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Ecotoxicity in LCA – A review of methods and an assessment of the ecotoxic impact of pesticide use in Swedish winter wheat and Brazilian soybean production.

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Summary

This study gave a review of some of the existing life cycle assessment (LCA) methods focusing on ecotoxicity, and made assessments of the ecotoxic impact of pesticide use in an example Swedish winter wheat field from a 2005 inventory and an example Brazilian soybean production field. Pesticides are used worldwide within agriculture and are under constant development aiming to increase the control of unwanted weeds, fungi and insects etc. Regulation occurs worldwide at various levels but the global usage of herbicides and insecticides etc. brings concern for the health of the environment from exposure to toxic substances. Although human toxicity is of equal importance, this thesis looked at ecotoxicity as an impact category within LCA. Currently ecotoxicity impact assessment within LCA is a difficult task due to a multitude of factors to consider, such as the vast number of active ingredients, which can cause impacts at a single organismal level or communal level, acting individually or synergistically. The consensus of a single method and subsequent impact unit to use has not been met globally, making ecotoxicity evermore harder to assess. In this thesis, assessment methods were compared on several aspects with the aim to choose one for use on the following two case studies. The results from the comparison and other factors presented USEtox as the method to continue with for the two case studies. A field in Egonsborg was chosen as the example Swedish wheat field as farmer practices were known, giving realism to the assessment on pesticide use and dosage. For the Brazilian soybean assessment the area of Mato Grosso, known for its extensive soybean farms and production was chosen. Although dosages were known for the Mato Grosso area, confidentiality in farmer practices meant an estimate on the combination of pesticides used had to be applied for the assessment. Results of this report bring to light the difficulty in directly comparing LCA methods showing how the number of active substances each method can assess differs greatly as well as the characterised unit and how the characterisation factors are derived. Points where LCA lacks and improvements could occur would be e.g. the assumption of linearity of substance exposure as background volumes or potential threshold levels of substances in the environment are not currently considered. The toxicity of winter wheat and soybean production is presented as 0.28 CTUe/kg and 1.3 CTUe/kg respectively although these results are not intended to be directly compared due to assumptions made on specific pesticide use on the example soybean field. Within the discussion the thesis questions are discussed and the current state of ecotoxicity in LCA is reviewed. Topics of method comparison and validation are examined as well as how farming habits, climate and geographical differences influence the intensity of an ecotoxic impact of pesticides. The thesis closes with ideas for future development, briefly describing other assessment methods such as risk assessment where aspects and ideas could be drawn from. Potential improvements such as those mentioned above are used in the suggestion of the creation of a transparent method for the assessment of ecotoxicity within an LCA of crop production.

Acknowledgements

CONTENTS

List of abbreviations:

2-4D	2,4-Dichlorophenoxyacetic acid
a.i	Active Ingredient
CDV	Critical Dilution Volume
CF	Characterisation Factor
CTUe	Comparative Toxic Units
DDT	Dichloro-diphenyl-trichloro-ethane
EC50	Effective Concentration for 50% of the Species
EEA	European Environmental Agency
EPA	Environmental Protection Agency
ERA	Environmental Risk Assessment
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
HC50	Hazardous Concentration for 50% of the Species
HCH	Hexachlorocyclohexane
ISO	International Organization for Standardisation
KEMI	Swedish National Chemicals Inspectorate
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
MCPA	2-methyl-4-chlorophenoxyacetic acid
MRI	Midwest Research Institute
PAF	Potentially Affected Fraction
PDF	Potential Disappeared Fraction
PNEC	Predicted No-Effect Concentration
PPD	PhysProp Database
PPDB	Pesticide Properties Database
RA	Risk Assessment
RED	Reregistration Eligibility Decision
SETAC	Society of Environmental Toxicology and Chemistry
SIK	Swedish Institute for Food and Biotechnology
SimaPro	System for Integrated Environmental Assessment of Products
SMILES	Simplified Molecular-Input Line-Entry Specification
TEG	Triethylene Glycol

1   Introduction

The historical background of pesticide use

Pesticides are used worldwide and are under constant development to counteract weed resistance or target additional species. Since around 4,500 years ago when the dusting of sulphur onto crops was practiced by the ancient Sumer in Mesopotamia (Miller 2004) the use of toxic substances has gone hand in hand with the large quantity production of harvestable plants. Regulations concerning pesticides differ from country to country around the globe and in the mass trade world of today it is inevitable that the pesticides produced will be used elsewhere in the world than in the place of creation. Due to the problems incurred by this the UN FAO created the International Code of Conduct on the Distribution and Use of Pesticides and implemented in 1985, subsequently updating it in 1998 and 2002 (Willson 1996).

In the history of pesticide use and regulation America has played a large role begging as early as 1901 where the state of California passed its first pesticide related law (CEPA 2001). In 1910 however was when America passed the Federal Insecticide Act by the federal government (Goldman. 2007). The 1940's is considered the start of the rise of the synthetic pesticide (Daly, Doyen et al. 1988); chemicals developed during wartime research were being rediscovered as having pesticide properties with the examples of chlorinated hydrocarbon (HCH) (Bowen 1952) and dichloro-diphenyl-trichloro-ethane (DDT) (Centers for Disease Control and Prevention). Between 1945 and 1950 the synthetic organic usage went from 45 thousand tons in 1945 to over 136 thousand tons (Finegan 1989). During the 20th century any pesticide legislation already created was updated and new regulations were developed. The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) was created in 1947 and has been updated many times as recently as 2007 (EPA).

Since 1965 when it became compulsory for handlers of acutely toxic pesticides in agriculture to complete a course to obtain a licence (Wiklund, Lindefors et al. 1988), the Swedish government has not stopped in lowering pesticide reliance and risk of exposure or to health. 1986 saw the Swedish government adopt a policy for the future reduction of pesticide use by weight and taking up of less hazardous pest management strategies, reported by Kemikalieinspektionen (Ekström and Bergkvist). As more concern grew about the environment the European Union increased its pesticide regulation and in 1990 formed the European Environmental Agency (EEA 2012) (European_Environment_Agency); now regulating Sweden since it became part of the EU in 1995.

Within Brazil there are regulatory federal agencies of Agriculture (MAPA), Health (ANVISA) and of the Environment (IBAMA), together handling policies and regulations concerning environmental topics such as pesticide registration and regulation having been about since 1909, 1999 and 1989 respectively. Although Brazil is said to have the most complete environmental legislations in the world the lack in enforcement of the laws in the past has compromised the overall effectiveness towards protection.

The ecotoxic problem

Damage at some level has always occurred from toxic substances entering the environment but it was not until 1960 that the true extent pesticides can impact an ecosystem was brought to the public eye through the book "Silent Spring" by Rachel Carson. Since then the field of ecological toxicology has been developed presenting a growing concern over the increase of toxicological substances within the environment. Pesticides are a large category of toxic

substances and are any substances or mixture of substances intended for preventing, destroying, repelling or mitigating any pest, such as plants (herbicides), fungi (fungicides) and insects (insecticides). This report looks at the three mentioned although there are substances against other organisms regarded as pests.

Aside from the many documented cases of human toxicity from pesticide use, notably Paraquat (EXTOXNET 1993) and Endosulfan (EXTOXNET 1993); the ecotoxic impacts affect individual organisms directly or indirectly with possible risk to entire populations or species. Studies have been conducted which in total give a general view on the ecotoxicological problems occurring from pesticide use, ranging from direct death from exposure as well as developmental and reproductive problems to subtle but just as damaging sub lethal changes (Balcomb 1984; Relyea and Hoverman 2006) (Baldwin, Spromberg et al. 2009). Indirectly, pesticides can have a much larger impact when they start affecting whole trophic levels in a food chain, the ramifications of eliminating a producer or prey species (Pimentel and Edwards 1982) could be a cascade of declining numbers of species due to the lack of food in the area (Poulin, Lefebvre et al. 2010).

In Sweden the use of phenoxy acid herbicides such as MCPA and 2,4-D has been increasing since first introduction in 1947 (Bäckström 1978). As the use of pesticides in Sweden shows no signs of long term decrease, fluctuating around 1.5 doses/ha[1] sold since the early 1980's (Kemikalieinspektionen & SCB, 2011, Växtskyddsmedel i jordbruket 2010. Statistiska meddelandenMI31 SM 1102), it is important to try to evaluate the effects pesticides have in the environment to have a better chance to reduce their negative impact.
The environmental effects caused by toxins can vary greatly, from the factors regarding a single substance, including its toxicity, the concentration reaching an organism and the time scale considered, to the lesser examined synergistic and other problems occurring when a mixture of chemicals interact with each other.

LCA

Life Cycle Assessment (LCA) is a methodology for assessing the environmental impacts of a product through its life cycle with one of the first being conducted, but unpublished, in 1969 by the Midwest Research Institute (MRI) for the Coca Cola Company. In order to gain this understanding the product is followed from 'cradle to grave' where each and every relevant step from raw material extraction, production and disposal are looked at with all the various inputs and outputs taken into consideration.
Depending on the product in question various impact categories are used to assess how the product will affect the environment. For example, how much land is used, the energy input and output, potential eutrophication effect and various gas emissions are some of the parameters used for assessment. By covering many important categories, as mentioned above, an LCA is an effective and commonly used way to assess the overall impact a product has on the environment. One point where an LCA lacks however is by its inability to illustrate the effect on the environment of using pesticides within production in a way accepted by all.

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[1] The quantity of active substance used per hectare, introduced by Statistics Sweden. SCB. and KEMI (2011). Plant protection products in Swedish agriculture. Number of hectare-doses in 2011 Final statistics.

Ecotoxicity handling within LCA

The ecotoxicity from chemicals is difficult to quantify using LCA due to, for example, the vast number of environmental effects caused by different chemicals. Unlike for example the assessment of energy consumption or global warming potential, there is no recognised consensus on the units to which results are presented and which environmental effects need to be included. (Reap, Roman et al. 2008) gives a good representation of how accurate assessment/representation is difficult to achieve within LCA, bringing light to things like data gaps in toxicity data, which are unlikely to be completely filled because of the sheer number of chemicals being used today.

From the mid 90's and through the following decade various LCA methods have been created or adapted allowing for the assessment of a substance's ecotoxic impact. Such methods include the EDIP methods (97/2003) (Wenzel, Hauschild et al. 1997) and (Hauschild and Wenzel 1998), IMPACT 2002 + (Jolliet, Margni et al. 2003), ReCiPe (Goedkoop M.J. 2009) and Eco-indicator (95-99) (Goedkoop 1995) among others. Even though these methods are all able to be used as standalone tools for assessment, software packages such as SimaPro used in this study (Consultants., Goedkoop et al. 2008) were developed for LCA practitioners. SimaPro groups such LCA methods together with a database of substances. Having the methods collected allows the user to either select the method best suited for the impact under investigation or easily run a product scenario with defined inputs and outputs through multiple methods, allowing for comparison of impact results of the same environmental impact category. Although there are many methods out there which have the capability to produce an environmental risk value for chemicals and substances, studies have shown that the variability between these values are high which gives an overall uncertainty of the true risk (Dreyer, Niemann et al. 2003).

2   Background

For a long time SIK has made LCAs on agricultural products with the impact categories most frequently analysed being energy use, acidification potential, eutrophication potential and climate change (formally global warming potential); ecotoxicity however has hardly been included. This is, for example, particularly a problem when conventional and organic agriculture is compared since pesticide usage is the principal difference between the two methods. What has been included is pesticide *use* and occasionally hectare doses which entails presenting the amounts of active ingredients used (grams/kg of product) of herbicide, fungicide and insecticide respectively. Pesticide use does not tell us anything about the frequency of pesticide application, since some pesticides are applied in a low dosage and some are applied in larger volumes throughout the course of crop production. Further, the amount of active ingredients does not give any information on the possible environmental effects from the pesticide use – one substance may be easily degraded, while others may be more persistent and stay harmful in the environment for a longer time. Ecotoxicity is an important impact category when assessing the environmental impact of all conventional agricultural products, since pesticide use is widespread in most agricultural systems of today.

In 2008, SIK published an LCA database on feed ingredients for conventional production (Emanuelsson, Flysjö et al. 2008). This database is successively updated and supplemented, and is used in most LCA's of animal production performed by SIK. The database contains both imported and domestically produced ingredients.

To be able to give a more complete view of the environmental impacts from food production, SIK needs a method which attempts to present how damaging a substance is with regards to the potential ecotoxicological impact it could cause should it be emitted at a predefined dose.

3   Aim and goal

Aim:
- Establish a transparent method which is accommodating to the ecotoxicity impact assessments, primarily of pesticide use within Life Cycle Assessments of crop production at SIK.

Goal:

- Present results for the ecotoxicity impact of pesticide use with Swedish winter wheat and Brazilian soybean production as case studies.

Questions:

- Which of the methods cover the most pesticides of interest in this study?
- Do the different LCA methods give similar results when estimating the ecotoxicity impact of the same pesticide use?
- What is the ecotoxicity impact of pesticide use in Swedish winter wheat production?
- What is the ecotoxicity impact of pesticide use in Brazilian soybean production?
- If the concordance between different methods is low; can the models be validated; are the results a good representation of the actual ecotoxicological impact to the environment?
- Is LCA a suitable method for assessing toxicity of pesticide use in agriculture?

3.1   Delimitations

Due to time constraints, the high volume of toxic substances and large number of LCA methods capable of expressing an ecotoxic impact had to be narrowed down. This report is limited to the coverage of only LCA methods which are available within the SimaPro (default v. 7.3) software and are also commonly used at SIK. As previous LCA studies at SIK have been only environmentally orientated the coverage of human toxicity has not been considered. With this report not being a full LCA of wheat and soybean production, substances used in preceding or processing methods such as fertiliser creation are not included; meaning solvents, fuels and metals among other substances will not be part of the total ecotoxic impact.

Key aspects when understanding an LCA method.

When assessing LCA methods it is important to be familiar with the terminology used; in doing so one is able to notice and understand where differences occur and to what extent they affect the results. Below are common concepts used in LCA described with example methods used in this report.

Compartmentalisation within LCA:

LCA models typically represent the environment as a group of compartments with the commonest being Air, Water and Soil (Mackay 1979). The complexity of the model also determines whether these compartments are further specified e.g. stratosphere/troposphere in the air or fresh/sea in the water compartment. Additional compartments may also be added such as the sediment or biota through which materials and energy is exchanged.

The Midpoint and Endpoint approach to LCA:

The scope of the LCA being carried out determines which results, either midpoint or endpoint, are the most useful. The midpoint technique involves looking at the hundreds of impacts to the environment as falling into environmental themes of interest such as acidification, toxicity or climate change based on their mechanism of impact. Midpoint categories are set between the emission inventory results and the endpoint issues of concern. The modelling is simpler in appliance than that of endpoint but can be difficult to interpret due to its inherent complexity though attempts to mimic reality.

The endpoint damage orientated approach groups all midpoint problems into larger damage categories such as human health, ecosystem quality and resources which are simplified representations of quality changes in reality. Due to its requirement for more complex models, the endpoint approach is more time consuming, at risk from uncertainties but gives simple to follow results allowing for easy comparison at an endpoint level e.g. human health impacts from climate change compared to those from toxicological exposure effects.

Spatial variation:

Within LCA are three levels of spatial differentiation, site-*generic*, site-*dependent* and site-*specific* which each require increasing levels of environmental information. The lowest level of spatial resolution is site-generic. Within this criterion no spatial differentiation about the source of the emission or receiving environments is considered. Increasing the resolution a little requires the practitioner to define the class of a source as well as the receiving environment to that source; for example if the source and receiving environment are defined as being within the range of 150-500km then the study will be spatially resolved to the levels of small countries or the regions within. It is this site-dependent level of spatial differentiation which is suggested for characterisation modelling within EDIP2003. The final and most detailed spatial differentiation works with sources of very local areas, for example a sewage treatment plant. By working at such proximity to the source the site-specific modelling gives the greatest accuracy but the receiving area may be at a considerably larger level, making the full impact difficult to calculate and define accurately. The choice to work at a specific resolution often has direct influence on impact categories governed by the geographical area the emission occurs in. The impact on human health for example, is directly linked to the population in the area defined by the spatial resolution chosen.

Characterisation factors:

A characterisation factor is a substance specific impact value calculated on the basis of how the substance interacts with the environment depending on its physiochemical properties. The factors are calculated per impact category per substance and are then multiplied with the mass of the substance emitted to calculate the relative contribution of that substance to the impact. For example, in ecotoxicity, specifically in the model IMPACT 2002+ the characterisation factor for triethylene glycol (TEG) is 1 where as the characterisation factor for DDT is 7.4. This means that 1kg of DDT is considered as toxic as 7.4kg of TEG.

Table 1: Methods covered in this report.[2]

Method	PestLCI	EDIP2003	IMPACT 2002+	ReCiPe midpoint (H)	USEtox
Midpoint / Endpoint	N/A	Midpoint with some damage orientation	Midpoint and Endpoint	Midpoint with option for Endpoint	Midpoint
Impact categories	Fraction emitted to: Air (f_{air}) Surface water (f_{sw}) Ground water (f_{gw})	Ecotoxicity: Water Acute, Water Chronic, Soil Chronic.	Ecotoxicity: Aquatic, Terrestrial.	Ecotoxicity: Terrestrial, Freshwater, Marine.	Freshwater Ecotoxicity
Characterised Unit	Grams	The volume needed to dilute 1 g of the emitted substance to a degree corresponding to its predicted no effect concentration (PNEC). m3 water/g emitted to Air	kg triethylene glycol-eq (TEG) into water/soil	kg 1,4-dichlorobenzene eq /kg into soil/water	Comparable Toxicity Units (CTUe)
Number of substances covered in ecotoxicity in database.	70	183	440	450	2600
Number of Characterisation factors for ecotoxicity within all compartments	N/A	2568	2568	4034	22603
How Characterisation factors are derived		EDIP 2003 keeps the same modular approach as seen in EDIP 97 by identifying properties of a substance which affect the potential for ecotoxicity, expressing them as a characterisation factor.	Analysis of mean impacts based on HC50 (geometric mean of EC50), Affected & Disappeared fraction of species	Calculated from the fate factor, exposure and the effect factor. Each calculated from physiochemical properties.	Uses physiochemical and biochemical properties as well as EC50 values (per m3 per day/kg of emission).

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[2] For further information see Annex 1.

4 Project Plan

The overall plan for the thesis was to:
1. Review/describe available LCA methods (according to delimitations)
2. Comparison of the LCA methods within version 7.3 of the LCA software SimaPro; EDIP, Impact, ReCiPe and USEtox
   a. The example field from the winter wheat case is run in all methods (EDIP, Impact, ReCiPe and USEtox)
   b. Commonly used pesticides and inputs found in all methods are run in EDIP, Impact, ReCiPe and USEtox to compare CFs, how they weigh substances differently.
3. Decide which method to use in the two case studies
4. Swedish winter wheat case run
5. Brazilian case study run
6. Compare how farming habits, climate and geography affect the ecotoxic impact of pesticides.

