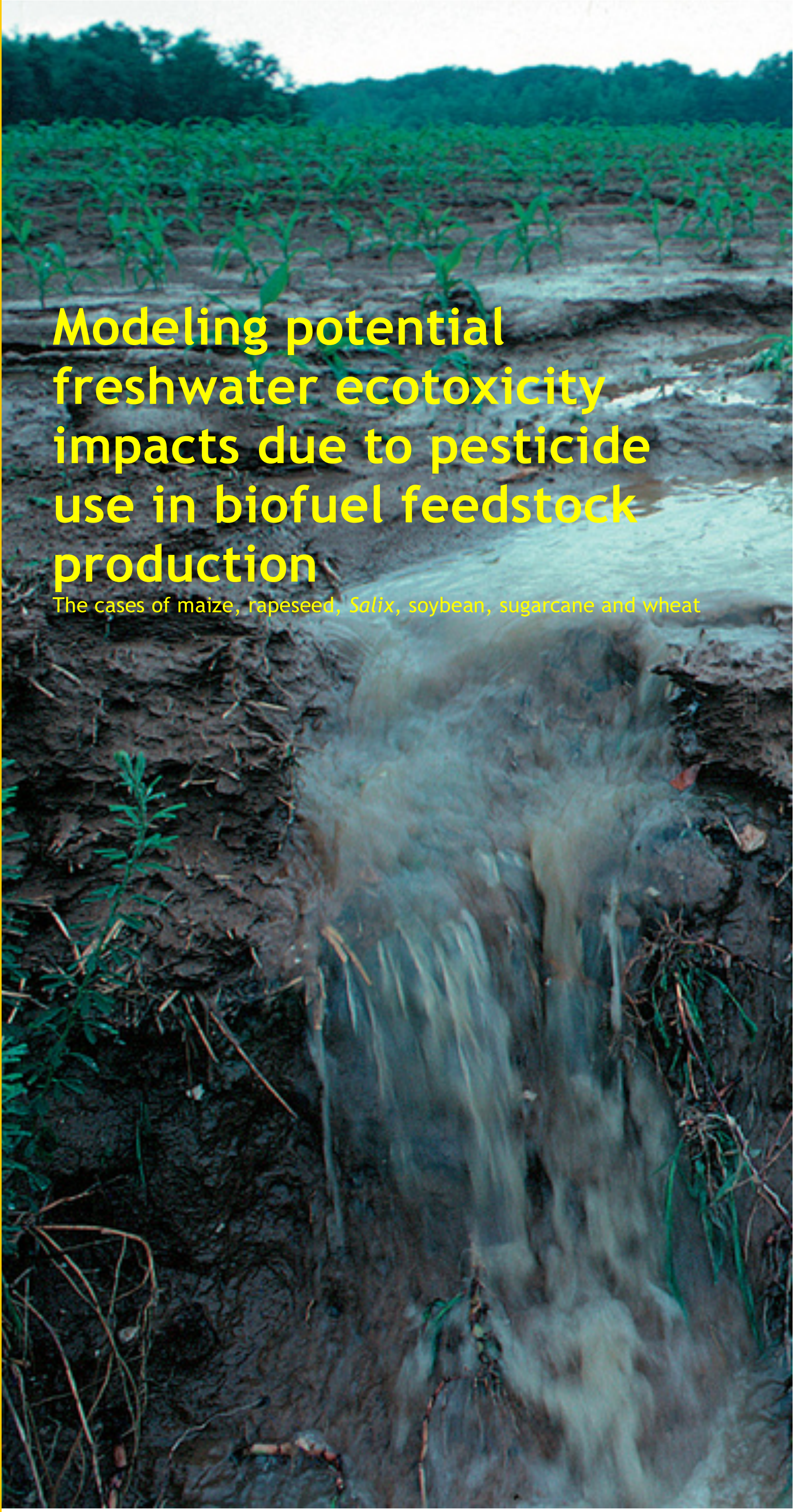
Modeling potential freshwater ecotoxicity impacts due to pesticide use in biofuel feedstock production

The cases of maize, rapeseed, *Salix*, soybean, sugarcane and wheat



Ecotoxicity impacts have seldom been included in Life Cycle Assessments of biofuels. This report demonstrates an approach to model the potential freshwater ecotoxicity impacts due to pesticide use, using the PestLCI and USEtox models. The method is applied to eight biofuel feedstock production cases: maize in the US (two cases), rapeseed and wheat in Germany, soybean (two cases) and sugarcane in Brazil, and Salix in Sweden. Potential freshwater ecotoxicity impacts vary by up to 3 orders of magnitude with Salix at the lower end and wheat and rapeseed at the higher end. Potential mitigation strategies include substitution to less toxic pesticides, and reduction of emissions to freshwater ecosystems, through improved management, e.g. the use of buffer zones.

IEA Bioenergy

IEA Bioenergy Task 43
Report 2015:TR04

This page is Reserved for copywrite information and ISBN number

Cover page photo credit: Lynn Betts, USDA
Photo:(flickr).www.flickr.com/photos/48722974@N07/4464667181/

MODELING POTENTIAL FRESHWATER ECOTOXICITY IMPACTS DUE TO PESTICIDE USE IN BIOFUEL FEEDSTOCK PRODUCTION

Authors

Maria Nordborg (Chalmers University of Technology), Göran Berndes (Chalmers University of Technology), Christel Cederberg (Chalmers University of Technology)

Summary report

KEY MESSAGES

Ecotoxicity impacts have often been excluded in Life Cycle Assessment studies of biofuels due to methodological challenges. However, pesticides are an integral part of the cultivation of biofuel feedstocks and much of the applied dose is dispersed in the surrounding environment where it may cause harm to non-target organisms.

The report gives an overview of the global use of pesticides, and their documented negative effects. Potential freshwater ecotoxicity impacts due to typical pesticide use is assessed for eight biofuel feedstock production cases; maize in the US, rapeseed and wheat in Germany, soy and sugarcane in Brazil, and Salix in Sweden.

The assessed potential freshwater ecotoxicity impacts varied greatly, by up to 3 orders of magnitude. Salix had the lowest impact score, both in relation to biofuel yield and in relation to area and time. Rapeseed and wheat had the highest impact scores. The uses of the insecticide beta-cyfluthrin (rapeseed) and the fungicide chlorothalonil (wheat) where responsible for 92 and 84% of the total impact scores for these crops.

Due to existing uncertainties and model limitations, results should be interpreted with caution, and foremost be used for ranking and identification of the highest-impact active substances. The results also show that amount of pesticide active substance is an inadequate indicator of ecotoxicity.

Mitigation strategies for reducing freshwater ecotoxicity impacts in biofuel feedstock production include substitution to pesticide products with lower toxic potency, and reduction of emissions to freshwater ecosystems, through improved management, e.g., application of buffer zones.

EXECUTIVE SUMMARY

Biomass-based transport fuels (biofuels) currently supply around 3% of global road transport fuel demand, a share that is projected to increase significantly in the future. Biofuels could supply up to 27% of global transport fuel demand by 2050, according to the IEA Technology Roadmap. Most Life Cycle Assessment studies of biofuels have focused on energy and greenhouse gas balances, while ecotoxicity impacts have often been excluded due to methodological challenges. Pesticides are an integral part of modern agriculture, also in the cultivation of biofuel feedstocks. However, only a fraction of the applied dose typically reaches the target pest, while the majority is dispersed in the surrounding environment where it may cause harm to non-target organisms. The report gives an overview of the global use of pesticides, and their documented negative effects.

We investigated typical pesticide use in selected biofuel feedstock production cases; expanded the pesticide database and the regional coverage of the pesticide emission model PestLCI v.2.0, combined it with the impact assessment model USEtox v.1.01, and assessed the potential freshwater ecotoxicity impacts due to pesticide use in the following eight cases: MZ-I/II (genetically engineered glyphosate tolerant maize cultivated in Iowa, US, with (MZ-I) and without (MZ-II) *Bt*-technology, i.e., ability of the crop to produce its own insecticidal toxin from the bacterium *Bacillus thuringiensis*); RS (winter rapeseed cultivated in Schleswig-Holstein, Germany); SX (*Salix* short rotation woody coppice cultivated in South Central of Sweden); SB-I (conventional soybean cultivated in Mato Grosso, Brazil); SB-II (GE glyphosate tolerant soybean cultivated in Mato Grosso, Brazil); SC (sugarcane cultivated in São Paulo, Brazil) and WT (winter wheat cultivated in Schleswig-Holstein, Germany).

We found that potential freshwater ecotoxicity impacts, expressed in the unit Comparative Toxic Units ecotoxicity (CTUe), varied greatly, by up to 3 orders of magnitude. In relation to biofuel yield, the SX case has a potential freshwater ecotoxicity impact score of about 3 CTUe TJ^{-1} (allocated with partitioning based on energy content), while impact scores for the cases SC, MZ-I, MZ-II, SB-II, SB-I, WT, and RS are about 30, 110, 270, 305, 310, 750, and 1000 times larger, respectively. In relation to area and time, the SX case has a potential freshwater ecotoxicity impact score of < 1 CTUe ha^{-1} yr^{-1} (unallocated value), while impact scores for the cases SC, MZ-I, SB-II, SB-I, MZ-II, RS, and WT are about 60, 205, 220, 220, 500, 1110, and 1115 times larger, respectively. The high scores of RS and WT are associated with the use of the insecticide beta-cyfluthrin in RS, and the fungicide chlorothalonil in WT, responsible for 92 and 84% of the total impact scores, respectively. Due to existing uncertainties and model limitations, results should be interpreted with caution, and foremost be used for ranking and identification of the highest-impact active substances (ASs). The results also show that amount of pesticide AS is an inadequate indicator of ecotoxicity.

The influence of management and local conditions on resulting impacts were tested in sensitivity analyses, and discussed. Mitigation strategies for reducing freshwater ecotoxicity impacts in biofuel feedstock production include substitution to pesticide products with lower toxic potency, and reduction of emissions to freshwater ecosystems, through improved management, e.g., application of buffer zones.

Much remains to be done before ecotoxicity due to pesticide use is routinely included in agricultural LCAs. Areas for future research and development include: expanding substance databases, expanding regionalization of PestLCI and validating it against non-European conditions, developing methods for including toxicity of degradation products and of mixtures, and reviewing the selection criteria of physico-chemical and ecotoxicity effect data to PestLCI and USEtox.

CONTENTS

GLOSSARY OF TERMS AND ACRONYMS

AS	Active Substance; the biologically active part of a pesticide product
Bt	*Bacillus thuringiensis*; genetic engineering of crops to produce insecticidal toxins from the *Bt*-bacterium
CAS-RN	Chemical Abstracts Service Registry Number: numerical identification system of chemicals
CFs	Characterization Factors
CTUe	Comparative Toxic Units ecotoxicity
DDGS	Dried Distillers Grains with Soluble: co-product from the ethanol production used as protein fodder for livestock
ECX	Effective Concentration X; the concentration of a substance that cause 50% of test organisms to be affected
F	Fungicide
GE	Genetically Engineered
GHG	Greenhouse Gas
H	Herbicide
HCX	Hazardous Concentration X: the concentration at which X% of species in a SSD are exposed above a certain effect level.
$HC50_{EC50}$	The Hazardous Concentration at which 50% of the species in a SSD are exposed above their EC50 effect-level.
I	Insecticide
IEA	International Energy Agency
ILCD	International Reference Life Cycle Data System
IPM	Integrated Pest Management
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCX	Lethal Concentration X; the concentration of a substance that cause a Lethal Effect in X% of test organisms
LOEC	Lowest Observed Effect Concentration
MZ-I	Maize-I case: Genetically engineered glyphosate tolerant maize with *Bt*-technology, cultivated in Iowa, USA
MZ-II	Maize-II case: Genetically engineered glyphosate tolerant maize without *Bt*-technology, cultivated in Iowa, USA

N	Nematicide
NOEC	No Observed Effect Concentration
RS	Winter rapeseed case: rapeseeds cultivated in Schleswig-Holstein, Germany
SB-I	Soybean-I case: conventional soybean cultivated in Mato Grosso, Brazil
SB-II	Soybean-II case: genetically engineered glyphosate tolerant soybean cultivated in Mato Grosso, Brazil
SC	Sugarcane case: sugarcane cultivated in São Paulo, Brazil
SMILES	Simplified Molecular Input Line Entry System; a chemical notation system in which molecular structure are represented by a linear string of symbols
SSD	Species Sensitivity Distribution
SX	*Salix* case: *Salix* short rotation woody coppice cultivated in South Central of Sweden
PAF	Potentially Affected Fraction
PEC	Predicted Environmental Concentration
PGR	Plant Growth Regulator
PNEC	Predicted No Effect Concentration
PPDB	Pesticide Properties Database
USDA	United States Department of Agriculture
WT	Winter wheat case: winter wheat cultivated in Schleswig-Holstein, Germany

CHAPTER 1. INTRODUCTION

The transport sector contributed an estimated 22% of global CO_2 emissions in 2011 (IEA, 2013a), and global demand for transport is expected to grow significantly over the coming decades. The International Energy Agency (IEA) projects that transport fuel demand will grow by nearly 40% between 2011 and 2035(IEA, 2013b). Biomass-based transport fuels (biofuels) currently supply around 3% of global road transport fuel demand (Chum et al. 2011), a share that is projected to increase substantially in the future. The World Energy Outlook 2013 projects that biofuel use will triple between 2011 and 2035, by which time it supplies 8% of road transport fuel demand, under the New Policies Scenario (IEA, 2013b). By 2050, biofuels could supply up to 27% of the global transport fuel demand, according to the IEA Technology Roadmap, based on cost effective strategies for climate change mitigation (IEA, 2011).

Currently, biofuels are over 99% derived from conventional agricultural crops (IEA, 2013b), such as sugarcane, maize, rapeseed, soybeans and cereals. Advanced biofuels, derived from e.g., fast growing trees, perennial grasses and agricultural residues, are potentially more environmentally benign and economically viable than conventional biofuels, but currently limited to pilot and demonstration plants (IEA, 2013b). Under the IEA New Policies Scenario advanced biofuels increase their market share from less than 1% of total biofuels in 2013, to almost 20% in 2035, and become commercially available around the year 2020 (IEA, 2013b).

Most studies of the environmental performance of biofuels have focused on energy and GHG balances (von Blottnitz and Curran, 2007; Wiloso et al. 2012). However, several studies (Kim and Dale, 2005; von Blottnitz and Curran, 2007; Kim and Dale, 2008; Bai et al. 2010; Emmenegger at al. 2012; Yang et al. 2012; Yang, 2013) have shown that biofuels can be associated with higher impacts than fossil fuels, in terms of e.g. acidification, eutrophication, ecotoxicity and human toxicity. Thus, broadening the scope to a wider range of impacts is essential to ensure that conclusions and recommendations are based on sufficiently comprehensive assessments and to avoid environmental burden-shifting (Bai et al. 2010; Guinée et al. 2011; Wiloso et al. 2012; Yang et al. 2012; Laurent et al. 2012).

Ecotoxicity impacts have received relatively little attention in biofuel-LCAs.von Blottnitz and Curran (2007) found that only one of 47 reviewed lifecycle-based studies of ethanol published between 1996 and 2004 considered ecotoxicity. Wiloso and co-workers (2012) found that only six of 31 Life Cycle Assessments (LCAs) of second generation bioethanol published between 2005 and 2011 considered ecotoxicity. It should also be noted that inclusion of ecotoxicity in LCA does not necessarily mean that the ecotoxic effects from pesticides are considered. Neither does inclusion of pesticides in the inventory necessarily mean that their ecotoxicity impacts are considered.

Chemical pesticides have become an integral part of agricultural systems since the middle of the last century (Edwards, 1993) and world production of formulated pesticide product increased by approximately a factor 50 between 1945 and 2005 (Carvalho, 2006). Since the beginning of the 21st century, global pesticide consumption has reached a maximum, and currently show a slightly decreasing trend (US-EPA, 1997; 1999; 2002; 2004; 2011). Pesticides protect crops from adverse impacts from weeds, pests and diseases, and have enabled the “Green revolution”, but are also associated with negative effects, such as contamination of surface and ground water (Arias-Estévez et al. 2008) and impacts on pollination services (van der Sluijs et al. 2013; Lu et al. 2014), farmland bird populations (Hallmann et al. 2014), biodiversity (Geiger et al. 2010; Beketov et al. 2013), community structure and ecosystem function (Schäfer et al. 2007) and human health (WHO, 1990; Mostafalou and Abdollahi, 2013). For more information on negative effects of pesticides, see Chapter 2.3. Large-scale and improper use of pesticides is also increasingly linked to problems with resistance development in weeds, insects, and fungi (Mortensen et al. 2012; Gilbert, 2013; Heap, 2014; IRAC Website, FRAC Website); see further in Chapter 2.4.

Amount of applied pesticide active substance (AS) is not an adequate indicator of the ecotoxic effect; an increasingly acknowledged fact (Audsley et al. 2003; de Vries et al. 2010). Recent scientific advances, in particular the launch of the USEtox-model (Rosenbaum et al. 2008; USEtox Website) make more sophisticated freshwater ecotoxicity assessments possible.

Traditional LCA is site-generic, i.e., does not take the location of emission sources or receiving compartments into account (Potting and Hauschild, 2006). This is an acceptable approach for impacts that are global in character and that are not influenced by local factors, such as global warming. It has however been known for well over a decade that the site-generic approach is less applicable to products of agricultural origin, and to impacts that are local or regional in character, since local agricultural practices and site-specific pedoclimatic factors influence results (Kim and Dale, 2005; Potting and Hauschild, 2006; Kim and Dale, 2008; Kim and Dale, 2009; Fazio and Monti, 2011; Tessum et al. 2012), not the least concerning pesticide emissions and toxicity impacts (Birkved and Hauschild, 2006; Wegener Sleeswijk and Heijungs, 2010; Wegener Sleeswijk, 2011; Dijkman et al. 2012; Kounina et al. 2014). Derivation of spatially differentiated ecotoxicity characterization factors (CFs) have shown that there are considerable regional variations due to differences in rain rates, distributions of lakes and rivers, and temperatures (Wegener Sleeswijk and Heijungs, 2010).

Pesticide emission fate modeling is currently handled inconsistently in agricultural LCAs, and typically builds upon simplified assumptions and generic fate-factors (van Zelm et al. 2014; Rosenbaum et al. 2015), e.g., that the pesticide dose is entirely emitted to agricultural soil (Nemecek and Schnetzer, 2011), or other weakly supported distribution patterns (Audsley et al. 2003).

In this study, we combine a state-of-the-art pesticide emission inventory model, PestLCI 2.0 (Dijkman et al. 2012), with the “best available” (Hauschild et al. 2013) model for impact assessment of freshwater ecotoxicity, USEtox (Rosenbaum et al. 2008), and assess the potential freshwater ecotoxicity impacts due to pesticide use in biofuel feedstock production.

1.1 Aim

The aim of this study is to examine and demonstrate a methodology for potential freshwater ecotoxicity impact assessment of pesticide use; apply it to a set of biofuel feedstocks; highlight the importance of performing a detailed and site-specific inventory of pesticide usage and emissions; identify the highest-impact ASs; discuss associated uncertainties and propose measures to reduce the environmental burden in freshwater ecosystems caused by biofuel feedstock production.

1.2 Scope

Seven cases comprising five conventional biofuel feedstocks are considered: maize (US, two cases; see below), winter rapeseed (Germany), soybean (Brazil, two cases; conventional and genetically engineered glyphosate tolerant soybean), sugarcane (Brazil) and winter wheat (Germany). The two maize cases represent genetically engineered (GE) glyphosate tolerant maize with and without *Bt*-technology, i.e., ability of the crop to produce its own insecticidal toxin from the bacterium *Bacillus thuringiensis*. The eighth case is an example of a potential future lignocellulosic feedstock for the production of second generation biofuels(*Salix*, Sweden; n.b. biofuel conversion technologies not yet commercially available).

The eight cases are presented in Table 1.1 along with their associated biofuel types, cultivation regions, fresh harvest yields and co-products. The list of possible co-products in Table 1.1 is exhaustive, but represent those co-products that we considered in the allocation, see further in Chapter 4.6.

Limitations

Only direct and intentional pesticide field application and associated emissions to air and surface water are considered. Accidental spills and emissions that originate from handling and storage of pesticides are not included, and neither are emissions that originate from other stages in the life cycle of pesticides. Emissions to other environmental compartments, other than air and surface water, are not considered. Only freshwater ecotoxicity is assessed, i.e., terrestrial and marine ecotoxicity are excluded.

USEtox allows for the quantification of impact on human toxicity, but existing methods only take into account the typically minor effects on the general public through diffuse exposure such as airborne emissions, contaminated drinking water, and food residues. The more adverse near-field impacts, affecting primarily field workers through direct exposure, are not taken into account. Toxic effects on humans are therefore not included in this study.

Only the ASs in herbicides (H), fungicides (F), insecticides (I), nematicides (N) and plant growth regulations (PGR) are included. Other pesticide product ingredients, such as solvents and surfactants, are not included. Pesticides used to treat seeds were not considered.

Toxicity of degradation products, as well as mixture toxicity, are beyond the scope of this study.

Table 1.1. Case definitions.

Case abbrev.	**Feedstock**	**Biofuel type**	**Cultivation region**	**Fresh harvest yield** [a] **(kg ha^{-1} yr^{-1})**	**Allocation factor** [b]	**Co-products considered**
MZ-I, MZ-II [c]	Maize	Ethanol	Iowa, US	10 700	0.62	DDGS [d]
RS	Winter rapeseed	Biodiesel	Schleswig-Holstein, Germany	4050	0.61	Rapeseed cake, refined glycerol
SX	*Salix*	Ethanol	South Central Sweden	20 000	0.94	Electricity
SB-I, SB-II [e]	Soybean	Biodiesel	Mato Grosso, Brazil	3030	0.33	Soy cake, refined glycerol
SC	Sugarcane	Ethanol	São Paulo, Brazil	84 300	0.98	Electricity
WT	Winter wheat	Ethanol	Schleswig-Holstein, Germany	8740	0.56	DDGS[d]

[a] Fresh harvest yields for the conventional feedstocks (all cases excluding *Salix*) represent 2006-2011 production averages in the defined cultivation regions. Fresh harvest yield data were derived from USDA NASS Quick Stats Database for maize, from Statistikamt Nord (2013) for rapeseed and wheat, and from SIDRA-IBGE for soybean and sugarcane. The following water contents at harvest were used: maize: 14%, rapeseed: 15%, soybean: 13%, sugarcane: 72.5%, wheat: 13.5% - all derived from JRC (2012). Fresh harvest yield for *Salix* represents a conservative estimate of the future yearly yield potential averaged over a plantation life cycle, assuming 50% water content at harvest, based on IEA (2012). More information in Chapter 4.5.

[b] Allocation factors were calculated using the partitioning method based on energy content considering output shares in representative production systems, more information in Chapter 4.6.

[c] Genetically engineered (GE) glyphosate tolerant maize with (MZ-I) and without (MZ-II) *Bt*-technology.

[d] Dried Distillers Grains with Solubles.

[e] Conventional soybean (SB-I) and GE glyphosate tolerant soybean (SB-II).

1.3 Structure of this report

This report starts with an introduction to pesticides in Chapter 2, followed by an introduction to the modeling of potential ecotoxicity impacts in LCA, in Chapter 3.

Chapter 4 contains a detailed presentation of the models and methods employed in this study, as well as the data used, aiming to enable reproduction of this study, and facilitate further assessments.

Chapter 5 introduces the eight cases and the associated pesticide application data.

Chapter 6 presents and discusses the results of the study, and of the sensitivity analyses, and includes a discussion of related uncertainties and options for reducing negative effects.

Chapter 7 ends with a summary of the main conclusions derived from this study.

CHAPTER 2. PESTICIDES

This chapter contains an introduction to pesticides (Chapter 2.1); an overview of the global use of pesticides (Chapter 2.2); an overview of documented negative effects of pesticides on the environment and on human health (Chapter 2.3) and a discussion of issues related to pesticide resistance (Chapter 2.4).

2.1 What are pesticides?

The term pesticide is defined by FAO (2003) as "*any substance or mixture of substances intended for preventing, destroying or controlling any pest, including vectors of human or animal disease, unwanted species of plants or animals causing harm during or otherwise interfering with the production, processing, storage, transport or marketing of food, agricultural commodities, wood and wood products or animal feedstuffs, or substances which may be administered to animals for the control of insects, arachnids or other pests in or on their bodies. The term includes substances intended for use as a plant growth regulator, defoliant, desiccant or agent for thinning fruit or preventing the premature fall of fruit, and substances applied to crops either before or after harvest to protect the commodity from deterioration during storage and transport*".

Pesticides used in agriculture are sometimes called plant or crop protection products. The biologically active part of pesticide products are referred to here as active substance (AS), but pesticide products typically contain a mixture of ingredients to make products useful and effective (FAO, 2003), e.g., surfactants, adjuvants, fillers or extenders, wetting agents, diluents or solvents, adhesives, buffers, preservatives and emulsifiers (FAO, 1996).Such "inert" ingredients are added to enhance the product performance (by e.g. making it easier to apply), but can also have toxic effects on their own (Geller, 2005). Adjuvants and fillers have for example been shown to be able to increase the biological efficiency and toxicity of pesticide products by up to a factor 10, by modifying spray droplet size, retention and crop uptake (van Zelm et al. 2014).

