solved by using the SimaPro COM interface and reading the uncertainty information (geometric square of the standard deviation) for each process. This way of importing a LCI database proved to work, but was however quite time consuming and not very flexible. Therefore a MATLAB script has been written to read in a single CSV LCI database file. This script reads and imports an entire ecoinvent 2.2 database within 60 seconds with one mouse click from the user.

The MATLAB script needs as input an Excel file with all the substances in the database, corresponding to the rows in the intervention matrix. The first thing the script does is searching for unit conversion factors. It then searches quickly for all processes in the database, to establish the size of the technology matrix. The CSV file is then read row by row and for each process part, e.g. ‘materials/fuels’, ‘resources’, ‘emissions to air’, it assigns the amount of a process or substance to the corresponding entry in the technology or intervention matrix. It finds the corresponding rows and columns by searching in the list of processes and substances, defined in the first part of the script. When the unit of a process or substance does not match with the unit as in the technology and intervention matrix, it uses the unit conversion factors to converse the amount to the proper unit. The script also builds two matrices with uncertainty information. The row and column indices of these matrices correspond to those of the technology and intervention matrix. When all is imported, the variables are stored to a binary MAT-file.

Another MATLAB script has been written to import an impact assessment method. At first, a specific script has been written, which was only able to import the ‘Australian indicator set 2.01’ IAM. Subsequently, an enhanced script has been written to be able to import any IAM. It reads in a single CSV file. It has been tested with the PIQET IAM v4. Input for this script is an Excel file with all substances, their compartments and their sub compartments, corresponding to the substances in the intervention matrix.

The first execution in the script is searching for the unit conversion factors and to store this in an array. These conversions are used when the unit of a substance in the list do not match with the unit of a substance specified in the impact assessment method. The script scans a CSV file row by row and builds the characterisation matrix $\boldsymbol{Q}$ by assigning the characterisation factors to the correct indices of the matrix. It does so by searching in the list of all substances. When finished, the matrix is stores in a binary MAT-file.

CH. 3.4.2 - ANALYSIS

The script MAIN.m performs LCA analysis and Monte Carlo simulations. It loads the binary MAT-files, containing the database and the IAM. The final demand vector $\boldsymbol{f}$ has to be defined by the user within the script. Each non-zero elements in this vector, results in an output of the corresponding product. The inventory problem is then solved by using MATLAB's left division operator. See the code below.

```
s=A\f;
g=B*s;
h=Q*g;
```

CH. 3.4.3 - MONTE CARLO SIMULATION

For the Monte Carlo simulation it is assumed that the amounts of all processes that have uncertainty information are all log normally distributed. For the ecoinvent database this is a valid assumption. For the Australian database this cannot be assumed, because a lot of the processes have a triangle or uniform distribution.

The build in MATLAB function 'lognrnd' is used to generate random numbers, which are log normally distributed with parameters mu and sigma. Inputs for this function are two vectors mu and sigma. The (mean) amount and square of the geometric standard deviation are stored in matrices, so to be able to use the lognrnd-function, these matrices need to be transformed to vectors. The variance is determined, using formula (7). The variance vector, together with the mean (amount) vector are input for formulas (3) and (4) to determine mu and sigma. The function 'lognrnd' generates then the random values for the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$. These matrices are built by back transforming the vectors to matrices. The inventory problem can now be solved and characterisation can be performed. A loop repeats this procedure for the number of simulation runs specified by the user.

A graphical user interface for the Monte Carlo simulation is shown in Figure 3. The user can select multiple products in a database and the number of runs for the simulation.

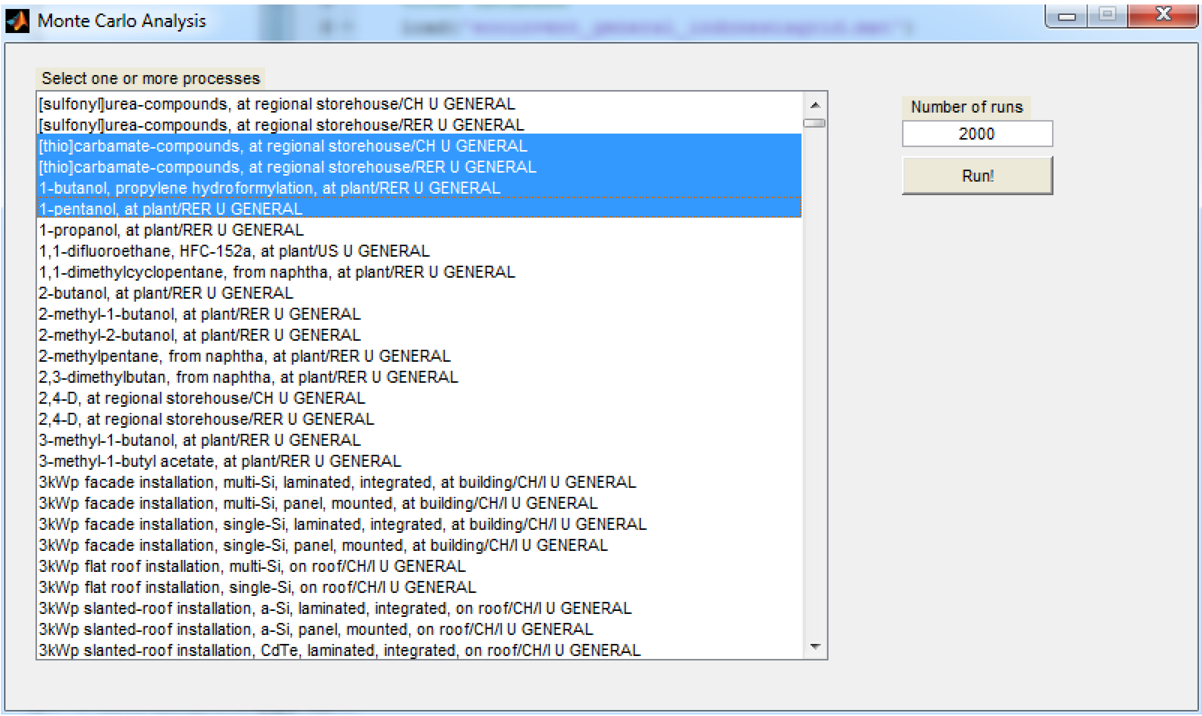

Figure 3 Screenshot: Monte Carlo simulation in MATLAB

CH. 3.5 - VALIDATION

The working and validation of the MATLAB LCA tool will be shown by comparing the results to the results of the same calculations conducted in SimaPro. This, for both an analysis and a Monte Carlo simulation. Also the convergence of the mean and standard deviation, estimated from the Monte Carlo simulation, will be evaluated.

CH. 3.5.1 - ANALYSIS

In this section, the results of the MATLAB LCA tool will be compared with the results from the same analysis conducted in SimaPro software. The LCI database used is the ecoinvent v2.2 database and the IAM used is PIQET IAM v4 (Verghese, Horne, & Carre, 2010). This IAM assesses nine indicators. The product to be compared is 1 kg of '[sulfonyl]urea-compounds, at regional storehouse/RER U'. This unit process is connected to 2000 processes in the ecoinvent database. The result of the analysis is shown in Table 2, with an accuracy of ten decimal places. There are some slightly differences after 7~8 decimal places. This could be caused by the different solving algorithms between SimaPro and MATLAB. SimaPro uses matrix inversion to solve the inventory problem, while MATLAB does not. Matrix inversion can cause slightly accuracy problems, which might explain the (very small) differences. It may also due to an error in the script.

Table 2 Analysis in MATLAB compared to analysis in SimaPro. Characterisation of 1 kg of product '[sulfonyl]urea-compounds, at regional storehouse/RER U', using PIQET IAM v4

Impact category	Unit	Analyse SimaPro	Analyse MATLAB
Global Warming	kg CO_2 eq.	10.7236115843	10.7236115817
Cumulative energy demand	MJ LHV	209.8938784845	209.8938784380
Minerals & fuel	MJ surplus	13.4478923604	13.4478923556
Photochemical oxidation	kg C_2H_4 eq.	0.0087800990	0.0087800990
Eutrophication	kg PO_4 eq.	0.0140719788	0.0140719788
Carcinogens	DALY	0.0000037056	0.0000037056
Land use	Ha a	0.0000293324	0.0000293324
Water Use	kL H_2O	0.7072218679	0.7072218678
Solid waste	kg	1.0166274508	1.0166274466

Remarkable is the big difference in calculation time between SimaPro and MATLAB. For SimaPro it took about 20 seconds to calculate the results, while it took MATLAB only 0.16 seconds. The calculation in MATLAB is thus about 125 times faster than SimaPro, using the ecoinvent v2.2 database. This would probably be even more on the latest generation dual and quad core processors, because SimaPro can only allocate a single core, while MATLAB allows for multi-threading.

CH. 3.5.2 - MONTE CARLO SIMULATION

The same product as in the analysis used as described in the former, is also used to compare the results in a 2000 run Monte Carlo simulation. The results are shown in Table 3.