The review and subsequent descriptions of the models used in this report can be found in the annex. The way to add new substances to the PestLCI and USEtox databases is also included as well as what data is required to regionalise a method for a climate/landscape different than that of the default.

5 Case Studies

5.1 Comparison of LCA methods

5.1.1 Method

The first component of this report was to assess how each of the four methods within SimaPro calculated and delivered, using their own parameters, the ecotoxicological impact 1kg of winter wheat has on the environment. Although acknowledged in this report that there are more methods which cover ecotoxicity, the ones chosen for this comparison was done so almost arbitrarily with influence from personal parameters. The main idea was to choose methods[3] which practitioners at SIK were familiar with using; as it turned out EDIP, IMPACT and ReCiPe also occurred frequently in comparative literature and each covered a wide range of substances in their databases. USEtox was included as it is the most recently created, a collaboratively built method with straightforward user input capabilities; and is also often found in the literature with a positive review.

In order to give a meaningful representation of ecotoxicity with regards to real world dosages one field was chosen where all application conditions were known. A field in Egonsborg in Skåne, Sweden from a 2005 inventory was chosen as an example wheat field. Although the herbicide Glyphosate was not included in the inventory, an average amount applied to a field in Sweden was assumed and added to the analysis as it is a commonly used pesticide. It must be noted that since the study is from 2005 it includes the use of Isoproturon, a herbicide which now has been completely banned since 2009 in part due to its extreme leachability.

To start, the correct dosage of each pesticide applied to 1 hectare of land was noted for each pesticide used. In SimaPro, a process was created and named accordingly wherein

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[3] See Annex 2 for a description of the methods used in this report.

the applied pesticides and their mass in each compartment were added; this process acts as a base which is then run separately through the methods where each then calculates the relative potential ecotoxic impact.

As only the dose per hectare value is known about the pesticides used on the fields, it is difficult to accurately divide and assign the value to each compartment ourselves through estimation without incurring massive inaccuracies in the results. For this reason the programme PestLCI[4] was used in this research as a tool to calculate the dispersion of a pesticide from its initial emission to the field to the environmental compartments.

One at a time, each pesticide was put into the PestLCI excel spreadsheet with appropriate parameters such as application method and month of application to derive how the pesticide is dispersed. Table 2 shows the distribution of active ingredients (a.i.). When spraying MCPA for example, PestLCI calculates how much of the applied dose reaches the environmental compartments of air and water. The amount reaching soil compartment is not noted as this is thought to be intentional; the field is considered part of the technosphere (an area heavily manipulated by human interaction) meaning only emissions leaving this zone are accounted for.

Table 2: Distribution of applied pesticide dose to each environmental compartment of air and water for one hectare winter wheat field in Skåne, H=herbicide; F=fungicide

a.i.	Dose g/ha	PestLCI distribution results	
		Air (g)	Water (g)
Diflufenican (H)	125	3.37E+01	2.37E+00
Florasulam (H)	1.75	4.42E-01	5.25E-04
Fluroxypyr (H)	101	2.68E+01	3.52E-02
Isoproturon (H)	1380	3.47E+02	5.99E-01
MCPA (H)	1130	5.66E+02	2.66E-01
Prothioconazole (F)	138	9.50E+01	1.55E-42
Pyraclostrobin (prop) (F)	25.0	1.72E+01	2.03E-01
Glyphosate (H)	1080	2.87E+02	2.62E+00

For this comparison run through, all extra inputs for the production of 7.5t of wheat yielded from 1 hectare of land was included and shown in Table 3. These inclusions were substances occurring from various sources, for example, tractors which require gasoline to run, may be used for processes like tillage, pesticide application and crop harvesting; the engine emits substances which could come up as being ecotoxicologically significant within one of the methods.

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[4] See Annex 2 for details on how pesticides reviewed in this report were added to the PestLCI database.

Table 3: Inputs for the general production of winter wheat.

Products	Amount	Unit
Wheat, winter, SE South, cultivation + drying	7470	kg
Resources		
Land use, höstvete	1.00	ha
Materials/fuels		
SIK fertiliser P with net energy	6.30	kg
SIK fertiliser K with net energy	7.60	kg
SIK fertiliser N SV MEDEL with net energy	135	kg
SIK Herbicide, average with net energy	800	g
SIK Fungicide, average with net energy	300	g
SIK Insecticide, average with net energy	12.0	g
SIK Glyfosat, average with net energy (same as herbicide)	1080	g
Electricity/heat		
SIK Diesel tractor with net energy	86.0	MJ
Lubricant oil (to be added to traction)	7.30	kg
SIK Electricity, medium voltage, at grid/SE S with net energy 2007	172	kWh
SIK Light oil with net energy	40.5	MJ

The process was analysed by EDIP 2003, IMPACT 2002+, ReCiPe Midpoint (H) and USEtox. Each method has its own impact categories to which it calculates how damaging a substance will be once it reaches the compartments at the mass given from PestLCI; for example the impact categories used in IMPACT 2002+ are the potential for aquatic and terrestrial ecotoxicity.

Following the initial comparison of pesticides used under an example wheat field scenario it was noted that some methods were lacking in their coverage of pesticides. The total substances were narrowed down to those only found within all methods, these being MCPA, Propiconazole and Glyphosate. For further comparative measures benzene (from tractor fuel combustion) and cadmium (mostly from fertilizer and pesticide production) were included in the assessment in order to see how the methods rate non-pesticide compounds (which could enter the life cycle) for toxicity. Within each method is a characterisation factor database, from this the respective characterisation factors from both the air and water sub-compartments were taken and summed from each impact compartment the method had.

5.1.2 Results

One finding was that with regards to the substances covered in this report, the ReCiPe method only calculates the ecotoxic impact using soil emission characterisation factors. As PestLCI considers the soil as part of the technosphere, any mass reaching this compartment is considered intended and it is only the mass reaching the ground water below after degradation/adsorption which is considered. As no "unintended" pesticide mass reaches the soil compartment, only air and water, ReCiPe cannot derive these substances' ecotoxic impact to the environment as it has no air or water characterisation factors to use for the substances we chose.

Table 4's results cannot be compared to each other primarily due to their use of different units; they act only to show the overall ecotoxic impact value the production of winter wheat has as calculated by each method.

Table 4: Ecotoxic impact of 1kg winter wheat as represented in each methods respective midpoint impact values and units.

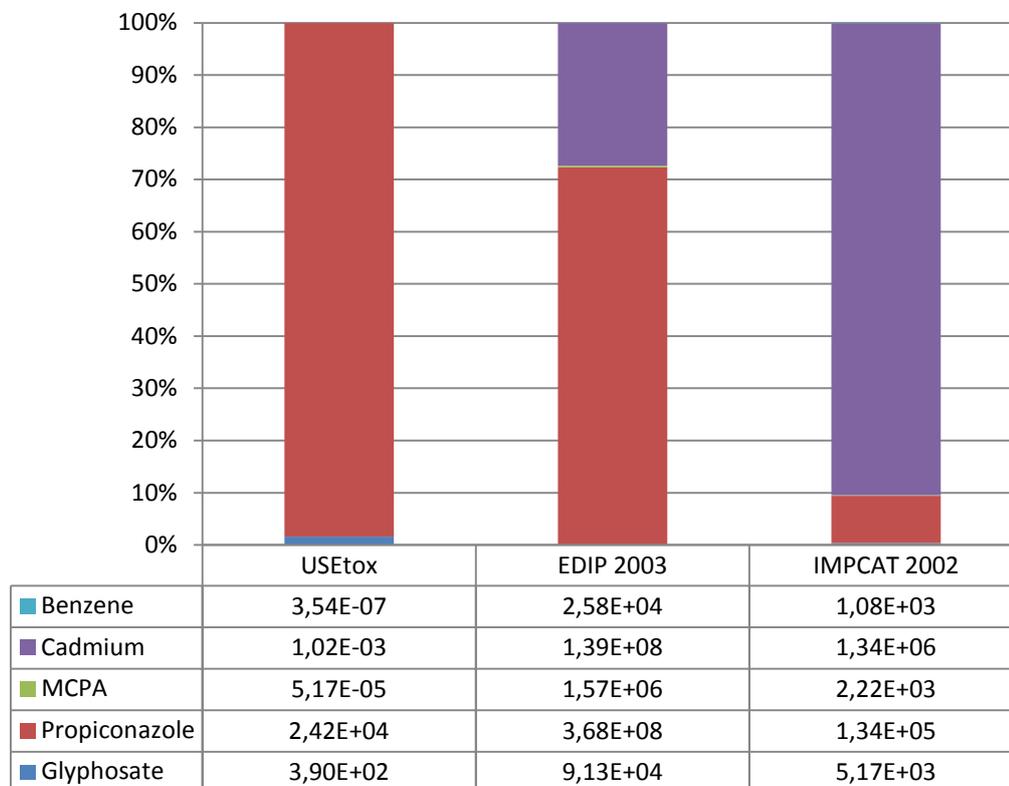|	Usetox	EDIP 2003	IMPACT 2002
	CTUe/kg	m3	kg TEG
Ecotoxicity	2.76E-01	7.59E-01	9.68E-01

The results from each method's toxicity impact calculations presented in Graph 1 and Graph 2: **Representative of the total characterisation factor value a method gives to a chemical as a sum of the characterisation factors used for emission to the air and water sub-compartment.** were represented in 100% stacked column graphs for an easy visual representation as to which impact category was most affected by the pesticide in question.

In Graph 1 we see the relative toxicity for each pesticide covered in each method, per compartment. This allows for comparisons of the potential for ecotoxicity between the pesticides within a method. As methods differ concerning the number of pesticides included, no thorough comparisons between methods can be done. Nevertheless it is clear however, that there are large differences between the methods when it comes to which substances are more toxic and in which compartment; see for instance Glyphosate whereby its overall toxicity not only varies between methods, which cannot be directly compared, its relative toxicity within a method's compartments has varying values e.g. comparing between aquatic and terrestrial toxicity in IMPACT, even having a higher impact than isoproturon regarding terrestrial toxicity. It is not clear why these results occur as the research regarding Glyphosate describes it as having a low toxicity to fish and wildlife when compared specifically in this case to isoproturon. It strongly adsorbs to soil increasing its time in and exposure of the environment compared to the easily leached isoproturon.

	Air	Water	Ecotoxicity	Water Chronic	Water acute	Soil Chronic	Aquatic ecotoxicity	Terrestrial ecotoxicity
	USEtox			EDIP			IMPACT	
	CTUe / kg	CTUe / kg	CTUe / kg	m3	m3	m3	kg TEGeq water	kg TEGeq soil
Glyphosate	5,14E-04	1,13E-04	6,27E-04	2,86E-02	3,51E-03		3,21E-02	6,41E-02
Pyraclostrobin	1,18E-04	3,27E-04	4,45E-04					
Prothioconazole	1,87E-03	4,20E-45	1,87E-03					
MCPA	7,44E-03	6,70E-05	7,50E-03	5,39E-02	2,21E-03		5,61E-02	5,29E-05
Isoproturon	2,54E-01	9,38E-03	2,63E-01				7,66E-01	4,80E-02
Fluroxypyr	1,70E-03	1,37E-05	1,71E-03	6,12E-04	5,56E-05		6,68E-04	1,34E-03
Florasulam	3,04E-04	1,83E-06	3,06E-04					
Diflufenican	1,36E-04	3,97E-04	5,33E-04	6,70E-01	4,12E-04	4,52E-05		

Graph 1: Analysis of the field by all methods representing total ecotoxic impact of pesticides per impact category per method. Impact to air and water are shown for USEtox but its only Impact category is Ecotoxicity, which is the sum of the compartment-specific toxicities.

Graph 2 shows the results from the comparison of the pesticides included in all methods as well as Cadmium and Benzene. It shows that non-pesticide substances included in an ecotoxic assessment are handled differently by each method, either the metal will vastly over shadow the toxicity of the pesticides (as seen in IMPACT), or will not be deemed as dangerous (as seen in USEtox).

	USEtox	EDIP 2003	IMPCAT 2002
■ Benzene	3,54E-07	2,58E+04	1,08E+03
■ Cadmium	1,02E-03	1,39E+08	1,34E+06
■ MCPA	5,17E-05	1,57E+06	2,22E+03
■ Propiconazole	2,42E+04	3,68E+08	1,34E+05
■ Glyphosate	3,90E+02	9,13E+04	5,17E+03

Graph 2: Representative of the total characterisation factor value a method gives to a chemical as a sum of the characterisation factors used for emission to the air and water sub-compartment.

5.1.3 Conclusion

Based on the results, the literature and the experience working with the models the decision was made that the USEtox method was most suited for calculating and presenting the ecotoxic impact of crop production. Other such positive traits were its collaborative creation, its extensive coverage of substances in the database as well as its high level of user straightforwardness regarding the manual addition of substances to the database not already included.

5.2 Case Study One: - Swedish winter wheat

5.2.1 Methods and data used

Figure 1 illustrates the flow of raw data input, through the methods and eventually leading to an output of an ecotoxic impact value.
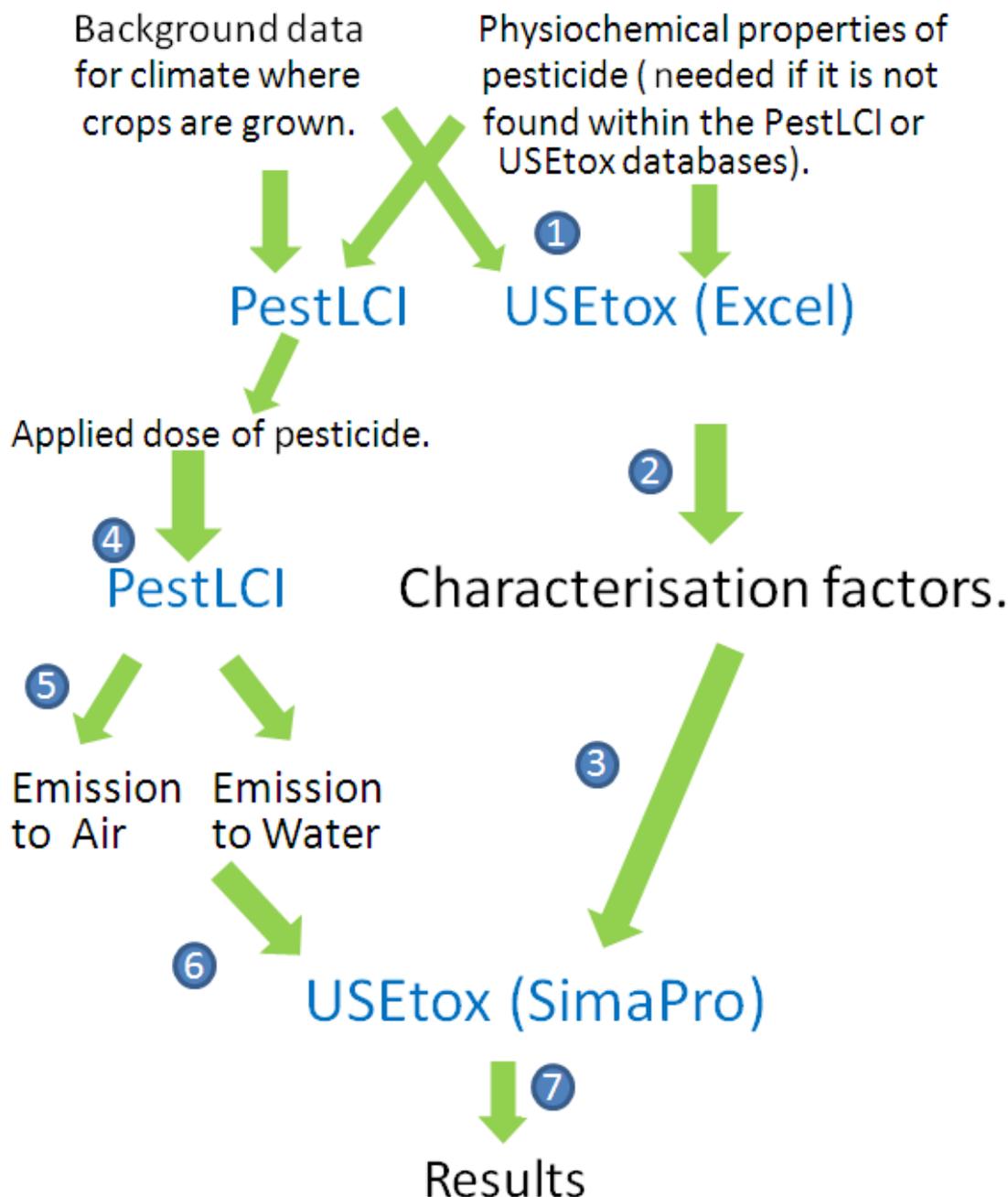

Figure 1:
1. Input of new pesticide and respectively required properties into the databases.
2. Calculation of Characterisation factors for new pesticide.
3. Transferral of new pesticide and its calculated CF's into the USEtox SimaPro database.
4. Input of dose, application time and crop development stage.
5. Applied emissions of pesticide to compartments.
6. Input of masses per compartment to respective USEtox (SimaPro) field boxes.
7. Calculation of Ecotoxicological impact, given in Cumulative Toxic Units (CTUe).

To start, an excel study analysis was first carried out on winter wheat production following the USEtox determined impact assessment method[5], this provided characterisation factors for the pesticides used.

The SimaPro process for the field was set up using the same distribution values used for the wheat case study as shown in Table 2 though this time removing the herbicide glyphosate. Once all parameters and emission values had been input, the process was run through the USEtox Recommended + Interim database[6] which had previously been adapted to include the pesticides missing from the initial USEtox database[7].

5.2.2 Results

Table 5 shows the results from the USEtox assessment of the field and represent the freshwater toxicity impact the pesticides have once they have been emitted and subject to various fate processes.

Table 5: USEtox toxicity results (CTUe/kg) for the example wheat field (without Glyphosate), H=herbicide; F=fungicide.