Pesticides can be classified based on target organism, toxic mode-of-action, or chemical composition (Arias-Estévez et al. 2008). Common terminology indicate a classification based on target organisms, as in herbicides (weeds), insecticides (insects), fungicides (fungi or fungal spores), molluscicides (slugs and snails), acaricides (mites and ticks), rodenticides (rodents) and nematicides (nematodes). For a review of the biological mechanisms of pesticides, i.e. toxic modes-of-action, refer to DeLorenzo et al. (2001).Another system of classifying pesticides is based on their potential human health hazard as in the ranking system developed by the World Health Organization (WHO, 2010).

2.2 Global use of pesticides

World production of formulated pesticide product increased by approximately a factor of 50 between 1945 and 2005 (Carvalho, 2006). Since the beginning of the 21st century, global consumption seems to have reached a maximum and has started to decrease slightly (US-EPA, 1997; 1999; 2002; 2004; 2011).

Global total pesticide use (all pesticides) amounted to 2.4 million metric tons of AS in 2007, the latest year for which the US Environmental Protection Agency produced global estimates (US-EPA, 2011). If only herbicides, plant growth regulators, insecticides and fungicides are included, global use amounts to 1.6 million metric tons of AS (US-EPA, 2011; FAOSTAT).

For comparison, the European Union (EU-25) consumed 0.2 million metric tons of herbicide, fungicide and insecticide AS in 2003, the latest year for which the Eurostat compiled the statistics (Eurostat, 2007).

2.3 Negative effects of pesticides

Negative effects of pesticides stem from the fact that pesticides are designed to be toxic, and intentionally released into the environment, where they may cause harm to non-target organisms. In fact, ten out of the 12 most dangerous and persistent chemicals as initially identified by the Stockholm Convention on Persistent Organic Pollutants (the so-called “dirty dozen”), are pesticides (POPS, 2001).

Environmental impacts

An early review by Pimentel and colleagues (1993) linked pesticide use with negative effects on a wide range of environmental and ecosystem functions, including domestic animal poisoning, destruction of beneficial natural predators and parasites, pesticide resistance in pests, reduced pollination, ground- and surface water contamination, fishery losses and impacts on microorganisms, invertebrates, wild birds and mammals. Since then, numerous studies have followed. A selection of recent studies on topical subjects is reviewed here.

Declining bee populations globally have recently been in the limelight, and several studies have linked bee disorders and negative population trends to the use of neonicotinoids, a class of systemic, and widely used, insecticides. van der Sluijs et al. (2013) reported that at field realistic exposure levels, neonicotinoids impaired bee foraging success, brood and larval development, memory, learning and hive hygiene, increased susceptibility to diseases and caused damage to the central nervous system. Lu et al. (2014) exposed honey bees to sub-lethal levels of neonicotinoids and observed that bees from six of twelve neonicotinoid-treated colonies abandoned their hives and died with symptoms resembling colony collapse disorder (CCD), while only one out of six untreated control hives were lost (due to parasite infection).

Recent evidence from the Netherlands indicates that neonicotinoids affect not only insects but also insectivorous birds (Hallmann et al. 2014).Based on data from 2003-2009 on 15 farmland bird species, and data on pesticide residues in surface water, it was found that surface water concentrations of the neonicotinoid imidacloprid were spatially, and negatively, correlated with bird populations. The proposed hypothesis by Hallmann and colleagues (2014) is that food source depletion is an explanatory factor, possibly in combination with toxic effects due to consumption of neonicotinoids-exposed insects.

Pesticides have also been linked to declining biodiversity. Geiger et al. (2010) reviewed the evidence on the links between agricultural intensification and biodiversity, in terms of species diversity of wild plants, carabids and ground-nesting farmland birds on farmland in eight European countries, and concluded that the use of insecticides and fungicides was associated with consistent negative effects on biodiversity.

Beketov et al. (2013) studied the effects of pesticides on regional biodiversity in terms of taxa richness of stream invertebrates in Europe (Germany and France) and Australia, and found a statistically significant negative effect in both regions.

Pesticides have also been linked to negative effects on community structure and ecosystem function. Schäfer et al. (2007) studied the effects of pesticide exposure on invertebrate community structure and ecosystem function in terms of leaf-litter breakdown, in France and Finland, and found that elevated pesticide levels were associated with lower relative abundance and number of sensitive species, and a reduction in the leaf-litter breakdown rate.

Human health impacts

Pesticides have also been linked to negative impacts on human health. Mostafalou and Abdollahi (2013)reviewed the literature on the correlation between pesticides and human chronic diseases, and concluded that there exists a huge body of evidence on the connection between pesticide exposure and different types of cancers, diabetes, Parkinson's disease, Alzheimer's disease, amyotrophic lateral sclerosis (ALS), birth defects, and reproductive disorders. They also concluded that there exist less conclusive, but yet indicative, evidence on the connection between pesticide exposure and some respiratory problems and cardiovascular and autoimmune diseases, including asthma, rheumatoid arthritis and chronic fatigue syndrome.

Several review studies are available that confirm the finding of Mostafalou and Abdollahi (2013) with regard to cancer (Van Maele-Fabry et al. 2006; 2013; Vinson et al. 2011; Alavanja et al. 2012) and Parkinson's disease (Freire and Koifman, 2012; Van Maele-Fabry et al. 2012; Allen and Levy, 2013).

Other recent review studies have linked pesticide exposure to neurodevelopmental effects in children, e.g. cognitive deficits, behavioral deficits and motor deficits (Muñoz-Quezada et al. 2013; González-Alzaga et al. 2014), hearing loss (Kós et al. 2013; Gatto et al. 2014), and reduced male fertility (Roeleveld and Bretveld, 2008).

The most recent estimate to our knowledge, of the number of people that become acutely pesticide poisoned each year, was made by the World Health Organization in 1990. According to this estimate, more than 1 million people become acutely pesticide poisoned each year unintentionally, and 2 million people become acutely pesticide poisoned each year intentionally (mostly suicide or suicide attempts) (WHO, 1990). Of the total 220 000 deaths due to acute pesticide poisoning, 91% were attributable to suicide, 6% to occupational exposure and 3% to other causes, in 1985 (WHO, 1990).

2.4 Pesticide resistance

Due to natural genetic variability, some organisms are less susceptible to pesticides, i.e., naturally resistant. In a given insect population e.g., the naturally tolerant share of the population is typically less than 1‰ of the total population, but increases in response to repeated insecticide treatments (Ekbom, 2002).

Crops genetically engineered (GE) to tolerate glyphosate has been called the "*most rapidly adopted technology in the history of agriculture*" (Green, 2012). While this technology offers several benefits, the rapid adoption of glyphosate tolerant crops has undoubtedly been associated with an increase in field-evolved glyphosate resistant weeds(Mortensen et al. 2012; Gilbert, 2013).

Pesticide resistance is not a new problem, nor limited to a specific technology. Development of resistance is mainly caused by excessive and repeated use of pesticides with the same toxic mode-of-action, and best avoided by employing a wide and varying set of strategies, including chemical (with different toxic modes-of-action), mechanical, biological and cultural options (Mortensen et al. 2012; Green, 2012). Although genetic engineering of crops to tolerate glyphosate *per se* is not responsible for causing pesticide resistance, the management practices associated with the cultivation of such crops favors the development. This is because weed management strategies in the cultivation of GE glyphosate tolerant crops are typically restricted to repeated use of glyphosate alone, year after year (Green, 2012; Owen and Hartzler, 2011; 2012; 2013).

Supporters of the GE technology claim that it can reduce pesticide use, among other benefits (Uzogara, 2000; Phipps and Park, 2002).That might be true in some cases, e.g., herbicide tolerant canola in Canada (Brimner et al. 2005). However, several recent studies have shown that cultivation of major GE crops has led to increased pesticide use. In the cases of US maize and cotton, Benbrook (2012) estimated that the *Bt*-technology reduced insecticide use by 56 million kg between 1996 and 2011, while with respect to herbicide tolerant crops (soybean, cotton and maize), herbicide use, in particular glyphosate, increased by 239 million kg, causing a net total pesticide increase of 7%.Lundgren et al. (2008) showed that the area of US soybean treated with glyphosate increased from 20% to nearly 100% between 1994 and 2006 in parallel with the introduction and large-scale adoption of GE glyphosate tolerant soybean varieties.

In the case of Brazil, Meyer and Cederberg (2010) found that herbicide use increased with 50%between 2003 and 2008, in parallel with the large-scale adoption of GE glyphosate tolerant soybean.

It should be noted that while cultivation of glyphosate tolerant crops may be associated with increasing use of glyphosate, it is typically at the expense of other, more toxic and persistent herbicides (Frisvold et al. 2009; Green, 2012), which is a strong reason for protecting the GE-technology against resistance development.

In the US, over-use of glyphosate in the cultivation of glyphosate tolerant crops has been linked to the development of very problematic glyphosate tolerant weeds such as Palmer amaranth (*Amaranthus palmeri*), horseweed (*Conyza canadensis*), and Johnsongrass (*Sorghum halepense*) (Mortensen et al. 2012), recently termed “superweeds” (Gilbert, 2013).

In total, 235 different weed species in 65 countries have developed herbicide resistance, to a total of 155 different ASs, primarily in the cultivation of wheat, maize, rice and soybean, according to the International Survey of Herbicide Resistant Weeds (Heap, 2014).

Among insect pests and crop pathogens there are also multiple documented cases of pesticide resistance, and hence important to use integrated pest and disease management strategies to slow the development. For many years, the *Bt*-technology was “saved” from development of resistance, which was interpreted as an indication of effective resistance prevention strategies (Bates et al. 2005). However, recently documented cases of field-evolved resistance against multiple *Bt*-toxins (Gassmann, 2012; Gassmann et al. 2014)show that resistance management strategies still need to be improved.

For more information on pesticide resistance in insect pests and crop pathogens, refer to the Insecticide Resistance Action Committee (IRAC Website) and the Fungicide Resistance Action Committee (FRAC Website).

CHAPTER 3. ECOTOXICITY IN LIFE CYCLE ASSESSMENT

Toxicity is defined by FAO (2003) as "*a physiological or biological property which determines the capacity of a chemical to do harm or produce injury to a living organism by other than mechanical means*".

It is common to differentiate between ecological toxicity (ecotoxicity) and human toxicity. Ecotoxicity can in turn be divided into aquatic and terrestrial toxicity, and aquatic toxicity can further be divided into freshwater and marine ecotoxicity. This report deals with aquatic freshwater ecotoxicity.

This chapter starts with a general introduction to Life Cycle Assessment (LCA) (Chapter 3.1), and is followed by an introduction to ecotoxicity impact assessment in LCA and the central concepts of fate, exposure and effect (Chapter 3.2). It ends with a review of ecotoxicity impact assessment models in LCA, with a special focus on different approaches to the modeling of effect (Chapter 3.3). The chapter deals with chemicals in general and pesticides in particular.

3.1 Life Cycle Assessment

LCA is an environmental systems analysis tool that aims to assess the potential environmental impacts associated with a product or service, throughout its life cycle. The LCA methodology has been standardized by the International Organization for Standardization (ISO) 14040 and 14044, and recently thoroughly described by the International Reference Life Cycle Data System (ILCD) in a handbook on LCA-methodology with guidance for good practice (JRC, 2010). The compulsory steps of an LCA include goal and scope definition; Life Cycle Inventory (LCI) and Life Cycle Impact Assessment (LCIA).

In the goal and scope definition, the intended audience, the system boundaries and the functional unit, to which all impacts are related, are defined; further, it is decided if the LCA is attributional or consequential, which impact categories should be included, and allocation strategies (JRC, 2010).

In the LCI, data regarding all flows, to and from all processes in the studied system, are collected, including elementary flows (resources, emissions and land use), product flows (good and services) and waste flows (JRC, 2010).

In the LCIA, inventory data are sorted, based on the environmental impacts to which they contribute, and transformed into impact indicators(JRC, 2010).In practice, transformation, also called characterization, consists of multiplying inventory data (emissions or extractions) with so-called characterization factors (CFs), which quantify how much each unit emission or extraction contribute to various environmental impacts, relative to each other (JRC, 2010).

Numerous impact assessment models exist. In a recent review of LCIA methods for the Joint Research Centre (JRC) of the European Commission (Hauschild et al. 2013), a total of 156 models were identified within the impact categories climate change, ozone depletion, human toxicity, particulate matter/respiratory inorganics, ionizing radiation (human health and ecosystems), photochemical ozone formation, acidification, terrestrial and aquatic eutrophication, freshwater ecotoxicity, land use and resource depletion (water, mineral and fossil). In the impact categories human toxicity and freshwater ecotoxicity, USEtox was identified as "the best".

Impact indicators can be located at any place along the chain that link emissions or extractions with impacts, and are commonly referred to as midpoint or endpoint indicators, depending on the proximity to damages of direct human concern, also called areas of protection (Jolliet et al. 2004; Hauschild et al. 2013). The ILCD handbook on LCA methodology (JRC, 2010) recognizes three areas of protection: human health, natural environment and natural resources. Sometimes man-made environment is also recognized as an area of protection (Jolliet et al. 2004). Generally, endpoint indicators are associated with higher interpretability and uncertainty than midpoint indicators (Jolliet et al. 2004). Radiative forcing e.g., is a more certain impact indicator of climate change than temperature rise, but temperature rise is more easily interpretable and more closely associated with the damages that ultimately should be avoided (Jolliet et al. 2004).

LCA-results should be interpreted as potential impacts, rather than actual environmental effects, in line with the comparative, rather than predictive, context in which LCA is typically used (JRC, 2010).

3.2 Ecotoxicity impact assessment

Three concepts are of fundamental importance for the modeling and assessment of potential ecotoxicity impacts in LCA, namely fate, exposure and effect. These concepts provide a conceptual link between chemical emissions and associated damages.

Fate

It has been estimated that often, less than 0.1% of the applied pesticide dose actually reaches the target pest (Pimentel and Levitan, 1986); in other words, most pesticide AS is dispersed into the surrounding environment, where it may contaminate soil, air and water, and cause harm to non-target organisms. That contamination is widespread is illustrated by the fact that 44% of US wells with potable groundwater contained detectable levels of pesticides in 2008 (USDA, 2009).

The specific “pattern of pollution” is called fate, and refers to the distribution (in time and space) of pesticides after application. Fate involves various processes of physico-chemical and biological nature, such as degradation, distribution, and sorption.

Degradation processes are biotic or abiotic and include processes such as metabolism, microbial degradation, hydrolysis, photolysis and oxidation (FAO, 1996).

Transportation and distribution processes include e.g. wind drift during spraying (spray drift),dispersion in the atmosphere, evaporation and volatilization from crop and soil surfaces, absorption into crops, adsorption by the soil surface, leaching through the soil, surface runoff and water-borne transport in drainage systems and ditches (van Zelm et al. 2014).

The contamination potential of pesticides depends to a large degree on two processes: soil sorption, i.e., the strength by which pesticide molecules bind to soil particles, and degradation, i.e., the break-down of pesticide molecules (Arias-Estévez et al. 2008). The pesticide-soil system is a complex and dynamic physico-chemical and biological system, in which the relative importance of various processes depend on the biological and physico-chemical properties of the soil, and the physico-chemical properties of the pesticide (Arias-Estévez et al. 2008).

Table 3.1 lists key physico-chemical properties of pesticides that influence environmental fate, and which were used in this study (see further in Chapter 4).

Table 3.1. Key physico-chemical parameters that influence environmental fate.

Parameter	**Interpretation (AGRITOX; PPDB, 2014)**
Vapor pressure	Indicator of a substance's tendency to vaporize, i.e. change phase from liquid to vapor. The higher the vapor pressure the greater the vaporization potential.
Log P/Log Kow	Log of the octanol – water partitioning coefficient: indicator of a substance's lipid solubility and hence its tendency to bioaccumulate. The higher the Log P, the greater the bioaccumulation potential.
DT50 soil	Soil half-life: the time it takes for 50% of the molecules to degrade and indicator of a substance's persistence in soil.
Solubility in water	Indicator of a substance's tendency to dissolve in water, and hence bioavailability.
pKa	Dissociation constant: defined as the negative logarithm of the acidity constant Ka and indicator of the strength of an acid and the potential to form ions in water. The lower the dissociation constant the stronger the acid.
Koc	Organic carbon - water partition coefficient: indicator of a substance's sorption to soil particles and hence mobility. Also called organic carbon sorption constant or soil adsorption coefficient.
Henry's Law constant	Indicator of a substance's preference for air relative to water, i.e., its volatility. The larger the constant, the higher volatilization potential.

Sorption, primarily to soil organic matter, depends on the physico-chemical properties of pesticides and the content and molecular structure of soil organic matter, and pH for ionic pesticides (Arias-Estévez et al. 2008).Sorption generally makes pesticides less accessible to soil microorganisms, slow the degradation rate, and reduce the mobility.

Pesticides may remain for long periods in ecosystems, and some have properties that enable them to biomagnify in food chains. For examples, organochlorine pesticides, most of which were banned in the US before 1992, were still detected in over 90% of fish tissue samples collected from streams in agricultural, urban and mixed landscape areas between 1992 and 2001 (Gilliom et al. 2006). The residence times in different environmental compartments depend on the degradation rate of substances, and the mobility. The persistence of pesticides in soil depends on the physico-chemical properties of the pesticide (e.g., its volatility and solubility), physico-chemical and biological properties of the soil (e.g., its content of clay, organic matter and moisture, and pH), the topography and history of the site (e.g., its elevation, slope, microbial population, drainage, tillage type etc.), the climate (e.g., the temperature, solar radiation, rainfall and evaporation), and management factors such as application method and time of year (Arias-Estévez et al. 2008).

The large number of parameters that affect fate, and their inter-dependency, make pesticide fate-modeling a challenging task, that consists of modeling the most relevant processes over time, from the emission sources to the final receiving compartments. Although fate processes are dynamic and may endure over considerable time after application, for modeling purposes they are assumed to reach some equilibria.

Several transport models have been developed over the years that model the run-off and/or the transportation of pesticide in soil (Arias-Estévez et al. 2008), most of which are not specifically designed for use in LCA. One example is MACRO v. 5.2 (Jarvis and Larsbo, 2012) which models the mobility and fate of pesticides in soil, and is widely used in regulatory risk assessment and authorization processes of pesticides in the EU.

To our knowledge, only one pesticide distribution model has been developed specifically for use in the inventory phase of LCA; namely PestLCI (Birkved and Hauschild, 2006; Dijkman et al. 2012). This is the model used in this study, introduced in detail in Chapter 4.3.

Exposure

Chemical exposure, i.e., the process of coming in contact with chemicals, is characterized by the time, the type, and the level of exposure, and the likelihood of being exposed depends on the persistence and bioavailability of chemicals to living organisms, including humans (Gilden et al. 2010).

It is common to separate between direct and indirect exposure. Human direct exposure includes dermal contact, inhalation and ingestion while indirect exposure includes e.g. residues in food and contaminated water.

The exposure of freshwater organisms to chemicals is not modeled in detail in ecotoxicity impact assessment in LCA, due to the multitude of different species that exists, and the specific exposure pathways that apply to different species. Rather, exposure is implicitly included in the effect factor (Jolliet et al. 2004), or potential exposure is modeled as the dissolved fraction as a measure of the bioavailable share, as in USEtox (Rosenbaum et al. 2008).

Conversely, in human toxicity impact assessment, exposure is often modeled in greater detail, and may include several exposure pathways, including inhalation of contaminated air, ingestion of contaminated drinking water and ingestion of residues in crops, meat, milk and fish, as in USEtox (Rosenbaum et al. 2008).

Effect

Toxicity effects refer to various impacts on living organisms, including humans, that result from exposure to toxicants. It is common to differentiate between acute and chronic effects, and between effects on humans and on other living organisms. Acute effects are typically associated with short-term exposure at high doses, while chronic effects are associated with long-term exposure at low doses.

The type of effects that result as a consequence of toxicant exposure depends on a range of factors, including the type of toxicant and its physico-chemical properties, (specifically its toxic mode-of-action); the exposure duration and the type of organism exposed and its sensitivity (see Chapter 2.3 for an overview of environmental and human health effects that have been linked to pesticide exposure).

Effect measures in ecotoxicology can be classified as effect based or no-effect based. One example of the latter is the No Observed Effect Concentration (NOEC). Commonly used effect-based measures include the Lowest Observed Effect Concentration (LOEC); the Effective Concentration (EC) to X% of test organisms (ECX), i.e., the concentration at which X% of organisms exhibit an effect, and the Lethal Concentration (LC) to X% of test organisms (LCX), i.e. the concentration that induces a lethal effect in X% of test organisms. Common endpoints in ecotoxicity tests include intoxication, mobility, mortality, generation time, biomass growth and weight (US-EPA ECOTOX Database). A large part of the existing effect data originate from a legislative context of chemical evaluation and authorization.

3.3 Ecotoxicity impacts assessment models in LCA

Several toxicity and ecotoxicity impact assessment models designed for use in LCA have been proposed over the years. Many of these differ in scope, fate modeling principles, exposure and effect, number of substances and compartments included, and not least in terms of the relative toxic weights assigned to different substances in the form of CFs (Hauschild et al. 2011).

Some of the most well-known toxicity impact assessment models include EDIP-97 (Wenzel et al. 1997), EDIP (Hauschild et al. 1998), CML2001 (Guinée, 2001), Eco-indicator 99 (Goedkoop and Spriensma, 2001), USES-LCA (Huijbregts et al. 2000), CalTOX (McKone and Enoch, 2002), IMPACT 2002+ (Jolliet et al. 2003), USEtox (Rosenbaum et al. 2008), USES-LCA 2.0 (Van Zelm et al. 2009) and ReCiPe (Goedkoop et al. 2009).

Most methods build on the modeling of fate, exposure and effects, but intuitively “simpler” methods exist e.g., the Critical Dilution Volume method (see e.g. Van Hoof et al. 2011)in which the volume of freshwater required to dilute a toxicant to a harmless concentration is used as an indicator of its toxic potency.

Inconsistencies in CFs proposed by different models indicate the complexities involved in ecotoxicity effect modeling, and partly explain why the freshwater ecotoxicity impact category has often been omitted from LCAs in the past. Refer to the work by Dreyer and colleagues(2003) and Van Hoof and colleagues(2011) for studies that apply and compare different ecotoxicity models, and exemplify these problems.

Inconsistencies between models has also been a source of incentive for further research. USEtox (Rosenbaum et al. 2008) is one of the most recent toxicity impact assessment models in LCA, officially launched in 2010,as the result of a scientific consensus process aimed at comparing and merging seven of the existing toxicity impact assessment models (Hauschild et al. 2008). USEtox is the model used in this study and is introduced in detail in Chapter 4.4.

Effect factor modeling in ecotoxicity impact assessment

Potential ecotoxicity impacts are generally assessed as the product of emissions and ecotoxicity CFs, summed over all emission compartments and substances. Ecotoxicity CFs indicate the relative toxic potency of individual substances, and generally consist of a fate part, an exposure part and an effect part, also called effect factor (Pennington et al. 2004) or effect indicator (Larsen and Hauschild, 2007a). There exist several approaches to the modeling of ecotoxicity effect factors – a topic that has been reviewed at least twice over the past decade (Pennington et al. 2004; Larsen and Hauschild, 2007a).

In regulatory risk assessment of chemicals, effect data are used to determine a chemical-specific Predicted No-Effect Concentration (PNEC) that is used together with a Predicted Environmental Concentration (PEC) to quantify risks (Pennington et al. 2006). The PNEC is estimated by dividing the lowest effect concentration (i.e., the effect concentration of the most sensitive species) with a so-called assessment factor, that typically varies between 10 and 1000. Assessment factors are used to provide safety margins and to account for uncertainties and/or lack of data. For more information on the similarities and differences between environmental risk assessment and LCA, refer to the work by Udo de Haes and co-workers (2006).

Larsen and Hauschild (2007a) noted that effect factor modeling approaches fall into one of two main categories: assessment factor-based approaches (also called PNEC-based approaches) and Species Sensitivity Distribution (SSD) -based approaches, also called Potentially Affected Fraction (PAF) -based approaches.

PNEC-based impact assessment approaches include USES-LCA (Huijbregts et al. 2000) and EDIP (Hauschild et al. 1998), in which effect factors are calculated as the reciprocal of the PNEC-value (Equation 3.1). Such effect factors are closely related to approaches used in chemical risk assessment (by their use of assessment factors, and ecotoxicity data based on the most sensitive species),and can be interpreted as conservative estimates of the toxic potency (Larsen and Hauschild, 2007a).

$$Effect\ factor = \frac{1}{PNEC}$$

Equation 3.1

A SSD is a statistical distribution describing the variation in sensitivity to a certain toxicant among a set of species, constructed with effect or no-effect data, e.g., NOEC or EC50-data (Posthuma et al. 2002). The share of species in a SSD that have a certain effect or no-effect level exceeded at a given environmental concentration of a toxicant is denoted PAF (Traas et al. 2002). The concentration at which X% of species in a SSD are exposed above a certain level (e.g., NOEC or EC50) is denoted the Hazardous Concentration X (HCX). The concentration at which 50% of the species in a SSD are exposed above their EC50-level is denoted $HC50_{EC50}$.