Table 3 Monte Carlo simulation in MATLAB compared to SimaPro. Properties of the distribution for characterisation of global warming

Properties for Global Warming	SimaPro	MATLAB
Mean [kg CO_2]	10.730	10.737
Median[kg CO_2]	10.661	10.673
Standard Deviation [kg CO_2]	0.9941	0.964
Coefficient of Variation [%]	9.264%	8.979%
2,5% boundary [kg CO_2]	8.9644	9.002
97,5% boundary [kg CO_2]	12.8344	12.684

The distribution as a result of the Monte Carlo simulation performed in SimaPro is shown in Figure 4. The outer red lines are the boundaries for the 95 per cent confidence interval. The red inner line is the median and the dashed line is the mean.

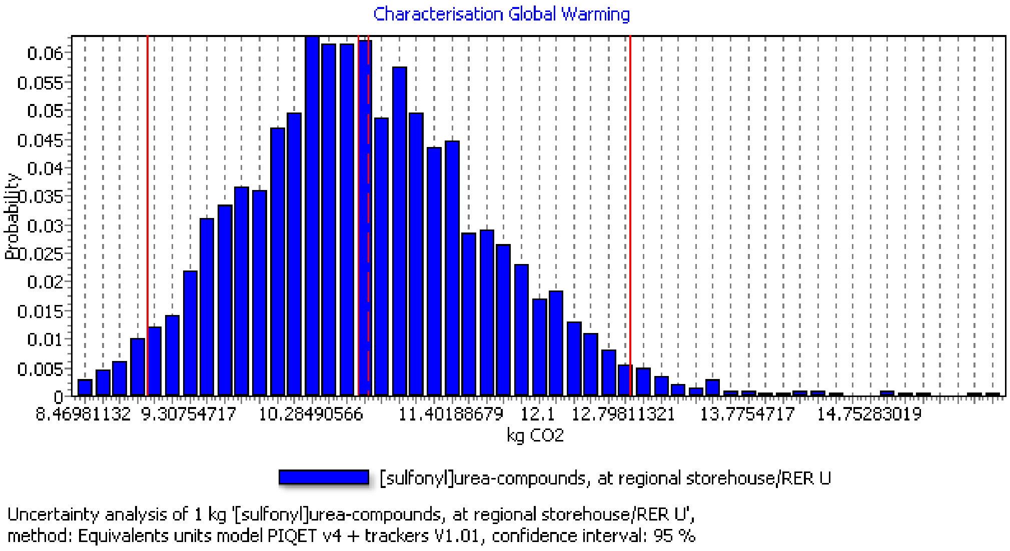

Figure 4 Monte Carlo simulation in SimaPro, 2000 runs

The distribution, as a result of the Monte Carlo simulation performed in MATLAB is shown in Figure 5. A fitted lognormal probability density function is also plotted with parameters μ and σ. These parameters for the lognormal distribution are maximum likelihood estimates, according to formulas (5) and (6). The boundaries for the 95% confidence interval are calculated using formula (12).

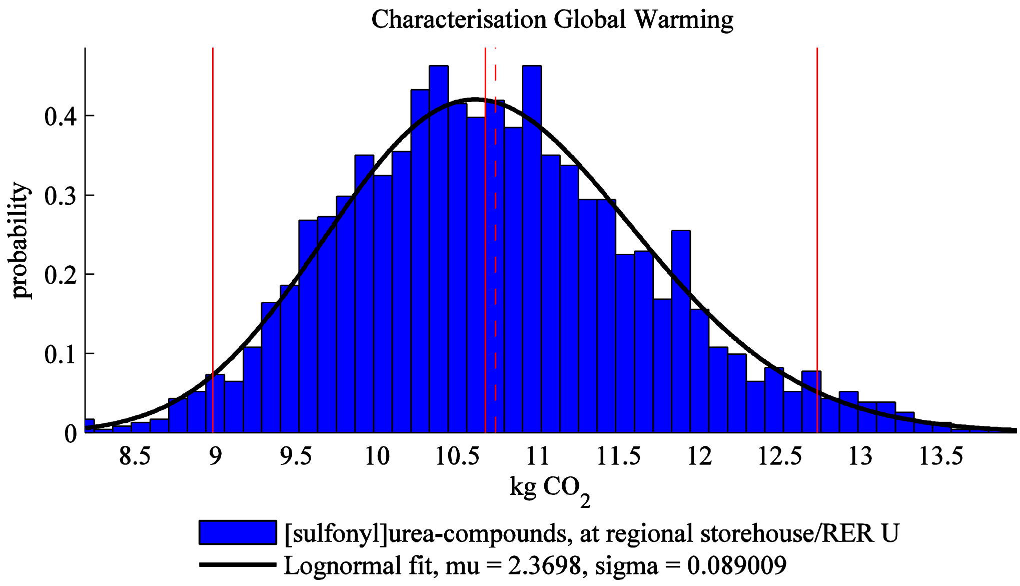

Figure 5 Monte Carlo Simulation in MATLAB, 2000 runs for 1 kg of product '[sulfonyl]urea-compounds, at regional storehouse/RER U', using PIQET Impact Assessment Method v4

Table 4 shows how much more efficient MATLAB is compared to SimaPro.

Table 4 Time comparison between SimaPro and MATLAB. Using the ecoinvent 2.2 database and a computer with a core 2 duo processor.

	SimaPro	**MATLAB**	**Speed increase**
Analyse single process	±20 s	0.16 s	125 times
Monte Carlo 2000 runs	14h, 55m, 45s	372s	144 times

Table 5 shows the statistics from the Monte Carlo simulation in SimaPro. This validates the assumption that almost all processes are defined as log normally distributed. It also shows that 28,1% of the processes do not contain uncertainty information.

Table 5 Statistics SimaPro Monte Carlo simulation

Statistics SimaPro Monte Carlo simulation	
Total calculation time	14:55:45
Parts of values that contain uncertainty data	71.9 %
Total distributions	68728
Undefined	19321
Lognormal	49399
Normal	6
Triangle	2
Uniform	0

CH. 3.5.3 - CONVERGENCE

The convergence of the mean value and the standard deviation in a Monte Carlo simulation performed in MATLAB is shown in Figure 6 and Figure 7 respectively. The scaling of the y-axis is such that the minimum and maximum value on the y-axis is ten per cent of the overall value.

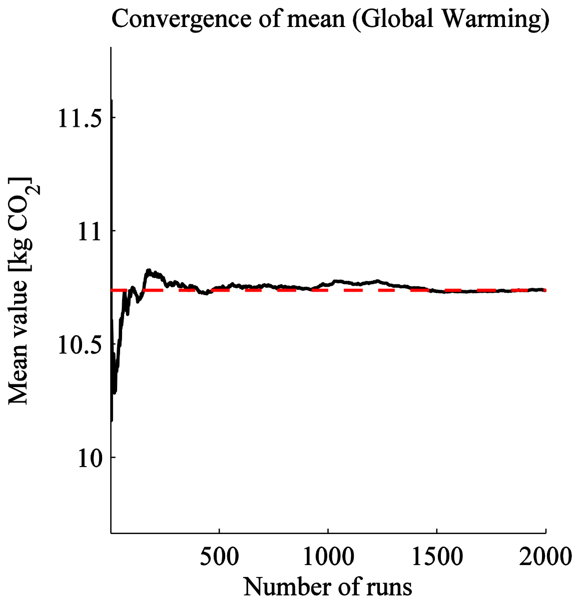

Figure 6 Convergence of the mean value for characterisation of global warming. (1 kg of product '[sulfonyl]urea-compounds, at regional storehouse/RER U', using PIQET IAM v4)

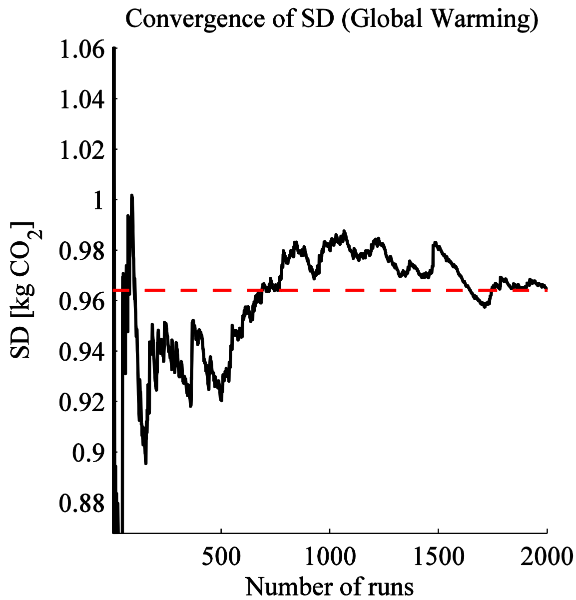

Figure 7 Convergence of the standard deviation for characterisation of global warming. (1 kg of product '[sulfonyl]urea-compounds, at regional storehouse/RER U', using PIQET IAM v4)

The convergence of the coefficient of variation is shown in Figure 8. The scaling of the y-axis is now 100 per cent under and above the red dashed line. After 50 runs, the coefficient of variation stays within a range of $\pm 4.1\%$ and after 100 runs it stays within a range of $\pm 2.1\%$.