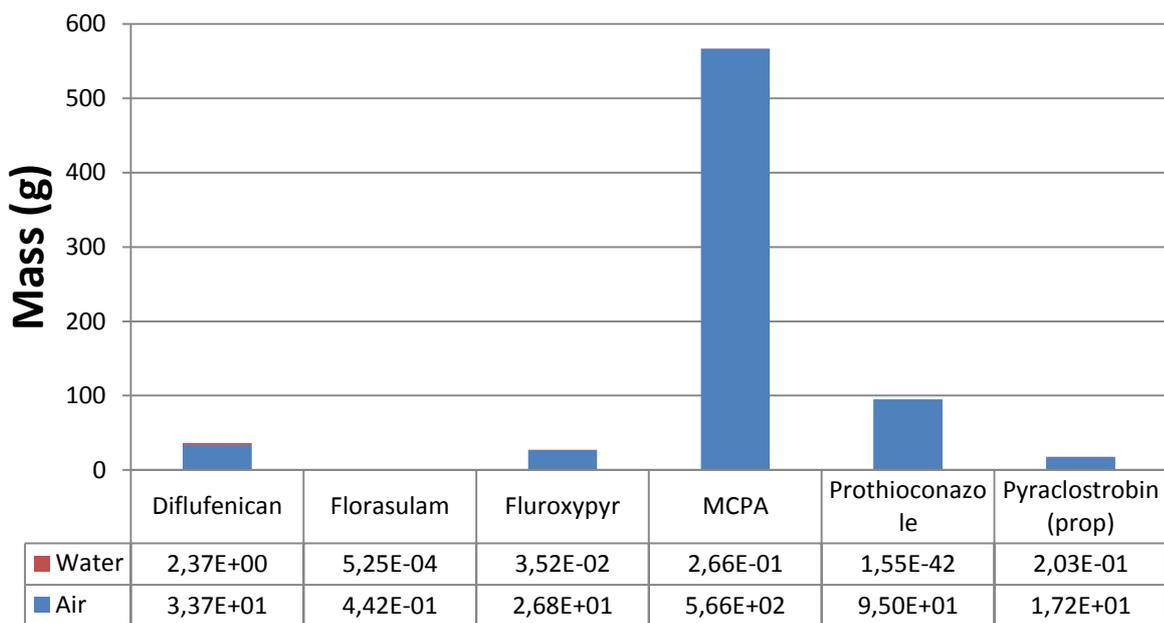| a.i.	SimaPro-USEtox (CTUe/kg)		
	Air	**Water**	**Total**
Diflufenican (H)	1.36E-04	3.97E-04	5.33E-04
Florasulam (H)	3.04E-04	1.83E-06	3.06E-04
Fluroxypyr (H)	1.70E-03	1.37E-05	1.71E-03
Isoproturon (H)	2.54E-01	9.38E-03	2.63E-01
MCPA (H)	7.44E-03	6.70E-05	7.50E-03
Prothioconazole(F)	1.87E-03	4.20E-45	1.87E-03
Pyraclostrobin (prop) (F)	1.18E-04	3.27E-04	4.45E-04
Ecotoxic impact			2.76E-01

Graph 3 and
Graph 4: Usetox calculated ecotoxicity impact (CTUe/kg) of pesticides used in the example field without Isoproturon. represent the ecotoxicity values from the USEtox analysis (Table 5) and the mass in each compartment, (Table 2) which served to show the relation between the mass and ecotoxicity of each pesticide. To enhance the distinction between the ecotoxicity values of the pesticides, Isoproturon has been removed from the graphs as its high values obscured the readability. As reference the Isoproturon ecotoxicity in this case amounts to 0.25 CTUe in air and 0.009 CTUe in water; with 350 g and 0.60 g reaching the air and water respectively. The general trend seen is that the more mass of chemical emitted, the higher the ecotoxicity impact will be. With regards to Diflufenican and Pyraclostrobin however, the mass reaching the air compartment is an order of magnitude larger than that reaching the water, but the ecotoxicity impact to the water is marginally higher, not seen with the other pesticides. As seen in Graph 4 MCPA has a high ecotoxic impact, this could be attributed to the mass reaching the environment being comparatively higher to the other pesticides.
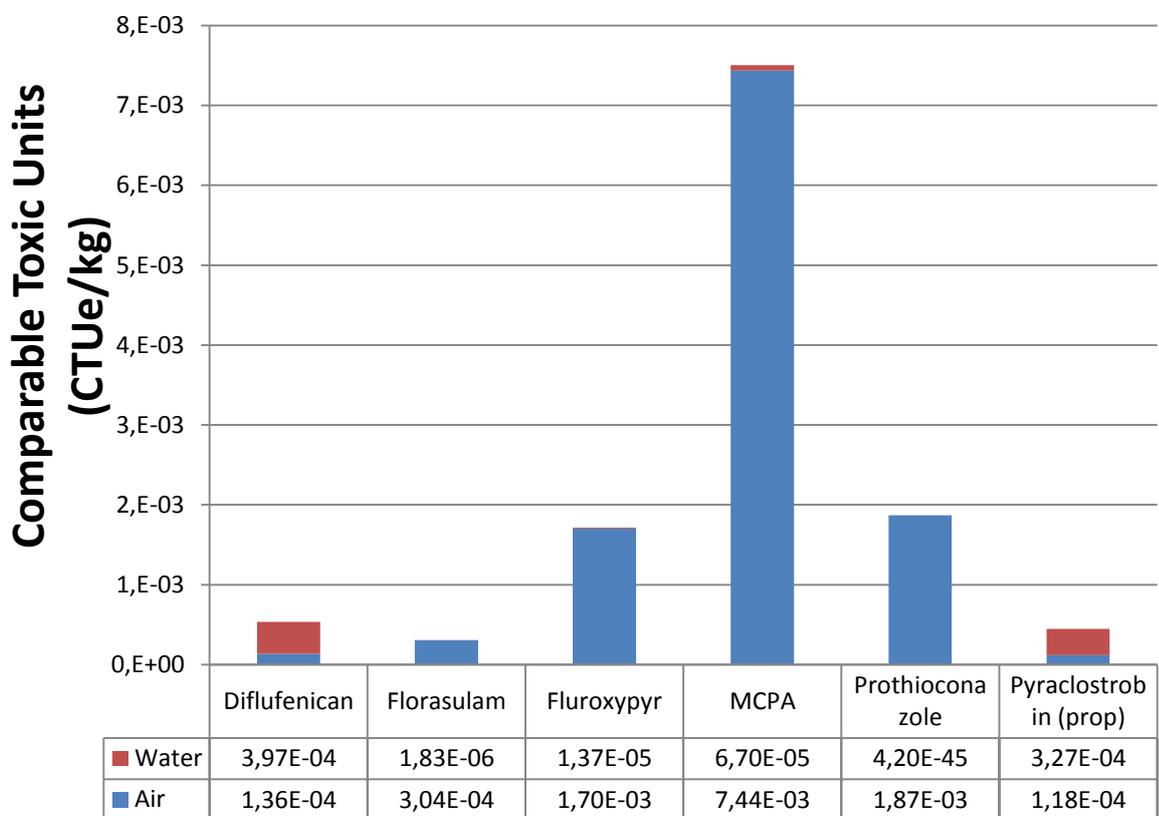
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[5] See previous comparison case study and Annex 4 for background on the method.
[6] See Annex 1 re: USEtox.
[7] See Annex 3 for data requirements on manual adding of substances to the database.

	Diflufenican	Florasulam	Fluroxypyr	MCPA	Prothioconazole	Pyraclostrobin (prop)
■ Water	2,37E+00	5,25E-04	3,52E-02	2,66E-01	1,55E-42	2,03E-01
■ Air	3,37E+01	4,42E-01	2,68E+01	5,66E+02	9,50E+01	1,72E+01

Graph 3: Mass of pesticide reaching each environmental compartment of air and water, through distribution of the applied dose to the example field by PestLCI.

	Diflufenican	Florasulam	Fluroxypyr	MCPA	Prothioconazole	Pyraclostrobin (prop)
■ Water	3,97E-04	1,83E-06	1,37E-05	6,70E-05	4,20E-45	3,27E-04
■ Air	1,36E-04	3,04E-04	1,70E-03	7,44E-03	1,87E-03	1,18E-04

Graph 4: Usetox calculated ecotoxicity impact (CTUe/kg) of pesticides used in the example field without Isoproturon.

5.3 Case Study Two: - Brazilian soybean

5.3.1 Methods and data used

Method for assembling soil data for Mato Grosso.

The state of Mato Grosso is found in the centre of South America and covers the third largest area within Brazil. With large flat areas in a tropical climate and a high number of rapidly expanding farms creating large scale production of soybeans, Mato Grosso is Brazil's largest soybean producing state, recording yields of 20.4 million tons in a year. In ongoing projects, SIK has visited farms in the state looking out for ways to make production more environmentally sustainable; due to this, data about farming habits and pesticide usage were available for assessment and comparison in this study.

The same method of using both PestLCI in conjunction with USEtox to calculate distribution and ecotoxicity was again applied for Brazilian soybean production[8]. PestLCI and USEtox however are both developed within Europe and have their default parameters concerning climate and landscape set for Danish and European temperate conditions respectively. For the calculation of the ecotoxic impacts within Brazil, the models had to be calibrated from the default so that geographical values used reflected those of the tropical environment found in Brazil.

Data required for the regionalisation of PestLCI to that of Brazil.

Table 6 lists the climatic condition parameters required for PestLCI to calculate the fate of a pesticide from an emission in a region. The sources given provide information specific to the state of Mato Grosso which are input to the 'METEROLOGY' tab of the method.

Table 6: Parameters required for regionalisation of PestLCI and accompanying sources. Any sources which provided daily values were averaged to give the required monthly values.

PestLCI parameters	Source website
Average temp	http://www.meoweather.com/history/Brazil/na/-15/-59.95/Mato%20Grosso.html
Average precipitation (mm)	http://www.meoweather.com/history/Brazil/na/-15/-59.95/Mato%20Grosso.html
Potential water balance (mm)	http://www.saecanet.com/20100716/saecanet_calculation_page.php?pagenumber=555
Number of days with precipitation > 1 mm	http://www.zoover.co.uk/brazil/brazil/pocone-mato-grosso-pantanal/weather
Average maximum rainfall in one day (mm)	http://www.meoweather.com/history/Brazil/na/-15/-59.95/Mato%20Grosso.html
Solar irradiation (MJ/m^2)	http://www.cpao.embrapa.br/clima/index.php?intervalo=1&dados=radia&Submit=Mostrar&pg=resultado_normal
Day length hrs/day	http://www.timeanddate.com/worldclock/astronomy.html?n=2395&month=9&year=2011&obj=sun&afl=-11&day=1

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[8] Refer to Case Study One: - Swedish winter wheat for details on using PestLCI together with USEtox.

Within PestLCI, under the 'SOIL_DATA' tab a new soil profile was created to reflect the composition of the region of interest: Mato Grosso. Each soil profile in PestLCI requires specific soil content data such as sand, silt and clay content etc. To collect this information the ISRIC-WISE soil database (ISRIC-WISE 1966) (Batjes 2006) was used.

In order to narrow down the extensive WISE3_SITE soil sample database to just those taken in the Mato Grosso region, Google maps was first used to identify the geographical spread of the Brazilian state. Coordinates were noted of the outskirts which gave a range of coordinates in which soil samples could be used from the database provided they fit within this established range depicting the Mato Grosso region.

All samples from the Mato Grosso region had their ID number noted so that the corresponding horizon data for that site could be taken from the accompanying WISE3_HORIZON spreadsheet.
Due to the inconsistency of the horizon depths per sample (i.e. several samples marked as "horizon level 2" having different depths in the soil), a range was created (Figure 2) from the most commonly used values for the top and bottom of a horizon.
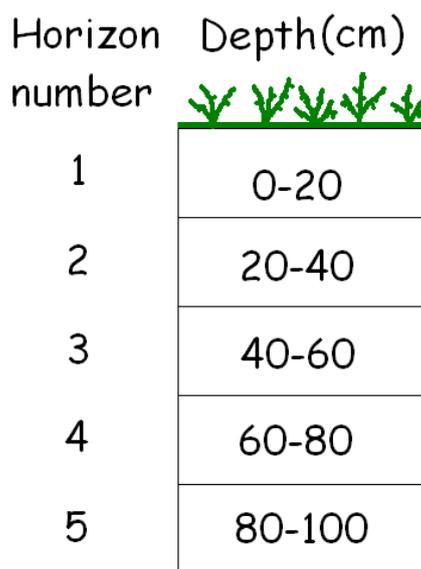

Figure 2: Diagram depicting the depth selected for each horizon from ground level to a maximum of 1 meter.

The narrowed down WISE3_HORIZON database, of samples only from Mato Grosso, were further narrowed down again to only horizons which fit into the ranges given in Figure 2. From these the average sand, silt, clay, organic carbon, pH and bulk density were calculated for each horizon based on information provided in the database. Once collected the values were input to the PestLCI spreadsheet 'SOIL_DATA'.

Data required for the regionalisation of USEtox to that of Brazil.

So that the characterisation factors were also calculated in accordance to the climate found in Mato Grosso, a USEtox regional profile was created for Brazil. The GLOBACK database was used from the Globox model (Wegener Sleeswijk 2011) which provides regional data values for 240 countries. From the Brazilian data the required parameters for a new USEtox profile (Area, agricultural fraction and wind speed etc. Table 7) were noted and input to the USEtox 'Landscape data' spreadsheet under the broad heading 'continental'; the values under the global heading were kept the same.

Table 7: Parameters required for the regionalisation of USEtox through the use of GLOBACK data (the area of the sea included coastline and arbitrary calculation using geographical information.

USEtox parameters			GLOBACK parameter	symbol in GLOBACK
Area	land	km^2	total area	SYSTEMAREA
Area	sea	km^2	coastline (+assumptions)	SYSTEMAREA
Areafrac	fresh water	[-]	Calculated by hand	AREA_water
Areafrac	nat soil	[-]	land use: assumed fraction natural soil of total surface area	Farea_nat
Areafrac	agr soil	[-]	land use: fraction agricultural soil (+assumptions) of total surface area	Farea_agr
Areafrac	other soil	km	land use: assumed fraction urban and industrial soil of total surface area	
Temp		^{o}C	assumed average temperature	RAINRATE
Wind speed		m,s-1	assumed average wind speed	WINDSPEED
Rain rate		mm,yr-1	average precipitation (+assumptions)	RAINRATE
Depth	fresh water	m	assumed total depth fresh water	TOTALDEPTH_lake
RiverFlow	reg-cont	[-]	N/A	
Fraction	run off	[-]	assumed volume fraction particles in soil runoff	Fsolid_runoff
Fraction	infiltration	[-]	N/A	
Soil erosion		mm,yr-1	N/A	

Once the models had been calibrated, other factors were decided to be tested. For example, a common method of application used in Mato Grosso is via aircraft. It was decided to see how using this method affects the ecotoxic impact the pesticides have, depicted in Graph 5.

The significant difference in the climate and soil composition between Brazil and Sweden was predicted to have noticeable effects on both the distribution and fate of a pesticide and ultimately its ecotoxic impact. In order to test this, several different procedures were conducted comparing various aspects.

In order to see how the higher temperature and soil composition affect the emissions to the air and water compartments the pesticides used in the winter wheat case study with their respective doses, application times, etc. were ran through PestLCI; once with the method calibrated for Scandinavia and again under Brazilian conditions.

The next comparison looked at how the overall ecotoxic impact differed between the newly calibrated methods and their outputs with the default Scandinavian methods. Pesticides used on the example Brazilian field were run in both versions of PestLCI and then the corresponding USEtox version.

An overall winter wheat and soybean production impact comparison of 1kg yielded crop was deemed appropriate to gain insight as to how the practices, climate, geographical conditions and specific pesticides used affected the overall impact to the environment.

5.3.2 Results

Table 8 shows the PestLCI distribution of the applied pesticide doses to the compartments of the example soybean field. As can be seen, aside from the doses varying greatly, not all pesticides reach the water compartment; or do so but in minute amounts. When spraying Bifenthrin for example, PestLCI calculates how much of the applied dose reaches the environmental compartments of air and water. The amount reaching soil compartment is not noted as this it thought to be intentional; the field is considered part of the technosphere (an area heavily manipulated by human interaction) meaning only emissions leaving this zone are accounted for.

Table 8: Distribution of applied pesticide dose to each compartment for the field, H=herbicide; F=fungicide; I=insecticide.

a.i.	Dose g/ha	PestLCI distribution results	
		Air (g)	Water (g)
2,4-Dichlorophenoxyacetic acid (2,4-D) (H)	160	3.82E+01	1.44E+01
Azoxystrobin (F)	60.0	3.56E+01	1.05E-13
Epoxiconazole BAS 480F (F)	27.5	1.62E+01	1.66E-113
Bifenthrin (I)	3.50	2.06E+00	
Chlorimuron-ethyl (H)	25.0	5.01E+00	2.63E+00
Beta-cyfluthrin (I)	7.81	4.61E+00	
Cyproconazole (F)	24.0	1.42E+01	1.91E-05
Endosulfan (I)	196	1.16E+02	
Glyphosate (H)	1040	2.15E+02	2.94E-16
Imidacloprid (I)	62.5	3.68E+01	4.95E-01
Methamidophos (I)	225	1.32E+02	2.70E+01
Methomyl (I)	86.0	5.07E+01	1.01E+01
Prothioconazole (F)	61.3	3.61E+01	
Pyraclostrobin (F)	73.2	4.31E+01	4.45E-09
Teflubenzuron (I)	7.50	4.42E+00	
Triflumuron (I)	14.4	8.49E+00	

Table 9 represents the USEtox assessment of the field and again represents the freshwater ecotoxicity impact the pesticides have once they have been emitted and subject to various fate processes. A graphical representation of the Usetox assessment was decided against in favour of a table; this was due to the ecotoxicity of Cyfluthrin being several orders of magnitude larger than that of the other pesticides resulting in an unclear representation. What can be seen through comparison of Table 8 and Table 9 is that although Bifenthrin was applied in a comparatively very low dose it has an ecotoxic impact higher than most others applied.