Larsen and Hauschild (2007a) identified three subcategories of PAF-based approaches: marginal PAF-increase approaches, average PAF-increase approaches and multi-substances PAF (ms-PAF) approaches, see Figure 3.1.

Marginal PAF-increase approaches are based on the tangential or marginal gradient at a chosen working point on the SSD-curve, i.e., the marginal change in the fraction of species that have a predetermined effect or no-effect level exceeded.

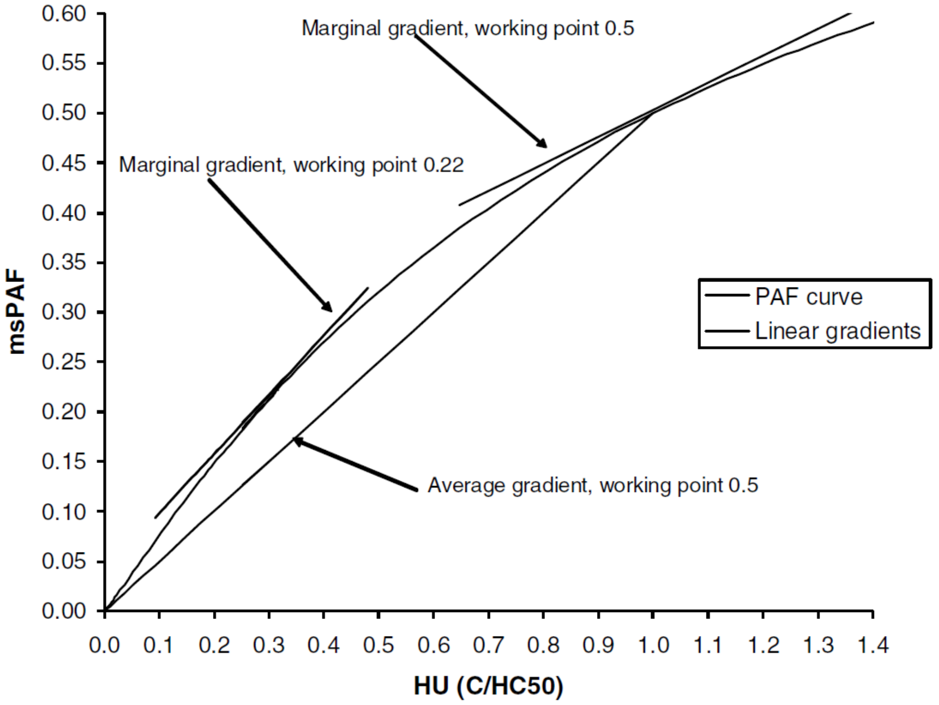


Figure 3.1. Three approaches to effect factor modeling shown in relation to a Potentially Affected Fraction (PAF) -curve based on a log-logistic Species Sensitivity Distribution (SSD). The x-axis is in Hazard Units (HU), i.e., the concentration scaled by the HC50. Figure adopted from Larsen and Hauschild (2007a), with kind permission.

The Eco-indicator 99 method (Goedkoop and Spriensma, 2001)belongs to the group ms-PAF approaches, and has been developed as a special case of a marginal PAF-increase approach. In this method, the average background impact level due to environmental toxicants is taken into account through mixture toxicity theory, but is limited to Dutch environmental conditions. The effect factor in Eco-Indicator 99 is expressed according to Equation 3.2,

$$Effect\ factor = \frac{0.59}{HC50_{NOEC}}$$

Equation 3.2

where 0.59 is the slope of the tangent at the working point PAF = 0.22 (shown in Figure 3.1) and $HC50_{NOEC}$ is the concentration at which 50% of the species are exposed above their NOEC-level.

Average PAF-increase approaches use the slope of a secant or average gradient from a chosen working point at the PAF curve to the origin as an indicator of the toxic potency(Larsen and Hauschild, 2007a). One example is the Assessment of the Mean Impact (AMI) method (Payet, 2004), which uses PAF = 0.5 as a working point (shown in Figure 3.1), and the HC50 based on acute and chronic EC50-data for species of different phyla. The effect factor in the AMI-method is expressed according to Equation 3.3.

$$Effect\ factor = \frac{0.5}{HC50_{EC50}}$$

Equation 3.3

The different PAF-approaches share a common effect factor expression (Equations 3.2 – 3.3). The only differences are the constant in the numerator (which is of no practical significance in a comparative context), the data on which the HC50 is based, and the averaging principle by which the HC50 is calculated (Larsen and Hauschild, 2007a).

Regarding the data on which the HC50 is based, Payet (2004) reported that the data availability, and hence the potential for estimating effect indicators, is by far greatest for EC50-data, and further that the EC50 is less dependent on the experimental design than the NOEC, and is associated with lower uncertainty than other effect measures.

Larsen and Hauschild (2007b) explored different averaging principles for the $HC50_{EC50}$(arithmetic mean, geometric mean and median),and found the geometric mean to be the most statistically robust, and compatible with the non-normal data distribution. They also stressed the importance of using ecotoxicity data from standardized tests (that use standardized organisms and follow explicit guidelines) to ensure reproducibility and robustness.

Pennington et al. (2004) argued a decade ago that PAF-based approaches are more "*consistent and environmentally relevant in LCA*" than PNEC-based approaches, and recommended the use of a single, average PAF-based, effect factor (Equation 3.4) as best practice in LCA, and further that it should be based on EC50-data.

$$Effect\,factor = \frac{0.5}{HC50}$$

Equation 3.4

Larsen and Hauschild (2007a) evaluated several different approaches to effect factor modeling against a set of assessment criteria and found that in their present form, none is optimal, but agreed that PNEC-based approaches are incompatible with the comparative framework of LCA.

PNEC-based as well as PAF-based approaches generally model to the level of potential impact in the ecosystem, i.e., midpoint in the chain linking emissions to impacts (Hauschild et al. 2013). Attempts exist to model all the way to damage (i.e., endpoint), although such attempts are all at an early stage of development, see further in Chapter 6.6.

CHAPTER 4. MODELS, METHODS AND DATA

The assessment method employed here involves two models: PestLCI v. 2.0.5 (Dijkman et al. 2012), and USEtox v.1.01 (Rosenbaum et al. 2008). In short, three consecutive steps in the assessment route can be identified, described in detail in the following chapter, and illustrated schematically in Figure 4.1.

1. Pesticide application inventory (Chapter 4.2)
2. Pesticide emission inventory with PestLCI (Chapter 4.3)
    - Expansion of PestLCI's pesticide database
    - Regionalization of PestLCI
3. Potential freshwater ecotoxicity impact assessment with USEtox (Chapter 4.4)
    - Calculation of new USEtox characterization factors (CFs)

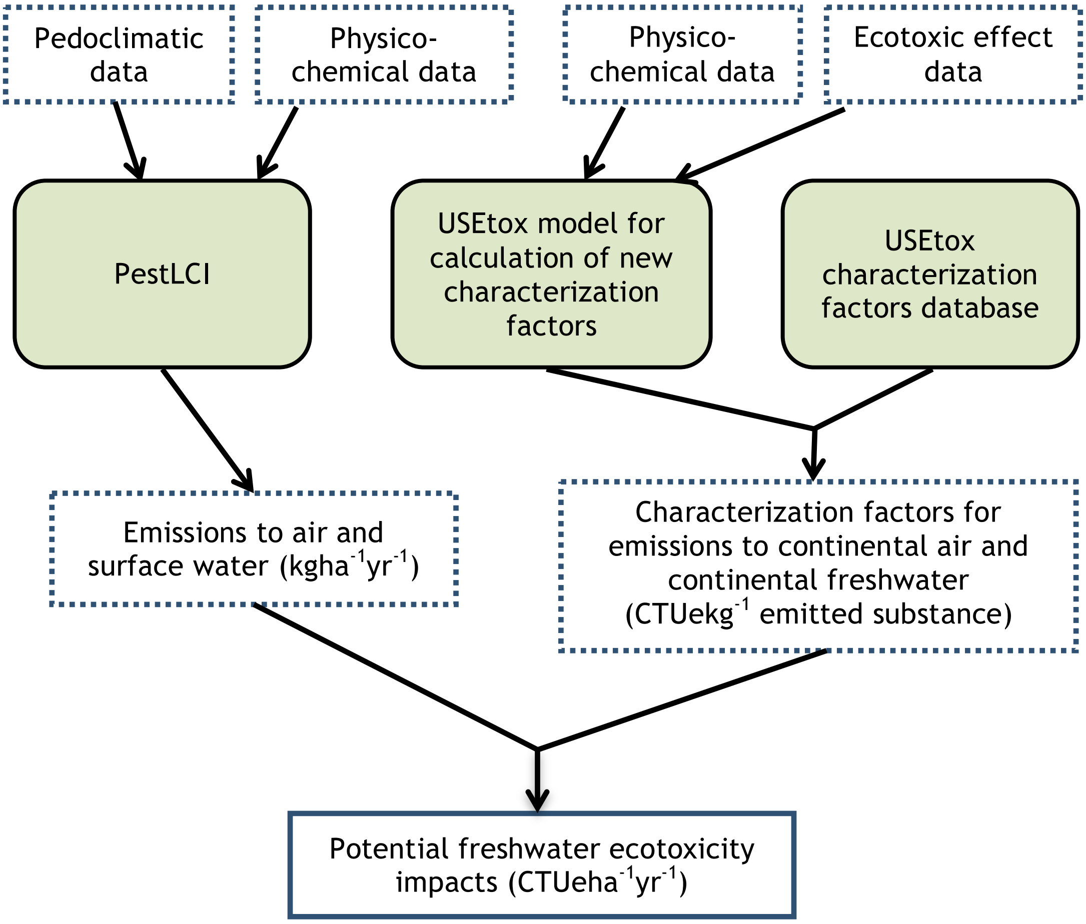


Figure 4.1. Flowchart illustrating the assessment method of potential freshwater ecotoxicity impacts employed here.

Chapter 4 also describes the impact metrics used (Chapter 4.1), the derivation of biofuel energy yields (Chapter 4.5), the selected allocation method and the derivation of allocation factors (Chapter 4.6), and the sensitivity analyses performed (Chapter 4.7).

4.1 Functional Units

Potential freshwater ecotoxicity impacts from pesticide use were determined in relation to

- hectare (ha) and year (yr), and
- biofuel yield (joule), as gross energy biofuel output per ha and year from the biofuel conversion plant, i.e., no deduction of energy inputs to produce the biofuel.

Biofuel energy yields were calculated based on fresh harvest yields, for typical transportation pathways and conversion efficiencies in biofuel conversion plants, see Chapter 4.5. All biofuels studied can be used as vehicle fuel, thus fulfilling the requirement for equivalent function in LCA.

4.2 Pesticide application inventory

Crop cultivation practices in the studied regions were investigated and pesticide application data were obtained from experts familiar with agricultural practices in the respective regions, and/or determined based on statistics or other literature. The data obtained were complemented or modified, when appropriate, by our own assumptions (see details in Chapters 5.1 – 5.6). Based on this, application scenarios were constructed aiming to represent realistic and typical agronomic practices and pesticide management in the respective regions. Rationales for pesticide application in terms of weeds, pests and diseases were also investigated.

The pesticide application scenarios contain data about the pesticides applied (mass AS per ha and application, i.e., dosage), method of application (ground, soil incorporation, or aerial), time of application (month), crop type and development stage at time of application, tillage type, and average frequency of application. Application frequencies can be interpreted as the share of a field treated in a year, or the variation in treatment between years, and were used to even out the pesticide application and resulting impacts scores over the years.

Chapter 5 presents the qualitative and quantitative data collected in this inventory.

Actual AS chemical formulations were used throughout the study, for example glyphosate isopropylamine salt (Chemical Abstracts Service Registry Number (CAS-RN) 38641-94-0)instead of glyphosate (CAS-RN 1071-83-6) as the AS in the herbicide RoundUp Ready. This approach was considered most appropriate in accounting for the potential impact.

4.3 Pesticide emissions inventory

We used PestLCI v. 2.0.5 (Dijkman et al. 2012) to estimate the mass of pesticide AS emitted from the agricultural field to the surrounding natural environment following application. This is the currently most advanced pesticide emission inventory model available, developed for use in agricultural LCAs (van Zelm et al. 2014).

PestLCI estimates pesticide emissions to the air, surface water, and ground water compartments, by modeling primary and secondary distribution processes following field application (Birkved and Hauschild, 2006; Dijkman et al. 2012).Primary distribution refers to the initial distribution to plant leaves, soil and the air. Secondary distribution processes refer to three processes that take place on leaves: volatilization, degradation and uptake; and seven processes that take place in the soil: topsoil volatilization, topsoil biodegradation, topsoil run-off, macropore flow and tillage, subsoil degradation, interception into drainage system and ground water leaching (Dijkman et al. 2012).

Distribution, transportation and degradation processes in PestLCI are based on fate modeling principles originating from Environmental Risk Assessment (ERA), with the difference that PestLCI models a realistic estimate of the average mass of AS emitted to the environment rather than a “worst-case” Predicted Environmental Concentration (PEC) as done in ERA (Dijkman et al. 2012). Emission distributions are pesticide-specific, as well as soil- and climate-specific, and depend on a range of field-specific parameters.

The agricultural field down to a depth of 1 m into the soil and 100 m up into the air is regarded part of the technosphere in the PestLCI model. Only pesticides that cross the technosphere-environment border are considered as environmental emissions – thus excluding emissions to agricultural soil. The rationale for this modeling approach is explained in Birkved and Hauschild (2006).

Crop type and development stage at time of application was determined for each application event from a suite of over 100 predefined options, based on the time of application and assumed sowing dates (Chapter 5).

PestLCI differentiates between application using aircraft, soil incorporation and several types of pesticide ground spray equipment depending on the morphology of crops. The different ground booms are associated with different ways of modeling wind drift. For every pesticide application event, an appropriate boom type was determined with regard to crop morphology and crop development stage.

PestLCI also enables the evaluation of the effect of buffer zones, i.e., safety areas between field and surface waters where pesticides are not sprayed.

Field data required in PestLCI include field size (length and width), slope, fraction drained, depth of drainage system, irrigation and tillage type. These data were set in each case based on information from the literature, agricultural experts, and our own assumptions, see Table 4.1.

It should be noted that no consensus exists in the LCA community on how to model the fate of pesticides after application. PestLCI is recognized as one inventory option but is not endorsed over other options. For a review of options, and a discussion of various modeling approaches, refer to Rosenbaum et al. (2015) and van Zelm et al. (2014). We selected PestLCI because it is recognized as the most advanced pesticide emission inventory model currently available, developed for use in agricultural LCAs (van Zelm et al. 2014), and because a detailed emission inventory can be expected to reduce uncertainties and increase precision in modeling.

Table 4.1. Field parameters used in emission inventory modeling in PestLCI.

Case abbrev. [a]	Size (ha) [b], width×length (m)	Slope [c] (%)	Fraction drained [d] (%)	Depth of drainage system [d] (m)	Annual irrigation [e] (mm)	Tillage type [f]
MZ-I/II	35 [g],418×837	1	0	not applicable	0	reduced
RS	10 [h], 224×447	1	0	not applicable	0	conventional
SX	10 [i], 224×447	1	0	not applicable	0	no-till [j]
SB-I/II	250 [i], 1118×2236	1	0	not applicable	0	no-till
SC	20 [k], 316×632	1	0	not applicable	0	no-till [j]
WT	10 [h],224×447	1	0	not applicable	0	conventional

[a] *MZ-I, MZ-II:*Genetically engineered (GE) glyphosate tolerant maize with (MZ-I) and without (MZ-II) *Bt*-technology cultivated in Iowa, US. RS: w*inter rapeseed cultivated in* Schleswig-Holstein, Germany. SX: *Salix short rotation woody coppice cultivated in* South Central of Sweden. SB-I: *conventional* soybean cultivated in Mato Grosso, Brazil. SB-II: GE glyphosate tolerant soybean cultivated in Mato Grosso, Brazil. SC: sugarcane cultivated in São Paulo, Brazil. WT: *winter wheat cultivated in* Schleswig-Holstein, Germany. For more information, refer to Chapter 5.

[b] We set the field length to twice the width in all case fields to maintain consistent shape and orientation with regard to pesticide application and wind direction (see further in Chapter 6.4).

[c] Emissions to air in PestLCI are independent of slope, while emissions to surface water, through top soil runoff, depend on the slope through an AS-independent correction factor (Dijkman et al. 2012). Sensitivity analyses that we performed for > 10 ASs showed that when the slope increased from 1 to 5%, emissions to surface water increased by a fixed factor of 6.24 for all ASs tested. In lack of region and crop-specific slope data and considering the rather crude modeling of the slope dependency, we set the slope to 1% in all cases.

[d] We collected data on drainage fractions in the various crops, but eventually chose not to include drainage due to that drainage systems are often installed below 1 m depth, while the soil compartment in PestLCI is only modeled down to a depth of 1 m (i.e. this modeling approach was judged insufficient with regard to drainage). We determined the following drainage fractions: SX: 0% (own assumption); SB-I/II: 0% (Meyer, pers. com. 2013); RS and WT: 80% (Gleser, pers. com. 2013) and MZ-I/II: 25% (Ertl, pers. com. 2013), but used 0% for all cases due to the reasons explained above.

[e] None of the crops were assumed to be irrigated in line with dominant cultivation practices in the studied regions.

[f] PestLCI includes three predefined tillage types: conventional, reduced or no tillage. Tillage types were determined based on dominant cultivation practices in the studied regions, see Chapter 5.

[g] Ertl, pers. com. (2013).

[h] Gleser, pers. com. (2013).

[i] Own assumption.

[j] Conventional tillage assumed for the first pesticide applications in conjunction with field establishment and no-till for all subsequent applications. See further in Tables 5.4 and5.7.

[k] Galdos, pers. com. (2013).

Pesticide addition route

The database of PestLCI v. 2.0.5 includes 101 pesticide ASs defined by their molecular mass, water solubility, vapor pressure, dissociation potential, bio-accumulation potential, soil adsorption potential, and degradation rates in soil and atmosphere. We added an additional 31 pesticide ASs to the model database to account for all pesticides identified during inventory (see Appendix 1). Table 4.2 lists the required data for addition of pesticides ASs to the model database.

PestLCI v.2.0.5 is based in Analytica® (Lumina Decision Systems), which requires a license to make adjustments to the model database. In this study, the PestLCI development team assisted in making the necessary adjustments.

Several databases were consulted to derive the required data. First priority was given to the Pesticide Properties Database (PPDB); second priority to the Physical Properties Database (PHYSPROP), third priority to experimental data from EPISuite (US-EPA, 2012), and fourth priority to estimated data from EPISuite, in accordance with guidelines obtained from the PestLCI modeling team (Dijkman, pers. com. 2013).That is, PHYSPROP and EPISuite were only consulted in case data were not available in the PPDB.

The PPDB is an online database developed by the Agriculture and Environment Research Unit (AERU) at the University of Hertfordshire. It contains an extensive set of physical-chemical data and a smaller set of ecotoxic effect data for around 1150 pesticides and 700 metabolites, including all ASs used in the EU.

The PHYSPROP is a database developed by the Syracuse Research Centre (SRC). It contains freely available estimated and experimental data of melting point, boiling point, water solubility, log Kow, vapor pressure, pKa, Henry's Law constant and atmospheric OH-rate for around 25 000 compounds.

The Estimation Program Interface Suite^{TM} (EPISuite) v. 4.11 is a “toolbox” of thirteen different estimation programs for various physical and chemical properties, developed by the US Environmental Protection Agency's (EPA) office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC) (US-EPA, 2012).

We used EPISuite primarily to collect data for the atmospheric OH-rate from the program AOPWIN. If experimental data were not available, we used the “overall OH rate constant”-estimate available under the AOPWIN Hydroxyl Radicals Page 2 (or for some pesticides only by accessing AOPWIN in single program mode). For a few compounds, Koc-values were also retrieved from EPIsuite (KOCWIN). In those cases the MCI-estimation method was used. For more information on EPISuite, refer to Chapter 4.4.

The full set of physico-chemical data used is available in Appendix 3.

Table 4.2. Pesticide data required for addition of new ASsin PestLCI.

Parameter (notation as in PestLCI)	**Unit**	**Explanation**
Type	-	Herbicide, insecticide, fungicide, etc.
CAS-RN	-	Chemical Abstract Services Registry Number.
SMILES	-	Simplified Molecular Input Line Entry System; a chemical notation system in which molecular structure are represented by a linear string of symbols.
Molecular weight	g $mole^{-1}$	Called molecular mass in the PPDB.
Molecular volume	cm^3 $mole^{-1}$	Calculated based on molecular weight and bulk density.
Solubility, ref. temp.	g l^{-1}, °C	Solubility in water, and reference temperature at which it was determined.
Vapor pressure, ref. temp.	Pa, °C	Vapor pressure, and reference temperature at which it was determined.
pKa	-	First dissociation constant (neutral to charged). Not applicable for non-ionizing substances.
log Kow	-	Log of octanol-water partition coefficient. Denoted log P in PPDB and PHYSPROP.
Koc	l kg^{-1}	Soil organic carbon-water partition coefficient. Denoted soil adsorption coefficient in EPISuite.
Soil t½,ref. temp.	days, °C	Soil biodegradation half-life, and temperature at which it was determined.We used “DT50 (lab at 20 ° C)" to be consistent with the data of pesticides already included in PestLCI.
Atmospheric OH rate	$cm^3molecule^{-1}$ s^{-1}	Overall OH-radical oxidation rate constant.
Bufferzone width	m	Width of the zone along the edges of the field in which pesticides are not sprayed. We used a default value of 0 m, in accordance with all other pesticides included in the model database.
E(a) Evaporation	kJ $mole^{-1}$	Activation energy for evaporation. We used a default value of 100 kJ $mole^{-1}$, in accordance with all other pesticides included in the model database.

Regionalization of PestLCI

PestLCI includes 25 pre-defined climate profiles that represent climate conditions throughout Europe. Climate profiles are defined by the location’s monthly and yearly averages in terms of average, maximum and minimum air temperatures, precipitation, number of days with rainfall and solar radiation as well as annual average potential evaporation and elevation above sea level, see Table 4.3. In addition, the climate data include two derived parameters that are calculated by the user: average rainfall on a rainy day (calculated as average monthly precipitation divided by number of days with >1 mm precipitation) and rain frequency (calculated as number of days in the month divided by number of days with >1 mm precipitation).

We developed four new climate profiles to account for conditions in São Paulo and Mato Grosso, Brazil; Iowa, US and northern Germany (data from Hamburg).Table 4.3. presents a summary of climate data. For Sweden, we used the predefined climate dataset for Linköping located in South Central Sweden (at 58.40° N, 15.62° E) already included in the PestLCI meteorological database (also included in Table 4.3).

Table 4.3. Summary of climate data for the five studied regions. The full set of climate data is available in Appendix 6.

	São Paulo, Brazil	**Mato Grosso, Brazil**	**Iowa, US**	**Northern Germany**	**South Central Sweden**
Elevation above sea level (m)	620 [a]	400 [a]	300 [a]	15 [a]	80 [a]
Average air temperature, year (°C)	21.7 [b]	25.2 [f]	8.8 [i]	8.7 [m]	6.9 [p]
Average minimum air temperature, year (°C)	16.4 [b]	19.5 [f]	3.0 [i]	4.9 [m]	2.6 [p]
Average maximum air temperature, year (°C)	28.9 [b]	32.6 [f]	14.7 [i]	12.4 [m]	11.1 [p]
Annual total rainfall (mm)	1465 [b]	1620 [f]	880 [i]	770 [m]	535 [p]
Rain days (> 1 mm), monthly average	10.8 [c]	13.6 [g]	13.4 [j]	10.9 [m]	8.4 [p]
Annual potential evaporation (mm) [d]	1065	1425	685	620	595
Average solar radiation, year (Wh m^{-2} day^{-1})	5455 [e]	5290 [h]	4030 [k]	2880 [n]	2520 [p]

[a] Average elevation in the defined regions from the Altitude Website.
[b] Weather Normals averages 1961-1990 for Sao Simao climate station (21.29° S, 47.33° W) from the Freemeteo Website.
[c] Average rain days for Ribeirao Preto (21.18° S, 47.81° W) from the World Weather Online Website.
[d] Calculated using the Thornthwaite equation (Thornthwaite, 1948) based on latitude, average daily number of hours with sunlight and average monthly temperatures. Hours of daylight per day derived from the Daylight Hours Explorer.
[e] Global horizontal solar radiation for the location 21°18 S, 47°36 W from INPE-LABSOLAR (2005).
[f] Weather Normals averages 1961-1990 for Diamantino climate station (14.24° S 56.27° W) from the Freemeteo Website.
[g] Average rain days for Diamantino (14.41° S 56.45° W) from the World Weather Online Website.
[h] Global horizontal solar radiation for the location 14.42° S, 57.25° W from INPE-LABSOLAR (2005).
[i] Weather Normals averages 1981 – 2010 for Waterloo Airport, Iowa (42.55° N 92.40° W) from National Climatic Data Center (NCDC).
[j] Average rainfall days for Waterloo, Iowa (42.49° N 92.34° W) from the World Weather Online Website.
[k] Global horizontal solar radiation for the location 42°20 N 92°30 W from the PVWatts Calculator, based on typical meteorological year weather data.
[m] Average climate data based on the years 1961-1990 for Hamburg (53.57° N, 10.00° E) from the WeltklimaDatabase.
[n] Horizontal solar radiation estimates of long term monthly averages for 53°2 N 10°1 E from PVGIS.
[p] Data according to the PestLCI predefined climate profile “North European and Continental I: Linköping”.