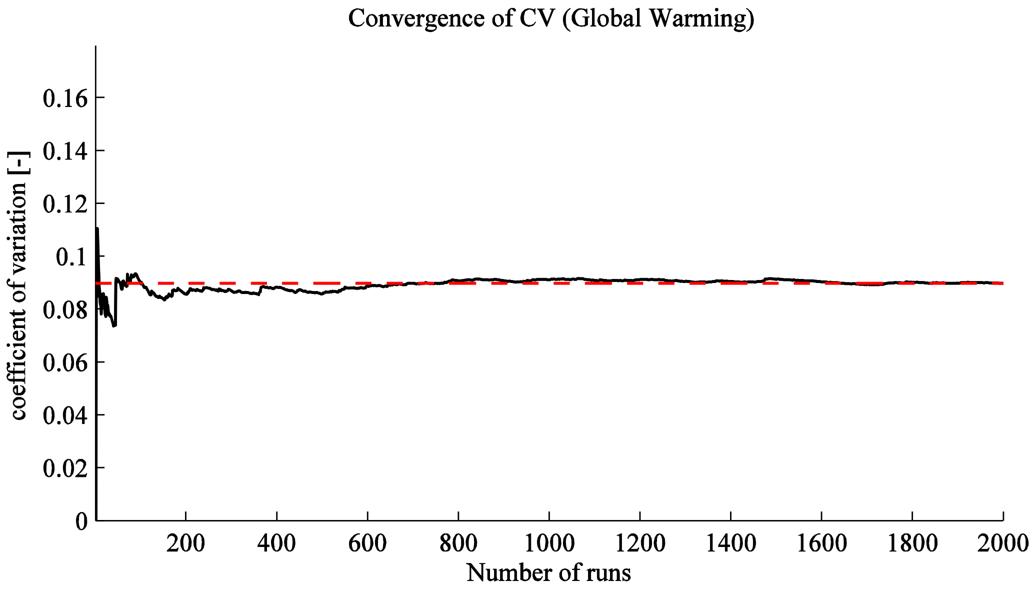

Figure 8 Convergence of the CV for characterisation of global warming. (1 kg of product '[sulfonyl]urea-compounds, at regional storehouse/RER U', using PIQET IAM v4)

CH. 3.6 - CONCLUSION AND DISCUSSION

The MATLAB LCA tool is a very powerful tool to perform LCA analysis and Monte Carlo simulations. It can import LCI databases and impact assessment methods in CSV format. Because of its efficiency, the tool can be used to calculate the uncertainty for all the products in a database fairly quickly. From this, the coefficient of variation can be determined. This normalised value can be used to compare different products in a database on their reliability of characterised results.

Furthermore, the coefficient of variation can be determined per impact category. So using these results, one might conclude that the calculated carbon dioxide emissions of a product might be very accurate and reliable, while the calculated water use for that product is very uncertain. One could think of benchmarking the products in a database on their uncertainty per impact category. A quality indicator per impact category for each product might be valuable information for streamlined LCA tools like PIQET and Greenfly.

The limitation for the tool is that it can only be used with the ecoinvent database. The first reason for that is that the tool does not account for allocation. For the ecoinvent there is no need to account for allocation, because all products have pre-allocated processes. Also, the import script cannot handle avoided products. Another reason is that for the ecoinvent database it can be assumed that all uncertainty is given as a lognormal distribution. This is the only probability distribution that is supported in the Monte Carlo simulation in the tool. Global and local parameters are also not supported. With SimaPro it is possible to export a database containing only constants and no parameters, but then uncertainty information within the parameterisation gets lost. The last issue is that the script for importing a LCI database only reads substances in the sub compartments ‘raw’, ‘air’, ‘water’ and ‘soil’. These are the substances as in the ecoinvent database.

CH. 4 - UNCERTAINTY WITH GENERIC ELECTRICITY GRIDS

This chapter shows a comparison between a product in a standard ecoinvent database and a modified ecoinvent database. In the modified dataset all the electricity processes are substituted by generic equivalents. The substitution tool is used for this, as described in chapter 2.

CH. 4.1 - PROCEDURE

First generic process cards for high, medium and low electricity are fed into an ecoinvent 2.2 database within SimaPro, using the substitution tool as described in chapter 2. Processes from Europe and Indonesia are plugged into these generic processes, using ‘iff-statements’ with parameters in SimaPro. Using this iff-statements with parameters, it is possible to quickly select which geographic grid is used, the Europe grid, or the Indonesia grid.

For the Europe grid, the product ‘Electricity, high voltage, production UCTE, at grid/UCTE U’ is used for high voltage and the medium and low equivalents for the ‘generic medium voltage’ and ‘generic low voltage’ cards respectively. The electricity production mix for Indonesia is modelled using data from (IEA Energy Statistics - Electricity for Indonesia, 2009). Table 6 shows how the electricity production mix is modelled within SimaPro. The square of the geometric standard deviation is based on the pedigree matrix, using Table 1 with indicators (2,5,4,5,4,5) and formula (1). The pedigree matrix is

Table 6 electricity Production mix Indonesia (2009)

	Product/ substance	**Amount**	**Unit**	**Distribution**	**SD_g^2**
Output	Production mix Indonesia	134575	kWh	-	-
Inputs	Electricity, hard coal, at power plant/CN U	64976	kWh	Lognormal	1.69
	Electricity, oil at power plant/CZU	35467	kWh	Lognormal	1.69
	Electricity, natural gas, at power plant/GB U	11381	kWh	Lognormal	1.69
	Electricity, hydropower, at plant/CH U	9295	kWh	Lognormal	1.69
Emissions	Heat, waste	20895	kWh	Lognormal	1.69

There is also accounted for energy losses according to (Dones, Bauer, Bolliger, Burger, Heck, & Roder, 2007)

- Production to high voltage: 1.1% (95% heat to air, 5% heat to soil)
- High voltage to medium voltage: 1.3% (55% heat to air, 45% heat to soil)
- Medium voltage to low voltage: 24.5% (25% heat to air, 75% heat to soil)

The modelled electricity grid for Indonesia is representative for the way the generic grids are modelled within the background database of PIQET.

CH. 4.2 - RESULTS

Now a product in the modified generic database will be analysed and compared using a Europe grid versus an Indonesia grid. Table 7 shows the characterised results and the coefficient of variation for both the Europe grid and Indonesia grid for product '[sulfonyl]urea-compounds, at regional storehouse/RER U'.

Table 7 Uncertainty using Europe electricity grids vs Indonesia electricity grid. 1 kg of product '[sulfonyl]urea-compounds, at regional storehouse/RER U' between Europe and Indonesia grid.

	Europe grid		**Indonesia grid**	
Impact category	**Characterisation**	**CV [%]**	**Characterisation**	**CV [%]**
Global Warming	11.1	9.2	16.3	18.1
Cumulative energy demand	213.1	10.3	241.2	28.5
Minerals & fuel	13.8	9.4	18.0	22.7
Photochemical oxidation	0.009	19.2	0.01	18.9
Eutrophication	0.01	14.9	0.02	14.7
Carcinogens	3.7e-6	58.5	3.6e-6	62.5
Land use	3.0e-5	57.4	4.6e-5	70.9
Water Use	0.7	8.3	1.0	22.1
Solid waste	1.0	50.4	1.3	42.4

Table 7 reveals some interesting information. Not surprisingly, the carbon dioxide emissions are higher for the Indonesia grids compared to the Europe grid. This is not shocking, because the Indonesia grid is far more 'dirty'. Far more interesting are the coefficients of variation. For instance, changing the grid from Europe to Indonesia almost doubles the uncertainty range for global warming. Other interesting indicators like cumulative energy demand, land use and water use show an increase in uncertainty with about a factor 2-3.

CH. 4.2.1 - BENCHMARKING PRODUCTS

The coefficient of variation can be calculated per impact category for each product in the database. All products can be benchmarked on their degree of uncertainty and this will be shown in the following.

Figure 9 shows a histogram of the coefficient of variation for global warming for the entire modified ecoinvent database. The CV for each process is determined using Monte Carlo simulation with 200 runs per process. It should be mentioned that not all processes contain uncertainty information, which is also reflected in the bar at $CV = 0$.