Table 9: USEtox toxicity results (CTUe/kg) for the example soybean field used in Mato Grosso, Brazil, H=herbicide; F=fungicide; I=insecticide..
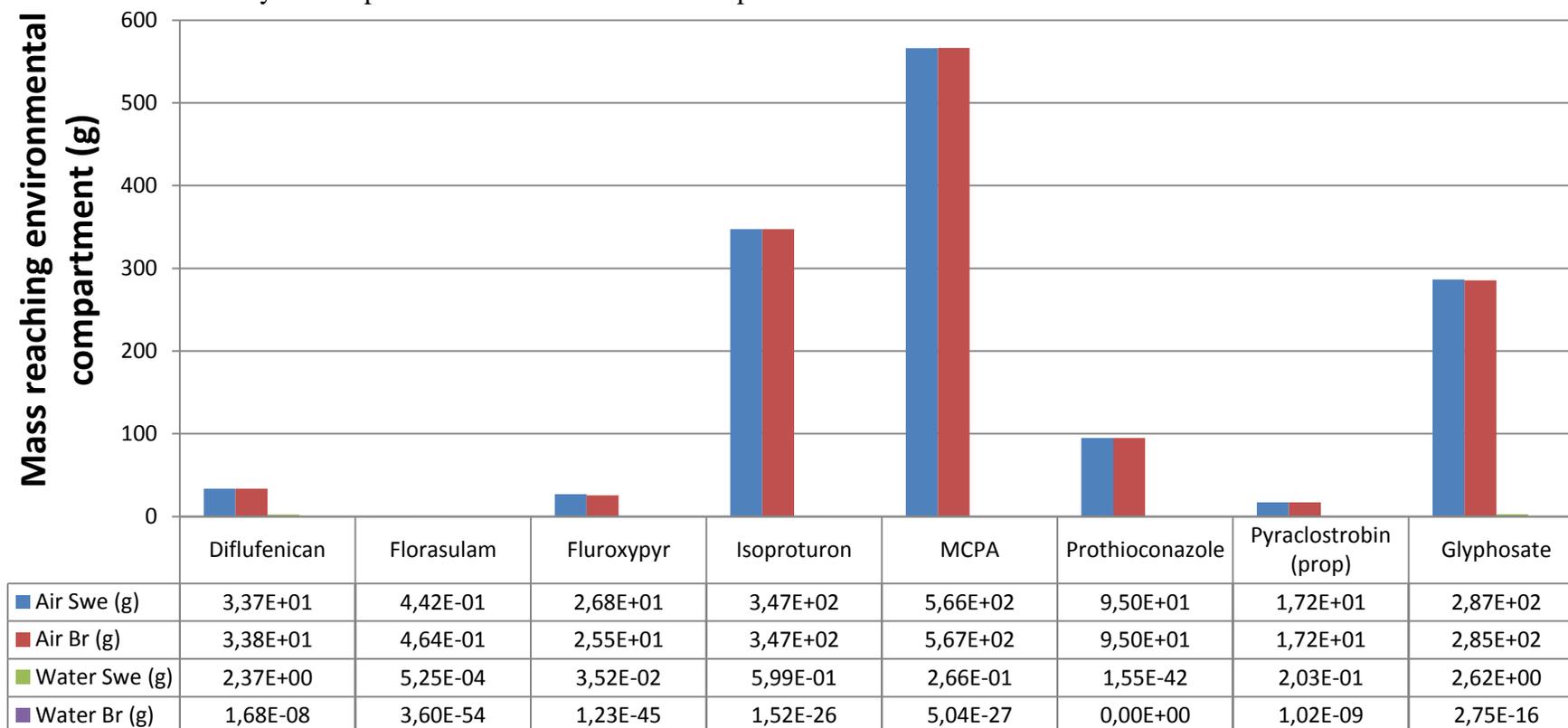
a.i.	USEtox (CTUe/kg)		
	Air	**Water**	**Ecotoxicity**
2,4-Dichlorophenoxyacetic acid (2,4-D) (H)	1,18E-05	6,04E-06	1,78E-05
Azoxystrobin (F)	8,73E-04	4,36E-18	8,73E-04
Epoxiconazole BAS 480F (F)	1,89E-04		1,89E-04
Bifenthrin (I)	3,46E-03		3,46E-03
Chlorimuron-ethyl (H)	1,30E-08	1,07E-08	2,37E-08
Beta-cyfluthrin (I)	1,24E+00		1,24E+00
Cyproconazole (F)	3,10E-05	1,03E-10	3,10E-05
Endosulfan (I)	8,41E-03		8,41E-03
Glyphosate (H)	7,54E-06	3,91E-23	7,54E-06
Imidacloprid (I)	2,71E-05	8,68E-07	2,79E-05
Methamidophos (I)	2,09E-04	1,12E-04	3,20E-04
Methomyl (I)	4,50E-04	1,22E-04	5,72E-04
Prothioconazole (F)	1,08E-04		1,08E-04
Pyraclostrobin (F)	6,02E-05	4,25E-14	6,02E-05
Teflubenzuron (I)	2,47E-03		2,47E-03
Triflumuron (I)	2,01E-02		2,01E-02

Graph 5 depicts the percentage difference in ecotoxic impact occurring from aerial application of the pesticide to the field as opposed to using a conventional boom spray. What is seen is an average increase of 9% in ecotoxicity with a noticeable outlier of the herbicide Glyphosate (+47.26%)
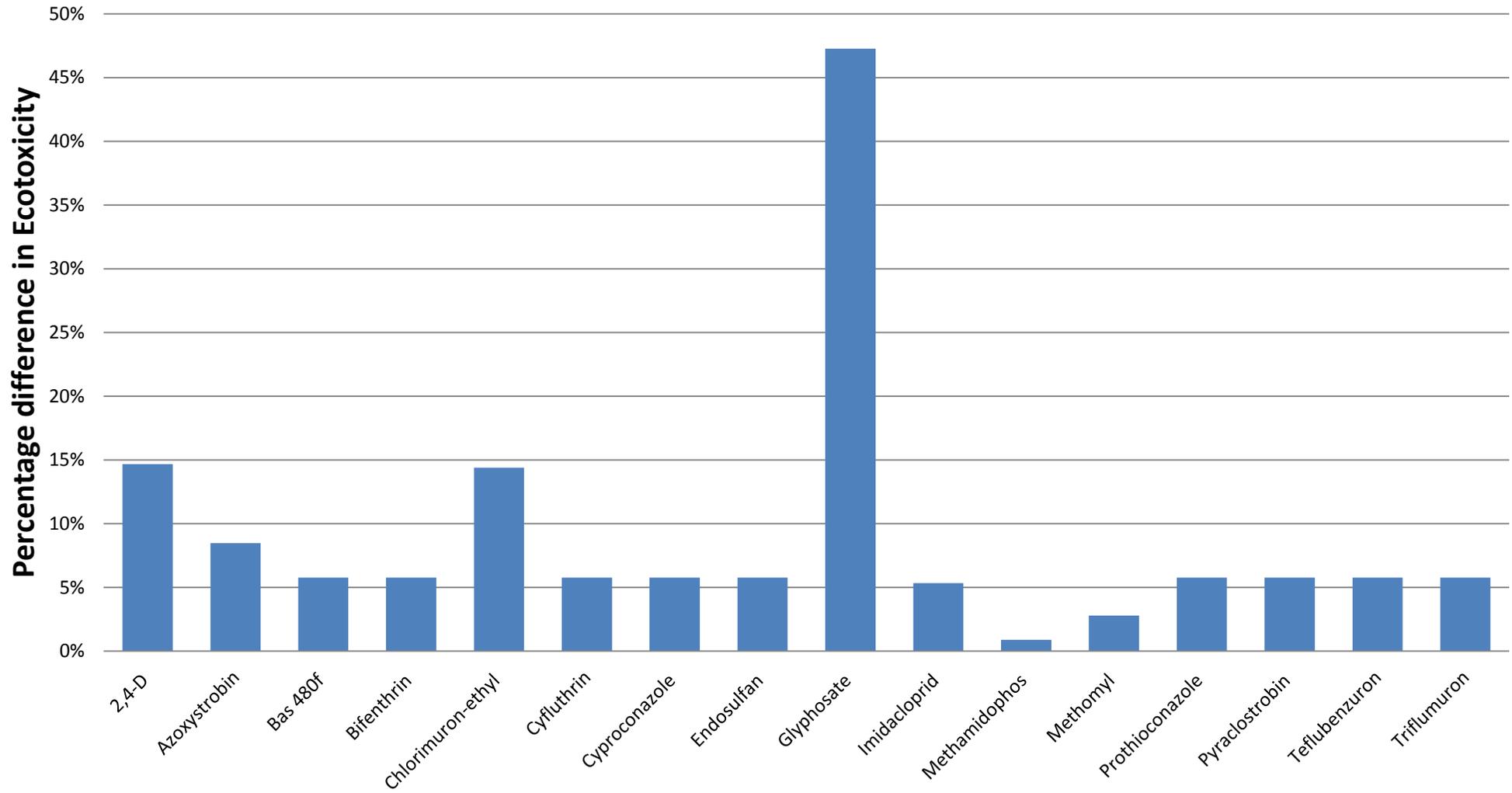
Graph 5: Percentage difference of Ecotoxic impact between aerial application method compared to boom application method.

Graph 6 shows how the pesticides and their respective doses used on the winter wheat field were distributed by PestLCI under both Scandinavian and Brazilian conditions using their region specific application parameters (time of the year and method of application etc.). Although there is no major difference in the distribution to the air compartment, the difference in distribution to the water compartment is significant; this however is not distinguishable in the graph as the amounts reaching the water are considerably lower than those in the air. On average there are several orders of magnitude between Sweden and Brazil, for example Florasulam (5.25E-04 vs. 3.60E-54g) and Fluroxypyr (5.25E-04 vs. 1.23E-45g). The main factors causing this are temperature and soil composition. Brazil has hotter days which increase degradation in the air/soil and soil mainly comprised of highly adsorbent clay. These factors make it less likely for the pesticide to reach the water compartment.

	Diflufenican	Florasulam	Fluroxypyr	Isoproturon	MCPA	Prothioconazole	Pyraclostrobin (prop)	Glyphosate
Air Swe (g)	3,37E+01	4,42E-01	2,68E+01	3,47E+02	5,66E+02	9,50E+01	1,72E+01	2,87E+02
Air Br (g)	3,38E+01	4,64E-01	2,55E+01	3,47E+02	5,67E+02	9,50E+01	1,72E+01	2,85E+02
Water Swe (g)	2,37E+00	5,25E-04	3,52E-02	5,99E-01	2,66E-01	1,55E-42	2,03E-01	2,62E+00
Water Br (g)	1,68E-08	3,60E-54	1,23E-45	1,52E-26	5,04E-27	0,00E+00	1,02E-09	2,75E-16

Graph 6: Mass (g) reaching each compartment for the pesticides used on the example wheat field emission values under Brazilian or Scandinavian conditions.

Graph 7 illustrates how different environments can affect the ecotoxic impact (CTUe/kg) a chemical can have. Although the pesticides used are found in soybean production this comparison did not measure the toxicity of the actual applications made to soybeans. Instead 1g/ha per pesticide was assessed under both Scandinavian and Brazilian climatic and geographical conditions in order to make the environment the only variable; this was then presented in stacked graphs for easy visualisation. Due to the use of a stacked graph format, Cyfluthrin was excluded because of its extremely high (in comparison) values of 1.82E-01 and 9.33E-01 CTUe/kg for Scandinavia and Brazil respectively leading to an overshadowing of the other pesticides visual representations.

What can be seen is that under Scandinavian conditions the ecotoxic impact is much lower compared to under Brazilian conditions of 6.52E-03 and 2.11E-02 CTUe/kg respectively. The highest contributors to the impact are Triflumuron (2.44E-03 vs. 1.01E-02 CTUe/kg) and Bifenthrin (3.35E-03 vs. 8.51E-03 CTUe/kg) for Scandinavia and Brazilian respectively. A suggestion for the lower ecotoxic impact under Scandinavian conditions compared to Brazilian could be due temperature and geographical makeup as described more in the discussion.
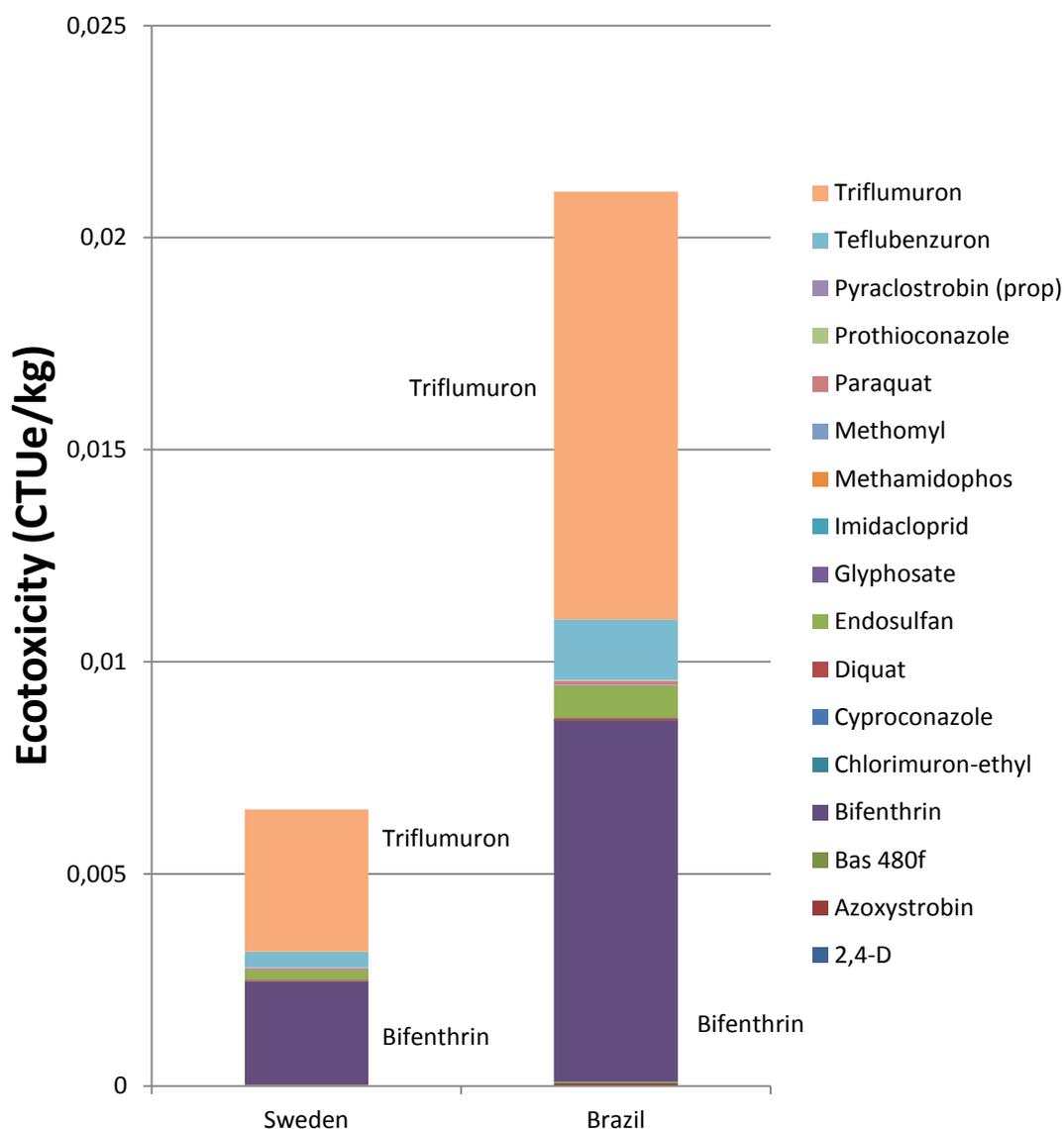
Graph 7: The ecotoxic impact (CTUe/kg) of pesticide (1g/ha) used for soybean production, both under Scandinavian and Brazilian climatic and geographical conditions. Triflumuron and Bifenthrin have been labelled due to their significant contributions to the bars.

Graph 8 shows the ecotoxic impact (CTUe/kg) of pesticide used for Swedish winter wheat and Brazilian soybean production. It must be noted that these results are purely for visualisation of each case study and not to be directly compared due to the soybean field being an example and not of accurate specific pesticide usage. What can be seen is a lower overall ecotoxic impact from the Swedish winter wheat (2.76E-01 CTUe/kg) compared to the Brazilian soybean (1.27E+00 CTUe/kg). The main contributors to the impact are Isoproturon (95% of total) for the winter wheat and Cyfluthrin (97% of total) for the soybean. As mentioned before, Isoproturon has been banned in Sweden since 2009; if this assessment were to be done again it could be assumed the ecotoxic impact from winter wheat would be significantly lower. As is stated in the case studies, the fate, distribution of the applied pesticides through PestLCI and the characterisation factors for the pesticides calculated by USEtox are done under Scandinavian temperate conditions and Brazilian tropical conditions for winter wheat and soybean respectively.
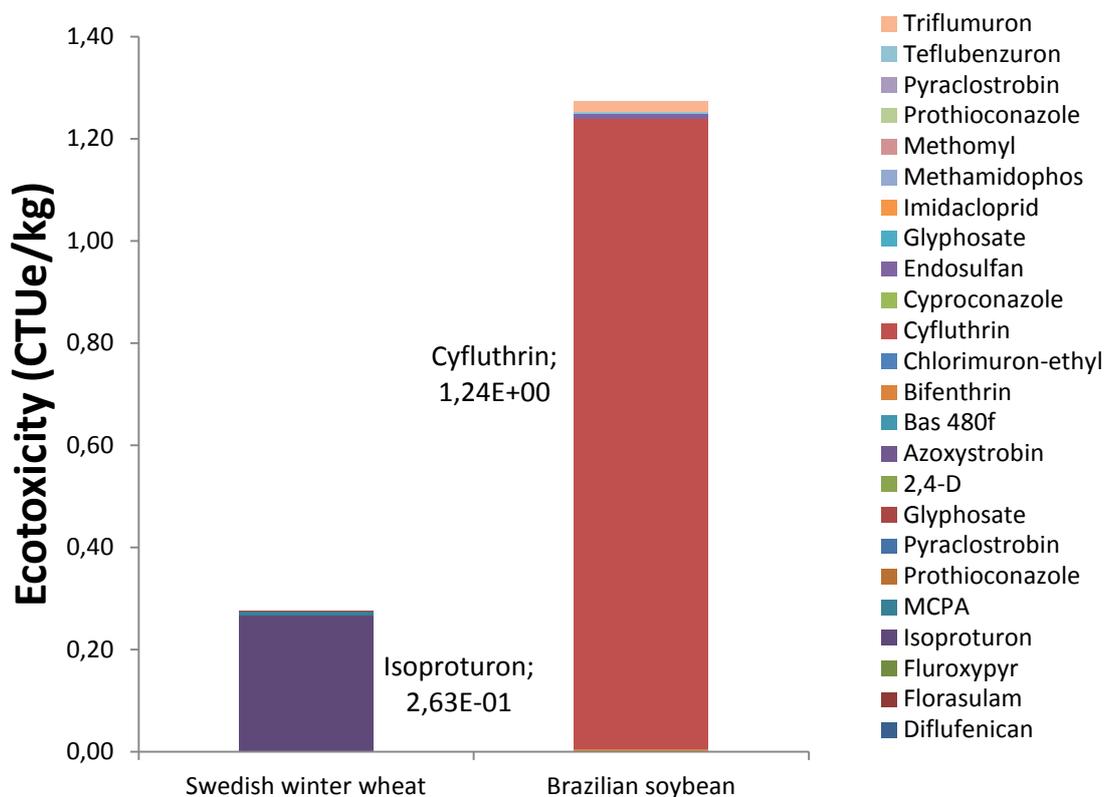
Graph 8: Comparison of ecotoxic impact (CTUe/kg) of pesticide use for 1kg yielded crop in the example Brazilian soybean and Swedish winter wheat fields. Isoproturon and Cyfluthrin have been labelled due to their significant contributions to the bars.