PestLCI includes seven pre-defined soil profiles that represent soils typical to Europe. Soil profiles are defined by their pH-H$_2$O (pH in water solution), composition of sand (particles > 50 µm), silt (particles 2-50 µm), clay (particles < 2 µm) and organic carbon content for each soil horizons to a depth of 1 m, as well as the overall soil bulk density, see Table 4.4.

We developed five new site and crop-specific soil profiles to represent pedoclimatic conditions in the studied regions. Soil conditions in the studied regions were investigated; representative soil samples from the ISRIC-WISE Harmonized Global Soil Profile Dataset v

3.1 (Batjes, 2008; 2009)were selected, and modified based on literature data and/or expert inputs to account for local crop- and site-specific conditions. Table 4.4 presents a summary of the soil data used.

The São Paulo soil is an Oxisol (Ferralsol in the FAO soil classification): a soil typically found under sugarcane in the Mid-South of Brazil. Based on over 27 000 soil samples from sugarcane fields in the Mid-South of Brazil taken by Cane Technology Center (CTC) between 1990 and 2009, 75.1% were identified as Oxisols (Joaquim et al. 2011). The top two layers of the selected soil were modified to correspond to average conditions specific to sugarcane, based on the CTC study (Joaquim et al. 2011).

The Mato Grosso soil is a clayey Oxisol corresponding to soils typically used for soybean cultivation in the Cerrado region of Mato Grosso (Jantalia et al. 2007). Its top layer was adjusted to correspond to average textural conditions as identified at the Tanguro Ranch, Mato Grosso (Scheffler et al. 2011).

The Iowa soil is an example of the official Iowa state soil series: the Tama; a set of highly productive, well-drained soils, covering nearly 380 000 ha in 28 counties in Iowa, widely cultivated with maize (Iowa State University Extension and Outreach Website).

The German soil is a Luvisol: a soil type widely found in the Eastern parts of Schleswig-Holstein and predominantly used as arable land (LLUR, 2006), in particular the crop rotation winter wheat – winter barley – winter rapeseed (Bless, pers. com. 2013).

The Swedish soil is representative of soils associated with agricultural crops in the South Central region of Sweden (Svealand), based on data from the most recent national soil inventory on arable land (Eriksson et al. 2010). It also matches the soil requirements of *Salix* (IEA, 2009).

Table 4.4. Summary of soil data for the five studied regions with datavalues in the top soil horizon and horizon weighted averages. Data originate from ISRIC-WISE Harmonized Global Soil Profile Dataset v 3.1 (Batjes, 2008; 2009) but were modified to improve representativeness based on expert consultancy and literature data. The full set of soil data is available in Appendix 7.

	São Paulo, Brazil	**Mato Grosso, Brazil**	**Iowa, US**	**Northern Germany**	**South Central Sweden**
ISRIC-WISE soil sample ID-number	BR0643	BR0578	US0323	DE0008	SE0013
No of horizons modeled	3	4	5	4	5
Depth of top layer (cm)	25	20	20	14	20
pH-H_2O top layer / average	6 [a] / 5.5	6 [a] / 5.7	6.1 / 6.1	6 [g] / 5.5 [g]	6.4 [h] / 7.1
Sand (%) top layer / average (particles > 50 µm)	52 [c] / 53	55 [e] / 43	3/ 4	47 / 42	23 [h] / 25
Silt (%) top layer / average (particles 2-50 µm)	15 [c] / 12	2 [e] / 7	66 / 65	37 / 33	36 [h] / 37
Clay (%) top layer / average (particles < 2 µm)	33 [c] / 35	43 [e] / 50	31 / 31	16 / 26	41 [h] / 38
Organic carbon (%) top layer / average	1.1 [c] / 1.1	2.7 [f] / 1.1	2.3 / 0.9	2.1 / 0.6	2.3 [h] / 0.9
Soil bulk density ($kg\ m^{-3}$)	1450 [d]	1350 [d]	1500 [d]	1580	1400 [d]
USDA soil texture classification [i]	Sandy clay	Clay	Silty clay loam	Loam	Clay loam

[a] pH in the top layer set to 6 assuming lime has been applied.

[c] Clay and organic carbon content in top layer (0-25 cm) and second layer (25-50 cm) adjusted to correspond to average conditions under sugarcane in the Mid-South of Brazil as identified by CTC (Joaquim et al. 2011) based on 27 552 soil samples. Composition of sand and silt determined based on expert judgment (Sparovek, pers. com. 2013).

[d] Bulk densities derived based on clay content, from Joaquim et al. (2011).

[e] Soil texture in the top layer based on data in Scheffler et al. (2011), representing average conditions in Tangaru Ranch, Mato Grosso.

[f] Organic carbon content in the top horizon based on Jantalia et al. (2007).

[g] Based on expert judgment (Bless, pers. com. 2013).

[h] pH, clay content and organic matter content in the top horizon (0-20 cm) of the Swedish soil based on data from the Swedish Arable Land- and Crop Inventory (Eriksson et al. 2010), representing measured averages from 398 mineral soil samples under agricultural crops in the plains of South Central Sweden (Svealand). Organic carbon content calculated as 58% of organic matter. Composition of sand and silt set based on own assumptions.

[i] Soil texture classification, based on the USDA soil texture calculator, is not needed for modeling purposes but included here for comparison.

4.4 Potential freshwater ecotoxicity impact assessment

LCIA refers to the assessment of potential impacts by multiplying emissions with CFs, see further in Chapter 3. We used USEtox v.1.01 (Rosenbaum et al. 2008) to calculate potential freshwater ecotoxicity impacts due to pesticide emissions to air and surface water.

USEtox is an emission route-specific impact assessment model for comparative assessment of chemicals and their toxic effects on humans and freshwater ecosystems. It was developed for use in LCIA in a “scientific concensus” process (Hauschild et al. 2008), and recently appointed “the best” among existing characterization models for freshwater ecotoxicity and human toxicity in a review study of LCIA models for the Joint Research

Centre of the European Commission (JRC) (Hauschild et al. 2013). It is also recommended by the US Environmental Protection Agency (Bare, 2011).

Potential freshwater ecotoxicity impact scores calculated by USEtox represent an estimate of the Potentially Affected Fraction (PAF) of species in time and (freshwater) space, and are expressed in the unit Comparative Toxic Unit ecotoxicity (CTUe). Ecotoxicity CFs(expressed in the unit CTUe per kg of an emitted chemical) are available for various emission compartments on the continental and global scales for nearly 2500 substances (Henderson et al. 2011). We obtained CFs from the Excel file “USEtox_results_organics”, available at the USEtox Website. CFs may also be obtained from databases incorporated in LCA software, but practitioners should be aware that LCA software may not contain the most recently updated CFs at all times.

Here, potential freshwater ecotoxicity impacts were assessed as the product of emissions to air and surface water and freshwater ecotoxicity CFs corresponding to emissions to continental air and continental freshwater (Equation 4.1).

$$Potential\ freshwaterecotoxicityimpact\ of\ pesticide = \left(e_{air,P} \cdot CF_{air,P} + e_{water,P} \cdot CF_{water,P}\right) \cdot f_P$$

Equation 4.1

where f_P denotes pesticide P’s frequency factor (yr^{-1}), $e_{air,P}$ and $e_{water,P}$ denote the mass of pesticide P emitted to air and surface water (kg ha^{-1}), respectively, and $CF_{air,P}$ and $CF_{water,P}$ denote freshwater ecotoxicity CFs for emissions to continental air and continental freshwater (CTUe kg^{-1}), respectively.

USEtox CFs are products of a fate-, an exposure-, and an effect factor, in accordance with the cause-effect chains that link emissions to impacts in the environment (Rosenbaum et al., 2008; for more information see Chapter 3).

Fate factors have the dimension days, and represent the persistence of chemicals in the environment, based upon substance-specific physico-chemical properties and site-generic landscape parameters. Landscape parameters in USEtox represent an average default continent, whichis not intended to resemble any particular real continent, such as Europe or the US. Hence, USEtox CFs are site-generic and represent global averages. The site-specificness referred to in this study is thus limited to the inventory of pesticide usage and emissions.

Exposure factors equal the dissolved fraction of chemicals (dimensionless), calculated based on their fate, and solubility in water. These fractions are used as simplified measures of the bio-available share.

Effect factors are inversely proportional to the geometric mean of ecotoxic effect data (EC50 and LC50-data) of freshwater organisms at different trophic levels in the ecosystem (see further detail below) (Huijbregts et al. 2010b).

USEtox CFs are classified as "recommended" or "interim" where the latter indicate that there is a lack of data or considerable uncertainties in the modeling of fate, exposure and/or effect. The USEtox model is primarily designed and valid for non-polar, non-ionic organic substances, while metals, organometallics, dissociating substances, amphiphilics (e.g. detergents) and organic substances with effect data covering less than three different trophic levels, are all classified as “interim” (Rosenbaum et al. 2008). We used CFs that are classified as “interim”, since they represent a currently best-estimate and are considered “better than nothing”. All CFs and their associated classification are available in Appendix 1.

Freshwater ecotoxicity impact assessment is an active research area, in particular with regard to regionalization (Kounina et al. 2014), for which reason updates in CFs, and methodology, can be expected (USEtox Website).

Some of the pesticides identified during inventory were not available in the USEtox database of CFs.For these, we derived new CFsto account for all substances identified during inventory (see Appendix 1). We derived new CFs for a total of 20 ASs by following the recommended procedure (Huijbregts et al. 2010a). The USEtox model requires physico-chemical and ecotoxic effect data for calculation of new CFs, summarized in Table 4.5.

Table 4.5. Physico-chemical and ecotoxic effect data required for calculation of new USEtox CFs(adopted from Huijbregts et al. 2010b).

Notation as in USEtox model	**Unit**	**Explanation**
MW	g·mole^{-1}	Molecular weight
Kow	-	Octanol – water partition coefficient
Koc	l kg^{-1}	Organic carbon - water partition coefficient
K_H25C	Pa·m^{3}mole^{-1}	Henry’s law constant
Pvap25	Pa	Vapor pressure at 25°C
Sol25	mg l^{-1}	Water solubility at 25°C
K_{DOC}	l kg^{-1}	Dissolved organic carbon – waterpartition coefficient
$kdeg_A$	s^{-1}	Degradation rate in air
$kdeg_W$	s^{-1}	Degradation rate in water
$kdeg_{Sd}$	s^{-1}	Degradation rate in sediment
$kdeg_{Sl}$	s^{-1}	Degradation rate in soil
avlogEC50	log mg l^{-1}	Measure of ecotoxic effect based on acute and chronic EC(L)50s.

Physico-chemical data collection for calculation of new USEtox CFs

We derived the required physico-chemical data from the Estimation Program Interface Suite^{TM} (EPISuite) for Windows v. 4.11 (US-EPA, 2012), in line with the recommendation in Huijbregts et al. (2010a).

EPISuite is a “toolbox” of thirteen different estimation programs for physico-chemical properties of chemicals, developed by the US Environmental Protection Agency’s (EPA) office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). The only input required for running EPISuite is the chemical’s SMILES (see Table 4.2). Besides estimation models, several of the programs have built-in databases with experimentally determined data. We prioritized experimental data and used estimated values only when experimentally determined data were not available, in line with the recommendation. Details of how the required data were obtained from EPISuite are given in Appendix 2.

Ecotoxic effect data collection for calculation of new USEtox CFs

Ecotoxic effect factors in USEtox are inversely proportional to the geometric mean of ecotoxic effect data of freshwater organisms at different trophic levels in the ecosystem, and calculated in the model according to Equation 4.2,

$$USEtox\ effect\ factors = \frac{0.5 \cdot 1000}{10^{avlogEC50}}$$

Equation 4.2

where the factor 1000 is a unit converter; 0.5 represents the working point on the PAF-curve, and the expression $10^{avlogEC50}$, sometimes also denoted $HC50_{EC50}$, is equivalent to the geometric mean of the availabe effect data (refer to Chapter 3.3 for more information on different effect factor modeling approaches).

The parameter avlogEC50 has to be calculated by the user and entered into the model. The input data required to calculate the avlogEC50are EC50data for freshwater organisms at different trophic levels in the ecosystem. Although the USEtox user manual does not explicitly state so, LC50-data may also be used, which is a common endpoint in toxicity tests on fish (Larsen and Hauschild, 2007b). The avlogEC50-parameter can be calculated in two equivalent manners:

1) by first calculating the logarithm of all chronic equivalent EC(L)50s and then calculating the arithmetic mean of all log-values – the middle term in Equation 4.3, according to the USEtox user manual (Huijbregts et al.2010b, p. 16 – 17), or

2) by first calculating the geometric mean of all chronic equivalent EC(L)50s and then calculating the logarithm of the geometric mean – the right term in Equation 4.3, according to Payet (2004, p. 65),

$$av_{logEC50} = \frac{\sum_{i=1}^{N} \log(x_i)}{N} = log\left(\sqrt[N]{\prod_{i=1}^{N} x_i}\right)$$

Equation 4.3

where $x_i$represent ecotoxic effect data in the form of EC50 and/or LC50 values in mg l^{-1} and N the number of unique species. That the right and middle term of Equation 4.3 are indeed equivalent follow from logarithmic rules.

If more than one effect data value exists for a species, a geometric mean should be calculated, according to the USEtox user manual. This requires that criteria for aggregation of test values are properly defined. In absence of such criteria, we aggregated test values that referred to the same ASs, species and test duration time. Refer to Larsen and Hauschild (2007b) for anin-depthanalysis of the effect of averaging (i.e., calculating the geometric mean) at different ecosystem levels.

In USEtox, acute effect data are converted to chronic equivalents, by applying an acute-to-chronic extrapolation factor of 2 (Huijbregts et al. 2010b), according to Equation 4.4.

$$Chronic\ equivalent\ EC(L)50 = \frac{Acute\ EC(L)50}{2}$$

Equation 4.4

The USEtox user manual does not explicitly state on what basis the differentiation between acute and chronic tests should be made. In fact, there is no scientific consensus or internationally accepted standard on the differentiation between acute and chronic tests (Payet, 2004). Here, we used the following differentiation approach: whenever a given database stated whether a test was acute or chronic, we used that classification. For cases when the test duration time was available, but not a classification into acute or chronic, we used a classification based on test duration time, modified from Payet (2004), presented in Table 4.6. For the few cases when the test duration time was not stated, the test was assumed to be acute, as are the majority of ecotoxicity tests.

Table 4.6. Differentiation between acute and chronic E(L)C50-tests based on test duration time (modified from Payet, 2004).

Type of organism	**Acute**	**Chronic**
Vertebrates	< 7 days	≥ 7 days
Invertebrates	< 7 days	≥ 7 days
Plants	< 7 days	≥ 7 days
Algae	< 3 days	≥ 3 days

The USEtox user manual does not explicitly recommend specific freshwater organisms, and for this reason we did not use any species selection criteria. However, freshwater ecotoxicity tests have been standardized (by e.g., the OECD, US-EPA and the European Union),and we acknowledge that using ecotoxicity effect data from such standardized tests would remove an unnecessary dimension of uncertainty and serve the purpose of comparative LCA, as pointed out by Larsen and Hauschild (2007b).

With regard to trophic levels, we followed the recommendations by Larsen and Hauschild (2007b) and aimed for representation at the algae, invertebrate and fish ecosystem level. In summary, we collected the following data:

- the species’ scientific name
- test duration time (h)
- classification of the test as acute or chronic
- trophic level; differentiating between algae, aquatic plants, aquatic invertebrates, fish, freshwater molluscs and freshwater insects
- data source

We derived ecotoxic effect data primarily from the Pesticide Properties Database (PPDB), AGRITOX, US-EPA ECOTOX Database, US-EPA OPP Pesticide Ecotoxicity Database and TOXNET. For a more extensive list of chemical toxicity databases, refer to the list published by the AltTox Website. The full set of ecotoxic effect data used for calculation of new CFs, as well as the calculated avlogEC50 parameters, are available in Appendix 5. LCA-pracitioners are recommended to make sure that data collected indeed refer to tests on freshwater species (and not e.g., marine species), since databases often lack this information.

4.5 Biofuel energy yields

Biofuel energy yields refer to the gross biofuel output per ha and year from the biofuel conversion plant (after conversion). Gross output refers to the total biofuel output, and excludes the deduction of energy inputs for feedstock production and transport, conversion of feedstock to fuel, and distribution of biofuels to the final consumer. Biofuel energy yields were calculated based on fresh harvest yields, typical transportation pathways and conversion efficiencies in biofuel conversion plants. Biofuel production pathways and conversion efficiencies for maize, rapeseed, soybean, sugarcane and wheat are based on data inJRC (2012). For*Salix*,ethanol production data are based on González-García et al. (2012b). Key data used in calculations and resulting gross biofuel outputs are presented in Table 4.7.

Table 4.7. Key data used to calculate gross biofuel output (also given in table).

Case [a]	**Fresh harvest yield** [b] **(kgha^{-1} yr^{-1})**	**Water content at harvest** [c]**(%)**	**Energy content of feedstock, LHV** [d] **(MJ kg$^{-1}_{\text{dry matter}}$)**	**Conversion efficiency** [e] **(MJ$_{\text{biofuel}}$ MJ$^{-1}_{\text{feedstock}}$)**	**Resulting gross biofuel output, energy (MJ$_{\text{biofuel}}$ ha^{-1} yr^{-1})**
MZ-I/II	10 700	14%	17.3	0.60	96 000
RS	4050	15%	27.0	0.61	56 800
SX	20 000	50%	19	0.41	78 800
SB-I/II	3030	13%	23	0.32	19 700
SC	84 300	72.5%	19.6	0.34	154 000
WT	8740	13.5%	17.0	0.54	69 600

[a] MZ-I, MZ-II: Genetically engineered (GE) glyphosate tolerant maize with (MZ-I) and without (MZ-II) *Bt*-technology cultivated in Iowa, US. RS: winter rapeseed cultivated in Schleswig-Holstein, Germany. SX: *Salix* short rotation woody coppice cultivated in South Central of Sweden. SB-I: conventional soybean cultivated in Mato Grosso, Brazil. SB-II: GE glyphosate tolerant soybean cultivated in Mato Grosso, Brazil. SC: sugarcane cultivated in São Paulo, Brazil. WT: winter wheat cultivated in Schleswig-Holstein, Germany. For further details, see Chapter 5.

[b] Fresh harvest yields for maize, rapeseed, soybean, sugarcane and wheat represent averages of production between 2006 and 2011 in the defined regions as follow: MZ-I/II: Iowa, US, from USDA NASS Quick Stats Database; RS and WT: Schleswig-Holstein, Northern Germany from Statistikamt Nord(2013); SB-I/II: Mato Grosso, Brazil, from SIDRA-IBGE and SC: São Paulo, Brazil, from SIDRA-IBGE. Yields of wheat and maize refer to the weight of clean, dry grains in the form usually marketed; of sugarcanes the weight of clean canes free of leaves in the stage they are sent to the sugar factories, and of soybean and rapeseed the weight of harvested seeds (FAO, 2011). Fresh harvest yield of *Salix* represents a conservative estimate of the future yearly yield potential averaged over a plantation life cycle, assuming 50% water content at harvest, based on IEA (2012) more information in Chapter 5.3.

[c] Water contents at harvest of maize, rapeseed, soybean, sugarcane and wheat from JRC (2012) and of *Salix* from IEA (2012).

[d] Lower heating values from JRC (2012).

[e] Conversion efficiencies represent conditions in typical biofuel conversion plants, and are based on JRC (2012) for maize, rapeseed, soybean, sugarcane and wheat and on González-García et al. (2012b) for *Salix*. Conversion efficiencies of maize, rapeseed and wheat include a transport loss factor of 1% from field to plant, while for soybean the loss factor is 2% (JRC, 2012). For *Salix* we assumed a loss factor of 1%.

4.6 Allocation and allocation factors

All biofuel production processes considered here are associated with co-products, see Table 4.8. We allocated through partitioning based on energy content as suggested by the EU Renewable Energy Directive (RED) (EC, 2009) where greenhouse gas emissions associated with biofuel production system are divided between the fuel and the co-product on the basis of their lower heating values. We allocated impacts expressed in relation to biofuel energy yield, while impacts expressed in relation to cultivated area and time were left unallocated. The rationale for not allocating impacts expressed in relation to ha and year is that we considered it more relevant, from the perspective of freshwater ecosystems and their protection, to account for the total impact at the cultivation stage. However, re-calculation to allocated results can be done using the allocation factors in Table 4.8.

Allocation factors were calculated considering output shares between biofuels and co-product(s) in representative production systems, see Table 4.8.

To illustrate the calculation procedure, consider the following example: based on the data in Table 4.8 it can be calculated that the gross energy output per kg dry rapeseed (0% moist) is 16.49 MJ FAME (= 14.02/0.85), 9.89 MJ rapeseed cake (= 0.538·18.38) and 0.723 MJ glycerol (= 101.87·16.0·14.02/(1000·37.2·0.85)). That is, the total gross energy output per kg dry rapeseed is 27.1 MJ (= 16.49+9.89+0.723), of which biodiesel, rapeseed cake and glycerol make up 60.8, 36.5 and 2.67%, respectively. Hence, 60.8% is used as allocation factor for biodiesel from rapeseed, according to the partitioning method based on energy content.

Table 4.8. Allocation factors calculated (this study) using the partitioning method based on energy content, and water contents at harvest as given in Table 4.7. Data for maize, rapeseed, soybean, sugarcane and wheat were derived from JRC (2012) and for *Salix* from González-García et al. (2012b). Heating values refer to lower heating values.

Input feedstock	**Output product**	**Data value**	**Unit**	**Allocation factor (%)**
Maize	Ethanol	8.935 [c]	MJ ethanol / kg maize at 14% moisture	61.6
	DDGS [a]	0.0334	kg dry DDGS / MJ ethanol	38.4
		18.70	MJ / kg dry DDGS	
Rapeseed	Biodiesel (FAME [b])	14.02 [c]	MJ FAME / kg feedstock at 15% moisture	60.8
		37.2	MJ / kg FAME	
	Rapeseed cake	0.5380	kg dry cake / kg dry rapeseed	36.5
		18.38	MJ / kg dry cake	
	Glycerol	101.9	kg glycerol / ton FAME	2.67
		16.0	MJ / kg glycerol	
Salix	Ethanol	59.41	ton ethanol / 200 ton oven dry feedstock	93.9
		26.80	MJ / kg ethanol	
	Electricity	103.7	GJ electricity / 200 ton oven dry feedstock	6.11
Soybean	Biodiesel	6.495 [c]	MJ biodiesel / kg soybeans at 13% moisture	32.7
		37.2	MJ / kg FAME	
	Soybean cake	0.7840	kg dry cake / kg dry soybean seeds	65.8
		19.14	MJ / kg dry cake	
	Glycerol	101.9	kg glycerol / ton biodiesel	1.43
		16.0	MJ / kg glycerol	
Sugarcane	Ethanol	1.828 [c]	MJ ethanol / kg fresh cane in	98.2
	Electricity	9.20	kWh excess electricity / ton fresh cane in	1.78
Wheat	Ethanol	7.963 [c]	MJ ethanol / kg wheat at 13.5% moisture	55.9
	DDGS	0.3740	kg wet DDGS at 10% moisture / kg wheat grain at 13.5% moisture	44.1
		18.70	MJ / kg dry DDGS	

[a] Dried Distillers Grains with Solubles.
[b] Fatty Acid Methyl Esters.
[c] Calculated based on data in Table 4.7 and included here for completion.

Allocation is a debated topic in LCA (Curran, 2007), and other valid bases for partitioning exist, e.g., economic value, although variable over time. Beyond partitioning, three conceptually different approaches exist for solving multifunctionality of processes in LCA, the first two of which avoid allocation (JRC, 2010):

1) constructing functionally comparable systems through system expansion,

2) identifyingthe displaced products, by answering the question "*if this co-product was not produced what would be produced instead?*", and subtracting the environmental impacts associated with the displaced products from the studied production system (referred to as substitution by system expansion), and

3) allocating the environmental effects between process outputs through partitioning based on some relationship, e.g., physical characteristics or economic value.

The ILCD Handbook, based on the ISO-standard for LCA, prescribes that multifunctionality in attributional LCAs should be solved by substitution through system expansion if the LCA takes into account "*existing benefits outside the analysed system*", and by allocation if the LCA "*accounts for the analysed systems in isolation*" (JRC, 2010). Partitioning based on energy or economic value are common approaches in biofuel LCA, and each has their strengths and limitations.