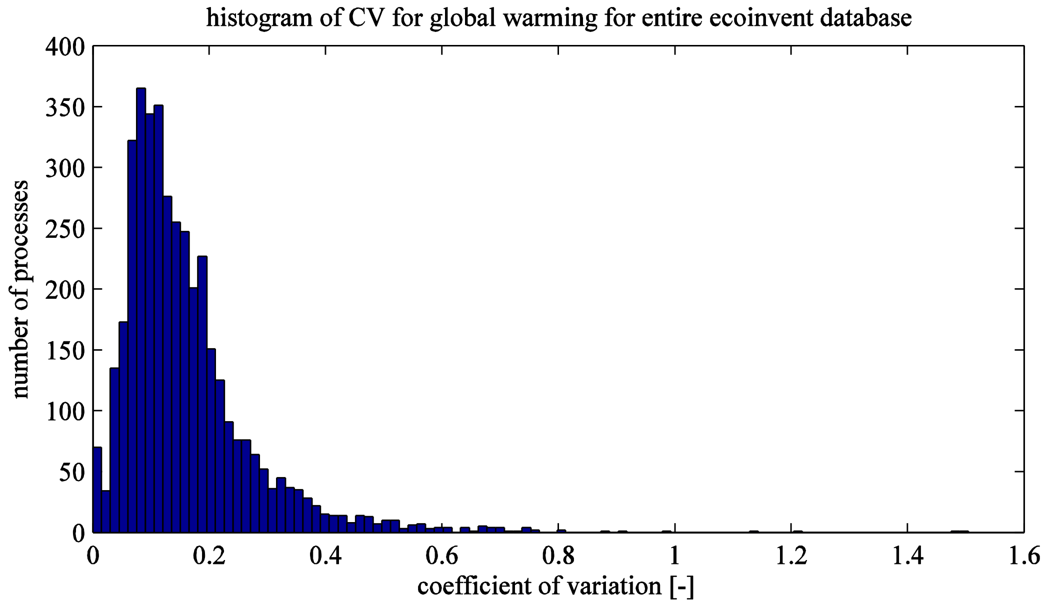

Figure 9 Histogram of CV for global warming for entire ecoinvent database

Figure 9 reveals for each product how reliable the results are for carbon dioxide emissions. The majority of the products have a coefficient of variation of about 10-15 percent, but there are also products with very high uncertainty. This is very useful information, especially if you want to evaluate the uncertainty in an assessment, but not want to perform a comprehensive Monte Carlo simulation.

CH. 4.3 - DISCUSSION AND CONCLUSION

The illustration in this chapter shows that uncertainty is important to consider when using generic electricity grids in a database. The illustration in this chapter shows for example that the coefficient of variation for carbon dioxide emissions for a product can almost double when switching between geographical electricity grids.

Benchmarking products on the degree of uncertainty in a LCA provides useful information to assess the reliability of LCA-based decisions. This is especially of interest when one does not want to conduct a comprehensive Monte Carlo simulation. This is for instance the case in online streamlined life cycle assessment tools like PIQET or Greenfly. Although benchmarking products does give information about the uncertainty between the products, it does not give the uncertainty of the model outcomes of an entire product system, consisting of several products. The next step is thus to investigate how the coefficient of variation of several products can be used to evaluate the uncertainty of a product system.

Benchmarking the product in a LCI database on the degree of uncertainty also reveals which products are unreliable. These products either should not be used any more or they need to be refined. This way you are improving the quality of your database.

CH. 5 - MINOR PROJECTS

CH. 5.1 - DEVELOPMENT ON GREENFLY

Greenfly is a new online tool that helps to design environmentally improved products (Greenfly: Design Greener Products, 2012). It is a streamlined life cycle impact assessment tool, which incorporates EcoDesign strategies. It has been developed at the Centre for Design together with WSP Environmental, a consultants company, to a point where it has been released as a beta version. The planning was that it could be released as a final completed version, Greenfly 2.0, after reviewing and updating the background life cycle inventory datasets. This should have been my major project during my internship at the Centre for Design. It turned out that more work has to be done, before a final version could be released.

In the second week of my internship we had a meeting about the progress of the development of Greenfly together with some people from the computer science department at the RMIT University. Two conclusions came out of that meeting; the first was that a test plan had to be written to check for bugs and browser compatibility in the current version of Greenfly. The second was that the long term maintenance of the website is a big issue. There was not someone dedicated to this task.

I have written a test plan and did some debugging and browser compatibility tests. The long term maintenance of the website was however a bigger issue. More work needed also to be done on solving bugs in the code. This had to be addressed before the background LCI datasets needed to be reviewed and updated. This implied that I could not do much regarding Greenfly. The Centre for Design has now joined forces with the computer science department of the RMIT University to further develop Greenfly. A group of computer science students are working on rewriting the code to develop and upgrade Greenfly into Greenfly 2.0. It can be concluded that there is a good potential for this online tool, but some work needs to be done before it can released as a final version.

CH. 5.2 - LAND USE CHANGE VALUES FOR CARBON STOCKS

A small project were I was involved in was about the calculation of land use change values for carbon stocks. I first assisted in this project, entering climate and soil data in Excel, but eventually I also set up the formulas and calculations in Excel and came up with results.

There is report available where the land use change values are calculated for several countries (BSI/Carbon Trust, 2011). These values needed also to be calculated for other countries, as part of the development work on PIQET, These countries are China, Japan, Mexico and New

Zealand and an Europe's average. The countries accounted for Europe are the countries that PIQET defines as Europe.

The purpose was to carry out the same calculations as done by Carbon Trust and to come up with the land use change values for the countries mentioned. The guidelines for these calculations are defined in (European Commission, 2010). The following land use change values needed to be determined

- From annual cropland to forest land
- From annual cropland to grassland
- From perennial cropland to forest land
- From perennial cropland to grassland

The land use change values are calculated as follows (Renewable Fuels Agency, 2011)

$$e_I = (CS_R - CS_A) \cdot 3.664 \cdot \frac{1}{20} \cdot \frac{1}{P} - e_B \tag{12}$$

where CS_R is the carbon stocks for the reference land and CS_A is the carbon stocks for the actual land. The factor 3.664 is the quotient of the molecular weight of carbon dioxide (CO_2) divided by the molecular weight of carbon (C) and the factor $1/20$ refers to the annualising over a 20 year period. The factor $\frac{1}{P} - e_B$ is not taken into account in the calculations, because the results Carbon Trust did not included this factor in their results. As the purpose was to come up with similar results for other countries, this factor is left out.

For the calculation of CS_R and CS_A the following rule applies (European Commission, 2010)

$$CS_i = (SOC + C_{VEG}) \cdot A \tag{13}$$

where CS_i is the carbon stock per unit area associated with the land use i, i.e. actual and reference. SOC is the soil organic carbon, C_{VEG} is the above and below ground vegetation carbon stock and A is a factor scaling to the area concerned, which is one in this case. For the calculation of SOC the following rule may be used

$$SOC = SOC_{ST} \cdot F_{LU} \cdot F_{MG} \cdot F_l \tag{14}$$

where SOC_{ST} is the standard soil organic carbon in the 0-30 centimetre topsoil layer, F_{LU} is a factor associated with the type of land use, F_{MG} is a factor associated with the principle management practice and F_l is a factor associated with the carbon input to the soil.

The value of SOC_{ST} in formula (12) is dependent on a combination of the climate region and the soil type of the area concerned. The European Commission report provides figures with the different climate regions and soil types in the world. A figure for the climate regions is shown in Figure 10, where each colour represents a different climate type. A similar figure is available for the soil type per area.

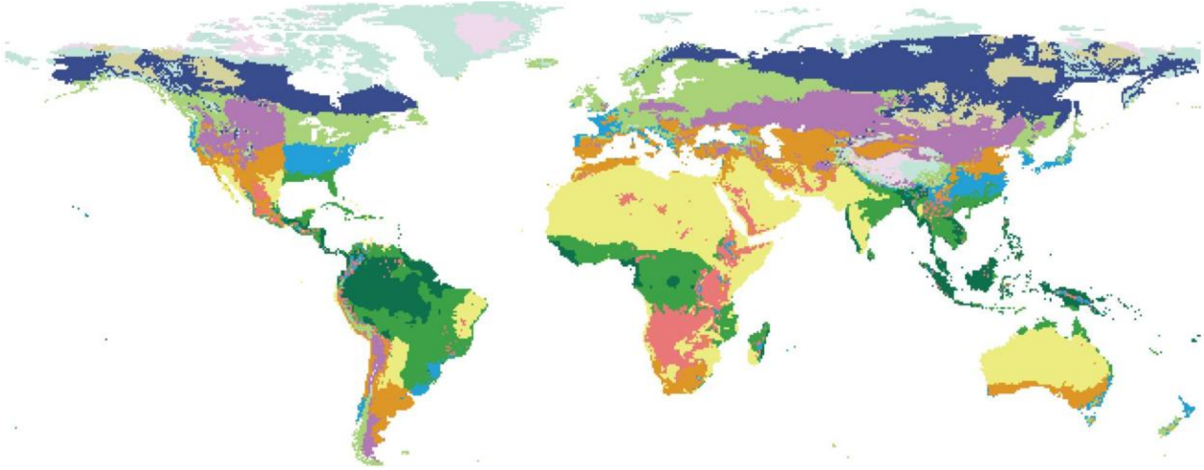

Figure 10 Climate regions

Although the information about climate and soil is thus available, it is not in a very useful form for calculations. We wanted the climate and soil data in Excel. We did this by importing the climate and soil figures in Excel, making them transparent such that the grid of cells was still visible. Now we were able to enter the soil and climate data within each cell of Excel, corresponding to an area on the figure. The grid was fixed, square and with the same resolution for all countries. As an indication, the grid for China counted approximately 5000 cells.