6 Discussion

This study aimed at establishing a transparent method which is accommodating to the ecotoxicity impact assessments, primarily of pesticide use within Life Cycle Assessments of crop production at SIK. The goal was to compare how different LCA methods assessed ecotoxicity, using examples of Swedish winter wheat and Brazilian soybean production. Results for the ecotoxic impact from production of 1 kg of wheat and soy were presented.

Which of the methods cover the most pesticides of interest in this study?

The problem with large data gaps in the LCA models can partly be explained by the large number of newly registered pesticides each year globally (Finnveden 2000). In North America, prior to 1994 there were an estimated 875 active ingredients registered in pesticides, with an average of 15-28 pesticides registered each subsequent year for the first time under the FIFRA(Arnold L. Aspelin 1997). As of July 2012 the number of pesticides sold in Brazil stands at 1,537 (Birkett 2012). Within Sweden, since being started in 1972, the latest pesticide registry of 2010, (Kemikalienspektionen) now includes a total of 3,068 pesticides denoting the 671 approved for use today in Sweden as well as their 503 active ingredients.

There are also examples of possible scientific and political pressures, such as problems with glyphosate resistance in weeds. This makes it likely that not all the data gaps will be filled as efforts are prone to be put towards chemicals which could act as a replacement such as 2-4-D or those seen as more of a concern than other less used substances which could be of just as much importance or even trending in use to become future problems (Finnveden, Hauschild et al. 2009). Data gaps were noticed in the review of the methods under comparison; as an example the chemicals Florasulam, Prothioconazole and Pyraclostrobin are not assessed in EDIP, IMPACT or ReCiPe so have no model specific calculated characterisation factors. Although not found initially in the USEtox database either, the model allows for additional characterisation factors to be calculated[9] though a user friendly spreadsheet built into the models Excel file. By being able to easily add new substances through input of properties and toxicity data to the USEtox database, the initial absence of the chemicals Florasulam etc. did not hinder the ecotoxic assessment but actually aided in the overall understanding of how USEtox calculates its characterisation factors. Undesirably though due to the time required for the gathering of the data and calculation of new characterisation factors for USEtox alone, it was decided that the addition of all the missing chemicals to the other three methods would not be feasible; and although possible through various spreadsheets and equations, the work would not have added significantly to the conclusions from the comparison of the methods.

With the main focus of this study being on pesticides alone, the toxicity caused when other substances reach the environment, such as emissions of benzene in the tractor fuel were not included. If this report were to be a whole life cycle assessment of winter wheat and soybean, all processes involved in crop production, including fertiliser production and means of application would be accounted for; in which case metals such as Cadmium and Manganese would be included. How metals are handled within LCA

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[9] It subsequently falls to the coverage of databases like those of the PPDB, the Hazardous Substance Data Bank (HSDB) and the PhysProp database which provide physiochemical and toxicological data for over 1700, 5000 and 25000 substances respectively acting as go-to sources when LCA practitioners have to calculate characterisation factors for their chemicals.

toxicity methods is an important point to touch upon as in a comparative report (Dreyer, Niemann et al. 2003) it was noted that nickel's characterisation factor for aquatic ecotoxicity from an emission to air was a million times higher in the LCA method CML2001 than in EDIP97. Although the goal of this report was to present results for the ecotoxicity impact of pesticide use alone, the inclusion of some metals occurred when later SimaPro runs were done to gauge just how the overall toxicity was affected by chemicals in crop production other than pesticide active substances. The inclusion of the aforementioned processes such as fertilizer production meant Cobalt, Cadmium and Mercury among others came up in the inventory, increasing the toxic impact. Although the results were only noted, Cadmiums impact is present in this result and corresponds to the findings of Dreyer (Dreyer, Niemann et al.) of metals having very high CF's; a suggestion of how to tackles this problem is mentioned later in this report.

After comprehension of the data gaps, consideration was given and the comparison could move forward to see how the methods handled the mock-up wheat field.

Can ecotoxicity impact results from different LCA models be compared?

Although organisations like the Society of Environmental Toxicology and Chemistry (SETAC) and the International Organisation for Standardisation (ISO) have had a huge impact to the field of LCA through their work on development, harmonisation and standardisation, detailed guidelines for impact assessment methodology have not been given. This was not the intention of the standards, since "there is no single method for conducting LCA studies" (ISO 2006). With no constraints aside from the ISO standards, ecotoxicity assessment can range from being very specific and intricate to fairly simple and basic, each with its own positive and negative aspects. The more detailed a method becomes, including more and more equations to account for the various fates of the substance, the lower the transparency becomes and the higher the chance of a mistake to occur. Conversely a broad method which may for example only use one reference species per impact compartment may have the transparency for its results allowing for easy explanation and presentation but it will be imprecise and possibly under estimate the potential damage.

Due to the dilemma of having many takes on toxicity assessment within LCA, comparison and analysis reports have been carried out which vary in method, level of detail and number of models covered. In the literature these reports range from simple breakdowns depicting many models(Hans-Jörg Althaus 2007) sometimes in a table format for easy analysis (Commission 2010) to directly comparing how a handful of models conduct analysis on a number of pre chosen substances and their impact on human and environmental categories (Dreyer, Niemann et al. 2003). Some comparisons have been as part of a consensus scheme in order identify and pick out central features of the models with the aim to incorporate them into an agreed upon model for recommended use such as those of OMNITOX (Pant, Hoof et al. 2004) and USEtox (Rosenbaum, Bachmann et al. 2008).

Through comparison of the results and conclusions given in the reports previously mentioned, similarities can be seen which bring to light the main points of variation between the current LCA methods (Finnveden, Hauschild et al. 2009). These common points of differentiation mentioned all have influence over the final results delivered and are described below.

Data requirements between methods can vary considerably, such as how the modest needs by EDIP, which tries to allow for all substances to be included, pale to the more demanding levels of IMPACT 2002+ which in turn are different to those of USEtox.

Fate and exposure modelling principles is a high variable between methods due to the vast number of factors which can be taken into account. Within ReCiPe for example fate modelling is achieved through the use of the USES-LCA software which includes a multitude of parameters, as opposed to the simpler method of EDIP which takes the simply calculated substance fraction reaching the impact compartment and potential for biodegradation as enough.

Lack of consensus on the characterisation method/unit plays a significant role in the inability to directly compare the impact predictions of LCA methods. LCA invokes many assumptions regarding the impact categories, meaning in model creation it is generally down to the developers as to what algorithms to build the model on (NAHB Research Center 2001) and what is to be included in the characterisation of a substance; this subsequently determines the scope and thus level of detail covered. In this process, consensus on simplifications may be hard to achieve leading to developers sometimes branching off to create a new model to cover toxicity. Although diverging develops the field it runs the risk of flooding practitioners with methods.

When commenting on any of the results presented in this report it must be remembered that the impact values cannot be directly compared between methods; only relations between substances, farms, crops etc. can be compared and commented on across methods. With the difficulty of comparison in mind, due to all the differences in the units used for characterisation of chemicals, further comparative analysis of the methods was not possible. For example, because no ratio of cumulative toxicity units (CTUe) to m^3 of soil/water was found between USEtox and EDIP respectively, it was not possible to directly compare which method found a chemical more toxic.

Within Graph 2 the results of the comparison exercise show the handling of metals within ecotoxic assessment vary significantly. Noticeable is the almost exclusion of the metal Cadmium, assumed to be presented as highly toxic within EDIP and IMPACT. The low coverage of Cadmium in USEtox is most likely because of how the method is not geared towards the handling of metals, dissociating substances and amphiphilics; this is handled by the method creators by classifying the substances as 'interim' as the extrapolation of the substances fate in the environment is uncertain (Rosenbaum, Bachmann et al. 2008). Of course the inclusion of other metals could bring about opposing results of the severity of the toxic impact of metals.

The ecotoxicity impact of pesticide use in Swedish winter wheat production

When looking at the analysis of Swedish winter wheat, the first point of interest shown in
Graph 4: Usetox calculated ecotoxicity impact (CTUe/kg) of pesticides used in the example field without Isoproturon. and Graph 3 is how the relatively low emission of Diflufenican and Pyraclostrobin to water compared to the mass emitted to the air resulted in a comparatively higher ecotoxic impact in water. Looking at the substance data, including physiochemical properties or toxicity data, etc, there is nothing significant regarding these two pesticides. Although research on chemical specific aquatic toxicity yields warnings of their potential harmful effect, the same is found for all other pesticides in the case.

The paper by Berthoud et al (Berthoud, Maupu et al.) used USEtox to carry out a full ecotoxic impact LCA of winter wheat under French agricultural practices. This assessment included transportation and storage of the wheat, with the aim to replace the most toxic pesticides with lower impact ones with the same mode of action and estimate the effect this will have on the overall impact.

The results of the report by Berthoud et al (Berthoud, Maupu et al.) has a higher sample of 6,679 separate fields compared to the one single example field used in this report; this would indicate a higher resolution of the average pesticide usage values and practices. Notably the active ingredients are not stated by name meaning comparison of individual chemical impact results/characterisation factors cannot occur. An approximate look and comparison of the calculated potential for freshwater ecotoxicity from both reports shows their impact from pesticide use is significantly higher.

There are however similar conclusions drawn from the report which agree with the findings commenting on how the characterisation factors vary hugely which "underlines the importance of the active ingredient choice by farmers on the impact of wheat production on the freshwater ecotoxicity indicator." (Berthoud, Maupu et al. 2011)

One thing to compare between the reports is the distribution method; they mention that in the future the use of PestLCI would yield improved results if required French pedo-climactic data could be found. Interestingly enough one of the chemicals used in the report Trifluralin with an application dose of 0,88kg/ha is within the PestLCI database. To gain an idea of how the use of PestLCI would influence the distribution, the default model was run with Trifluralin using 0,88kg/ha. Although not set up for French conditions nor calibrated to crop type and application practices in any way, it has been noticed that the emission to the air compartment is on average relatively high and the emission would be higher than the use of a fixed 50% aerial emission value dependant on vapour pressure as in the report. The emission predicted by PestLCI was 825g of Trifluralin reaching the air compartment, compared to the 440g predicted and used in the Berthoud report (Berthoud, Maupu et al.).

The ecotoxicity impact of pesticide use in Brazilian soybean production

The Brazilian case study results primarily showed how large an effect the composition of the receiving environment has on the distribution of the pesticide from its initial application. The default PestLCI and USEtox methods are initially set to cover Danish and European temperate conditions respectively such as precipitation, temperature, wind speed, pH and soil composition. These variables were seen as important in the case studies introducing a difference between the predicted ecotoxic impact of a pesticide's use within Sweden and Brazil. The default methods are open to user input which allows for regional specification. Making use of this, the climactic and soil parameter values used in this report were attained from various sources and used to calculate values and factors specific for Brazil conditions. This could lead to variations in values should the same regional figures be obtain by another practitioner from a more reputable source, thus making the values used in this report only as reliable as the sources used.

Due to aerial application practices not being mentioned in the data received from Brazilian farmers, the aerial method was not included in this report as a case study example. What was done was an arbitrary comparison in which the case study dosages were applied by air and boom in order to see how the application method affects the distribution and subsequent ecotoxic impact. Not considered in this comparison

however is the idea that if aerial application is used, it is likely that the farmer will have to use a higher dose to correct for the wind drift factor; this could ultimately increase the ecotoxic impact more so than what was seen in the arbitrary comparison in this study.

Graph 5 showing the percentage difference in ecotoxicity between aerial and boom application show a noticeable outlier, using the Reregistration Eligibility Decision (RED) factsheets provided by the EPA (EPA) which describe the environmental fate of chemicals from laboratory testing, this results is explained. The first point to clarify is that when aerial application occurs, there is an increase and subsequent decrease in the mass of pesticide reaching the air and soil compartments respectively. The high increase in the ecotoxic impact Glyphosate is predicted to have is likely to be caused by more mass reaching the air and thus water compartment directly where it is not broken down easily by hydro or photolysis. In boom application a higher fraction will reach the soil directly where its chemical properties make it strongly adsorbed and thus highly immobile, lowering the potential freshwater ecotoxic impact.
Although Methamidophos does have an increase in toxicity, possibly due to less reaching the soil where it is rapidly broken down and more reaching the water where it is solubilised, due to its tendency to volatize and get degraded the increase is slight. Methamidophos is however highly toxic to humans and it can be assumed that if human toxicity were covered, it would rate higher for toxic impact.

The differences in mass reaching each compartment seen in Graph 6 and to a degree Graph 7 can be attributed to the meteorological and pedo-climatic differences which each directly affect the pesticide. Looking at Graph 6, generally during the crop production/pesticide application period, Sweden has a temperate climate with cooler days, moderate levels of rain and moderate sunlight. The soil is mainly comprised of sand, silt and clay in decreasing percentages of composition respectively. Brazil however, specifically the area of Mato Grosso, has a more tropical climate of higher temperatures, likely to increase photolysis and volatilization. Although having a higher average rainfall, the soil primarily consisting of sand and clay mean it is less likely for pesticide leeching to water sources; clay being a strong retainer of water and nutrients. Results in Graph 7 could possibly be down to the lower temperatures and less average rain under temperate conditions in Sweden; this could lessen the mobility of the applied pesticides through run off and leaching. Also USEtox considers the fractions of the area which is agricultural soil, natural soil and freshwater etc. when calculating a CF for a chemical. Brazilian conditions has larger fractions of freshwater and natural soil making the chance of unintentional environmental exposure to a chemical higher than under Scandinavian conditions, overall increasing the potential to cause ecotoxicity. Interestingly enough is that although USEtox covers chemical persistence in the calculation of a characterisation factors, Endosulfan did not come out with having a very high potential for ecotoxicity as predicted considering it stands to be a banned pesticide in Brazil in 2013.

Finally, Graph 8 comparing the two example fields in this report gave results which were as predicted. It was assumed that soybean production in Brazil would be more ecotoxic due to the use of such EU banned human toxic chemicals as the endocrine disrupter Endosulfan. The results agreed showing that the winter wheat production example field had around 4.5 times less ecotoxic potential. As stated earlier in the report, isoproturon is now banned in Sweden, the removal of this from the dataset would indeed lower the impact further but not change the overall idea that wheat production in Sweden is less ecotoxic. Aside from the pedo-climatic factors described above which would lead to a lower distribution of the Brazilian pesticides, the winter wheat field had

eight active ingredients applied compared to the sixteen used on the soybeans; however almost an extra 2kg/ha pesticide was applied to the wheat.

Although the findings of the comparison deem soybean production as having a more ecotoxic impact, we cannot categorically state this. In this report the data gathered for the winter wheat field was collected from reputable sources from known locations and is to the best of our knowledge accurate. Conversely the example soybean field and dosages used are of less accuracy due to the difficulty from confidentially of the practices of farmers in Brazil. Visits to Mato Grosso soybean farms yielded a large number of active ingredients used however their individual dosages had to be derived from how much pesticide product was applied and then subsequent calculation of how much active ingredient would make up that applied dose of product. Also to be considered is that the combination of pesticides applied to one field was based on assumption and so do not accurately represent a real Brazilian soybean production scenario.

It must also be mentioned that the area of Mato Grosso is twice as large as the country of Sweden; due to this an average soil composition was taken, however it is likely that the soil conditions vary between the agriculturally used areas of region making the pesticide fate and ultimately its ecotoxic impact differ from north and south for example.

Can the models be validated; are the results a good representation of the actual ecotoxicological impact to the environment?

Ecotoxicity has a wide range of causes and impacts which all fall under the 'toxicity' heading and cannot be focused upon when summarising the impact. An example problem is how the mode of action of a herbicide differs from that of an insecticide, meaning impact cannot be used as a means of toxicity measurement as the impact to insects would be significantly lower than that to plants. If a model such as USEtox, uses the potentially affected fraction of species as a unit to quantify the toxic potential, the requirements (trophic level of organisms considered); resources and time scale needed to validate this would range significantly depending on the detail wanted to fully confirm or not the change in the number of organisms. This presents problems when defining units and calculating characterisation factors for ecotoxicity in LCA.

But even if LCA does not properly reflect or predict the ecotoxic effects from production of a commodity, the method can still be of value for comparisons between different ways of production. To use the words of Olsen, Christensen et al. (2001): 'LCA is not suited for absolute assessments... it is an investigation of marginals, the emissions are aggregated, it is not a prediction of real effects, and the results cannot be validated'(Olsen, Christensen et al. 2001)(Olsen, Christensen et al. 2001)(Olsen, Christensen et al. 2001)(Olsen, Christensen et al. 2001)(Olsen, Christensen et al. 2001)(Olsen, Christensen et al. 2001)(Olsen, Christensen et al. 2001). One way of thinking however, as reported by the NAHB Research Centre (NAHB Research Center) revolves around repeatability to be a means of validation.

The timing and rate of an emission significantly affects the level of impact. Examples given in (Reap, Roman et al. 2008) describe how a single release of a volatile compound during midday will have a higher rate of degradation than if the same amount was continuously emitted throughout 24 hours; as well as how the time-dependent environmental processes such as toxicant accumulation could lead to future problems.

These sort of factors are not covered in the current LCA methodology regarding ecotoxicity which assumes linearity, looking at the ecotoxic impact with regards to the mass of active ingredient entering a compartment at a given instant, not considering background levels from prior exposures or the notion of tipping points/threshold levels.

Taking a look at the predicted distribution of the pesticide from initial application, the PestLCI results being presented in grams/hectare of active substance emitted mean it has potential to be tested for validity. The paper by (Berthoud, Maupu et al. 2011) uses the experimental volatilisation measurements from (Bedos, Génermont et al. 2009) to compare their EMEP–CORINAIR method (EMEP/EEA 2009) with calculated emission factors to the air. The differences are quite high which could be down the imprecise nature of the EMEP method of calculation through use of the vapour pressure alone. Although PestLCI was not implemented in Berthoud (Berthoud, Maupu et al.) it stands to reason that if PestLCI, the more data demanding method compared to EMEP was used, the results could possibly be more realistic giving a better idea of the dispersion.

It was decided that although important for improvement to the LCA method of ecotoxic impact assessment, development of a validation method of the results within ecotoxicity is not within the scope of this report. The belief that having something, such as calculated values which correspond to the relative potential for ecotoxicological impact a chemical has, attributed to its physiochemical properties is a reasonable starting point open to improvement.