The main advantage of substitution by system expansion is that is avoids allocation. In the context of attributional LCA, substitution by system expansion is also related to a number of problems:

- difficulty with identifying the displaced product
- approach is not constant over time
- co-products may displace products that are produced far away from the studied production system. This is especially problematic if effects are dependent on local conditions
- difficulty with interpreting and communicating results where avoided emissions are counted as credits, especially in the case of negative results
- limited applicability of results in consumption accounting or emission reporting.

For these reasons and others, it has been suggested that the substitution method should not be permitted in attributional LCA; refer to Brander and Wylie (2011) for the extended arguments.

The substitution method by system expansion has been identified as most commonly employed in biofuel LCAs (Wiloso et al. 2012). We did not consider it appropriate here, since the eight cases are parts of coupled fuels and feed systems. In this case, the system expansion method would be considered speculative by requiring assumptions about product displacement that have weak empirical support and are sensitive to changes in policy, markets, and production systems.

The main advantage of the partitioning method based on energy content is that it is predictable over time and easy to apply. In addition, it produces results that are generally comparable to those produced by the substitution method, according to the EU Renewable Energy Directive (EC, 2009). One disadvantage of the energy allocation method is that the same biofuel production system can score differently for some impact categories depending on how by-flows are used. For example, if bagasse from sugarcane ethanol production was sold as fuel, or used to generate electricity for export to the grid, a significantly lower allocation factor would be obtained for cane-ethanol compared to the case where the bagasse is instead used to meet internal energy demand at the ethanol mill. The scoring for some impact categories, notably GHG emission, might become worse (depends on GHG intensity of the heat and power used at the ethanol mill). But for other impact categories, such as those associated with pesticides, the scoring will improve.

4.7 Sensitivity analysis

A number of parameters that we identified as uncertain or subject to large temporal or spatial variation were tested in sensitivity analyses, in order to quantitatively measure their effects on results. In particular, we analyzed the effects of field size, buffer zones, method of application, soil parameters, site, and tillage type on pesticide emissions to air and surface water, and resulting impact-scores, in selected test cases. This was done by varying one parameter at a time while keeping all other parameters constant.

CHAPTER 5. INTRODUCTION TO CASES: CULTIVATION PRACTICES AND PESTICIDE APPLICATION DATA

Chapter 5 introduces the studied cases, in terms of agronomic practices and pesticide management in the studied regions. Pesticide application data were obtained from specialists familiar with agricultural practices in the studied regions, or determined based on statistics or other literature, and complemented or modified, when appropriate, with our own assumptions. Application scenarios were constructed with the aim to represent realistic and typical farm practice in the defined regions.

5.1 Maize (Zea mays)

Two maize cases were defined based on data for the state of Iowa, US; the top US state both in terms of planted area (5.75 Mha in 2012) and production (47.7 million metric tons in 2012) (USDA NASS Quick Stats Database). In 2012, 31% of US maize harvest was utilized for fuel ethanol production (NCGA, 2013).

Genetically engineered (GE) varieties of maize with traits such as glyphosate tolerance and ability to produce insecticidal toxins from the bacterium *Bacillus thuringiensis* (*Bt*) against primarily European corn borer and corn rootworm, are widely adopted by US farmers. In 2012, 52% of US maize in terms of planted area were GE with multiple traits; 21% were equipped with herbicide tolerance and 15% with insect resistance (*Bt*-maize) while only 12% were “conventional”, i.e. non-GE (NCGA, 2013). In Iowa, adoption of GE maize was even higher, with only 9% conventional maize in 2012 (NCGA, 2013).

The most recent pesticide use survey on maize was performed by the United States Department of Agriculture (USDA) in 2010, in selected program states that together represent 93% of US maize acreages, the results of which are available in a short report format (USDA NASS, 2011), and in a searchable online database (USDA NASS Quick Stats Database). Data presented below originate from this survey and were derived from USDA NASS Quick Stats Database unless otherwise stated.

Insecticides, a total of 67.1 metric tons, were applied to 8% of Iowa maize acreage in 2010. Due to confidentiality, it is not possible to identify the most widely used substances in Iowa, but in all program states included in the survey, the top three insecticides were chlorpyrifos (29%), tefluthrin (15%) and tebupirimphos (12%) (percentages referring to share of total insecticide use). Insecticides are either soil incorporated by the planter in conjunction with planting or applied later during tassling by aircraft (Ertl, pers. com. 2013). The most devastating insect pests are corn rootworms such as the western (*Diabrotica virgifera virgifera)* and the northern corn rootworms (*Diabrotica barberi*)(Benbrook, 2012).

Insecticide use on US maize decreased between 1996 and 2011 in parallel with a shift towards *Bt*-maize, partly due to adoption of new substances active in lower doses, and partly due to the *Bt*-technology (Benbrook, 2012). However, documented cases of field-evolved resistance in western corn rootworm against multiple *Bt*-toxins, have recently been reported (Gassmann, 2012; Gassmann et al. 2014), suggesting that this trend might not continue, unless the *Bt*-technology is integrated into a wider set of pest management strategies. In fact, the discovery of field-evolved resistance in western corn rootworm took place in Iowa, in 2009.

Fungicides, a total of 67.6 metric tons, were applied to 11% of Iowa maize acreage in 2010, of which pyraclostrobin represented a 62% share.

Herbicides, a total of 11 900 metric tons were applied to 100% of Iowa maize acreage in 2010. In Iowa, four herbicide ASs made up 90% of total herbicide use: glyphosate isopropylamine salt (34%), atrazine (26%), acetochlor (21%) and s-metolachlor (9%), applied to 68%, 65%, 32% and 19% of Iowa maize fields, respectively.

The introduction of glyphosate tolerant maize varieties has been associated with an over-reliance of glyphosate as weed management strategy;a practice that has favoured the development of herbicide resistance in weeds across the US (Mortensen et al. 2012; Green, 2012), as well as in Iowa (Owen and Hartzler, 2011; 2012; 2013). This has led to the emergence of so-called "superweeds" (Gilbert, 2013). The currently most problematic weed in Iowa is glyphosate resistant common waterhemp (*Amaranthus tuberculatus* syn: *rudis*) (Owen and Hartzler, 2011; 2012) while glyphosate resistant Palmer amaranth (*Amaranthus palmeri*), recently discovered in Iowa, may become the next big problem (Owen and Hartzler, 2013).

The two maize cases were constructed to represent maize with and without the *Bt*-technology. We did not include fungicides in any of the cases since it is not commonly used, but included one insecticide to capture the difference between maize with and without the *Bt*-technology. The two cases are:

1. MZ-I: GE glyphosate tolerant maize with *Bt*-technology (Table 5.1), and
2. MZ-II: GE glyphosate tolerant maize without *Bt*-technology (Table 5.2).

Pesticide application scenarios were constructed based on pesticide use statistics for the years 2010, retrieved from USDA NASS Quick Stats Database, in combination with agricultural recommendations for specific products. The two cases differ only by one insecticide, chlorpyrifos, which is applied in the MZ-IIcase.

The MZ-I pesticide application scenario amounts to a total of 3.34 kg AS ha^{-1} yr^{-1}, while the MZ-II pesticide application scenario amounts to a total of 4.18 kg AS ha^{-1} yr^{-1}.

A 62% share of US maize acreage was under no-till or minimum-till practice in 2010 (USDA NASS, 2011) and irrigation was practiced on 15% of US maize acreage in 2007, according to the latest agricultural census (USDA NASS Quick Stats Database). Therefore, both maize cases were assumed to be under reduced tillage without any irrigation input.

Table 5.1. Pesticide applications in GE glyphosate tolerant maize with *Bt*-technology (MZ-I) grown in Iowa, US (H = herbicide).

Active substance (AS)	**Frequency (yr^{-1})**	**Dose per application (g AS ha^{-1})**	**Application method**	**Crop type and development stage**	**Application month**
Atrazine (H)	1	1305	Conv. boom	Bare soil	April
Acetochlor (H)	1	1052	Conv. boom	Bare soil	April
Glyphosate isopropylamine salt (H)	1	982	Conv. boom	Maize II	June

Table 5.2. Pesticide applications in GE glyphosate tolerant maize without *Bt*-technology (MZ-II) grown in Iowa, US(H = herbicide, I = insecticide).

Active substance (AS)	Frequency (yr^{-1})	Dose per application ($g\ AS\ ha^{-1}$)	Application method	Crop type and development stage	Application month
Atrazine (H)	1	1305	Conv. boom	Bare soil	April
Acetochlor (H)	1	1052	Conv. boom	Bare soil	April
Glyphosate isopropylamine salt (H)	1	982	Conv. boom	Maize II	June
Chlorpyrifos (I)	1	841	Aircraft	Maize III	July

5.2 Winter rapeseed (Brassica napus)

One winter rapeseed case (referred to as RS) was defined based on data for rapeseed cultivation in Schleswig-Holstein, Northern Germany, with sowing in August and harvest the following summer (Table 5.3). Europe is the largest rapeseed producing region in the world and Germany, together with France, are the two largest producers in Europe, measured as average production between 2008 and 2012 (FAOSTAT). Around 60% of the global output of biodiesel is produced in the EU with rapeseed oil as the most important feedstock (Milazzo et al. 2013). Schleswig-Holstein produced an average of 435 000 metric tons of rapeseed between 2006 and 2011, on 107 000 ha Statistikamt Nord(2013), corresponding to 8.2% of the national output of rapeseeds during the same period (FAOSTAT).

The pesticide application scenario was set based on information from the Chamber of Agriculture in Schleswig-Holstein, Northern Germany (Gleser, pers. com. 2013) and represent typical practice in intense rapeseed cultivation in the region. Application doses are in line with recommended doses, see e.g. BASF (2013).

Some of the most serious fungal diseases affecting rapeseed in Europe include three soil borne diseases: Sclerotinia stem rot (*Sclerotinia sclerotiorum*), Verticillium wilt (*Verticillium longisporum*) and clubroot (*Plasmodiophora brassicae*); two foliar diseases: light leaf spot (*Pyrenopeziza brassicae*) and Phoma leaf spot (*Leptosphaeria* spp.) and one seed borne disease: dark leaf and pod spot (*Alternaria* spp.) (Berry et al. 2012).

Six major insect pests are of concern to winter rapeseed growers in Europe: cabbage stem flea beetles (*Psylliodes chrysocephala*), pollen beetles (*Meligethes aeneus*), cabbage seed weevils (*Ceutorhynchus assimilis*), cabbage stem weevils (*Ceutorhynchus pallidactylus*), rape stem weevils (*Ceutorhynchus napi*) and Brassica pod midge (*Dasineura brassicae*) (Williams, 2010).

The RS case includes three applications with insecticides: beta-cyfluthrin in the autumn against cabbage stem flea beetles; etofenprox in the flower bud stage against pollen beetles and thiacloprid in the flowering stage against biting insects and Brassica pod midge. These insecticides represent some of the most commonly used insecticides on rapeseed in Germany (Rossberg, 2013). The RS case also contains three fungicide treatments applied between the leaf development stage and the flowering stage against black leg (*Phoma lingam*) and Sclerotinia stem rot, and two applications of plant growth regulators; once in the fall to improve the winter hardiness and once in the spring to increase the plant stability. A range of herbicides are applied in the autumn from August to November to control weeds. All pesticides are applied with a conventional tractor pulled boom.

The RS pesticide application scenario amounts to a total of 2.36 kg AS ha^{-1} yr^{-1}. Pesticide use on oilseeds cultivated in Germany has fluctuated between 0.6 and 1.8 kg AS ha^{-1} between 1992 and 2002, and was 1.2 kg AS ha^{-1} in 2003, the latest year for which the statistical office of the European Union (Eurostat) compiled statistics (Eurostat, 2007).

Compared to North and South America, European farmers and authorities have shown greater resistance towards adoption of no-till and/or reduced tillage management systems, and the adoption rate in Germany has been particularly low with less than 5 000 ha cultivated under such schemes, while in Europe as a whole, only 1.1% of the total agricultural land is under no-till (Derpsch and Friedrich, 2009). For this reason, conventional tillage was assumed here.

Table 5.3. Pesticide applications in rapeseed (RS) grown in Schleswig-Holstein, Northern Germany (H = herbicide, F = fungicide, I = insecticide, PGR = plant growth regulator).

Active substance (AS)	**Frequency (yr^{-1})**	**Dose per application (g AS ha^{-1})**	**Application method**	**Crop type and development stage**	**Application month**
Glyphosate isopropylamine salt[a] (H)	0.25	2187	Conv. boom	Bare soil	Aug.
Metazachlor (H)	0.8	400	Conv. boom	Oilseed rape I	Aug.
Quinmerac (H)	0.8	200	Conv. boom	Oilseed rape I	Aug.
Dimethenamid-P (H)	0.8	400	Conv. boom	Oilseed rape I	Aug.
Quizalofop-P-ethyl (H)	0.67	40	Conv. boom	Oilseed rape I	Sept.
Beta-Cyfluthrin (I)	1	8	Conv. boom	Oilseed rape I	Sept.
Mepiquat-chlorid (PGR)	1	147	Conv. boom	Oilseed rape I	Oct.
Metconazole (F)	1	21	Conv. boom	Oilseed rape I	Oct.
Propyzamid (H)	0.67	500	Conv. boom	Oilseed rape I	Nov.
Mepiquat-chlorid (PGR)	1	147	Conv. boom	Oilseed rape II	April
Metconazole (F)	1	21	Conv. boom	Oilseed rape II	April
Etofenprox (I)	1	58	Conv. boom	Oilseed rape III	April
Thiacloprid (I)	0.67	72	Conv. boom	Oilseed rape III	May
Boscalid (F)	1	100	Conv. boom	Oilseed rape III	May
Dimoxystrobin (F)	1	100	Conv. boom	Oilseed rape III	May

[a] Addition to data retrieved from the Chamber of Agriculture in Schleswig-Holstein; based on Glyphosate Website (2013), stating that 75% of the arable land in the northern and eastern regions of Germany is treated with glyphosate.

5.3 Salix spp.

One *Salix* case, referred to as SX (Table 5.4), was defined based on data for *Salix* cultivation in Uppsala county in the South Central region of Sweden (Svealand) – one of the major *Salix* cultivation counties in Sweden(SCB, 2013). Pesticide application data were obtained from Salix Energy Europe (Åsheim, pers. com. 2012).

Salix is a genus of fast-growing trees and shrubs, native to the Northern Hemisphere. It is presently cultivated as a bioenergy crop on relatively small areas in a limited number of countries. Two breeding programs (one European and one Swedish) have developed several hybrid varieties of *Salix* for cultivation as short rotation woody coppice (SRWC) over the past decades (IEA, 2012). Sweden is one of the pioneering countries that cultivate *Salix* commercially on a relatively large-scale: 12 600 ha in 2012 (SCB, 2013), primarily for use as fuel in combined heat and power plants. Several options for producing biofuels from lignocellulosic feedstocks are under development, while none is commercially available yet (IEA, 2009). Advanced ethanol fuels from lignocellulosic biomass are projected to become commercially available within a 10-20 year time frame (IEA, 2009; 2012).

Typical cultivation practice, as described in González-García et al. (2012a), consists in short of the following steps: field preparation in the autumn prior to planting by disking, deep-ploughing and application of a broad-spectrum herbicide for weed removal; a second herbicide application in the spring “year 0” and planting of *Salix* coppice; cutting of sprouts year 1 to stimulate growth, followed by harvesting every three or four years over the plantation life cycle. Yields in the order of 10 dry metric tonsha^{-1} yr^{-1} can currently be expected from plantations cultivating improved varieties on better sites (IEA, 2012). Higher future yields can be expected to follow from improvements in agronomic management and from breeding efforts devoted to dedicated bioenergy crops - akin to the historic development in major food crops. Therefore, this yield level is considered a conservative estimate of the future yield potential of *Salix*.

In this study a plantation life length of 22 years is used, and the field is assumed to be harvested every third year, from year 4 onwards, resulting in seven harvest cycles in total.

In Sweden, only herbicides are allowed for use on *Salix* (KemI Pesticides Register). The severity of insect pests and fungal diseases typically do not motivate the use pesticides, nor is it practicable on fully grown *Salix* shrubs (IEA, 2012).

Glyphosate isopropylamine salt is applied once over the plantation life cycle in connection with field establishment, while a mix of flurtamone and diflufenican is applied once in connection with planting, and after every harvest, except the last one (i.e., a total of seven applications). Coppice typically requires herbicide application (IEA, 2012). Conventional tillage is assumed in connection with planting and no-till for all subsequent applications.

The SX pesticide application scenario amounts to a total of 0.24 kg AS ha^{-1} yr^{-1}. This can be compared with the 0.34 kg AS ha^{-1} yr^{-1} as reported in González-García et al. (2012b).

Table 5.4. Pesticide applications in *Salix* (SX) grown in South Central of Sweden (H = herbicide).

Active substance (AS)	**Frequency (yr^{-1})**	**Dose per application (g AS ha^{-1})**	**Application method**	**Crop type and development stage**	**Application month**
Glyphosate isopropylamine salt (H)	0.05	2187	Conv. boom	Bare soil	Oct.
Flurtamone (H)	0.32	313	Conv. boom	Bare soil	April
Diflufenican (H)	0.32	125	Conv. boom	Bare soil	April

5.4 Soybean (Glycine max)

Two soybean cases were defined based on data for soybean cultivation in Mato Grosso (and complemented with data from Bahia, see below). Brazil is the second largest producer of soybean in the world next to the US(FAOSTAT). Mato Grosso is the largest soybean producing state in Brazil with 21.8 million metric tons of soybean in 2012, grown on 7 million planted ha (IBGE, 2013), corresponding to 33.2% of the national production.

Genetically engineered (GE) soybean varieties, primarily equipped with glyphosate tolerance, have been cultivated in Brazil since the late 1990s (de Castro, 2008). The share of Brazilian soybean acreage cultivated with GE soybeans grew dramatically from 8 to 92% through the years 1998 to 2013(Soy Stats Website). The adoption of glyphosate tolerant varieties has changed agricultural practices, allowing glyphosate to be applied on top of growing crops. This has led to an increase in herbicide use and development of resistance (Meyer and Cederberg, 2010). Brazil increased its herbicide use on soybeans by 50% between 2003 and 2008, reaching on average 4.2 kg herbicide AS ha^{-1} in 2008, of which glyphosate was the most widely used herbicide (Meyer and Cederberg, 2010). The International Survey of Herbicide Resistant Weeds (Heap, 2014) has so far documented resistance against EPSP synthase inhibitors (the herbicide group to which glyphosate belongs)in six weed species in Brazil: horseweed (*Conyza canadensis*), hairy fleabane (*Conyza bonariensis*), Sumatran fleabane (*Conyza sumatrensis*), sourgrass (*Digitaria insularis*), Italian ryegrass (*Lolium multiflorum*) and tall windmill grass (*Chloris elata*).

The most important fungal disease is Asian soybean rust (*Phakopsora pachyrhizi*) and the most important insect pests are the velvet-bean caterpillar (*Anticarsia gemmatalis*) and three types of stink bugs: *Euschistus heros, Piezodurus guildinii* and *Nezara viridula* (Meyer and Cederberg, 2010). In response to fungal diseases and insect pests, Brazil increased its fungicide and insecticide use on soybean by 70%each between 2004 and 2008, reaching on average 0.55 kg AS fungicides ha^{-1} and 1 kg AS insecticides ha^{-1} in 2008 (Meyer and Cederberg, 2010).

Here, we consider two cases to account for differences in weed management strategies with and without GE seed technology:

1. SB-I: Conventional (not GE) soybean (Table 5.5), and
2. SB-II: GE glyphosate tolerant soybean (Table 5.6).

Application data for the SB-I case was provided by a conventional farmer in Mato Grosso through the Mato Grosso State Soy and Corn Producers Association, APROSOJA (Azevedo, pers. com. 2013), and correspond to the actual practice (sowing in October and harvest in February, after approximately 130 days) at a typical farm during the 2011 – 2012 growing season. Herbicide application data for the SB-II case was collected from a farm in Bahia (growing season 2012/2013) that cultivate GE soybean (Meyer, pers. com. 2013) and extrapolated to Mato Grosso under the assumption that herbicide application on this farm is representative of standard practice. Further, it was assumed that fungicide and insecticide applications in the SB-II case are the same as in the SB-I case. The SB-I pesticide application scenario amounts to a total of 1.92 kg AS ha^{-1} yr^{-1} while the SB-II pesticide application scenario amounts to a total of 3.75 kg AS ha^{-1} yr^{-1}.This can be compared with the average total pesticide use on Brazilian soybeans that Meyer and Cederberg (2010) estimated to be 6.6 kg AS ha^{-1}in 2008, including herbicides, fungicides, insecticides and other pesticides. This indicates that the pesticide application scenarios used here are underestimated.

No-till cropping systems have been adopted by Brazilian farmers at an exponential rate since the early 1990s and covered more than 50% of the total cultivated area in Brazil in the growing season of 2010/2011 (FEBRAPDP Website). In Mato Grosso, the adoption of no-till has been even more massive with 90% the cultivated area under such practice (APROSOJA, n.d.). For that reason, no-till was assumed in both soybean cases. Drainage systems are not widely used in soybean cultivation in Brazil (Meyer, pers. com. 2013) and were therefore not considered here.

Table 5.5. Pesticide applications in conventional soybean (SB-I) grown in Mato Grosso, Brazil (H = herbicide, F = fungicide, I = insecticide).

Active substance (AS)	Frequency (yr^{-1})	Dose per application (g AS ha^{-1})	Application method	Crop type and development stage	Application month
Paraquat [a] (H)	1	300	Conv. boom	Bare soil	Sept.
Lactofen (H)	1	72	Conv. boom	Soybean I	Oct.
Alpha cypermethrin (I)	1	30	Conv. boom	Soybean I	Oct.
Methomyl (I)	1	151	Conv. boom	Soybean I	Oct.
Bentazone (H)	1	540	Conv. boom	Soybean I	Oct.
Lactofen (H)	1	60	Conv. boom	Soybean I	Oct.
Chlorimuron-ethyl (H)	1	10	Conv. boom	Soybean I	Oct.
Chlorantraniliprole (I)	1	5	Conv. boom	Soybean I	Oct.
Clethodim (H)	1	84	Conv. boom	Soybean I	Nov.
Pyraclostrobin (F)	1	75	Conv. boom	Soybean I	Nov.
Chlorantraniliprole (I)	1	5	Conv. boom	Soybean I	Nov.
Pyraclostrobin (F)	1	67	Conv. boom	Soybean II	Nov.
Epoxiconazole (F)	1	25	Conv. boom	Soybean II	Nov.
Chlorantraniliprole (I)	1	10	Conv. boom	Soybean II	Nov.
Pyraclostrobin (F)	1	67	Conv. boom	Soybean II	Dec.
Epoxiconazole (F)	1	25	Conv. boom	Soybean II	Dec.
Teflubenzuron (I)	1	23	Conv. boom	Soybean II	Dec.
Thiamethoxam (I)	1	42	Conv. boom	Soybean III	Jan.
Lambda-cyhalothrin (I)	1	32	Conv. boom	Soybean III	Jan.
Paraquat [a] (H)	1	300	Conv. boom	Soybean III	Feb.

[a] Addition to original data obtained from Azevedo (pers. com. 2013), based on Meyer and Cederberg (2010) and Meyer (pers. com. 2013), which support that the use of paraquat in soybean is widespread.

Table 5.6. Pesticide applications in genetically engineered glyphosate tolerant soybean (SB-II) grown in Mato Grosso, Brazil (H = herbicide, F = fungicide, I = insecticide).

Active substance (AS)	**Frequency (yr^{-1})**	**Dose per application (g AS ha^{-1})**	**Application method**	**Crop type and development stage**	**Application month**
Paraquat [a] (H)	1	300	Conv. boom	Bare soil	Sep.
Glyphosate isopropylamine salt (H)	1	1296	Conv. boom	Soybean I	Oct.
Alpha cypermethrin (I)	1	30	Conv. boom	Soybean I	Oct.
Methomyl (I)	1	151	Conv. boom	Soybean I	Oct.
Chlorantraniliprole (I)	1	5	Conv. boom	Soybean I	Oct.
Glyphosate isopropylamine salt (H)	1	1296	Conv. boom	Soybean I	Nov.
Pyraclostrobin (F)	1	75	Conv. boom	Soybean I	Nov.
Chlorantraniliprole (I)	1	5	Conv. boom	Soybean I	Nov.
Pyraclostrobin (F)	1	67	Conv. boom	Soybean II	Nov.
Epoxiconazole (F)	1	25	Conv. boom	Soybean II	Nov.
Chlorantraniliprole (I)	1	10	Conv. boom	Soybean II	Nov.
Pyraclostrobin (F)	1	67	Conv. boom	Soybean II	Dec.
Epoxiconazole (F)	1	25	Conv. boom	Soybean II	Dec.
Teflubenzuron (I)	1	23	Conv. boom	Soybean II	Dec.
Thiamethoxam (I)	1	42	Conv. boom	Soybean III	Jan.
Lambda-cyhalothrin (I)	1	32	Conv. boom	Soybean III	Jan.
Paraquat [a] (H)	1	300	Conv. boom	Soybean III	Feb.

[a] Addition to original data obtained from Azevedo (pers. com. 2013), based on Meyer and Cederberg (2010) and Meyer (pers. com. 2013), which support that the use of paraquat in soybean is widespread.