The value for SOC_{ST} could now be determined, knowing the climate and soil type for each area per country. Next the carbon stock per unit area C_{VEG}, associated with the land use, had to be determined. This value depends on the type of land use and the climate type. Values for this can be found in (European Commission, 2010). The vegetation values for forest land are countries averages, which can be found at (Metadata and data sources, 2012).

The only thing that remains is the determination of the management and input factors for each type of land use, see formula (14). In (European Commission, 2010) all the management and input factors are given for each type of land use and climate region, but it is not clear how to apply them. In total, there are 33 possible combinations of land use, management and input factors per climate type, which are also quite sensitive to the end result. We contacted Carbon Trust, about how they came up with the land use change values and how they handled the management and input factors but they were not transparent in this and actually did not come up with a proper answer. The best result we could come up with was averaging all possible combinations of management and input factors given a type of land use. Figure 11 graphically shows the change in carbon stocks for the land use change from forest land to annual cropland for Mexico.

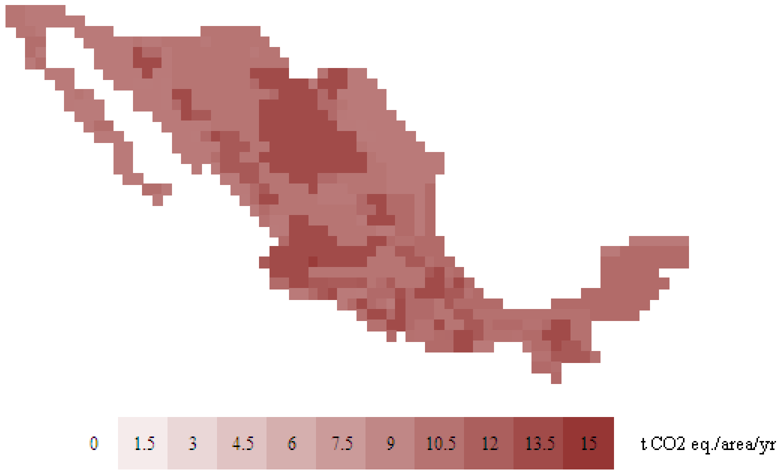

Figure 11 Land use change values for carbon stocks for Mexico.

All land use change values for carbon stocks for the countries China, Japan, Mexico and New Zealand and Europe are shown in Table 8. These are the values for the average outcome per country. Note that the average outcome is taken for all possible combinations of management and input factors.

Table 8 Land use change values for carbon stocks

Country	Current land use	Previous land use	GHG emmissions [t CO2 eq/ha/yr]
China	Annual cropland	Forest land	9.8
		Grassland	2.8
	Perennial cropland	Forest land	-0.5
		Grassland	-7.5
Europe	Annual cropland	Forest land	32.1
		Grassland	3.8
	Perennial cropland	Forest land	19.6
		Grassland	-8.6
Japan	Annual cropland	Forest land	24.9
		Grassland	4.8
	Perennial cropland	Forest land	11.3
		Grassland	-8.8
Mexico	Annual cropland	Forest land	11.2
		Grassland	4.3
	Perennial cropland	Forest land	1.4
		Grassland	-5.5
New Zealand	Annual cropland	Forest land	53.5
		Grassland	4.3
	Perennial cropland	Forest land	40.7
		Grassland	-8.5

CH. 5.3 - CAPABILITIES AND LIMITATIONS OF OPENLCA

I started my internship with a small project which was about exploring the features and capabilities of openLCA. openLCA is a freely available open source software for life cycle assessments. The purpose of exploring the software was to examine whether it could be used in student courses about life cycle assessment at the RMIT University. Now SimaPro software is used, but a major drawback of using this is that students are limited to use the software due to license restrictions. I have rewritten a tutorial about a comparison LCA study between a KeepCup and a typical disposal coffee cup over their entire life cycle, for modelling this in openLCA instead of SimaPro.

CH. 5.3.1 - LCA MODELS IN OPENLCA

Features of openLCA are

- import and export for EcoSpold and ELCD format
- goal and scope, inventory, impact assessment, and interpretation are covered
- graphical modelling of product systems
- Sankey and piece diagrams for visualising the effects of processes in the network on the overall result

- parameters on various levels, from process to project
- different allocation methods and system expansion modelling

The two most important elements in openLCA to build a model are ‘flows’ and ‘processes’. Processes illustrate the production or a modification of a substance or product. Two processes can be connected to each other by defining the output flow of one process, as the input flow for another process. There are three types of flows; elementary flows, product flows and waste flows. A product system is needed to actually model and calculate case studies. Basically, a product system is a network of processes, connected to the reference process, which has the required flow as output, i.e. functional unit. You need a project if you want to compare different products systems regarding.

An overview of the graphical modeller is show in Figure 12, where the life cycle model for the KeepCup study is shown. Note that the waste is modelled as input. This allows the reference output to bear the whole waste burden.

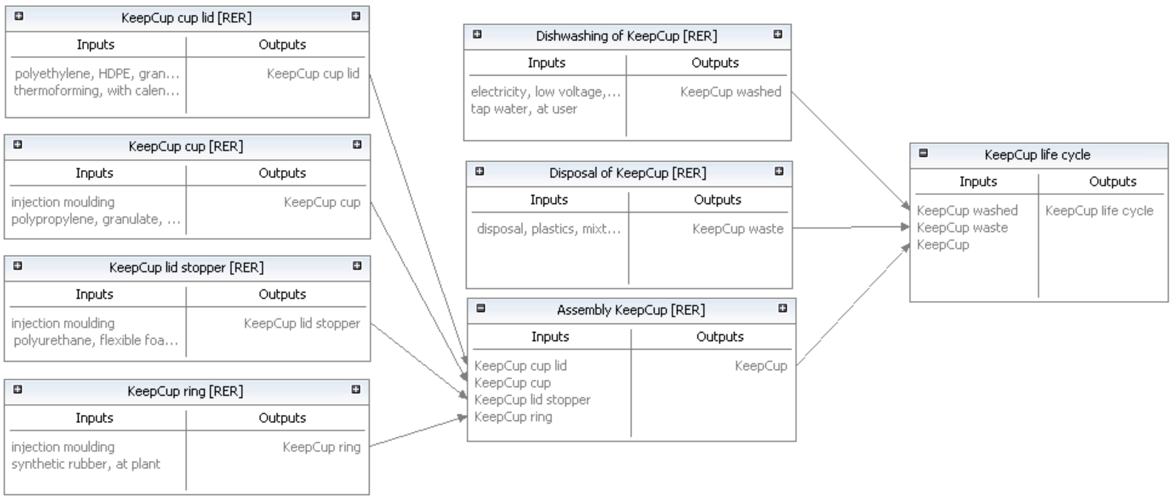

Figure 12 The modelling of a KeepCup life cycle in openLCA software

CH. 5.3.2 - CONCLUSIONS

The first conclusion is that openLCA is not compatible with the Australian LCI database. I struggled quite a lot to get it working, but there seems to be a problem with either how the Australian database is structured or how openLCA imports the database. Differences in the Australian database compared to the ecoinvent database include the use of multi output processes, avoided products and a lot of the values are parameterised. I have tried importing the Australian database from a CSV file with all values converted to constants, but that does not solve the problem. At first it seems that openLCA imports it well, but the calculations will not work. The sequential calculation solver does give results, but they are not correct. The matrix calculation method in openLCA is not even able to solve the inventory problem, which probably means that the process matrix is singular and at least one of the equations has no solution.

The second conclusion is that openLCA is compatible with the ecoinvent database. All features work quite well but the calculations run very slowly. Calculation time can even be more than three times of the calculation time in SimaPro. The program is also not very responsive. Even loading one single process card can take between 10 to 20 seconds. openLCA allows to adjust the settings for RAM allocation, but that does not make it must faster.

A more subjective conclusion is that modelling in openLCA is not very intuitive. It can also be quite annoying to adjust processes within a product system. You have to build your product system bottom up, but it can be troublesome to adjust processes down the chain. The program does namely not allow you to delete reference flows or processes that are linked upstream.

CH. 6 - DISCUSSION

The majority of the projects described in this report are somehow related to development work on streamlined life cycle assessment tools. The developed substitution tool can already be used to modify background databases and to speed up processes. The MATLAB LCA tool is a first exploration to incorporate uncertainty in streamlined life cycle assessment tools.

The developed tools give also rise to new opportunities or innovation in the field of LCA. The potential of the SimaPro COM interface is for instance larger than only substituting processes in a database. One could think of making the SimaPro database more dynamically or to extend the power of SimaPro to other software programs like Excel or MATLAB.

The MATLAB LCA tool has also potential. The computational power of MATLAB can be used to decrease the calculation time of computational intensive calculations. Besides Monte Carlo simulations, the tool can also be used to run batch analyses of products. When it is further developed, it can be a full LCA software package. Because MATLAB is used in most engineering environments, it could be a powerful tool in the design process.

The results of the benchmarking of products on their degree of uncertainty and reliability might also be interesting for new development work on Greenfly. It will be interesting to incorporate uncertainty in streamlined life cycle assessment tools. This report describes the first steps towards that.