Is LCA a suitable method for assessing toxicity of pesticide use in agriculture?

Although LCA is a widely used tool within environmental protection, it is difficult to say whether it is the best means for evaluation of toxicity impacts to the environment. Due to the issues brought up earlier in this report (such as lack of consensus), it would be wise to examine alternative means to assess and present ecotoxicity.
One such method is the process of Risk Assessment (RA); in its simplest terms it is the careful examination of something in order to determine the possible negative occurrences; this allows for weighing up to see if necessary precaution has been taken or if more should be done to minimize damage. Since researchers such as Cowell (Cowell, Fairman et al.), Sleeswijk (Sleeswijk, Heijungs et al.) and more recently Payet (Payet) have compared LCA with RA and present findings and key differences, only a brief out line will be provided in this report.

Ecological risk assessment (ERA) is the process by which stressors and impacts to the environment as imposed by humans are assessed in order to evaluate the types of effects which could or are occurring due to them. Unlike LCA, ERA can be used with either a prospective predictive approach or as a means to retrospectively evaluate how the effects of today were caused by past exposure to stressors (EPA 1998). Before any major construction project is carried out (such as the building of a marina) it is good practice to take a step in the planning stage for ERA to attempt to predict the environmental impacts which may occur. Similar to LCA, ERA conducts characterisation of effects and exposure which provide focus for the assessment; unlike LCA however this is often carried out under legislation circumstance. Initially, a precautionary standpoint is taken to help ensure for no unacceptable environmental risk, for example, considering the maximum concentrations of any harmful substances at the defined point of interest; a detailed RA will only be conducted if there is an indication for unacceptable risk.

It is important also to understand the differences in the goals of the methods. LCA has the "less is better" approach, comparatively assessing, using functional units, the impacts different products and scenarios have on the environment, aiming for environmental improvement of products to have an ideal emission level of zero (Olsen, Christensen et al. 2001; Payet 2008). ERA however works with a threshold value or reference site (for substance regulation or polluted site remediation respectively) to see if the impact which will occur from the project (a construction etc.) will be of an acceptable risk level; if not, what improvements could be made to get the impact under the threshold (Payet 2008).

LCA and ERA are not interchangeable but can benefit each other as they are complementary; each leading itself to be a subset of the other providing additional information which leads to a richer assessment of the situation at hand.

7 Future ideas for development

Within the literature it can be seen that the current methods for the assessment of ecotoxicity within an LCA have room for improvement. Some areas which would benefit from being focused on in future development are described below.

The assumption of linearity as mentioned in the description of the EDIP method[10] causes a lack in realism to the results derived from an LCA. Similar emissions from past or present surrounding processes not being included, means knowledge of background concentrations present in the receiving environment does not affect the predicted damage an emission will have. The exclusion of processes causing dilution or dispersion means in the eyes of an LCA the toxicity of an emission is only proportional to the mass emitted; no environmental thresholds are considered either, meaning a potential underestimation of the severity of the impact. This is an area of LCA which needs improvement upon.

The effects caused by single substances are to a greater degree more researched and tested than synergistic effects and ecotoxic potential of multiple substance interaction. Due to this lack of information LCA cannot yet account for this occurrence which ultimately may lead to a lower impact predicted by LCA than that which could/is occurring in reality.

As a result of the fugacity-based MacKay multimedia environmental fate model (Mackay 1979) being best suited for the assessment of organic chemicals, its prevalent use as a backbone within LCA methods means the coverage of metal toxicity is not optimal and could perhaps be better handled. Currently "the most widely used ecological toxicity models suggests that it is better to empty a jerrycan (5 gallons or 19 liters) of benzene into a fountain than to throw two pennies into it" (Heijungs 2004). This example brought from the calculations by Guinée (Guinée) whereby 10g of nickel received a 32kg 1,4DB equivalent value compared to 5kg benzene scoring only 0.45kg 1,4DB equivalent freshwater toxicity. As a reference for future LCA development, the paper by Gandhi, (Gandhi, Diamond et al.) used the method created by Gandhi, (Gandhi, Diamond et al.) to modify the USEtox method to include metal speciation and bioavailability. This modification gave results that were several orders of magnitude lower when considering freshwater metal ecotoxicity compared to the un-modified model.

When evaluating the potential for ecological damage, it would be wise to take into consideration factors which perhaps cannot be directly measured but never the less affect the ecotoxic impact. An example of such a factor would be the competency of the people responsible for pesticide application. Although manufacturer guidelines and regulatory procedures are set in order to minimize unnecessary exposure, it is not wrong to think that in some cases adherence to these could be lax. Improper disposal of excess or old pesticide mixture, inadequate cleaning of used pesticide drums and negligent filling of the drums on soil and not a concrete floor are some examples where exposure outside the technosphere could occur. Further development to account for these factors would be a difficult, if not impossible task, but inclusion of such factors could increase the realism of the scenario and thus predicted ecological impact.

Within the subject of predictive tools, a common point of debate, as mentioned above, is that between detail and realism against broadness and transparency. Although USEtox is

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[10] See Annex 1 re: EDIP 2003

a detailed and user friendly method, promoting its consensuses background and transparency; it does however require 15 parameters to calculate the impact score which in all cases may not be available, and is heaped in background calculations, perhaps lowering the overall clarity of the method. A future idea which is out of the scope of this report would be to create a method which made transparency and ease to convey how the results were calculated paramount. Possibly this could be achieved through limitation of the data needed and inclusion of only common toxicity test species (bumble bee, trout and worm for example). During the formulation of such a method, ideas from risk assessment would be discussed and attempted to be incorporated to LCA practice, possibly by presenting PAF toxicity results as a concentration allowing for easy comparison against PNEC values. This method would deliver a risk assessment style result which could then be compared with benchmarks calculated from surface water concentrations in that region (Andersson) leaving the practitioner to determine if there is an unacceptable risk. As a preliminary task for this, models such as SYNOPS (Gutsche and Rossberg 1997) and PRoMPT(Whelan, Davenport et al. 2007) would be reviewed; although PRoMPT has been looked at, it is not within the scope of this report for a detailed review and so no conclusive findings have been derived from its use.

Alternatively it may be that the future of ecotoxicological impact assessment might not be so suited for analysis through LCA and a simpler method may prove sufficient. The study by Saouter (Saouter, Perazzolo et al.) compared 69 chemical impact score rankings by USEtox with critical dilution volume (CDV) scores from the European Ecolabel (Ecolabel 1992) finding a "fair" agreement Spearman correlation coefficient ρ of 0.74 between the two models. This method requires just two parameters of degradation and toxicity to calculate the CDV of a substance. Also mentioned is that "any chemical can be assessed with CDV", presumably because of its simplistic means, however as elemental metals are not included nor spoken of it is not clear if this method can sufficiently predict their toxicity. Although the Saouters study brings up multiple points against USEtox such as how due to its detailed nature it could incur errors, the CDV method could also be viewed upon as lacking, or being too cautious in using only most sensitive species; both points coinciding with the argument mentioned above.

The results presented in this thesis are what we believe to be a step towards a useable method at SIK for the assessment of ecotoxicity in crop production, although it is somewhat lacking in transparency. However should sufficient time be dedicated, a more transparent method can be created which attempts to include the points for future development mentioned above.

8 Conclusion

- Of the LCA methods covering ecotoxicity reviewed in this report, it was found that the USEtox method covered the most pesticides. It is the only method which it created for ecotoxicity assessment and allows for new chemicals to be added to its assessment database; with more ease than the other methods studied.

- The results obtained from the methods did not agree on the ranking of ecotoxic impact of single chemicals within a sample; regardless of the difference in units used between the methods, all calculated using different means of modelling.

- The ecotoxic impact from pesticide use in Swedish 2005 winter wheat production, regarding a case study of an actual field located in the south of Sweden, is in this study reported to be 0.28 CTUe/kg. Calculated in future assessments to be lower since the banning of Isoproturon in 2009.

- The ecotoxic impact from estimated pesticide use in Brazilian 2011 soybean production, for a case study of a modelled field located in the state of Mato Grosso, Brazil, is in this study reported to be 0.022 CTUe/kg. Results however including the soon to be banned in Brazil 2013 Insecticide Endosulfan.

- Ecotoxicity covers many toxic effects in the environment. Due to the inherent complexity of nature and the simplistic outcome of LCA, presenting one result, it is difficult through LCA to predict and thus validate the effects that substances have in the environment.

- Alone LCA is not ideal for the definitive assessment of ecotoxic impacts within agriculture, due to the points mentioned in the discussion. However improvements and influence from other assessment methods, e.g. ERA and CDV, could lead to more transparent results allowing for comparison to actual environmental measurements such as chemical water concentrations.

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Annex 1: Description of LCI/LCA methods used in this report

PestLCI version 1.1.16

Aim

With partial basis on an earlier pesticide emission model for LCI at its core (Hauschild 2000), PestLCI was developed as a preliminary aid to the LCIA phase of an LCA. It is a modular model which estimates how much of an applied substance ends up in each of the four pre-determined environmental compartments of air, surface water, soil and ground water; these volumes can then be used as input for the LCIA phase.

Compartments included

Unlike models designed to support environmental risk assessment (ERA) PestLCI collectively estimates emissions to air, ground water and surface water. In doing this, the model aims to alleviate some of the problems which might occur when using separate models per compartment. Such problems may be the total mass balance of the field being disproportionate whereby the mass of the pesticide entering the field may not all be accounted for in accumulation or removal processes if multiple models are used per environmental compartment.

Figure 3 from Birkved (Birkved and Hauschild) shows the flow of the model and its structure in its entirety. Starting from the initial mass applied to the field area, a fraction of the pesticide will be deposited on the soil and will make its way into the air, surface water and eventually the ground water.
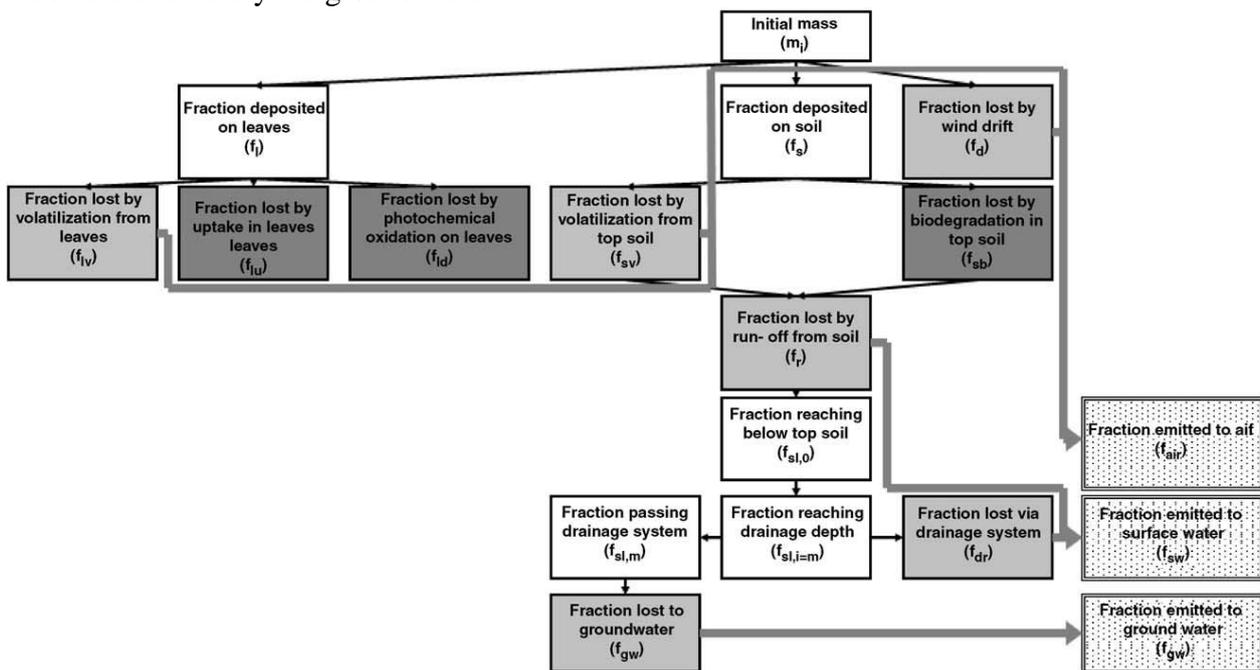

Figure 3: This is the overall model structure of PestLCI depicting how mass flows within the system. Dark grey boxes are terminal processes not leading to emissions from the field. Light grey boxes are terminal processes leading to an emission. Dotted boxes are emissions to compartments outside the field. Black arrows indicate flows; thick grey arrows indicate emissions to final compartments analysed taken from Birkved (Birkved and Hauschild).

Site
The default setting for PestLCI is valid for Denmark though through input of relevant parameters (rain fall and temperature etc.) it can be calibrated by the user so that any area on the planet can be assessed.

Time
PestLCI does not have a single timescale to which is adheres to, most modules for calculating the fate of a substance are considered isolated with the results from each module feeding in to the next link in the chain. For example the time scale considered for the volatization of a pesticide from the leaves of the crop is in hours whereas when looking at runoff from soil potential, three days are assumed to have gone by allowing for the pesticide to have been washed into surface water affecting the mass of substance left to leech deeper into the soil.

No of substances covered
70

Comments
The 1.1.16 version of PestLCI used in this report covers a wide range of fate processes though inclusion of more is proposed for the nest update, for example the uptake and loss though the root system. Another point of consideration is how the soil down to a depth of 1m is considered part of the technosphere due to it being highly manipulated soil, with a low biodiversity; seen as the same as a factory floor which is never considered in an LCA as an area of protection.

As of the finishing of this report PestLCI 2.0 was released which features such updates as macro pore flow and effects of tillage, an expanded pesticide database and an expanded soil and meteorological database for a range of European areas (Dijkman, Birkved et al. 2012).

EDIP 2003

Aim

EDIP 2003 is the latest version of the EDIP LCA methodologies extending the EDIP97 method into the field of exposure assessment.

Impact categories included (ecotoxicity)

EDIP2003 has 19 midpoint impact categories in total; this study will look at the three ecotoxicity categories named: water (acute and chronic) and soil chronic. Additionally both the chronic water and soil compartments each have three sub-compartments of air, water and soil.

Midpoint-endpoint

Although not having true endpoints EDIP2003 has midpoints set late in the impact pathway. By doing this it includes exposure factors for the characterisation modelling of the main non-global impact categories (e.g. acidification, eutrophication and ecotoxicity); thus giving more environmental relevance, making damage potential easier to interpret. A layout of the model can be seen in Figure 4 referenced from (Hauschild and Potting 2003).

Site

EDIP2003 is a spatially differentiated method; it allows for optional spatial resolution, whereby the environmental risk can be calculated for a smaller than global area. Within EDIP 2003 spatial differentiation can be done for 44 different regions or countries within Europe (Hauschild and Potting 2003), however it must be noted that the program SimaPro v. 7 only implements site-generic characterisation factors which do not take spatial variation into account (Consultants., Goedkoop et al. 2008). Where EDIP 2003 improves upon EDIP97 is with regards to spatial variations, such as fluctuations in background concentrations between regions and how climactic conditions can differ significantly.
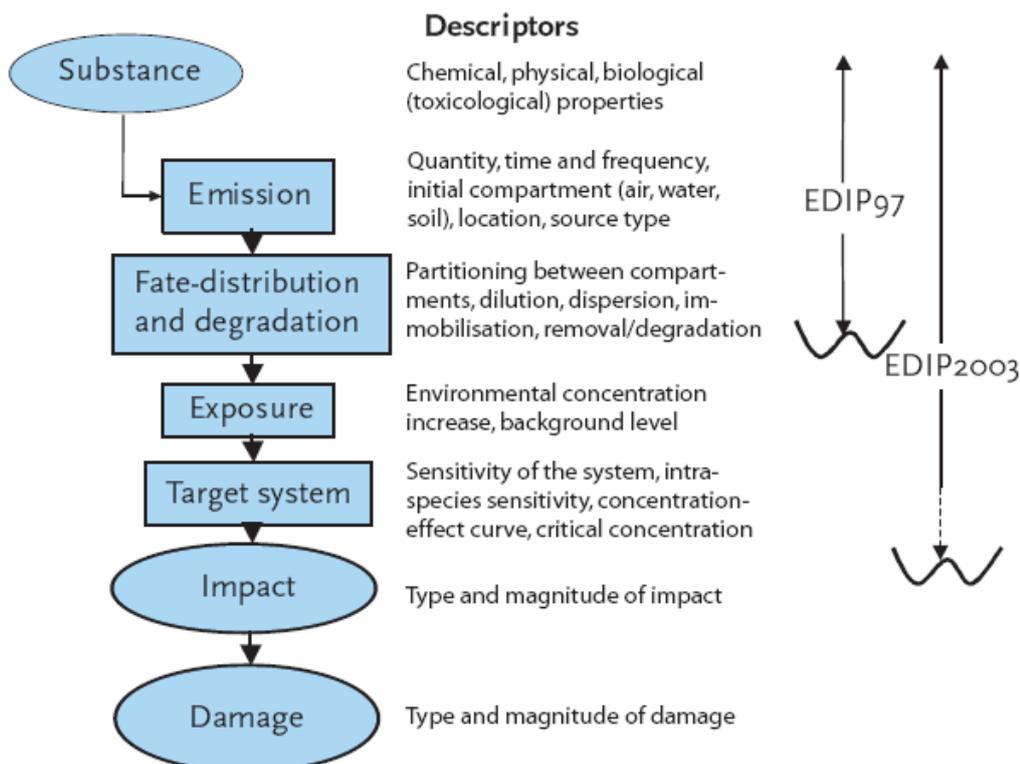

Figure 4: Overall module causality chain structure of the EDIP methods, depicting the extra considerations of EDIP2003 over EDIP97 (Hauschild and Potting 2003).

Time
Due to having an infinite timeframe certain assumptions have to be made when considering the fate of a substance. For example EDIP assumes that deposition of a substance from the atmosphere only occurs if the half-life of that substance exceeds 1 day, acute water toxicity is thought more likely to be caused by direct emission to the water compartment alone. The reasoning is that the substance will be degraded before it can be deposited and cause toxicity in the water within the short time frame of acute toxicity.

Units used, how to calculate CFs
The potential ecotoxic effects are defined by (Hauschild and Wenzel 1998) and are expressed as the critical volume which is the volume of a certain media (water or soil) required to absorb a specific emission without resulting in adverse effects (Stranddorf, Hoffmann et al. 2004). Within the sub-compartments the units of m^3water/g emitted to air, water or soil and m^3soil/g emitted to air, water or soil are used respectively.