5.5 Sugarcane (Saccharum officinarum)

One sugarcane case, referred to as SC, was defined based on data for sugarcane cultivation in the state of São Paulo, Brazil (Table 5.7). Brazil is by far the largest global producer of sugarcane (FAOSTAT), and São Paulo is the largest producing state in Brazil, with an output of 358 million metric tons in 2012 on 5.5 million planted ha, corresponding to about 53% of the total national production (IBGE, 2013).

Sugarcane is as a semi-perennial ratoon crop that regrows multiple times after harvest (Ometto et al. 2009). The first harvest takes place approximately 18 months after planting and is followed by annual harvests for four to five years (Joaqium et al. 2011) before the crop is removed mechanically or chemically. Field establishment consists of deep-ploughing, followed by planting of cane stalk seedlings in furrows (typically in April – May), and application of pesticides. During the first month after plantation the canes usually compete well with weeds, after which herbicides are applied, 30 – 120 days after plantation. Plant canes are always pesticide treated (Smith et al. 2008). Herbicide application is repeated 30-60 days after each harvest, on 70% of ratoon crops on average (Smith et al. 2008) and insecticides may be applied at any time of the year, when judged necessary (Meyer, pers. com. 2013). Aerial application may be used when ground application is not possible (i.e., when canes have grown tall).

In this study a plantation life-time of five and a half years is assumed, with a total of five harvests, all in August. Canes are assumed to be planted in April. The pesticide application scenario was provided by The Brazilian Bioethanol Science and Technology Laboratory

(CTBE) (Cavalett, pers. com. 2013) and is representative of typical use in São Paulo state (Barizon, pers. com. 2014).

Table 5.7. Pesticide applications in sugarcane (SC) grown in São Paulo, Brazil (H = herbicide, N = nematicide, I = insecticide, PGR = plant growth regulator).

Active substance (AS)	**Frequency (yr^{-1})**	**Dose per application ($g\ AS\ ha^{-1}$)**	**Application method**	**Crop type and development stage**	**Application month**
Fipronil [a] (I)	0.18	200	Soil incorp.	Bare soil	April
Carbofuran [a] (N)	0.18	2100	Soil incorp.	Bare soil	April
Tebuthiuron [b] (H)	0.18	500	Conv. boom	Maize II	June
Hexazinone [b] (H)	0.18	132	Conv. boom	Maize II	July
Diuron [b] (H)	0.18	468	Conv. boom	Maize II	July
Imazapic [c] (H)	0.73	175	Conv. boom	Maize II	Oct.
Trinexapac ethyl [d] (PGR)	0.91	125	Aircraft	Maize III	June
Glyphosate isopropylamine salt [e] (H)	0.18	1296	Conv. boom	Maize I	Sept.

[a] 1st year, in conjunction with planting.
[b] 1st year, after planting.
[c] 2nd to 5th years, approximately 45 days after harvest.
[d] 2nd to 6th year, approximately 45 days before harvest.
[e] 6th year, ratoon removal.

The SC case amounts to a total of 1.09 kg AS ha^{-1} yr^{-1}.This can be compared with the national average pesticide application rate on sugarcane in Brazil that has increased from an average of 2.5 kg AS ha^{-1} yr^{-1} between 2000 and 2003 (including herbicides, insecticides, fungicides and other pesticides) (Arrigoni and de Almeida, 2007; Ricci, 2007), to 3.05 kg AS ha^{-1} yr^{-1} in 2008 (Seabra et al. 2011) (estimated based on the total pesticide use divided over the total area planted with sugarcane), and up 3.7 kg AS ha^{-1} yr^{-1} on average between 2008 and 2012 (estimated based on total national pesticide sale statistics and sugarcane´s share in terms of economic value, see Figure 5.1. This indicates that the pesticide application scenario used here is underestimated.

In 2008, 91% were herbicides, 7% insecticides, close to 0% fungicides and 2% other pesticides (Seabra et al. 2011).

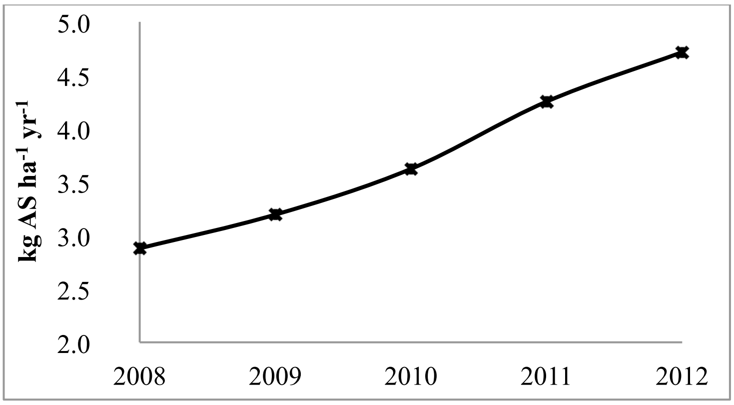


Figure 5.1. Pesticide use on sugarcane in Brazil in kg AS ha^{-1} yr^{-1} from 2008 to 2012, estimated (this study) based on total national pesticide sale statistics and sugarcane´s share in terms of economic value from the São Paulo Institute of Agricultural Economics (IEA-APTA), and the area planted with sugarcane in Brazil from FAOSTAT.

The two most important insect pests on sugarcane in Brazil are the sugarcane borer (*Diatraea saccharalis*), also known as the sugarcane beetle, and the sugarcane weevil (*Sphenophorus levis*) (Arrigoni and de Almeida, 2007). Some of the most widely used insecticides on sugarcane include fipronil, thiamethoxam, terbufos and imidacloprid (Ferreira Fernandes et al. 2012; Lehtonen and Goebel, 2009). Fungicide use on sugarcane is close to zero (Arrigoni and de Almeida, 2007; Seabra et al. 2011).

Only a very small fraction of Brazilian sugarcane is under irrigation (de Sousa, 2007) for which reason irrigation was not assumed here. Sugarcane plantations are typically not drained (Meyer, pers. com. 2013). Conventional tillage was assumed for the first pesticide applications in conjunction with planting and no-till for all subsequent applications.

5.6 Winter wheat (Triticum spp.)

One winter wheat case was defined based on data for winter wheat cultivation in Schleswig-Holstein, Northern Germany, with sowing in September and harvest the following summer (Table 5.8). Schleswig-Holstein produced 1.77 million metric tons of wheat on average between 2006 and 2011, on 203 000 ha (Statistikamt Nord, 2013), corresponding to 7.5% of the national production of wheat during the same time period (FAOSTAT).

Pesticide application rates were set based on information from the Chamber of Agriculture in Schleswig-Holstein, Northern Germany (Gleser, pers. com. 2013) and represent typical practice in intense wheat cultivation in the region. Application amounts are in line with recommended doses, see e.g. BASF (2013).

Weeds constitute the largest single cause of yield losses in European wheat cultivation, but in Western Europe fungal diseases are nearly as important, while insect pests overall are of lesser importance and more uneven between years (Jørgensen et al. 2008). Pesticide use is in accordance with this pattern. Herbicides represent a majority of pesticide AS input in European cereal cultivation, followed by a smaller share of fungicides and a very small share of insecticides (Eurostat, 2007). Pesticide use on cereals cultivated in Germany has been associated with a rising trend between 1992 and 2002, from 1.7 to 2.4 kg AS ha^{-1}. In 2003, the latest year for which the statistical office of the European Union (Eurostat) compiled the statistics, pesticide use had dropped to 1.9 kg AS ha^{-1} (Eurostat, 2003). According to the ENDURE wheat case study, the most important fungal diseases on wheat in Germany is septoria leaf blotch (*Septoria tritici*), tan spot (*Drechslera tritici-repentis*), brown rust (*Puccinia triticina*) and powdery mildew (*Blumeria graminis*) (Jørgensen et al. 2008).

The WT case includes two applications with insecticides: alpha-cypermethrin in the autumn against aphids as virus vectors and lambda-cyhalothrin in the spring against aphids in the ear. Three fungicide treatments are included, containing seven different fungicide ASs, applied between the stem elongation stage and the head emergence stage, and two applications of plant growth regulators to avoid lodging. A range of herbicides are applied between September and Mayto control weeds. All pesticides are assumed to be applied with a conventional tractor pulled boom. The WT pesticide application scenario amounts to a total of 5.14 kg AS ha^{-1} yr^{-1}.

Compared to North and South America, European farmers and authorities have shown greater resistance towards adoption of no-till and/or reduced tillage management systems, and the adoption rate in Germany has been particularly low with less than 5 000 ha cultivated under such schemes, while in Europe as a whole, only 1.1% of the total agricultural land is under no-till (Derpsch and Friedrich, 2009). For this reason, conventional tillage was assumed here.

Table 5.8. Pesticide applications in winter wheat (WT) grown in Schleswig-Holstein, Northern Germany (H = herbicide, F = fungicide, I = insecticide, PGR = plant growth regulator).

Active substance	**Frequency (yr^{-1})**	**Dose per application (g AS ha^{-1})**	**Application method**	**Crop type and development stage**	**Application month**
Glyphosate isopropylamine salt [a] (H)	0.25	2187	Conv. boom	Bare soil	Sept.
Diflufenican (H)	1	120	Conv. boom	Cereals I	Sept.
Flufenacet (H)	1	240	Conv. boom	Cereals I	Sept.
Alpha cypermethrin (I)	0.33	13	Conv. boom	Cereals I	Oct.
Iodosulfuron methyl sodium (H)	1	3	Conv. boom	Cereals II	April
Mesosulforon methylester (H)	1	15	Conv. boom	Cereals II	April
Florasulam (H)	0.5	3	Conv. boom	Cereals II	April
Fluroxypyr 1-methylheptyl ester (H)	0.5	144	Conv. boom	Cereals II	April
Chlormequat chlorid (PGR)	1	1440	Conv. boom	Cereals III	April
Trinexapac ethyl (PGR)	1	50	Conv. boom	Cereals III	April
Fenpropimorph (F)	1	260	Conv. boom	Cereals III	April
Epoxiconazole (F)	1	81	Conv. boom	Cereals III	April
Metrafenone (F)	1	98	Conv. boom	Cereals III	April
Clorothalonil (F)	1	500	Conv. boom	Cereals III	April
Florasulam (H)	0.5	3	Conv. boom	Cereals III	May
Fluroxypyr 1-methylheptyl ester (H)	0.5	144	Conv. boom	Cereals III	May
Trinexapac ethyl (PGR)	1	50	Conv. boom	Cereals III	May
Ethephon (PGR)	1	165	Conv. boom	Cereals III	May
MCPA dimethylamine salt (H)	1	918	Conv. boom	Cereals III	May
Epoxiconazole (F)	1	125	Conv. boom	Cereals III	May
Fluxapyroxad / Xemium (F)	1	125	Conv. boom	Cereals III	May
Tebuconazole (F)	1	125	Conv. boom	Cereals IV	June
Prothioconazole (F)	1	125	Conv. boom	Cereals IV	June
Lambda cyhalothrin (I)	1	8	Conv. boom	Cereals IV	June

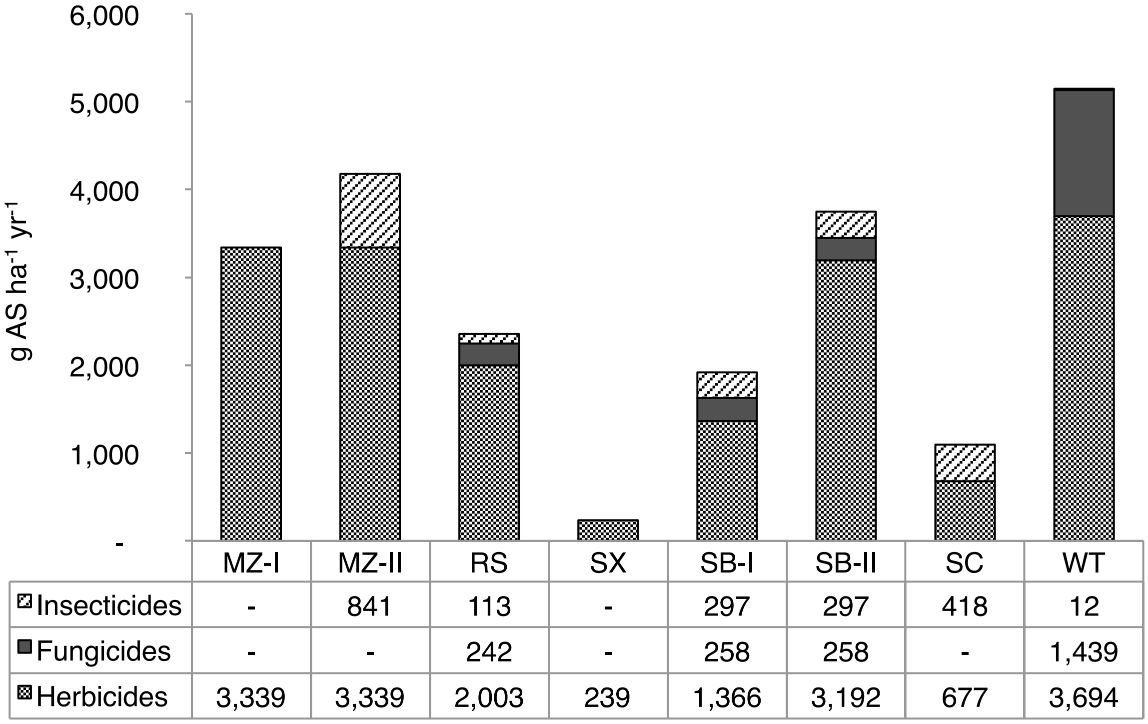
[a] Addition to data retrieved from the Chamber of Agriculture in Schleswig-Holstein; based on Glyphosate Website (2013), stating that 75% of the arable land in the northern and eastern regions of Germany is treated with glyphosate.

CHAPTER 6. RESULTS AND DISCUSSION

This chapter contains an integrated presentation and discussion of results, in terms of pesticide application rates (Chapter 6.1), potential freshwater ecotoxicity impacts, and the pesticide ASs associated with the largest impact scores (Chapter 6.2). Uncertainties(Chapter 6.3) and sensitivity analyses(Chapter 6.4) are discussed, and measures that could help bring down impact levels are proposed (Chapter 6.5). The chapter ends with identifying some key areas for future research (Chapter 6.6).

6.1 Pesticide application rates

Figure 6.1 presents the total yearly average pesticide application rates, and the distribution between herbicides, fungicides and insecticides. It shows that total yearly average pesticide application rates vary by more than a factor 20 between cases. In comparison, AS-specific application rates vary by almost 3 orders of magnitude (Chapter 5). The perennial woody crop *Salix* is associated with substantially lower pesticide use than the other crops; fungicides and insecticides are not used at all, and herbicides are, on average, applied only once every third year. In all annual crops except maize, all three major pesticide groups – herbicides, fungicides, and insecticides – are used every year. Insecticides are not applied in MZ-I (*Bt*-maize) due to the crop's ability to produce its own insecticidal toxin; however, this favourable situation could now be jeopardized due to emerging resistance (see further in Chapter 2.4).



	MZ-I	MZ-II	RS	SX	SB-I	SB-II	SC	WT
▨ Insecticides	-	841	113	-	297	297	418	12
■ Fungicides	-	-	242	-	258	258	-	1,439
⊠ Herbicides	3,339	3,339	2,003	239	1,366	3,192	677	3,694

Figure 6.1. Total yearly average pesticide application rates, and the distribution between herbicides (including plant growth regulators), fungicides and insecticides (including nematicides). MZ-I/II: Genetically engineered (GE) glyphosate tolerant maize with (MZ-I) and without (MZ-II) *Bt*-technology cultivated in Iowa, US. RS: winter rapeseed cultivated in Schleswig-Holstein, Germany. SX: *Salix* short rotation woody coppice cultivated in South Central of Sweden. SB-I:conventionalsoybean cultivated in Mato Grosso, Brazil. SB-II: GE glyphosate tolerant soybean cultivated in Mato Grosso, Brazil. SC: sugarcane cultivated in São Paulo, Brazil. WT: winter wheat cultivated in Schleswig-Holstein, Germany. For further details on cases, see Chapter 5.

That amount of pesticide AS is an inadequate indicator of ecotoxicity is illustrated by the fact that the potential freshwater ecotoxicity impact in relation to applied AS vary by 7 orders of magnitude across all assessed substances, i.e., one applied unit of an AS potentially causes up to 7 orders of magnitude larger impact, than one applied unit of another AS (Figure 6.2).

To further indicate that amount of pesticide AS is an inadequate indicator of ecotoxicity , consider the following example: glyphosate isopropylamine salt is applied at a rate almost 300 times higher than beta-cyfluthrin in RS – despite this, beta-cyfluthrin causes a potential freshwater ecotoxicity impact score more than 500 times larger than glyphosate isopropylamine salt, per application (244 and 0.5 CTUe ha^{-1} yr^{-1}, respectively).

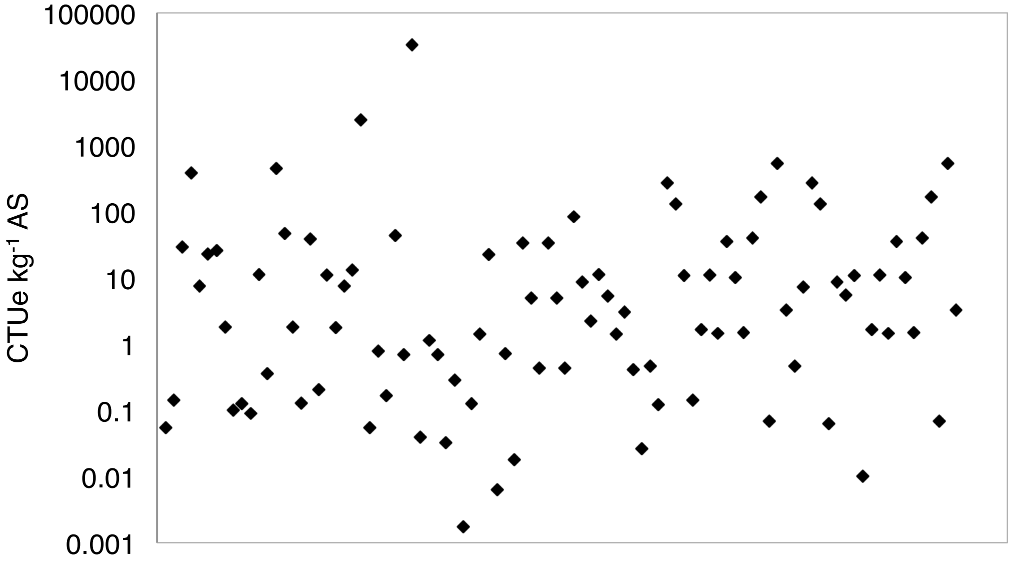


Figure 6.2. Potential freshwater ecotoxicity impact per kg applied AS, on a logarithmic scale. Each mark represents one unique combination of AS, crop, time of application and site.

6.2 Potential freshwater ecotoxicity impacts

Figure 6.3 presents the potential freshwater ecotoxicity impact scores, in relation to biofuel output (allocated values), and in relation to area and time (ha·yr; unallocated values), and shows that the impact scores vary substantially between the different cases, by up to 3 orders of magnitude (in both impact metrics). Figure 6.3 also shows that WT and RS are associated with considerably higher impacts than the other cases, regardless of impact metric. Placed in relation to biofuel yield, the SX case has a potential freshwater ecotoxicity impact score of about 3 CTUe TJ^{-1} (allocated value), while impact scores for the cases SC, MZ-I, MZ-II, SB-II, SB-I, WT, and RS are about 30, 110, 270, 305, 310, 750, and 1000 times larger, respectively. In relation to area and time, the SXcase has a potential freshwater ecotoxicity impact of < 1 CTUe ha^{-1} yr^{-1} (unallocated value), while impact scores for the cases SC, MZ-I, SB-II, SB-I, MZ-II, RS, and WT are about 60, 205, 220, 220, 500, 1110, and 1115 times larger, respectively.

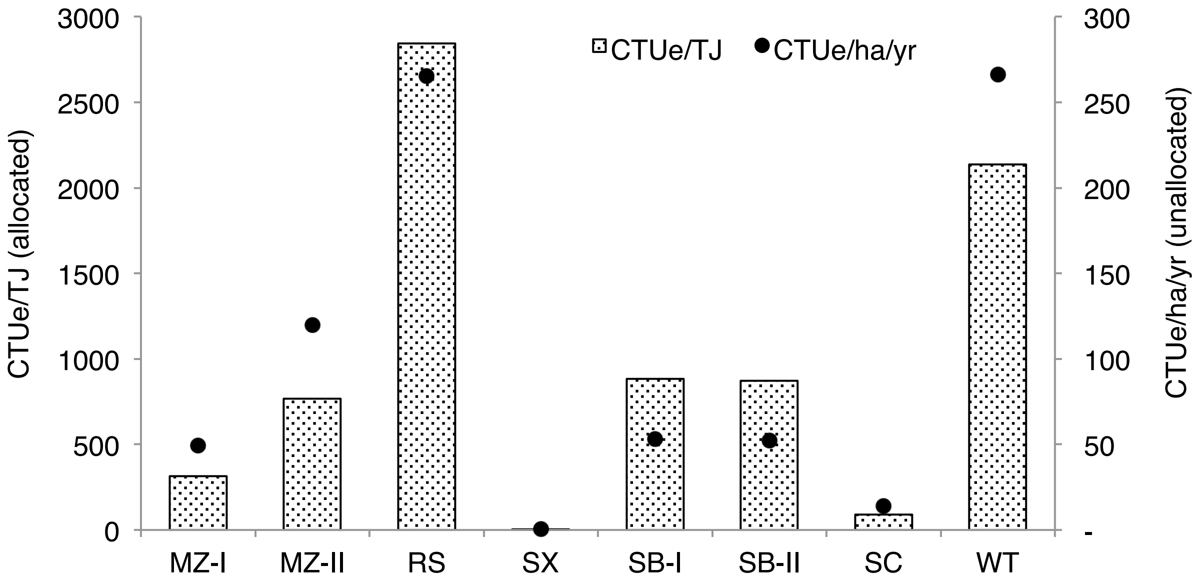


Figure 6.3. Potential freshwater ecotoxicity impacts in CTUe per biofuel gross energy output (allocated) and per ha and year of cultivated crop (unallocated).MZ-I, MZ-II: ethanol from genetically engineered (GE) glyphosate tolerant maize with (MZ-I) and without (MZ-II) *Bt*-technology cultivated in Iowa, US. RS: biodiesel from winter rapeseed cultivated in Schleswig-Holstein, Germany. SX: ethanol from *Salix* short rotation woody coppice cultivated in South Central of Sweden. SB-I: biodiesel from conventional soybean cultivated in Mato Grosso, Brazil. SB-II: biodiesel from GE glyphosate tolerant soybean cultivated in Mato Grosso, Brazil. SC: ethanol from sugarcane cultivated in São Paulo, Brazil. WT: ethanol from winter wheat cultivated in Schleswig-Holstein, Germany. For more information on cases, see Chapter 5.

The favorable results for *Salix* are explained by the relatively low pesticide use in cultivation, both in terms of application rates (0.24 kg AS ha^{-1} yr^{-1}) and frequency of application (see Chapter 5.3), and the use of pesticides (glyphosate isopropylamine salt, flurtamone and diflufenican) with relatively low CFs (see Appendix 1).Considering that biofuel from lignocellulosic crops are not yet commercially available, the results for *Salix* should be interpreted as an indication of the future potential.

The results indicate positive effects of using *Bt*-maize (MZ-I), due to the *Bt*-technology that eliminates the need for otherwise commonly used insecticides. The use of the insecticide chlorpyrifos in MZ-II is responsible for the 2.4 times larger impact score of MZ-II compared to MZ-I. In contrast, there is no substantial difference between the two soybean cases. The pressure of pests and diseases is high in South American soybean cultivation and the present GE-technology includes only herbicide-tolerant soybean, i.e., insecticides and fungicides are used every year regardless of seed technology (see Chapter 5.4).

It should be noted that pesticide application in the Brazilian cases (SB-I, SB-II and SC) may be underestimated (see Chapters 5.4 and 5.5), indicating that the associated impacts are in fact higher, than indicated here.

An intuitive interpretation of the potential freshwater ecotoxicity impact score follow from the definition of the ecotoxicity unit: CTUe = PAF·m^3·day. Consider e.g. 1 ha of wheat (WT) and the freshwater species in a 50 m^3 pond over the course of one week (for simplicity assuming that all pesticides are applied at the same time). In this example, the definition gives that 76% of the freshwater species are potentially affected. The same calculation for 1 ha of sugarcane (SC) gives that only 4% of the freshwater species are potentially affected.

Pesticide ASs with the largest potential impact scores

Table 6.1 presents the pesticide ASs associated with the largest potential freshwater ecotoxicity impact scores(≥ 1 CTUe ha^{-1} yr^{-1}) as identified in this study, and shows that the high scores of WT and RS are associated with the use of the insecticide beta-cyfluthrin in RS and the fungicide chlorothalonil in WT. In fact, these ASs are responsible for 92 and 84% of the total impact scores, respectively. It should be noted that field size is also an important explanatory factor to the high impact scores in the cases of RS and WT, see Chapter 6.4.