CH. 7 - CONCLUSIONS

The developed substitution tool can be used to substitute processes in a SimaPro databases. It takes less than half an hour to substitute processes in an ecoinvent 2.2 database containing about 4000 products. Besides substituting processes, the tool can also adjust the uncertainty parameters that might accompany with substituting processes. The tool is only compatible with the ecoinvent database.

The developed MATLAB LCA tool can perform LCA analysis and Monte Carlo simulations using an ecoinvent 2.2 database. The tool performs more than 100 times faster than SimaPro. The coefficient of variation can be calculated per impact category for each product in an ecoinvent 2.2 database. This coefficient of variation is a quality indicator per impact category of a product.

Using generic geographical processes in a LCI database affects the uncertainty and reliability of a life cycle assessment. The coefficient of variation for carbon dioxide emissions for a product can almost double when switching between geographical electricity grids.

Further development needs to been done on Greenfly, before it can be released as a final version. The online tool still contains bugs, which need to be fixed. Also the long term maintenance of the website is an issue what need to be addressed.

The land use change values for carbon stocks for the countries China, Europe, Japan, Mexico and New Zealand have been calculated. The procedure to calculate these values need to be validated, before the numbers can be used.

openLCA software is not compatible with the Australian LCI database. It is compatible with the ecoinvent database and all features work well. The calculations are quite time consuming compared to SimaPro.

CH. 8 - RECOMMENDATIONS

The tool cannot 'read' in the SimaPro database -using the COM interface- which probability distribution is defined for a process. Now it is assumed that all distributions are lognormal. It needs to be investigated how the COM interface can be used to determine the kind of probability distribution defined for a process.

The substitution tool can be used to feed in generic processes in a LCI database. It is not very clear how the pedigree matrix needs to be adjusted when generic processes are substituted. Generic processes are substituted to be able to quickly change between geographic areas. The geographic correlation –in the pedigree matrix- is therefore 'data from unknown or distinctly different area'. One could however argue that technological correlation is also affected by the geographic area. How much this is affected and how this will change has to be investigated further more.

The MATLAB LCA tool can now only import an ecoinvent database. The code for importing a database needs to be enhanced to be able to import other databases. The code behind the calculations of the analysis and the Monte Carlo simulations also need to be developed in order to work with other databases. Allocation and avoided products are not supported yet. Also, the Monte Carlo simulations only work with lognormal distribution. Functionality to incorporate other distributions like uniform and triangle distributions need to be added.

How the coefficient of variation -per impact category- of a product could be useful to the user needs to be addressed. A solution might be a star rating, but how that will say something about the uncertainty of a product system will be interesting to investigate.

Regarding the work conducted on the minor projects: it would be valuable to incorporate uncertainty in Greenfly. The work described in this report might be useful for this. The procedure for calculated the land use change values for carbon stocks need to be validated. And about openLCA: the efficiency of the calculations needs to be increased, because calculation time is large and the program is not very responsive. It would also be nice to see compatibility with more LCI databases.

CH. 9 - REFERENCES

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A I - BASIC UNCERTAINTY FACTORS

Basic uncertainty factors from (Goedkoop, Schryver, & Oele, 2008).

generic uncertainty of exhanges:	**Code**	U_b
demand of:		
thermal energy	1	1.05
electricity	2	1.05
semi-finished products	3	1.05
working materials	4	1.05
transport services	5	2.00
waste treamtent services	6	1.05
Land use, occupation	7	1.50
Land use, transformation	8	2.00
Infrastructure	9	3.00
resources:	10	1.05
primary energy carriers	11	1.05
metals, salts,	12	1.05
emission to air of:	13	1.05
CO2	14	1.05
SO2	15	1.05
From combustion: NOx, NMVOC total, methane, N2O and NH3	16	1.50
From combustion: CO	17	5.00
From combustion: individual hydrocarbons, TSM	18	1.50
From combustion: PM10	19	2.00
From combustion: PM2.5	20	3.00
From combustion: polycyclic aromatic hydrocarbons (PAH)	21	3.00
From combustion: heavy metals	22	5.00
Process emissions: individual VOCs	23	2.00
Process emissions: CO2	24	1.05
Process emissions: TSM	25	1.50
Process emissions: PM10	26	2.00
Process emissions: PM2.5	27	3.00
From agriculture: CH4, NH3	28	1.20
From agriculture: N2O, NOx	29	1.40
Radionuclides (e.g. Radon)	30	3.00
Process emissions: other inorganic emissions	31	1.50
emission to water of:		
BOD, COD, DOC, TOC	32	1.50
inorganic compounds (NH4, PO4, NO3, Cl, Na etc.)	33	1.50
individual hydrocarbons, PAH	34	3.00
heavy metals	35	5.00
From agriculture: NO3, PO4	36	1.50
From agriculture: heavy metals	37	1.80
From agriculture: pesticides	38	1.50
Radionuclides	39	3.00
emission to soil of:	40	1.05
oil, hydrocarbon total	41	1.50

pesticides	42	1.20
heavy metals	43	1.50
Radionuclides	44	3.00

A II - GUIDE TO THE SUBSTITUTION TOOL

File: SimaPro processes sub.xls

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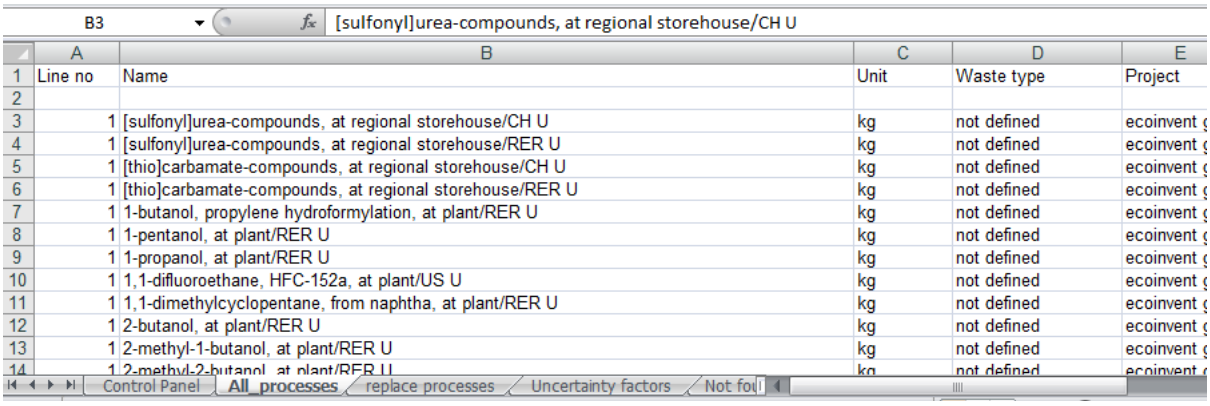
CAPABILITIES

The file contains a macro called 'processes_sub', written in Virtual Basic for Applications, which uses the SimaPro COM interface (Gelder & Moore, March 2010) to substitute processes in the SimaPro database. It has been written to 'feed in' generic processes in a database. What the macro basically does is searching within every process card that is specified, whether it can find an electricity or natural gas process card and if so, it substitutes that card with a generic equivalent. When generic processes are substituted in a process card, the name of the process card is changed to include a string 'GENERAL' and all the uncertainty information of all the processes and substances within that process card is increased by changing the pedigree matrix to account for the fact that it is now a general process card with one or more generic processes.

STRUCTURE

The Excel file contains several sheets were the user can give input to the macro. The most important are the sheets: 'control panel', 'All_processes' and 'replace processes'.


B3 [sulfonyl]urea-compounds, at regional storehouse/CH U

	A	B	C	D	E
1	Line no	Name	Unit	Waste type	Project
2					
3	1	[sulfonyl]urea-compounds, at regional storehouse/CH U	kg	not defined	ecoinvent
4	1	[sulfonyl]urea-compounds, at regional storehouse/RER U	kg	not defined	ecoinvent
5	1	[thio]carbamate-compounds, at regional storehouse/CH U	kg	not defined	ecoinvent
6	1	[thio]carbamate-compounds, at regional storehouse/RER U	kg	not defined	ecoinvent
7	1	1-butanol, propylene hydroformylation, at plant/RER U	kg	not defined	ecoinvent
8	1	1-pentanol, at plant/RER U	kg	not defined	ecoinvent
9	1	1-propanol, at plant/RER U	kg	not defined	ecoinvent
10	1	1,1-difluoroethane, HFC-152a, at plant/US U	kg	not defined	ecoinvent
11	1	1,1-dimethylcyclopentane, from naphtha, at plant/RER U	kg	not defined	ecoinvent
12	1	2-butanol, at plant/RER U	kg	not defined	ecoinvent
13	1	2-methyl-1-butanol, at plant/RER U	kg	not defined	ecoinvent
14	1	2-methyl-2-butanol, at plant/RER U	kg	not defined	ecoinvent

Control Panel | All_processes | replace processes | Uncertainty factors | Not fou

CONTROL PANEL

In the sheet 'control panel' information must be given about the SimaPro database and it must be specified how the data in the sheets 'all processes' and 'replace processes' is organised, e.g. start row and end row. The information under DATABASE DETAILS speaks for themselves. Under ALL PROCESSES it must be specified what the first row and last row in the sheet ‘All processes’, i.e. the rows with processes. Under REPLACE PROCESSES information must be given about which processes must be replaced and what the substitution processes are. See for example the figure below.