EDIP 2003 identifies properties of a substance which affect the potential for ecotoxicity and expressing them in the form of a characterisation factor. These toxicity properties however are not all that is needed as exposure must also be taken into account. Exposure is not just the released quantity of the substance, but the fate of the substance in the environment, e.g. biodegradation, ability to accumulate in organism and how it gets distributed between the environmental compartments.
Using Equation 1, as introduced in EDIP 97, the characterisation factor is calculated for substance (i)'s ecotoxicological impact (**et**) to compartment (**n** (Water **a**cute/**c**hronic or Soil chronic)) from first emission to compartment (**m**). This modelling takes the substances redistribution between the environmental compartments (given as factor f^{mn}) as well as its potential for biodegradation (BIO_i) as separate factors.

<p align="center">**Equation 1**</p>

The PNEC values for substances for water acute/chronic and soil chronic are determined from relevant laboratory work for the substance under investigation. If the PNEC is determined from acute results its bioconcentration potential will not be reflected and so will need to be corrected as directed by Wenzel (Wenzel, Hauschild et al.)

Biodegradation is only considered for chronic exposure and is established though laboratory tests of the substance, the lower the biodegradability, the higher the factor used in the equation.

Characterisation factors for site-*generic* impacts are maintained in EDIP2003 as they were defined in EDIP97. They disregard spatial variation concerning variation in distribution and dispersion of the substance exposure and the target systems. The EDIP97 model is however able to accommodate a very simple form of spatial differentiation which has the redistribution factor (   ) calculated as the fraction of the emission for which either an acute or chronic ecotoxicity potential in water is to be calculated (f_{wa} and f_{wc} respectively) or the fraction for which chronic ecotoxicity

potential in soil it to be calculated (f_{sc}). These factors are representative of which compartment the emission was made to and which compartment the impact is being calculated for, as well as being dependent on the physiochemical properties of the substance; primarily its half life and volatility (defined as having a Henry's Law constant greater than 10^{-3} atm.m^3/mol or not).

For a specific emission and impact compartment combination f can be set as 1, 0, 'a' or 1-a, with 'a' being the spatially determined fraction of which the area of deposition is water. It is defined in (Hauschild and Wenzel 1998) as being 0.5 for emissions in Denmark with a global default as 0.2.

Number of substances covered in ecotoxicity in database.
183

Number of Characterisation factors for ecotoxicity within all compartments
736

Comments
The EDIP method goes under the assumption of linearity (as also found in other LCA methods) by which it calculates the effect dependent only on the mass of the substance emitted and not of the concentrations found already in the receiving environment. It therefore has the impact being relative to only the quantity emitted after fate modelling has taken place, not in relation the mass already possibly in the receiving compartment. The slope of the quantity impact curve is as a result a straight line. With this in mind only fate processes which cause a reduction in the amount of substance reaching the ecosystem can be considered; any dilution or dispersion processes allowing for exposure concentration calculation are not. Among the many fate factors covered in EDIP there are a number which are not included; for a full list regarding these and spatial variation descriptors consult Potting (Potting and Hauschild).

IMPACT 2002+

Aim

Impact 2002+ is a Swiss created combined midpoint and damage categorisation method, putting LCI results into a midpoint category, then linking these 14 types of midpoints to four damage categories.

Impact categories included (ecotoxicity)

The aquatic and terrestrial ecotoxicity midpoint categories of IMPACT2002+ are divided into three sub-compartments of air, water and soil for both. In addition, the water sub-category is further divided into ground water, ground water long term and ocean.

Midpoint-endpoint

In Figure 5 the overall scheme framework of IMPACT 2002+ can be seen with all mid and endpoint categories presented. This study will focus on the Aquatic ecotoxicity and Terrestrial ecotoxicity midpoint categories.
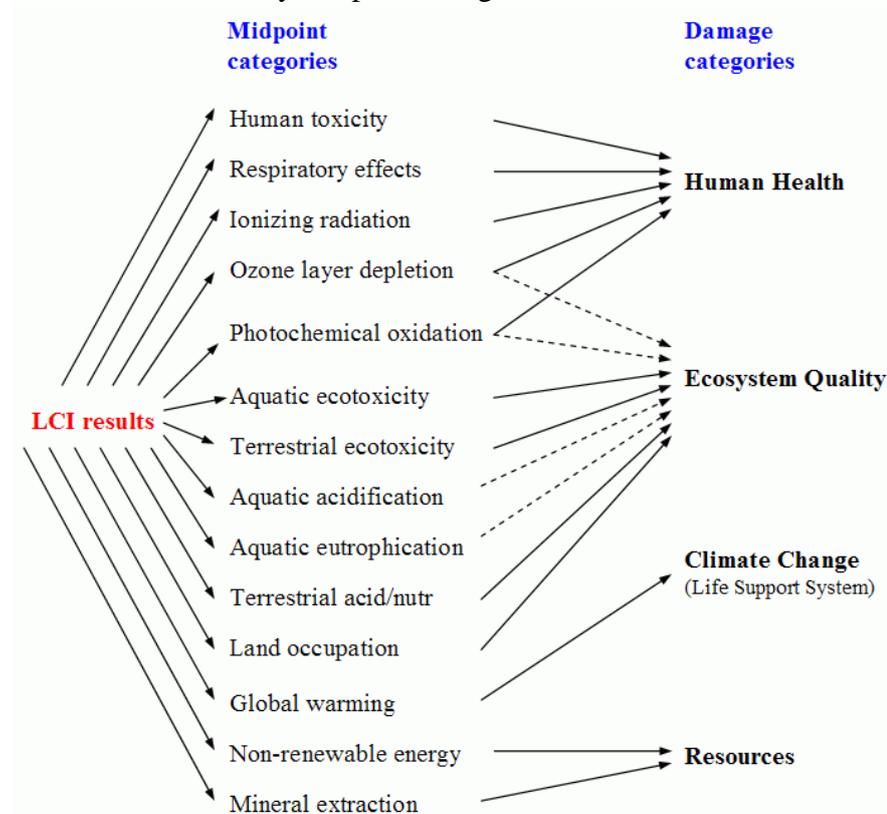

Figure 5: Layout of IMPACT 2002+ categories (Jolliet, Margni et al. 2003).

Site

Although a little spatial differentiation is included it is through the recognition that the impact of polluting a small lake is not the same as pollution occurring in all the lakes of Europe; this is done through the inclusion of the volume (V) of water which is polluted and to what extent. Spatial differentiation is only really spoken about within the human toxicity midpoint category. For spatially generic factors, a continental level for Western Europe is used in the calculation. When a more local insight is needed there is spatial differentiation for 50 watersheds and air cells in Europe.

Time

When considering the scope of the effect for long term scenarios, an infinite time horizon (approximately 500 years) is used.

Units used, how to calculate CFs

Based on principles of equivalency, the midpoint characterisation factors for ecotoxicity are expressed in kg-equivalents of the given substance to the reference substance triethylene glycol (TEG) in water or soil respectively.

At the mid-point level the aquatic ecotoxicity potential (AEP) is calculated by using a substances fate   and effect factors (based on EC50 values, in PAF m^3/kg). In order to calculate the fate factor, the two parameters **F** and   must be calculated using the IMPACT2002 model.

       =The dimensionless fraction of the emission of substance **i** in compartment **m** transferred to freshwater compartment **w**.

     = In years, this is the equivalent residence time of substance **i** in water, equal to the inverse of the overall decay rate constant in water (k).

β_i is calculated from the geometric mean of available EC50s on individual species to be calculated (Jolliet, Margni et al. 2003)

With the fate and effect values calculated, the time and space integrated potentially affected fraction (APAF, in PAF·m^3·year/kg) of species per unit of emission is estimated using Equation 2:

Equation 2

The APAF is then normalised to give the freshwater Aquatic Ecotoxicity Potential (AEP). By using Equation 3 the APAF for substance **i** is compared to the APAF of the reference substance for this compartment, triethylene glycol.

––––––––––

Equation 3

For terrestrial ecotoxicity within IMPACT2002+ HC50 values for soil (HC50^s) are available by extrapolation from aquatic HC50$_{water}$ values through the use of the method by Wenzel (Wenzel and Hauschild). This is calculated using Equation 4 with regards to various factors concerning the adsorption coefficient of the substance **i** (K_{di} in m^3/kg), the dimensionless volumetric water content of soil (f^w) and the density of the soil itself (ρ^s, in kg/m^3).

Equation 4

Number of substances covered in ecotoxicity in database.
440

Number of Characterisation factors for ecotoxicity within all compartments
2568

Comments
The practice of using the mean response value (HC50), and not a conservative EC50 value of the most sensitive species, was developed specifically for the IMPACT 2002+ model and provides an improved method for comparative assessment of ecotoxicity effect

ReCiPe Midpoint (H)

Aim

The ReCiPe method is considered to be the next step from the methods Eco-indicator and CML 2002; aiming to harmonize both midpoint and endpoint approaches in a consistent way (Commission 2010).

Impact categories included (ecotoxicity)

This report will cover the midpoint categories of terrestrial ecotoxicity (TET), Freshwater ecotoxicity (FET) and Marine ecotoxicity (MET) depicted in the flow diagram Figure 6.
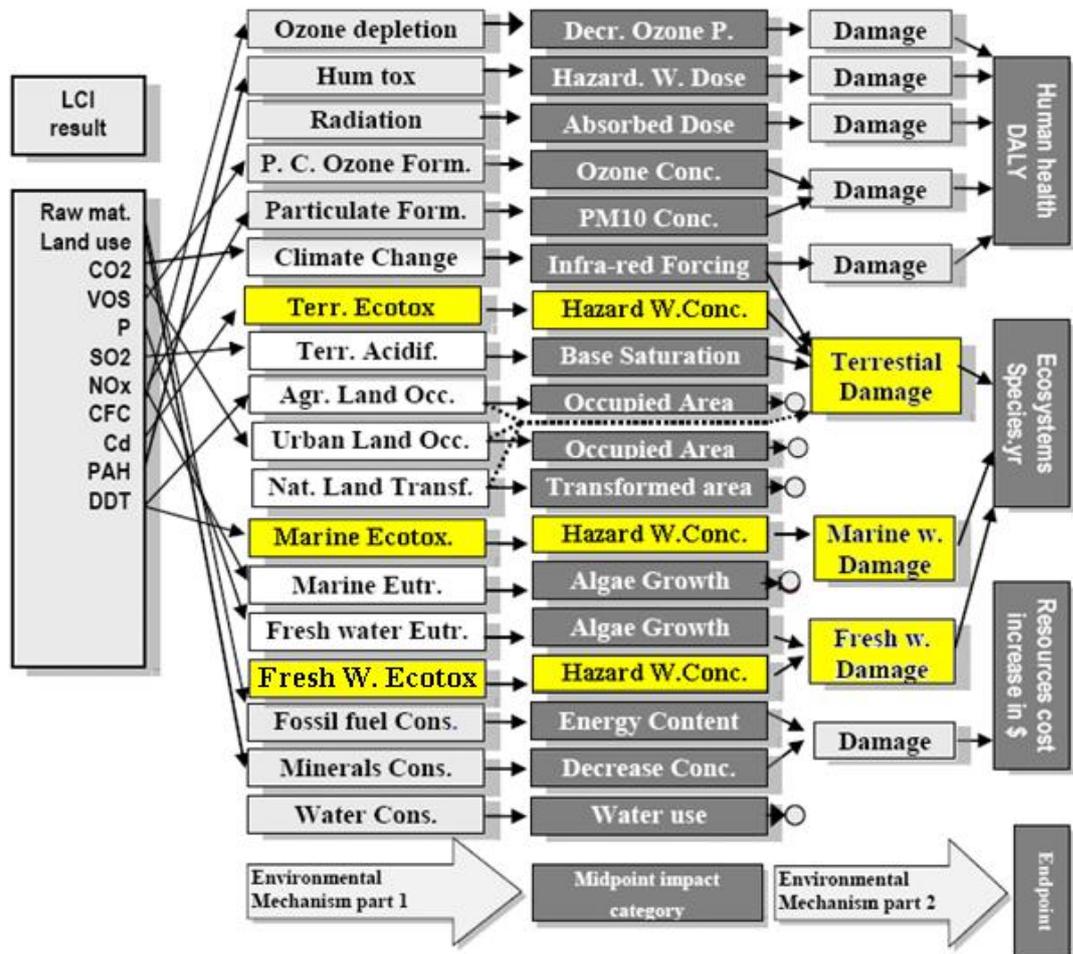

Figure 6: Flow through schematic of ReCiPe 2008, adapted from Goedkoop M.J. (Goedkoop M.J.).

Midpoint-endpoint

Composed of two sets of impact categories, ReCiPe 2008 covers 18 categories at the midpoint level which condense down into three at endpoint level. ReCiPe assumes that it is the diversity of the species within the environment which sufficiently represents the health and quality of the ecosystem; it thus represents the endpoint characterisation factor as the potentially disappeared fraction of species (PDF) integrated over area/volume (m^2/m^3) and time (years).

Site
The European scaled models used have been generalised to a high degree in order for them to be appropriate for all developed countries in temperate climates giving ReCiPe a limited validity for regions not within these conditions.

Time
Three perspectives can be taken when using ReCiPe which were developed not to represent standard human behaviours but simply group similar choices and assumptions together. This report will look from the hierarchist (H) perspective as it is based on the most common policy principles with regards to time-frame and other issues; dealing with ecotoxicity it takes the 'infinite' time frame for example. The other two perspectives, individualist (I) and egalitarian (E) are of opposite ends of the scale. The (I) perspective is concerned with only the short-term interest, often with a time span on the near future up to 100 years when concerning ecotoxicity. On the other hand the (E) perspective regards the future as important as the present and is the most precautionary point of view; it looks at an impact over a very long time span. When dealing with ecotoxicity both the H and E perspectives have the same assumptions and choices.

Units used, how to calculate CFs
Characterisation factors for midpoint ecotoxicity of a substance are derived from fate and toxicity data. The ReCiPe method relies on the multimedia fate, exposure and effect model USES-LCA (Uniform System for the Evaluation of Substances adapted for LCA purposes (Huijbregts, Guinée et al. 2001)to derive such data from substances under investigation within an LCA.

The characterisation factors $C_{j,i,x}$ specific for each substance dependent on the compartment of emission **i** and the compartment impact is being calculated for **j** (year.kg–1) involves the previously derived fate and effect factors input to Equation 5.

<div align="center">

Equation 5

</div>

$F_{j,i,x}$ = The fate factor of the substance x emitted regarding transport efficiency between defined compartments **j** and **i**.
$E_{j,x}$ =Toxicity of substance x in impact compartment j.

Details as to how the fate and effect factors above re calculated are found in (Huijbregts, Rombouts et al. 2005)

Similar to the IMPACT2002+ methodology the expression of characterisation factors are based on an equivalent substance. For ReCiPe the substance is kg-equivalents of 1, 4-dichlorobenzene.

Number of substances covered in ecotoxicity in database.
450

Number of Characterisation factors for ecotoxicity within all compartments
4034

USEtox

<u>**Aim**</u>
In 2003 the Life Cycle Initiative, comprised of the United Nations Environment Program (UNEP) and SETAC (Hauschild, Huijbregts et al. 2008) (the namesake of the model) initiated the international LCA model comparison and consensus project. Under the belief that the current situation of pesticide damage estimation was able to be improved upon, they aimed to give rise to a commonly used method. By 2006 during a workshop in Bilthoven, The Netherlands, the first prototype which was easy to use, clear with its results and parsimonious, allowing for easy manipulation depending on the detail needed for the investigation, was ready. The USEtox method evolved and is now a composite of several already existing and widely used LCA methods including: CalTOX, Fh-IUCT, Ecopoints, IMPACT 2002, GLOBOX, USES-LCA, EPS 2000, BETR, EDIP, WATSON, OMNIITOX and EcoSence. USEtox strives to achieve the goals set out by its creators though refining aspects from each of the methods it encompasses to give a useful model.

<u>**Impact categories included (ecotoxicity)**</u>
Ecotoxicity is comprised of six emission impact compartments under the headings: Urban Air, Rural Air, Freshwater, Seawater, Natural Soil and Agricultural Soil; each, except for Urban Air, are given at the global scale or the nested continental scale. Figure 7 is a representation of the nested USEtox model.
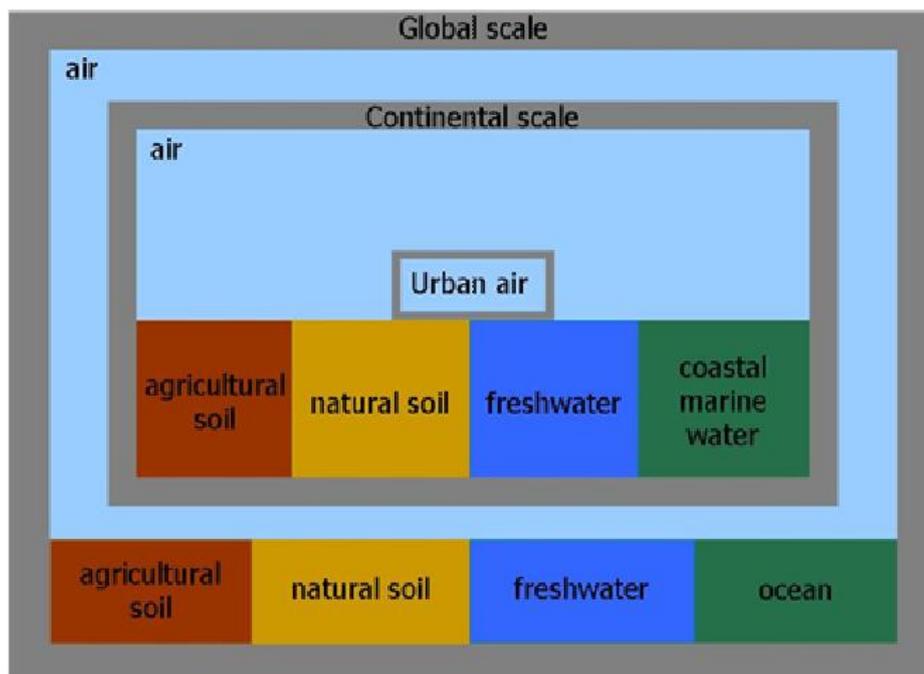

Figure 7: Nested structure of the USEtox model adapted from Mark Huijbregts (Huijbregts, Hauschild et al.).