Table 6.1. Pesticide ASs with the largest (≥ 1 CTUe ha^{-1} yr^{-1}) potential freshwater ecotoxicity impacts.

ASs with an unallocated impact score ≥ 10 CTUe ha^{-1} yr^{-1} and corresponding impact scores in CTUe TJ^{-1}

Pesticide AS [a]	CTUe ha^{-1} yr^{-1} unallocated	Case [b]	CTUe TJ^{-1} allocated
Beta-cyfluthrin (I)	244	RS	2620
Chlorothalonil (F)	223	WT	1793
Chlorpyrifos (I)	71	MZ-II	453
Atrazine (H)	44	MZ-I/II	279
Methomyl (I)	20	SB-I/II	327
Lambda-cyhalothrin (I)	18	WT	145
Dimethanamid-P (H) ×	18	RS	188
Lambda-cyhalothrin (I)	17	SB-I/II	281

ASs with an unallocated 1 ≤ impact score < 10 CTUe ha^{-1} yr^{-1} (descending order)

Pesticide AS [a]	Case [b]
Alpha-cypermethrin (I) ‡	SB-I/II
Flufenacet (H)	WT
Ethephon (PGR) ‡	WT
Tebuthiuron (H)	SC
Acetochlor (H)	MZ-I/II
Alpha-cypermethrin (I) ‡	WT
Carbofuran (N)	SC
Teflubenzuron (I) ‡	SB-I/II
Epoxiconazole (F) ×	WT
Dimoxystrobin (F) ×	RS
Epoxiconazole (F) ×	SB-I/II
Fipronil (I)	SC
Prothioconazole (F) ×	WT
Paraquat (H) ‡	SB-I/II
Lactofen (H) ×	SB-I

[a] Pesticide ASs that did not originally have USEtox CFs, but that we calculated, are marked with ×. CFs of pesticide ASs that are marked as interim in USEtox are marked with ‡. H = herbicide, F = fungicide, I = insecticide, N = nematicide, PGR = plant growth regulator.

[b] MZ-I, MZ-II: Genetically engineered (GE) glyphosate tolerant maize with (MZ-I) and without (MZ-II) *Bt*-technology cultivated in Iowa, US. RS: winter rapeseed cultivated in Schleswig-Holstein, Germany. SB-I: conventional soybean cultivated in Mato Grosso, Brazil. SB-II: GE glyphosate tolerant soybean cultivated in Mato Grosso, Brazil. SC: sugarcane cultivated in São Paulo, Brazil. WT: winter wheat cultivated in Schleswig-Holstein, Germany. For further details on cases, refer to Chapter 5.

Beta-cyfluthrin is a pyrethroid insecticide, used against cabbage stem flea beetles (*Psylliodes chrysocephala*) and other biting insect pests, in rapeseed cultivation. Of the applied dose beta-cyfluthrin in RS, 0.4% is emitted to air (intermediate fate, as calculated by PestLCI), which is the emission pathway responsible for 99.7% of the total impact score. A very low share (<0.01%) of the applied dose is emitted to surface water. Both emission fractions, as well as the applied dose, are relatively low (in fact, beta-cyfluthrin is applied at a very low dose of 7.5 g AS ha^{-1}); it is rather the very high CFs of beta-cyfluthrin that explain this result. In fact, beta-cyfluthrin has higher CFs than any other substance included in this study (see Appendix 1).

Beta-cyfluthrin is non-persistent and non-mobile in soil, and non to moderately volatile, according to the Pesticide Properties DataBase (PPDB), indicating that the high CFs of this substance is mainly due to its ecotoxic potency, which is consistent with the fact that the substance is classified as highly toxic to fish and aquatic invertebrates, while moderately toxic to algae (PPDB). The CFs of beta-cyfluthrin in USEtox are based on ecotoxicity data from 16 species at three trophic levels, and classified as “recommended”.

Chlorothalonil is a broad-spectrum fungicide, used against a wide range of diseases on many crops (PPDB).Of the applied dose chlorothalonil in WT, 0.6% is emitted to air, which is the emission pathway responsible for 98% of the total impact score. A very low share, 0.01% of the applied dose, is emitted to surface water, and is responsible for 2% of the total impact score. These emission fractions are not particularly high; it is rather the high CFs of chlorothalonil (see Appendix 1), in combination with the rather high dose (0.5 kg AS ha^{-1}), that explain the large impact of this substance.

Chlorothalonil is non-persistent and slightly mobile in soil, and non to moderately volatile (PPDB), indicating that the high CFs of this substance is mainly due to its ecotoxic potency, which is consistent with the fact that the substance is classified as highly toxic to fish and aquatic invertebrates, while moderately toxic to algae (PPDB). The CFs of chlorothalonil in USEtox are based on ecotoxicity data from 36 species at three trophic levels, and classified as “recommended”.

The third are fourth most highly impacting ASs are found in the cultivation of maize: chlorpyrifos in MZ-II and atrazine in both maize cases, responsible for 59%(chlorpyrifos in MZ-II) and 36-89% (atrazine in MZ-II and MZ-I, respectively) of thetotal impact scores, respectively. The range in impact scores of atrazine is due to the use of chlorpyrifos in MZ-II that takes a relatively larger share of the total impact.

Chlorpyrifos, an organophosphate insecticide, is the most widely used insecticide in the agricultural sector (defined as 21 major crops) in the US in 2008, the latest year for which summary statistics are available (Fernandez-Cornejo et al.2014).Of the applied dose chlorpyrifos in MZ-II, 3% is emitted to air, which is the emission pathway responsible for >99% of the total impact score. A very low share,<0.01%of the applied dose, is emitted to surface water. It should be noted that 3% emitted to air is a relatively high emission fraction compared to other pesticides included in this study, of which the large majority have air emission fractions <0.5%.

The high emissions fraction to air is consistent with the fact that chlorpyrifos is known to be rather volatile, as indicated by its Henry’s Law constant (PPDB). The CFs of chlorpyrifos are not particularly high (compared to other substances included in this study, see Appendix 1); it is rather the relatively high air emission fraction in combination with moderately high CFs that explain this result. Chlorpyrifos is moderately persistent and non-mobile in soil, highly toxic to fish and aquatic invertebrates and moderately toxic to algae (PPDB).The CFs of chlorpyrifos in USEtox are based on ecotoxicity data from 162 species at three trophic levels, and classified as “recommended”.

Atrazine is a triazineherbicide, and the second most widely used herbicide, after glyphosate, in the agricultural sector in the US in 2008 (Fernandez-Cornejo et al.2014).Of the applied dose atrazine in MZ-I and MZ-II, 0.3% is emitted to air, and causes one quarter of the total impact score, while 0.03% of the applied dose is emitted to surface water and causes three quarters of the total impact score.

It should be noted that 0.03% emitted to surface water is a relatively high emission fraction compared to other pesticides included in this study (in fact only exceeded by glyphosate isopropylamine salt). The water contamination potential of atrazine can be explained by its physico-chemical properties: its low sorption to organic soil particles, as indicated by its organic carbon - water partition coefficient (Koc), contribute towards making it mobile, and its slow soil degradation rate and hydrolysis contribute towards its persistence. Based on this, it has been classified as highly leachable (PPDB), and is frequently detected in surface water. In a pesticide residues inventory from 2008 conducted by the USDA, atrazine was found in 5% of ground water samples, and in 94% of treated drinking water samples, making atrazine the most frequently detected drinking water pollutant in the US (USDA, 2009). In Sweden, atrazine has been banned since 1989 (KemI Pesticides Register), and in the EU since 2004 due to its groundwater contamination potential (EC, 2004). Despite this, atrazine was found in 7% of ground water samples in a pesticide residues inventory from south of Sweden, due to its slow degradation rate (Länsstyrelsen Skåne, 2012).

The CFs of atrazine are not particularly high (compared to other substances included in this study, see Appendix 1), which is consistent with the fact that it is classified as moderately toxic to fish, aquatic invertebrates and algae (PPDB). It is rather the relatively high surface water emission fraction in combination with moderately high CFs that explain the large impact score of this pesticide. The CFs of atrazine in USEtox are based on ecotoxicity data from 128 species at four trophic levels, and classified as “recommended”.

The emission pathway from field to surface water via air is the dominant emission route for all ASs included in this study, and range from ≈0 to 13.4% (trinexapac-ethyl in SC) of the applied dose. The emission fraction from field to surface water is at most 0.03% of the applied dose (glyphosate isopropylamine salt, closely followed by atrazine). For the three substances with largest impact scores (beta-cyfluthrin, chlorothalonil and chlorpyrifos), the emission route via air is responsible for the greater part of the potential impact (>98%), while atrazine is associated with a particularly high surface water emission fraction, that is responsible for three quarters of the potential impact.

6.3 Uncertainty and variation

The results depend on hundreds of parameters of physico-chemical and pedoclimatic character, with varying uncertainty. Henderson and co-workers (2011) have shown that among the most influential and uncertain input parameters for CFs are substances' half-lives in different environmental compartments, and ecotoxic effect factors that are based on substance-specific ecotoxic effect data.

The uncertainty range of CFs has been determined to 1 – 2 orders of magnitude (Rosenbaum et al. 2008); consequently, a substance with CF = 100 may not be (but probably is), more toxic than a substance with CF = 1. The uncertainty in final impact scores also depend on the uncertainty in emissions, which has not been quantified previously, and is beyond the scope of this study. However, pesticide emissions as given by PestLCI have been shown to be in “*acceptable accordance*” with results produced by state-of-the-art pesticide risk assessment models (Dijkman et al. 2012).Therefore, a full-scale, quantitative, uncertainty analysis is not possible at this time.

Perhaps even more important and probably overshadowing uncertainty ranges is the fact that many of the input parameters display large temporal and/or spatial variability due to natural variations in the real world. This applies especially to pedoclimatic parameters, but also to some physico-chemical parameters, such as chemical substances´ half-lives in soil that can vary substantially depending on, e.g., microbial activity and pH (Bending et al. 2006). Consideration of such variations is highly data-demanding and thus impractical in most LCAs. Pesticide application in terms of product choices and doses can also have high variability in time and space and depend on a range of factors that vary between farms, regions and years, such as climate and weather, pressure from weeds, pests and diseases, legislation, certification schemes, and commodity prices. The pesticide application scenarios considered here are based on fairly common pesticides but not designed to represent any sort of national or regional average or to cover all possible alternatives. This approach was judged as the most appropriate considering limitations set by data availability and quality and by difficulties translating pesticide statistics (if available) into realistic use scenarios.

Site-generic pedoclimatic data are usually used in LCA, if pedoclimatic conditions are at all considered. We used site- and crop-specific data to improve accuracy and reduce uncertainties compared to conventional emission inventory approaches. However, due to existing uncertainties and model limitations, and the fact that quantitative uncertainty ranges have yet to be determined, results should be interpreted with caution, and foremost be used for ranking, and identifying the substances associated with the largest impacts; as done in Table 6.1.It is thus not possible to determine at this time if there is any significant difference between e.g., the RS and the WT case, while the results clearly indicate that the SX case (and possibly the SC case) offer potential benefits compared to the other cases. Also, it is beyond doubt that improvement measures should be directed at the ASs associated with the largest impact scores, as identified in Table 6.1.

6.4 Sensitivity analyses

Previous sensitivity analysis of PestLCI 2.0 for the herbicide MCPA (Dijkman et al. 2012) showed that the most influential input parameters concerning emissions to air were field width, solar radiation, and average temperature. Concerning emissions to surface water the most influential input parameters were soil pH, soil texture, and potential evaporation. We performed sensitivity analyses for additional ASs, the results of which are presented and discussed in the following.

Field size

In line with previous findings (Dijkman et al. 2012), we found field size (or field width to be more precise) to be a critical parameter for emissions to air and consequently, impact scores. This is due to the modeling of wind drift in particular, and the assumption that the wind always blows in parallel with the field width (Dijkman, pers. com. 2014). The spray equipment is modeled as moving in parallel to the field length. In effect, pesticides that are applied close to the field border perpendicular to the wind direction dominate the wind drift emissions (Dijkman, pers. com. 2014). Hence, emissions to air measured as kg ha^{-1} (averaged over the entire field area), decrease with increasing field width, whereas in absolute terms, total emissions to air (kg) are practically invariant under field width but increase in proportion to field length (if length remains constant). We used field sizes in the range from 10 to 250 ha to represent typical site- and crop-specific conditions (see Table 4.1), but kept all modeled fields of the same shape (the length twice the width) and orientation with regard to pesticide application and wind direction, to minimize influence due to varying field size.

We tested the effect of changing the field size in the SB-I case from 250 to 10 ha, while maintaining field shape and orientation, i.e., we decreased both width and length by a factor 5. This caused the potential freshwater ecotoxicity impact score

to increase by a factor 2.7, due to up to 5 times larger per-ha air emissions on the smaller field. However, emissions to surface water were practically unaffected, since emissions due to runoff are modeled as a function of the applied mass per surface unit (Dijkman, pers. com. 2014). The intuitive interpretation is that the larger the field, the lower the emissions as a fraction of total mass applied, due to decreased ratio of circumference to area. The significance of the field size parameter partly explains why the European cases (RS and WT, cultivated on 10 ha fields), are associated with relatively high per-ha impacts, and the soybean cases (SB-I/II, cultivated on 250 ha fields) are associated with relatively low high per-ha impacts. The fact that field sizes vary greatly in reality is one of several reasons why caution should be taken before generalizing the results presented here.

Buffer zones

Buffer zones are protective strips of land where pesticides are not sprayed, located between fields and surface water to prevent e.g. pesticides from reaching these water bodies (de Snoo and de Wit, 1998). Fields in PestLCI are modeled to have a ditch containing surface water along one side and a slope that results in runoff to this ditch (Dijkman, pers. com. 2014). We tested the effect of adding product-specific buffer zones for the 13 highest-impact ASs in the WT, RS, and MZ-II cases, i.e., substances with a potential freshwater ecotoxicity impact ≥ 1 CTUe ha^{-1} yr^{-1}, listed in Table 6.1. Buffer zones extended in the range from 5-20 m for ground application (0 m; one substance) to 46 m for aerial application (one substance), see Table 6.2.

Table 6.2. Buffer zones used in sensitivity analysis for the WT, RS and MZ-II cases, for the 13 most highly impacting ASs. Buffer zones are product specific regulations in the studied countries for ground application and aerial application (one substance). For Germany, first priority was given to buffer zones as specified for sprayers without drift reducing technology, and second priority to buffer zones as specified for fields with a slope > 2%.

Pesticide active substance (AS)	Buffer zone (m)	Sources and notes (sources in {} given below table, all accessed Jan 8, 2014).
Acetochlor	20.1	{1}: data for product Harness Xtra.
Alpha-cypermethrin	10	BASF (2013): data for product Fastac SC Super Contact.
Atrazine	20.1	{1}: data for product Harness Xtra.
Beta-cyfluthrin	15	{2}: data for product Bulldock.
Chlorothalonil	10	{3}: data for product Bravo.
Chlorpyrifos	45.7	{4}: data for product Chlorpyrifos 4E, aerial application.
Dimoxystrobin	5	BASF (2013): data for product Cantus Gold.
Dimethenamid-P	5	BASF (2013): data for product Butisan Gold.
Epoxiconazole	10	BASF (2013): data for product Capalo.
Ethephon	0	{3}: data for product Camposan.
Flufenacet	20	{3}: data for product Herold SC.
Lambda-cyhalothrin	15	{5}: data for product Karate Zeon.
Prothioconazole	10	{6}: data for product Prosaro.

{1} http://www.monsanto.com/products/Documents/MSDS-Labels/harness_xtra_5_label.pdf
{2} http://www.fcs-feinchemie.com/index.php?id=969&no_cache=1&tx_fcspromasconnect_pi1%5Bproduct%5D=23
{3} http://www.landhandelspartner.de/psberatung/SPE_NW_PSBeratung.pdf
{4} http://www.agrian.com/pdfs/Chlorpyrifos_4E_(Epa_060906)_Label.pdf
{5} http://www.raiffeisen.com/pflanzen/psm-manager/splitParams/4/l/f/0/004675-60/004675-60_00-002
{6} http://www.lwk-niedersachsen.de/index.cfm/portal/pflanze/nav/504/article/21743.html: see pfd: Fungizideinsatz im Winterweizen 2013.

As a result of the addition of buffer zones, impact scores for the WT, RS, and MZ-II cases were reduced by 68, 91, and 78%, respectively. These substantial improvements were due to air and surface water emissions associated with the analyzed ASs, reducing on average 76 and 86%, respectively. That buffer zones are indeed effective in protecting aquatic ecosystems has been shown also by other studies. Experimental research in the Netherlands by de Snoo and de Wit (1998) on the effect of buffer zones of varying width showed that a 3 m unsprayed strip of land reduced drift deposition in an adjacent ditch by a minimum of 95%, and Bunzel et al. (2014) analyzed over 600 sampling sites in Germany, and found that riparian buffer strips at least 5 m in width mitigated the effects and exposure of pesticides.

Method of application

Method of application is an important parameter for emissions to air. Most pesticides are applied using equipment for ground application; however, on tall crops in the Americas, aircraft are frequently used. We tested the effect of using ground application instead of aerial application on the ASs chlorpyrifos and trinexapac-ethyl, used in the MZ-II and SC cases, and found that it brought down air emissions by 37 and 10%, respectively.

Soil parameters

A soil sensitivity analysis was performed for three ASs (atrazine, glyphosate, and metazachlor), using an application scenario with tillering cereals cultivated in Görlitz, Germany (a PestLCI predefined climate profile), 1 kg AS of pesticide per ha applied in August with a conventional boom. The field size was set to 5 ha and the slope to 5%. Conventional tillage and no drainage were assumed. A default soil was constructed, see Appendix 8. Various soil parameters were then varied, one at a time, while all other modeling parameters were kept constant, and the response in emissions to air and water (kg ha^{-1}), was recorded. Since air emissions are relatively insensitive to changes in soil parameters, only emissions to surface water are presented here (Figure 6.4).

The soil sensitivity analysis showed that texture is the most influential parameter concerning emissions to surface water, i.e., composition of sand, silt, and clay. Emissions to surface water were 3 – 4 times lower for a sandy soil with low clay content (57% sand and 16% clay) compared with soils with clay and sand content > 20% and < 45%, respectively. This may seem counterintuitive but has been confirmed by others (Tiktak et al. 2012; Jarvis et al. 2007) and is explained by the fact that soils with high clay content may form macropores upon cracking, which act as shortcut transport routes for pesticides.

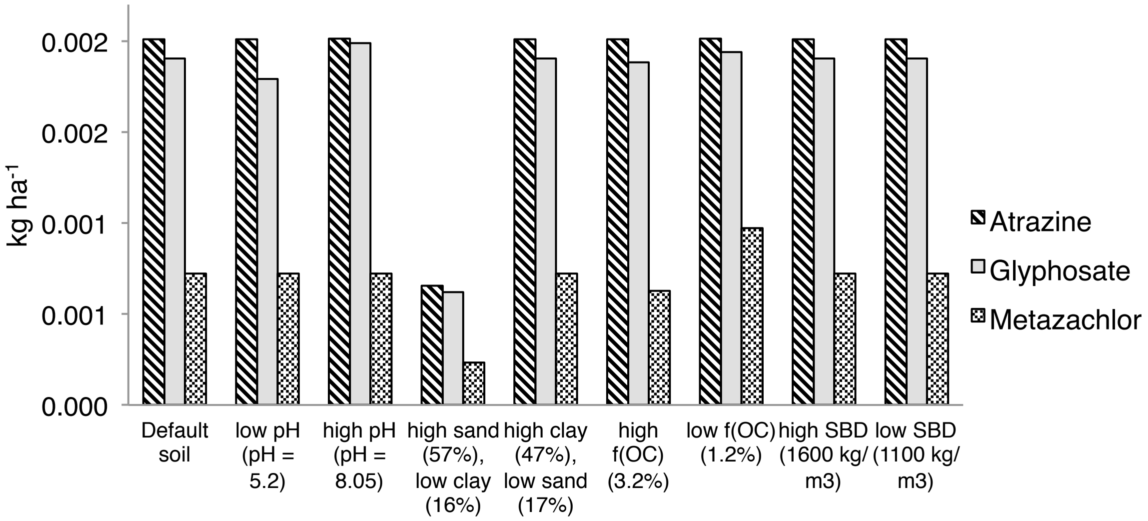


Figure 6.4. Emissions to surface water on soils with different characteristics. OC = organic carbon. SBD = soil bulk density.

Site

Atrazine is the second most widely used herbicide on maize in Iowa (USDA NASS Quick Stats Database) and included in both maize cases (see Chapter 5.1). We evaluated the (combined) influence of pedoclimatic parameters by changing the siteof application. When the same atrazine dose was applied to maize cultivated in either of the two Brazilian locations (Mato Grosso or São Paulo) instead of Iowa (keeping all other parameters as in the MZ-I case), the potential freshwater ecotoxicity impact score associated with atrazine increased by on average 70%, primarily due to four times higher air emissions of atrazine in Brazil, compared to Iowa. In fact, air emissions are responsible for two thirds of the total impact score of atrazine in Brazil, compared to one quarter in Iowa. The increase in air emissions is principally associated with climate parameters, and most probably an effect of April temperatures in Brazil being considerably higher than in Iowa (see Appendix 6), as increased temperature has been shown to increase the volatilization potential of atrazine (Burt, 1974). It should be noted that this analysis does not take into account that maize grown in Brazil and the US may be at different stages of growth in April.

Tillage type

Tillage can be defined "*any mechanical operation on the soil and crop residues that aims at providing a suitable seedbed where crop seeds are sown*" (Alletto et al. 2009). In PestLCI, tillage management effects on pesticide fate in soil are modeled based on principles derived from the review study by Alletto et al. (2009). More specifically, tillage is modeled to reduce macropore flow, which in turn affect emissions to ground and surface water, while emissions to air remain unaffected. More specifically, conventional and reduced tillage reduce macropore leachingby a factor 7.5 and 3.5, respectively (Dijkman et al. 2012).

We evaluated the influence of tillage type in the case MZ-II, by comparing emissions and resulting freshwater ecotoxicity impact scores under no tillage, reduced tillage and conventional tillage management regimes. In this case, tillage type had no influence on results, since emissions to surface water were unaffected by tillage type.

It should be noted that this modeling approach, in which tillage only affects macropore flow, overlooks the potential influence of tillage on soil erosion and surface runoff. In fact, reduced or no tillage management is often introduced with the objective to reduce soil erosion and surface runoff (Alletto et al. 2009). For example, it can be expected that reduced tillage would reduce soil-borne emissions for pesticides with strong soil sorption, see Chapter 3.2. However, studies show that the influences of tillage on soil erosion and surface runoff in general are mixed, and sometimes inconsistent (Alletto et al. 2009), which partly explain why these effects have not been included in PestLCI to date.

The importance and challenge of developing site-specific inventories

The sensitivity analyses demonstrate that potential freshwater ecotoxicity impacts are by no means a function of application doses alone. They also highlight the importance of taking into account site-, crop- and field-specific conditions in emission modeling and indicate the large uncertainties inherent in site-generic default fate-factors. In fact, archetypical emission fraction values with high geographic resolution do not reduce the need for comprehensive sensitivity analyses and can give LCA practitioners a false sense of precision. Up to now, the influence of parameters such as soil texture, buffer zones and method of application, have not been easily modeled in LCA.

However, we acknowledge that such specific inventories are difficult to develop due to limited data availability. In fact, data on pesticide use are, in the words of Repetto and Baliga (1996), “*remarkably difficult to find*” and seldom disaggregated to the level of different ASs, regions, and crops; but rather given in highly aggregated form, as in the FAOSTAT pesticide statistics database, if at all available.

The statistics collected regularly by the USDA and made publicly available by the National Agricultural Statistics Service (USDA NASS Quick Stats Database) are a positive exception. USDA NASS data is disaggregated to the level of states, major crops, and ASs. However, USDA has recently decided to decrease the inventory frequency in response to budget cuts (Benbrook, 2012), which seriously limit the potential for up-to-date analysis and monitoring. For Brazil, no USDA NASS-equivalence in terms of pesticide statistics exists (Meyer and Cederberg, 2010), making data acquisition a challenging endeavor.

In terms of site- and crop-specific field data and agronomic practices, availability is even more restricted.

6.5 Possibilities for reducing ecotoxicity impacts in biofuel feedstock production

Generally, mitigation strategies to reduce freshwater ecotoxicity impacts include substitution to pesticide products with lower toxic potency, and reduction of emissions to freshwater ecosystems.

Choice of pesticide product largely controls the potential freshwater ecotoxicity impact, as demonstrated by the large range in CFs associated with the ASs included here (up to 7 orders of magnitude, see Appendix 1). Where only one AS dominates the impact score, as in the cases of RS and WT (Table 6.1), possibilities for reducing impacts are straightforward. The insecticide beta-cyfluthrin used in RS against the cabbage stem flea beetle (*Psylliodes chrysocephala*) could for example potentially be substituted to another pyrethroid, e.g., lambda-cyhalothrin, alpha-cypermethrin, tau-fluvalinate or esfenvalerate (Yngveson, pers. com. 2013). We tested the effect of switching to an equivalent dose of lambda-cyhalothrin (LKSH Website) and found that it lowered the impact score of RS by 85%; clearly demonstrating the possibilities that exist for reducing impacts.