In this setup, there are four substitutions; the processes specified in the rows 3 to 71 in the sheet ‘replace processes’ will be substituted with the process ‘Generic electricity grid, high voltage/PIQET’ The generic process card will be added in the ‘TProcessPart’ ‘Electricity/Heat’ (=2) and the process is of type ‘Energy’ (=1). For the reference of these numbers see (Gelder & Moore, March 2010).

The second sub replaces the processes specified in the rows 72 to 138 in the sheet ‘replace processes’ with the process ‘generic electricity grid, low voltage/ PIQET’. Etc.

DATABASE DETAILS		
	Server	local server
	Alias	D:\GENERAL DATABASE
	Database	ecoinvent_general_test2
	Username	
	Password	
	Project name	general
	Method location	
	Method name	
	Output	
ALL PROCESSES		
	First row	3
	Last row	3582
REPLACE PROCESSES		
	number of substitutions	4
sub 1	begin row	3
	end row	71
	name general processes	Generic electricity grid, high voltage/PIQET
	TProcessPart	2
	TProcessType	1
sub 2	begin row	72
	end row	138
	name general processes	Generic electricity grid, low voltage/PIQET
	TProcessPart	2
	TProcessType	1
sub 3	begin row	139
	end row	206
	name general processes	Generic electricity grid, medium voltage/PIQET
	TProcessPart	2
	TProcessType	1
sub 4	begin row	207
	end row	218
	name general processes	Generic natural gas/PIQET
	TProcessPart	2
	TProcessType	1

UNCERTAINTY FACTORS

The macro changes the pedigree matrix for each process in a process card that contains a generic process. So if a substitution has been made, all the uncertainty information will be changed. The sheet ‘uncertainty factors’ is used as a lookup table for the uncertainty factors. In the macro the square of the geometric standard deviation is calculated as follows

$$SD^2{}_{g95} = \sigma_g^2 = e^{\sqrt{\ln^2(U_1)+\ln^2(U_2)+\ln^2(U_3)+\ln^2(U_4)+\ln^2(U_5)+\ln^2(U_6)+\ln^2(U_b)}}$$

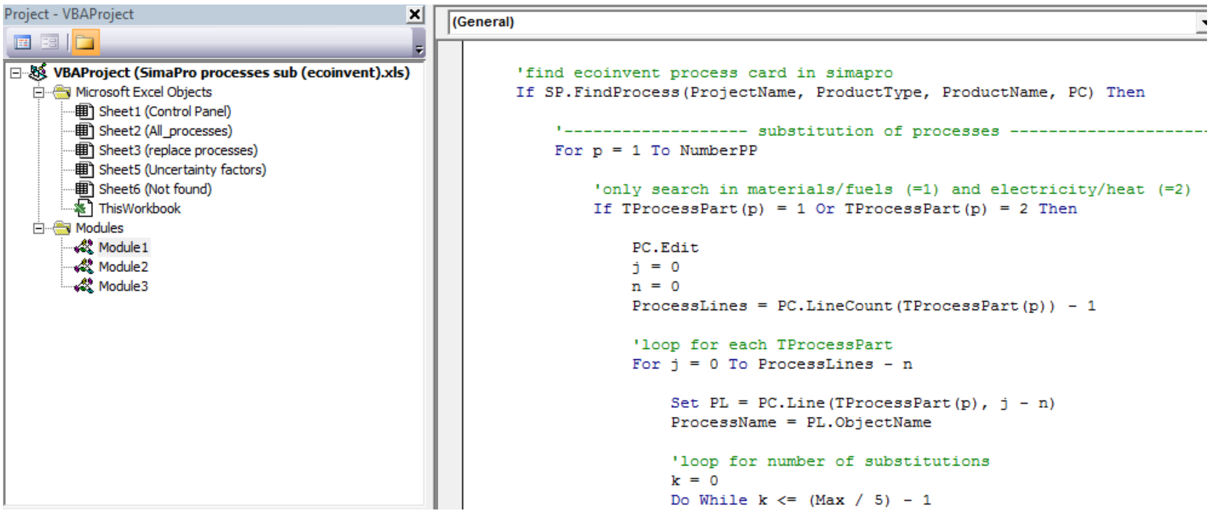
Were U1-U6 are derived from the pedigree matrix, and Ub is the basic uncertainty factor. The factor U4 (geographical correlation) is changed to 1.10 for all general processes. For more information about the pedigree matrix see (Rolf Frischknecht; Jungbluth, Niels; Althaus, Hans-Jörg; Doka, Gabor; Dones, Roberto; Heck, Thomas et. al., December 2007) and (Goedkoop, Schryver, & Oele, 2008).

RUNNING THE MACRO

1) Export a list of all processes from the SimaPro database and put them in the sheet ‘all processes’. The names must be in the second column and the type of process must be in column 8!
2) Remove the processes were you don’t want to substitute processes. e.g. if you want to substitute a generic electricity grid, you don’t want that this will be substituted in electricity processes. Also take care that the substitution processes itself are not in this list.
3) Export a list of processes that must be substituted (by their generic equivalents) and put them in the sheet ‘replace processes’. Enter the database details in the sheet ‘control panel’
4) Specify the start and end row in the sheet ‘control panel’ (for all processes)
5) Specify the number of substitutions in the sheet ‘control panel’
6) For each substitution, specify the start row, end row, name of substitution process, in which field this process must be added (e.g. ‘electricity/heat’) and what type of processes it is (e.g. Energy). There can be as many subs as you want, as long as it is properly specified.
7) Check that the processes to be substituted are in the SimaPro database
8) Run the macro, you can see the progress in the excel status bar.

THE CODE

The first loop is to loop over all the processes. A process is ‘picked’ from the sheet all processes and the function ‘SP.Findprocesses’ finds this process in the database and stores it in the object ‘PC’. Then there are two for-loops. The first loop is the substitution loop (it only searches in the fields Materials/Fuels and Electricity/Heat, but this can be adjusted), the second loops only runs if changed = true (so if a substitution has been made) and this loop changes all the uncertainty in the fields as defined in the array TprocessPart.



The substitution loop: process card is set in edit mode. The number of process lines is determined for the current field (e.g. materials/ fuels). Then there is a loop for each process line. The name of a process is stored in ProcessName. Then there is another loop '*Do While k <= (Max / 5) – 1*' which is a loop for each substitution. This searches if a replaces process matches the ProcessName. If so, it deletes the replace process and adds the substitution process in the field as defined in the control panel. If a pedigree is specified in the comment, the function ChangePedigree is called to change the pedigree. The function 'ChangePedigree' can be found in Module 2. If a standard deviation is specified, the distribution is set to LogNormal. This is because it is not (yet) possible to know what the distribution is by using the COM interface. Probably you need to add a library as reference in Virtual Basic. For the ecoinvent database this can however be assumed. Then the standard deviation is calculated by calling the function 'standarddeviation'. The OldComment is given as input to this function, but within this function the pedigree matrix is also changed, so it returns the standard deviation based on the new pedigree matrix

Change pedigree loop: this loop only runs if changed = true. So if you don't want this to run, just add changed= false, just before this block of code. Basically what is does is changing each standard deviation for each process. (as defined in the array TprocessPart)

Notes:

- The macro can only deal with lognormal
- The SimaPro and borland standard VCL type library must be added in the reference list in VBA. Tools→references: add 'Borland standard VCL type library' (stdvcl32.dll) and add 'SimaPro library'.

A III - GUIDE FOR MATLAB LCA TOOL

Folder: MATLAB LCA
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In the folder MATLAB LCA, there are three folders:

- Australian database
- Ecoinvent
- Ecoinvent CSV import

All the three folders contain MATLAB files which basically have the same functionalities, these are

- Import a life cycle inventory database and an impact assessment method
- running a Life Cycle Assessment analysis and show characterised result
- performing a Monte Carlo analysis for each impact category

The major difference between the folders is the way the LCI database and IAM are imported. The folders 'Australian database' and 'Ecoinvent' use the process matrix export from SimaPro to build the process matrix and the SimaPro COM interface is used to get all the uncertainty information (standard deviation). The folder 'Ecoinvent CSV import' contains MATLAB files which can read a entire CSV database file in once (thus process matrix and matrix with standard deviations are build in once) and also a CSV with the IAM be read in once. A brief overview of their capabilities is shown below

Folder 'Australian database':
It imports the AustralasianLCI_2011_10N and the Australian indicator set 2.01 IAM. The file *CreateAndSaveProcessMatrix.m* imports the process matrix from the file processmatrixAUS.xlsx, which is an export from simapro (File→Export to Matrix). The file *CreateAndSaveCharacterisationMatrix.m* imports the Australian indicator set 2.01 IAM from the folder 'Impact Categories'. Within the folder Impact Categories, where each impact category is saved in a separate excel file. There is also a file 'All_substances.xlsx' which is needed to build the characterisation matrix. The function *characterisationvector.m* is called to actually 'build' the characterisation matrix. The file *CreateAndSaveVarianceMatrix.m* imports the matrix with standard deviations from the file Get_uncertaintyAUS.xlsx. This file contains a macro which uses the SimaPro COM interface to read all the uncertainty information from the database. How it works is explained later. The file *MAIN.m* is the

matlab file that performs the LCA and Monte Carlo analysis. It loads the processmatrix, the characterisationmatrix and the variancematrix.