<u>**Midpoint-endpoint**</u>
There are currently two versions of USEtox available which work differently from each other but can be used in combination to deliver midpoints and endpoints. The first used in this report is the primary version of the model; based in Excel, it uses many properties of the pesticide to create two sets of midpoint characterisation factors concerning Human health and Freshwater Ecotoxicity summarised as Comparable Toxicity Units (CTUh/CTUe) to emphasise the comparativeness of the factors, for each fate defined by

the user. The other version is more recent, having only been added to the 7.3 update of the software tool SimaPro in March 2011; it uses the characterisation factors and the emitted mass values to deliver endpoint results in the form of Impact Scores to each compartment in the investigation.

Site
Continental scale and Global scale available.

Time
Infinite

Units used, how to calculate CFs
The impact a chemical has per mass unit reaching the freshwater environment is represented by the characterisation factor quantified as the Potentially Affected Fraction (PAF) of species due to a change in concentration of the pesticide (m^3.day/$kg_{emission}$). This is calculated from the multiplication of the fraction of substance emitted to compartment (i) and received by freshwater ($_{i,w}$), the Fate (FF[day]), the Exposure Factors (XF_w) and the Effect (EF_w), as seen in Equation 6 (Henderson, Hauschild et al. 2011).

Equation 6

$F_{i,j}$ = the fraction of the initial emission of the substance to compartment **i** reaching the freshwater impact compartment w.

FF = the persistence of a substance (in days) within a specific compartment

XF = the exposure factor calculates the dissolved and bioavailable fraction of a chemical to aquatic organisms. Within USEtox this factor is calculated as described in the USEtox manual (Huijbregts, Hauschild et al. 2010).

EF = From effect concentrations obtained through laboratory research on different species with regards to toxicity, this factor brings a substances inherent environmental toxicity into the calculation of a characterisation factor. Expressed as the change in PAF due to a change in the concentration of a substance; given as (PAF.m3/kg-1in water).

The USEtox SimaPro version can be seen as somewhat of an endpoint model, delivering substance impact scores (IS) in comparative toxic units; these are dependent on its characterisation factor and the mass of which it's emitted. Inputting the mass of the substance which reaches each environmental compartment of air, water and soil will allow for the calculation of the impact score dependent on the volume of the product the LCA is being carried out for. With regards to Ecotoxicity the excel version delivers to the user an Impact Score for each substance as calculated below with the example of glyphosate:

Equation 7

$IS_{ecotoxicity}$ = Impact Score for ecotoxicity
CFe = Characterisation factor (environmental) (CTUe/kg)
M = Mass of substance reaching the compartment (kg)

Number of substances covered in ecotoxicity in database.
2600

Number of Characterisation factors for ecotoxicity within all compartments
22603

Comments

The USEtox model has two databases of characterisation factors. One database is comprised of only "recommended" factors which the developers consider to be sufficient enough to provide an appropriate toxicity impact value through the USEtox model; they also have sufficient underlying data to support a recommendation. The second database goes under the belief that having some form of characterisation factor is better than not having one at all. Included are both recommended factors and "interim" factors which serve as temporary values until further research provides an improvement. These interim factors are used when there is either a lack in data or there is high uncertainty in the effects, exposure or fate of the chemical. Metals, inorganic chemicals, organometallic chemicals, amphiphilic chemicals and those dissociating under environmental conditions are currently given an interim characterisation factor; this is also the case for any aquatic ecotoxic characterisation factors if the effect factor is derived from species toxicity data covering less than three different trophic levels (Hauschild, Huijbregts et al. 2008) (Huijbregts, Hauschild et al. 2010).

Annex 2: Pesticide data required for PestLCI.

Through various methods including calculation, assumption, extrapolation and experimentation, the fate of a pesticide once it has been emitted into the environment can be predicted to a degree of accuracy. In order to make such predictions a database is required for each chemical under investigation which includes various physiochemical and environmental properties relevant to the type of predictions the program is going to make; for example the pesticide's air/water coefficient being needed to calculate its rate of volatilisation.

PestLCI aims to deliver to the user the volume of the emitted pesticide which ends up in three specified compartments of air, surface water and ground water, after a mixture of removal processes have occurred.

The Pesticide Properties Database

The database used in this report for all general properties such as Name, Type, CAS no., SMILES and Molecular weight, is the Pesticide Properties Database (PPDB) created by the Agriculture & Environment Research Unit (PPDB 2009). On occasion it would also have to be consulted for other properties as shown in Table 10: Properties acquired from the PPDB.

Table 10: Properties acquired from the PPDB.

Input parameter	Abbreviation	Unit
Molecular weight	Mol Wt	g/mol
First dissociation constant (neutral to charged)	pKa	
Soil half life	$t_{1/2}$	(days) (temp.)

PhysProp
The main source of pesticide properties in this report is the PhysProp database. Created by the Syracuse Research Corporation (PPD 2003) it is the preferred source of information by PestLCI and is the most prolifically used source within the calculation reference spreadsheet. Table 11: Properties acquired from the PhysProp database gives the input parameters and units required for PestLCI which can be found specifically in the database and should be used if available.

Table 11: Properties acquired from the PhysProp database

Input parameter	Abbreviation	Unit
Molecular weight	Mol Wt	g/mol
Solubility	Sol	g/l (temp.)
Vapour pressure	Vp	mm Hg (temp.)
First dissociation constant (neutral to charged)	pKa	
Log octanol-water partition coefficient	Log P	
Henrys law constant	K_H	atm*m3/mol
Air-water partition coefficient	K_H'	Calculated within PestLCI from the K_H
Atmospheric OH rate	AtmOH	(days) (cm3/molecules*sec) (temp.)

EPIsuite

Some of the pesticides investigated in this report were not covered in the PhysProp database leading to the use of other methods to determine the relevant properties. The properties in Table 12 were determined using the software EPIsuite, the other source recommended for use with PestLCI.

EPI (Estimation Programs Interface) suite is a collection of estimation programs developed by the EPA and uses the simplified molecular-input line-entry specification (SMILES) of chemicals to estimate a multitude of physiochemical and environmental properties (EPA 2011).

Table 12: Pesticide properties obtained through the EPIsuite software.

Input Parameter	Abbreviation	Unit
Solubility	Sol	mg/l
Vapour pressure	Vp	mm Hg
Log octanol-water partition coefficient	Log P	
Atmospheric OH rate		(days) (cm3/molecules*sec)

Taking Florasulam as an example pesticide in this description, the properties in Table 12 were acquired in the proceeding way:

Solubility (mg/l) (at 25°C) - Within EPIsuite is a program called WSKOWNT which estimated the solubility of Florasulam at 25°C by using the Kow and regression equation calculation. It must be noted however that if there is a value in the "Exper. Database Match" box, this value should be used as any experimental values have preference over estimated ones.

Vapour pressure (mm Hg) - The tab marked MPBPVP covers the melting point, boiling point and vapour pressure of the chemical and provides estimated and experimental values where possible. As noted above, unless an experimental value is available, the estimated vapour pressure value shall be used; for Florasulam this value is 4.33E-09 mm Hg at 25 deg C.

Log Kow – As the experimental value is unavailable, the estimated log Kow for Florasulam is taken as 2.13 and can be found under the KOWWIN tab.

*Atmospheric OH rate (days) (cm3/molecules*sec)* - Under the AOPWIN tab/Hydroxyl Radicals Page 2, the overall OH rate constant of 6.2713E-12 for Florasulam can be found.

ChemSketch
Using the pesticide's SMILES, the software ChemSketch, developed by ACD labs (ChemSketch 2010), generates the structure of the pesticide then calculates the Molecular volume, given in units of cm^3/mol Table 13.

Table 13: Molecular volume calculated in ChemSketch

Input parameter	Abbreviation	Unit
Molecular volume	Mol Vol	cm^3/mol

WIN PST
Keeping close to the sources used in the Pest LCI database, the software WIN PST (Windows Pesticide Screening Tool) was also used (WIN-PST 2011). As Flurtamone however was not covered in WIN PST its Koc (l/kg) value and soil half life was reference from EPIsuite Table 14.

Table 14: Properties acquired from WINPST

Input parameter	Abbreviation	Unit
Soil Organic Carbon-Water Partitioning Coefficient	Koc	l/kg
Soil half life	$t_{1/2}$	(days) (temp.)

OECD REPORT
A final piece of pesticide specific information used within the PestLCI program was obtained from an OECD report which provided the "No Spray Zone width (m)" under Annex D (Møhlenberg, Gustavson et al. 2000).

Annex 3: Pesticide data required for USEtox

Method for calculating characterisation factors for pesticides missing from USEtox and implementation into SimaPro to calculate toxicity.

When wanting to calculate the characterisation factors of a toxic substance, specific physiochemical and ecotoxicological properties must be obtained. Ranging from the molecular weight of the chemical, to the HC50 value, each can be found through a variety of methods which may involve the use of various databases or extrapolation estimation software.

In this report specifically, the Pesticide Properties Database (PPDB) and the EPI suite software was used for each of the missing chemicals. The following are the properties needed and how they were acquired for this report for the pesticides not already defined within the USEtox database.

Using Florasulam as an example pesticide, the properties have been divided into two groups, those which were obtained through the PPDB and those obtained via EPIsuite extrapolation.

The Florasulam page within the PPDB database provided the needed properties in Table 15; these were then entered into the USEtox Excel spreadsheet model with no calculations necessary.

Table 15: Pesticide properties obtained through the PPDB, exemplified by Florasulam.

Input parameter	Abbreviation	Unit
Molecular weight	MW	g/mol^{-1}
Partitioning coefficient between octanol and water	K_{OW}	-
Henry law coefficient (at 25°C)*	K_H25C	$Pa*m^3/mol^{-1}$
Vapour pressure (at 25°C)	Pvap25	Pa

*If experimental data for the Henry law coefficient is unavailable calculation is done by (Pvap25*MW)/ Sol25) = K_{ow}.

The properties in Table 16 were obtained through use of the EPIsuite software.

Table 16: Pesticide properties obtained through the EPIsuite software.

Input parameter	Abbreviation	Unit
Partitioning coefficient between organic carbon and water	Koc	L/kg
Solubility (at 25°C)	Sol25	Mg/L
Degradation rate in air	$kdeg_A$	s^{-1}
Degradation rate in water	$kdeg_W$	s^{-1}
Degradation rate in sediment	$kdeg_{Sd}$	s^{-1}
Degradation rate in soil	$kdeg_{Sl}$	s^{-1}
Bioaccumulation factor in fish/biota	BAF_{fish}	l/kg

Partition coefficient between organic carbon and water- Following the guide of USEtox, the Koc was estimated from the MCI (Molecular connectivity index) of Florasulam. This was calculated within EPIsuite by the KOCWIN program to be 160.7 $L.kg^{-1}$.

Degradation rate in air, water, soil and sediment – In order to calculate these degradation rates for Florasulam, the K_{OH} (the overall hydroxyl radical rate constant in units of cm^3/molecule per sec) is needed.

This can be found under the "Hydroxyl Radicals Page 2" tab of the AOPWIN tab in EPIsuite and is given as $6.27e^{-12}$.

This is then multiplied with the hydroxyl radical concentration ([OH] given as molecules (or radicals) per cm^3) with the default value for the [OH] as $1.5x10^6$ molecules (radicals)/cm^3 per 12h of daylight. For Florasulam this equation is:

$6.27e^{-12}*1.5x10^6 = 9.41e^{-6}$

This $9.41e^{-6}$ is assumed to be the degradation rate in air for a full 24 hour period of daylight as it is not until it is divided by two do we get the same value as used in the main USEtox database as created by the developers. The reason for the division by two is to account for only 12 hours of daylight as found in the environment and thus 12 hours of effective removal per day.

$kdegA = 9.41e^{-6}/2$

kdegA Florasulam thus equals $4.7e^{-6}$

For water, soil and sediment, the degradation rates are extrapolated differently using the biowin3 Ultimate Survey Model, found under the BIOWIN tab within EPIsuite. Next to the numerical value a reference output notation is given which can be used in combination with table 3 to give a biodegradation rate (1/s). For example with

Florasulam "Recalcitrant" is given, consultation of Table 17 indicates it has a biodegradation rate of around $4.5.10^{-8}$.

Table 17: The relation between the BIOWIN3 output and assigned half-lives and biodegradation rates. Adapted from Mark Huijbregts (Huijbregts, Hauschild et al.).

BIOWIN3 Output	Assigned Half-Life (days)	Biodegradation rate (1/s)
Hours	0,17	$4,7.10^{-5}$
Hours to Days	1,25	$6,4.10^{-6}$
Days	2,33	$3,4.10^{-6}$
Days to Weeks	8,67	$9,3.10^{-7}$
Weeks	15,5	$5,3.10^{-7}$
Weeks to Months	37,5	$2,1.10^{-7}$
Months	60	$1,3.10^{-7}$
Recalcitrant	180	$4,5.10^{-8}$

To extrapolate the biodegradation rates of Florasulam in water, soil and sediment, division factors of 1:2:9 are used respectively on the given degradation rate as recommended by EPIsuite. These are calculated as $kdeg_W 4.5*10^{-8}$, $kdeg_{Sl} 2.2*10^{-8}$ and $kdeg_{Sd} 5*10^{-9}$.

Bioaccumulation factor in fish/biota – This parameter is not necessarily required for the calculation of the ecotoxicological characterisation factors as it is more relevant to human toxicity; however the BAF can be included as it is easily acquired from the BCFBAF tab in EPIsuite under the heading "Log BAF (Arnot-Gobas – Upper Trophic)" where the BAF is noted in brackets as 13.4.

The final set of information needed for the pesticide is the average logEC50 which requires a different method from those above. The effective concentration (EC50) value is the amount of a chemical needed to invoke a predetermined response in 50% of the tested population; other notations such as EC5 or EC20 account for responses in 5% and 20% respectively. In order to get a minimal representation of the chemicals toxicity, these experiments are usually carried out with three species, each occupying a different trophic level. For some chemicals there may be multiple EC50 values for one species; to get one value for the species the geometric mean is taken. The hazardous concentration (HC50) value is the geometric mean of all the available EC50 values for each species in each trophic level. By taking this value instead of the most sensitive species (as done in risk assessment) the average sensitivity of the species is seen allowing for an easier comparison between the chemicals under investigation as a broader sense of the chemicals environmental impact is taken into account. If there is more than one data set for a species, the geometric mean of that species data is first taken before being averaged with the other species data. Chronic values are preferred to acute values as long as they are represented in terms of an EC50 value. More often than not acute EC50 values can be found for each chemical to satisfy the minimal requirements.
In this report both the Pesticide Properties Database and the ECOTOX database (ECOTOXdatabase 2011), created by the U.S. Environmental Protection Agency were used to gather available aquatic acute EC50 values for the chemicals not covered in the USEtox database. Table 18 is a representation of how the HC50 value for Florasulam was calculated.

The preferred unit for the EC/HC50s to be represented in is mg/l; due to this, any EC50 value given in µg/l is converted before the geometric mean is taken. With regards to Florasulam there is only one EC50 value given per species which are all given for an acute experiment. It must be noted that acute 96h LC50 (lethal concentration) values are more commonly used as a representation of toxicity for fish than EC50 values. Once all the EC50 values for the species have been grouped the geometric mean (found as GEOMEAN in Excel) is taken to give the corresponding HC50acute for Florasulam (Equations 8 and 9). To get the HC50chronic value, an acute to chronic ration value of 2 is used as suggested by the USEtox organic chemical manual (Huijbregts, Hauschild et al. 2010).The value derived from this calculation is then placed in the avelogEC50 column (20) in the work sheet.

Table 18: Effective concentration (EC50) values for Florasulam with required steps to calculate the hazardous concentration (HC50) chronic from the geometric mean (GM) of the species EC50s.

145701-23-1	FLORASULAM	
Trophic level/ Taxa	**Species**	**EC50acute (mg/l)**
Primary producers		
Freshwater algea	*Selenastrum capricornutum*	0.00894
Algea	*marine diatom*	47.6
aquatic plant - Inflated Duckweed	*Lemna gibba*	0.00118
aquatic plant - Duckweed	*Lemna spp*	0.001
Primary consumers		
Crustation	*Daphnia magna*	292
Secondary consumers		
Fish	*Oncorhynchus mykiss*	100
	HC50acute (mg/l)	0.494729972
	HC50chronic (mg/l)	0.247364986

Equation 8

Equation 9

Annex 4: From USEtox Excel to USEtox SimaPro.

Provided all the required parameters of USEtox have been included (all relevant chemical properties and climactic data), the Excel program can be run which will calculate the characterisation factors. Once finished, the results page will be displayed presenting the characterisation factors for each chemical selected.

The SimaPro version of USEtox works differently to the Excel version and acts as a next step to the process, providing Impact scores per compartment based on the characterisation factor and the amount of the chemical emitted to each compartment. Another noticeable feature is that the compartments from USEtox Excel are no longer found exactly in the SimaPro version. Instead the three main compartments of air, water and soil are divided up into various sub-compartments which correspond to those in Excel. Table 19: Correlation between sub categories in USEtox excel and Usetox SimaPro. Taken from (Consultants., Goedkoop et al. 2010) (Consultants., Goedkoop et al. 2010) shows how the sub-compartments of those used by the Excel version correspond to those used in the SimaPro version.

Table 19: Correlation between sub categories in USEtox excel and Usetox SimaPro. Taken from (Consultants., Goedkoop et al. 2010)

	SimaPro compartments	USEtox (excel) compartments		
Air	(unspecified)	50 Em.airU / 50 Em.airC	50/50 urban/continental	Estimated
Air	high. pop.	Em.airU	Urban air	Calculated
Air	low. pop.	Em.airC	Continental air	Calculated
Air	low. pop., long-term	Em.airC	Continental air	Estimated
Air	stratosphere + troposphere	Em.airC	Continental air	Estimated
Water	(unspecified)	Em.fr.waterC	Freshwater	Estimated
Water	river	Em.fr.waterC	Freshwater	Calculated
Water	river, long-term	Em.fr.waterC	Freshwater	Estimated
Water	lake	Em.fr.waterC	Freshwater	Calculated
Water	ocean	Em.sea waterC	Sea water	Calculated
Soil	agricultural	Em.agr.soilC	Agri. Soil	Calculated
Soil	(unspecified)	Em.nat.soilC	Natural soil	Estimated
Soil	forestry	Em.nat.soilC	Natural soil	Calculated

In this report, it was decided that the compartments focused on are Air - Stratosphere + Troposphere and Water - (Unspecified). These compartments were chosen as they best accommodate the data incoming from the PESTLCI dispersion model; previously used to calculate the emissions to each compartment from the point of application.
Once the USEtox SimaPro database has been updated with the characterisation factors of the chemical under investigation, the volumes released to each compartment (previously calculated by PESTLCI) can be entered into the current process allowing for analysis and calculation of the Impact scores. Once calculated, the impact scores of each chemical can be compared and the environmental impact of the chemicals used and which are more hazardous can be ascertained.