Folder 'Ecoinvent':

It imports the ecoinvent 2.2 LCI database and both the australian indicator and PIQET v4 IAM can be imported and loaded. The ecoinvent database is much larger (about 4000 processes) than the australian database (about 1000 processes) and therefore the scripts had to be adjusted because of memory issues. The matrices are now imported in submatrices and concatenated afterwards. Regarding the import of an IAM: the file *CreateAndSaveCharacterisationMatrix_AustralianIndicator.m* is the same as in the folder Australian database. The file *CreateAndSaveCharacterisationMatrix_PIQET_CSVimport.m* imports the PIQET IAM from a single comma separated CSV file. Both scripts save the characterisation matrix in *CharacterisationMatrix.mat* So before running the MAIN.m file, you have to run either one of these scripts to import an IAM. The MAIN.m file loads a graphical user interface for the Monte Carlo analysis (popup.m)

Folder Ecoinvent CSV import:

This folder contains a new file compared to the folder 'Ecoinvent' and that is the file *DatabaseImport.m.* This file reads a comma separated CSV file containing a LCI database (export from SimaPro). The advantage of this is that both the process matrix and the matrix with standard deviations are build 'at once' and the SimaPro COM interface is therefore not needed anymore. The CSV file containing the LCI database must be in the folder 'Databases'. Also a file Substances.xls is needed. This is the list of all substances with compartments, sub compartments and units exactly the same as in the processes matrix export from SimaPro. Limitations of this script are:

- no avoided processes possible
- no multi output and allocation
- only lognormal distribution
- no parameters and their distributions (only constants)

For the ecoinvent database these limitations are no problem, this is however a problem for the Australasian LCI.

Procedure for Ecoinvent CSV import folder

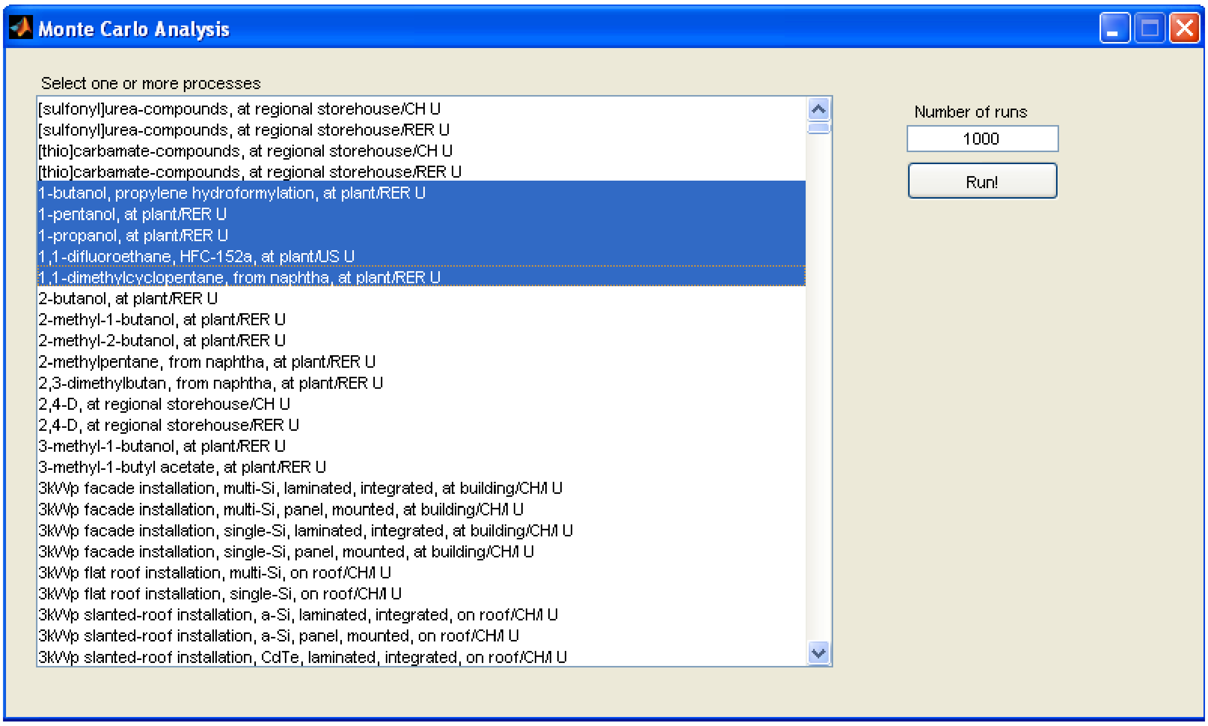
De database is imported in the first lines of the script

```
%load database
load('ecoinvent22_db.mat')
```

The file ‘ecoinvent22_db.mat’ is created by the file ImportDatabase.m. The final demand vector for the analysis (characterisation) is created at

```
%define output vector
f=zeros(size(A,1),1);
f(2,1)=1;
```

There is a graphical user interface for the Monte Carlo analysis, see figure below. Select as many processes as you want, or select all (ctrl+A), give the number of runs and press ‘Run!’. The coefficient of variation for each process is saved in the variable ‘CV’. The distribution of the last calculated process is saved in the variable ‘H’ for each impact category. The variable ‘processes’ contains all the names of the processes



Note: The process “Sulphate pulp, from eucalyptus ssp. (SFM), unbleached, at pulpmill/TH U GENERAL” has two inputs of medium electricity with the same amount. When a generic electricity grid is feed in to this process, it gives the following result:

Known inputs from technosphere (electricity/heat)

Name	Amount	Unit
Generic electricity grid, medium voltage/PIQET	-0.238	kWh
Generic electricity grid, medium voltage/PIQET	0.238	kWh

So, the net amount in the process matrix is zero and therefore the same element in the matrix with uncertainty has also to be zero. Therefore the following code is added.

```
var_A(1802,3598)=0;     %Electricity drops out
```

This needs to be active for the following databases

```
'ecoinvent_general_indonesiagrid.mat
'ecoinvent_general_europegrid.mat
```

It is a bit tricky workaround, but it works. A better solution would of course be improving the code.

Procedure to import database and uncertainty information (<u>without</u> CSV import script)

The following procedure is only for the folders Australian database and ecoinvent! It shows how to import the process matrix and how to import the matrix with uncertainty.

1) Export process matrix from SimaPro (File→Export to matrix). There are a lot of empty rows and columns in these matrix, delete these rows and columns.
2) The file CreateAndSaveProcessMatrix.m imports the matrix in step (1). Check for empty cells in the most upper left and lower right corner of each submatrix that is imported. So for example

```
A1 =
sparse(xlsread('processmatrixECO.XLSX','Sheet1','E7:FDE1000'))
;
```

   So check cells E7 and FDE1000, if they are empty, put a value in that cell. After the import, the most upper left and lower right element of the matrix have to be deleted, that is

```
A1(1,1)=0;    A1(size(A1,1),size(A1,2))=0;
```

3) Run CreateAndSaveProcessMatrix.m, the process matrix is stored in ProcessMatrix.mat

Now the uncertainty matrix is build using the file get_uncertainty.xlsm. This contains a macro that communicates with SimaPro through the COM interface.

4) Export a list of all processes from SimaPro (summary)
5) Copy and Paste this list of all processes in the sheet 'all_processes' in the file Get_uncertainty. Check that the names are in column 2 and the type of process is in column 7.

6) Copy and paste the process matrix as in step (1) in the sheet 'uncertainty_matrix' in the file Get_uncertainty.
7) Run the macro sub: setAllUncertaintyToOne. Check that the proper range is specified within the macro code. That is the range of the matrix. The reason for doing this is that the matrix with uncertainty has now the same size and number of elements as the process matrix.
8) In the sheet 'control panel', check the settings for the database details and the first and last row of all processes.
9) Run the macro sub getAndStoreUncertainty. This might take a while; the progress can be seen in the status bar.

Now the matlab file CreateAndSaveVariance.m is used to import the matrix in the excel file Get_uncertainty.

10) Run the matlab script CreateAndSaveVariance.m. The script is basically the same as in step (2) for the process matrix, so also for this yields: check the corners of the submatrices if they are empty.
11) Run the matlab script CreateAndSaveCharacterisationMatrix.m to import the IAM.

Note: Australian database→Process card: "Quickline, in pieces…" has a space character at end of the name. this space must be removed, otherwise the macro cannot find this process.