Substitution of chlorothalonil, a broad-spectrum fungicide with a multi-site mode-of-action (FRAC Website), is however not as straightforward. Due to recent shifts in sensitivity in Septoria leaf blotch (*Septoria tritici*) - the most important fungal disease on wheat in Germany (see Chapter 5.6) - agricultural advisors across Europe now recommend tank mixing with multi-site fungicides (e.g., chlorothalonil), to protect important fungicide groups, such as azoles, from losing their effect (HGCA, 2012). Chlorothalonil is considered to have a low risk of causing resistance development (FRAC Website). Based on this, it is likely that the use of chlorothalonil will continue. One possible replacement option is the fungicide mancozeb (Yngveson, pers. com. 2014).

Besides product substitution, impacts can be reduced by reducing emissions to freshwater, through management. Reichenberger et al. (2007) reviewed mitigation strategies to reduce pesticide inputs into ground and surface water, and found several management options with more or less documented efficiency, for example: creating grassed buffer strips, constructing wetlands, reducing application rates, reducing spray drift, shifting application date, and increasing farmers' awareness of risks associated with handling and applying pesticides.

The sensitivity analyses indicate that emissions could be reduced if, e.g., buffer zones are used where fields abut surface water and aircraft application is avoided. These measures and others that aim to control pests while reducing risks are already well-known within Integrated Pest Management[1] but, until now, not easily assessed within LCA.

Imposition of buffer zones on agricultural lands raises issues related to private property and economic impacts, and enforcing compliance with legislation mandating buffer zones can be a challenge (Sparovek et al. 2010). Implementation may require that farmers receive economic compensation for both the costs of conversion and lost production revenues. Streamside zones that are actively managed and harvested present alternatives to buffer zones that are allowed to exist passively as "hands-off" reserves (Neary et al. 2011). Studies have shown that some plants can be cultivated along water ways to provide biomass while also providing similar protective functions as unharvested buffer zones (Börjesson and Berndes, 2006; Gopalakrishnan et al. 2012; Skenhall et al. 2013).

The results also indicate that impacts would be lower if biofuels were produced from lignocellulosic crops subject to similar pesticide treatment as in the SX case. As mentioned previously, several studies (von Blottnitz and Curran, 2007; Kim and Dale, 2005; 2008; Bai et al. 2010; Emmenegger et al. 2012; Yang et al. 2012; Yang, 2013) have shown that the production of biofuels can be associated with environmental burden shifting compared to fossil fuels, i.e., a net gain in GHG emissions, at the expense of other environmental impact categories. Biofuels based on intensively cultivated crops (high inputs and yields) can have low GHG (and other) emissions per energy output, yet cause high local impacts (e.g., acidification, eutrophication and ecotoxicity). The cultivation of lignocellulosic perennial crops generally involves less pesticide input than conventional biofuel crops, due to lower economic incentives for application (associated with less damage caused by pests), and to fewer approved substances (at least in Sweden).

Wiloso and co-workers (2012)reviewed 31 LCAs of second generation bioethanol produced from lignocellulosic energy crops, biomass residues and biomass wastes and found that – in

---

[1] Integrated Pest Management is defined by the FAO (2003) as "*the careful consideration of all available pest control techniques and subsequent integration of appropriate measures that discourage the development of pest populations and keep pesticides and other interventions to levels that are economically justified and reduce or minimize risks to human health and the environment". IPM emphasizes the growth of a healthy crop with the least possible disruption to agroecosystems and encourages natural pest control mechanisms.*"

the 9 cases where a full comparison was possible – the overall environmental impact was consistently lower for second generation ethanol than for a conventional fossil oil reference system. Plausible explanations why second generation bioethanol perform well in LCA-studies is that lignocellulosic crops require relatively low inputs in the cultivation, or that feedstocks are considered as residues or wastes, and hence not attributed with impacts.

Studies have also shown that integration of lignocellulosic crops (willow, poplar and switchgrass) into agricultural landscapes can reduce the eutrophication load (Schmidt-Walter and Lamersdorf, 2012; Parish et al. 2012). However, the pesticide use (and other inputs) might increase in a scenario with increased feedstock prices in which biofuel demand causes higher pressure on land – indirectly causing higher ecotoxicity impacts as well as further expansion of the agriculture frontier into natural ecosystems. Since agricultural frontiers are concentrated in tropical habitats, a very large number of species can potentially be affected due to pesticide use in these areas (Schiesari et al. 2013), although ecotoxic effects are far from the only impacts associated with expansion of agricultural frontiers.

GE-technology has been shown to be able to bring down pesticide use levels in some cases. Benbrook (2012) estimated that GE *Bt*-maize and cotton reduced insecticide use in the US by 56 million kg between 1996 and 2011. However, it is uncertain if this positive development will continue as documented cases of field-evolved resistance in western corn rootworm (*Diabrotica virgifera virgifera*) against multiple *Bt*-toxins have recently been reported (Gassmann, 2012; Gassmann et al. 2014).

Other crops have seen an increase in pesticide use. Benbrook (2012) estimated that herbicide use in GE herbicide tolerant soybean, cotton and maize increased by 239 million kg in the US between 1996 and 2011.Also, growing problems with spread of glyphosate resistant weeds resulting from excessive use seriously challenge the potentially positive effects of the GE-technology (Mortensen et al. 2012; Gilbert, 2013), see further in Chapter 2.4.

Our findings do not indicate a reduced potential freshwater ecotoxicity impact in glyphosate tolerant soybeans compared with conventional. That is, our results do not support the notion that glyphosate tolerant crops are associated with increasing use of glyphosate, at the expense of other, more toxic and persistent herbicides, as sometimes claimed (Frisvold et al. 2009; Green, 2012).

6.6 Future research

Much remains to be done before ecotoxicity due to pesticide use is routinely included in agricultural LCAs. The French Environmental Foot printing with USEtox project has recently contributed to expanding the substance database by calculating new USEtox CFs (http://usetox.tools4env.com/), and further expansion is critical in overcoming one of the main barriers for inclusion of toxic impacts in LCA. Expansion of substance databases is however a highly challenging task since there are approximately 100 000 chemicals in commerce today, including 600 pesticide ASs, and thousands of new chemicals are synthesized every year (Harrison and Pearce, 2000).

A site-specific approach is needed in ecotoxicity impact assessment, since chemicals typically cause regional or local impacts. A regional pesticide emissions model, such as PestLCI, is therefore valuable to LCA practitioners, but needs to be expanded beyond Europe and validated against non-European soils and climates, e.g., tropical conditions. With regard to drainage, there is a need to model the soil down to a greater depth than 1 m, since drainage systems are often installed below this depth.

With regard to impact assessment, several updates of USEtox are foreseen (USEtox Website) and regionalization of USEtox is an active research area (Kounina et al. 2014).Employing regionalized CFs would increase the accuracy of ecotoxicity studies, but, as indicated in the study by Kounina and colleagues, probably not significantly change the results. Further, impact assessment methods for the marine, terrestrial and groundwater compartments need to be developed, for which no recommended impact assessment models exist to date (Hauschild et al. 2013).

Present models lack capabilities to account for degradation products, which is a potentially serious shortcoming that needs further attention. This simplification is especially troublesome for compounds that rapidly degrade into more stable compounds, some of which are more toxic than the parent compound. A recent study showed that the inclusion of degradation products may increase freshwater CFs by up to 5 orders of magnitude (van Zelm et al. 2010). It has also been reported that the main degradation product of chlorothalonil is about thirty times more acutely toxic than the parent compound (Cox, 1997).

Also, chemical emissions seldom take place in isolation, and the environment is simultaneously exposed to a mixture of chemicals. Studies have shown that surfactants, a common pesticide ingredient, may increase toxicity of ASs (Sharma and Singh, 2001; Lee et al. 2009). Methods that deal with the mixture toxicity of chemicals exist (Backhaus and Faust, 2012), and have been validated for pesticide mixtures (Belden et al. 2007; Coors and Frische, 2011), but have yet to be integrated in USEtox for toxicity assessment of chemical emissions in LCA.

Further, studies that link pesticide use to effects on biodiversity exist (see Chapter 2.3), but models that link midpoint indicators of ecotoxic effects (LCIA-results), to endpoint indicators representing impacts on biodiversity, are all at an early stage of development (Hauschild et al. 2013). The development of such models would ideally take into account all impact categories, including ecotoxicity, that may potentially impact biodiversity, and would facilitate interpretation of LCIA-results (although at the expense of increased uncertainty). Research is ongoing, in particular within the field of Land Use Impact Assessment, regarding the inclusion of impacts on biodiversity in LCA, see e.g. de Baan et al. (2013), Milà i Canals et al. (2014), Knudsen et al. (2013) and Knudsen et al. (*in preparation*).

An ongoing debate in the LCA community deals with system boundaries in agricultural LCAs; more specifically whether the agricultural field is part of the ecosphere, or part of the technosphere (Rosenbaum et al. 2015). This modeling choice may impact how pesticide emissions are calculated, since LCA only takes into account emissions to the natural environment. In PestLCI, the agricultural field is regarded as part of the technosphere (Birkved and Hauschild, 2006); hence emissions to agricultural soil are not accounted for – in contrast to the dominating practice in which the entire pesticide dose is assumed to be emitted to soil, under the implicit assumption that the field belongs to the ecosphere. It should be noted that no consensus exists in the LCA community, on how to model the fate of pesticides after application. For a review and a discussion of various modeling approaches, refer to Rosenbaum et al. (2015) and van Zelm et al. (2014).

The physico-chemical input data to PestLCI and USEtox are currently, on the recommendations from the respective development teams, derived from different data sources (see Chapter 4), which causes some deviation in the input data used by the respective models (see Appendices 2 and 3).This unfortunate situation, the implications of which have yet to be quantified, urgently needs to be resolved to bridge the gap between inventory and impact assessment in LCAs of biobased products, and to increase consistency between models. Other potential mismatches between models also need to be revealed and resolved (van Zelm et al. 2014).

In addition, there is a need for more stringent ecotoxic effect data requirements in calculation of new USEtox CFs. Currently, USEtox gives limited guidance on selection criteria in collection of ecotoxic effect data, which promoteshaphazard collection of ecotoxic effect data and possible bias in CFs. It is desirable to develop more specific guidelines for data collection, that promoteuse ofdata from standardized tests,in line with the proposals by Larsen and Hauschild (2007b).

Finally, beyond pesticides and toxicity impacts, research is needed to improve our understanding of trade-offs associated with bioenergy expansion and how integration of bioenergy crops into agricultural landscapes could foster multiple ecosystem services and mitigate impacts from existing crops (Berndes et al. 2008; Meehan et al. 2013). Implementation of beneficial integration strategies also require dissemination tools (Busch, 2012) to support the broad stakeholder processes that are needed to capture synergies and strike a balance between socioeconomic and environmental objectives.

CHAPTER 7. CONCLUSIONS

To summarize, we have investigated pesticide use and constructed realistic and typical pesticide application scenarios for eight cases comprising five current and onefuture biofuel feedstock. The pesticide application scenarios are based on fairly common pesticides but not designed to represent any sort of national or regional average or to cover all possible alternatives. Further, we have expanded the regional coverage and pesticide database of PestLCI, derived new USEtox CFs, and assessed the potential freshwater ecotoxicity impacts caused by pesticide use in biofuel feedstock production. We have used site- and crop-specific data in emission inventory to improve accuracy and reduce uncertainties compared to conventional approaches. We have also identified the ASs associated with the largest impacts; performed sensitivity analyses on the influence of field size, buffer zones, method of application, soil parameters, site and tillage type; discussed uncertaintiesand proposed measured that could assist in reducing impacts. These are the main conclusions derived from this study:

- Total yearly average pesticide application rates vary by more than a factor 20 between cases (from 0.24kg AS ha^{-1} yr^{-1} in SX to 5.14 kg AS ha^{-1} yr^{-1} in WT).
- Amount of pesticide AS is an inadequate indicator of ecotoxicity: one applied unit of an AS potentially causes up to 7 orders of magnitude larger impact, than one applied unit of another AS.
- Potential freshwater ecotoxicity impact scores (expressed as CTUe TJ^{-1} and CTUe ha^{-1} yr^{-1}) vary substantially between the different cases, by up to 3 orders of magnitude (in both impact metrics).
- Placed in relation to biofuel yield, the SX case has a potential freshwater ecotoxicity impact score of about 3 CTUe TJ^{-1} (allocated value), while impact scores for the cases SC, MZ-I, MZ-II, SB-II, SB-I, WT, and RS are about 30, 110, 270, 305, 310, 750, and 1000 times larger, respectively. In relation to area and time, the SXcase has a potential freshwater ecotoxicity impact of < 1 CTUe ha^{-1} yr^{-1} (unallocated value), while impact scores for the cases SC, MZ-I, SB-II, SB-I, MZ-II, RS, and WT are about 60, 205, 220, 220, 500, 1110, and 1115 times larger, respectively.
- The WT and RS cases are associated with considerably higher potential impacts than the other cases, regardless of impact metric, due to the use of the insecticide beta-cyfluthrin in RS, and the fungicide chlorothalonil in WT, responsible for 92 and 84% of the total impact score, respectively.
- The results depend on hundreds of parameters of physico-chemical and pedoclimatic character, with varying uncertainty. Some parameters also display large temporal and/or spatial variability due to natural variations in the real world (e.g. application rates, soil conditions and field sizes). The uncertainty range of CFs has (previously) been determined to 1 – 2 orders of magnitude, while the uncertainty range of pesticide emissions has yet to be determined. Therefore, a full-scale, quantitative, uncertainty analysis could not be done.
- Due to existing uncertainties and model limitations, results should be interpreted with caution and foremost be used for ranking, and identifying the substances associated with the largest potential impacts.

- The top-four ASs associated with the largest potential freshwater ecotoxicity impacts (CTUe ha^{-1} yr^{-1}) are: beta-cyfluthrin (RS), chlorothalonil (WT), chlorpyrifos (MZ-II) and atrazine (MZ-I/II).

- The emission pathway from field to surface water via air is the dominating emission route for all ASs included in this study. For the three ASs with largest potentialimpact scores (beta-cyfluthrin, chlorothalonil and chlorpyrifos), the emission route via air is responsible for the greater part of the potential impact (>98%), while atrazine (the AS with the fourth largest potential impact score) is associated with relatively high emissions directly to surface water, which are responsible for three quarters of the potential impact. This is consistent with atrazine's documented water contamination potential.

- Generally, mitigation strategies to reduce freshwater ecotoxicity impacts include substitution to pesticide products with lower toxic potency, and reduction of emissions to freshwater ecosystems. The wide range in CFs, by up to 7 orders of magnitude, indicate that choice of pesticide product largely controls the potential freshwater ecotoxicity impact. For example,substitution of beta-cyfluthrin to an equivalent dose of lambda-cyhalothrin could bring down the impact score by 85% in the RS case.

- Emissions to freshwater ecosystems can be reduced through management, for example: creating buffer zones (unsprayed field margins), constructing wetlands, reducing application rates, reducing spray drift, shifting application date, and increasing farmers' awareness of risks associated with handling and applying pesticides.

- Sensitivity analyses indicate that ecotoxic effects could be reduced considerably if buffer zones are used where fields abut surface water. The addition of product-specific buffer zones for the 13 highest-impact ASs in the WT, RS, and MZ-II cases resulted in reduction of impact scores, by 68, 91, and 78% respectively.

- Sensitivity analyses reveal (in line with previous findings) that field width is a critical parameter for emissions to air and consequently, impact scores. A change in the field size parameter in the SB-I case from 250 to 10 ha caused the potential freshwater ecotoxicity impact to increase by almost a factor3. The importance of the field size parameter partly explains why the European cases (RS and WT, cultivated on 10 ha fields), are associated with relatively high per-ha impacts, and the soybean cases (SB-I/II, cultivated on 250 ha fields) are associated with relatively low low per-ha impacts. The fact that field sizes vary greatly in reality is one of several reasons why caution should be taken before generalizing the results presented here.

- The results indicate that impacts would be lower if biofuels were produced from lignocellulosic crops subject to similar pesticide treatment as in the SX case. The cultivation of lignocellulosic perennial crops generally involves less pesticide input than conventional biofuel crops. However,considering that biofuel from lignocellulosic crops are not yet commercially available, the results for *Salix* should be interpreted as an indication of the future potential.

- Our findings do not indicate a reduced impact in GE glyphosate tolerant soybeans compared with conventional, in contrary to popular claims that the cultivation of glyphosate tolerant crops is associated with increasing use of glyphosate at expense of other, more toxic and persistent herbicides.

- Potential freshwater ecotoxicity impacts are not a function of application doses alone, but depend on site-specific parameters. It is therefore important to develop site-, crop- and field-specific inventories of pesticide usage and emissionsin order to improve accuracy and reduce uncertainties, rather than to use site-generic default fate-factors. Such specific inventories are however difficult and time consuming to develop due to limited data availability.

- Areas for future research and development include: expanding substance databases; developing impact assessment methods for the marine, terrestrial and ground water compartments; expanding regionalization of PestLCI and validating it against non-European conditions; developing methods for including toxicity of degradation products and of mixtures; reviewing the selection criteria of physico-chemical and ecotoxicity effect data to PestLCI and USEtox, and investigating the trade-offs associated with bioenergy expansion in agricultural landscapes.

REFERENCES

AGRITOX. Database on active plant protection substances, French National Institute for Agricultural Research. http://www.dive.afssa.fr/agritox/index.php (accessed Sept 3, 2014).

Alavanja, M. C. R.; Bonner, M. R. (2012) Occupational pesticide exposure and cancer risk: a review. *J. Toxicol. Environ. Health, Part B 15* (4), 238-263.

Allen, M. T.; Levy, L. S. (2013) Parkinson's disease and pesticide exposure - a new assessment. *Crit. Rev. Toxicol. 43*(6), 515-534.

Alletto, L.; Coquet, Y.; Benoit, P.; Heddadj, D.; Barriuso, E. (2010) Tillage management effects on pesticide fate in soils. A review. *Agron. Sustainable Dev. 30* (2), 367-400.

Altitude Website. http://www.altitude.nu/ (accessed March 14, 2014).

AltTox Website. Chemical Toxicity Databases;

http://alttox.org/resource-center/databases/#CT (accessed March 30, 2015).

APROSOJA (n.d.) Mato Grosso, Brazil: on the road to sustainability (Cartilha Sustentabilidade Bilingue). The Mato Grosso State Soy and Corn Producers Association, APROSOJA. Downloaded from http://www.aprosoja.com.br/publicacoes-impressas (accessed Oct 21, 2014).

Arias-Estévez, M.; López-Periago, E.; Martínez-Carballo, E.; Simal-Gándara, J.; Mejuto, J-C.; García-Río, L. (2008) The mobility and degradation of pesticides in soils and the pollution of groundwater resources. *Agric., Ecosyst. Environ. 123* (4), 247-60.

Arrigoni, E. D. B.; de Almeida, L. C. (2007) Agrochemicals (pesticides and others). In *Sugar Cane's Energy: twelve studies on Brazilian sugar cane agribusiness and its sustainability;* Macedo, I. C., Ed.; second edition, São Paulo Sugar Cane Agroindustry Union, UNICA: São Paulo; 149-156.

Åsheim, P. SalixEnergi Europa, Svalöv, Sweden. Personal communication, 2012.

Audsley, E.; Alber, S.; Clift, R.; Cowell, S.; Crettaz, P.; Gaillard, G.; Hausheer, J.; Jolliet, O.; Kleijn, R.; Mortensen, B.; Pearce, D.; Roger, E.; Teulon, H.; Weidema, B.; van Zeijts, H. (2003) *Harmonisation of environmental life cycle assessment for agriculture;* Final Report concerted action AIR3-CT94-2028, European Commission: Silsoe.

Azevedo, S. The Mato Grosso State Soy and Corn Producers Association, APROSOJA, Cuiabá, Mato Grosso, Brazil. Personal communication, 2013.

Backhaus, T.; Faust, M. (2012) Predictive Environmental Risk Assessment of Chemical Mixtures: A Conceptual Framework. *Environ. Sci. Technol. 46* (5), 2564-2573.

Bai, Y.; Luo, L.; van der Voet, E. (2010) Life cycle assessment of switchgrass-derived ethanol as transport fuel. *Int. J. Life Cycle Assess.15* (5), 468-477.

Bare, J. (2011) TRACI 2.0: the tool for the reduction and assessment of chemical and other environmental impacts 2.0. *Clean Technol. Environ. Policy13* (5), 687-696.

Barizon, R. Brazilian Agricultural Research Corporation (EMBRAPA), Jaguaríuna, São Paulo, Brazil.Personal communication, 2014.

BASF (2013) *Kulturenratgeber Schleswig-Holstein 2013;* BASF SE Agricultural Products Germany, Region North-East: Seelze-Lathwehren. http://www.agrar.basf.de/agroportal/de/media/migrated/de/infothek_neu/kulturenratgeber_2013/Kulturenratgeber_Schleswig_Holstein.pdf (accessed Dec 19, 2013).

Bates, S. L.; Zhao, J. –Z.; Roush, R. T.; Shelton, A. M. (2005) Insect resistance management in GM crops: past, present and future. *Nature biotechnology 23* (1), 57-62.

Batjes, N. H. (2008) *ISRIC-WISE Harmonized Global Soil Profile Dataset (Ver. 3.1);* Report 2008/2, ISRIC - World Soil Information: Wageningen, 2008 (with dataset).

Batjes, N. H. (2009) Harmonized soil profile data for applications at global and continental scales: updates to the WISE database. *Soil Use Manage. 25* (2), 124-127.

Beketov, M. A.; Kefford, B. J.; Schäfer, R. B.; Liess, M. (2013) Pesticides reduce regional biodiversity of stream invertebrates. *Proc. Natl. Acad. Sci. 110* (27), 11039-11043.

Belden, J. B.; Gilliom, R. J.; Lydy, M. J. (2007) How well can we predict the toxicity of pesticide mixtures to aquatic life? *Integr. Environ. Assess. Manage. 3* (3), 364-372.

Benbrook, C. M. (2012) Impacts of genetically engineered crops on pesticide use in the U.S. – the first sixteen years. *Environ. Sci. Eur. 24* (1), 1-13.

Bending, G. D.; Lincoln, S. D.; Edmondson, R. N. (2006) Spatial variation in the degradation rate of the pesticides isoproturon, azoxystrobin and diflufenican in soil and its relationship with chemical and microbial properties. *Environ. Pollut. 139* (2), 279-287.

Berndes, G.; Börjesson, P.; Ostwald, M.; Palm, M. (2008) Multifunctional biomass production systems —an overview with presentation of specific applications in India and Sweden. *Biofuels, Bioprod. Biorefin.2* (1), 16-25.

Berry, P.; Cook, S. M; Ellis, S.; Gladders, P.; Roques, S. (2012) *Oilseed rape guide - Summer 2012*; Cereals and oilseeds division (HGCA) of the Agriculture and Horticulture Development Board (AHDB): Warwickshire.

Birkved, M.; Hauschild, M. Z. (2006) PestLCI - A model for estimating field emissions of pesticides in agricultural LCA. *Ecol. Modell.198* (3-4), 433-451.

Bless, H. G. Chamber of Agriculture in Schleswig-Holstein, Rendsburg, Germany. Personal communication, 2013.

Börjesson, P.; Berndes G. (2006) The prospects for willow plantations for wastewater treatment in Sweden. *Biomass Bioenergy 30* (5), 428-438.

Brander, M.; Wylie, C. (2011) The use of substitution in attributional life cycle assessment. *Greenhouse Gas Meas. Manage. 1* (3-4), 161-166.

Brimner, T.A.; Gallivan, G. J.; Stephenson, G. R. (2005) Influence of herbicide-resistant canola on the environmental impact of weed management. *Pest Manage. Sci. 61* (1), 47-52.

Bunzel, K.; Liess, M.; Kattwinkel, M. (2014) Landscape parameters driving aquatic pesticide exposure and effects. *Environ. Pollut. 186*, 90-97.

Burt, G. W. (1974) Volatility of Atrazine from Plant, Soil, and Glass Surfaces. *J Environ Qual.3* (2), 114-117.

Busch, G. (2012) GIS-based tools for regional assessments and planning processes regarding potential environmental effects of poplar SRC. *BioEnergy Res. 5* (3), 584-605.

Carvalho, F. P. (2006) Agriculture, pesticides, food security and food safety. *Environ. Sci. Policy 9* (7–8), 685-692.

Cavalett, O. Brazilian Bioethanol Science and Technology Laboratory, CTBE, Campinas, São Paulo, Brazil. Personal communication, 2013.

Chum, H.; et al. (2011) Bioenergy. In *IPCC Special Report on Renewable Energy Sources and Climate Change Mitigation;* Edenhofer, O.; Pichs-Madruga, R.; Sokona, Y.; Seyboth, K.; Matschoss, P.; Kadner, S.; Zwickel, T.; Eickemeier, P.; Hansen, G.; Schlömer, S.; von Stechow, C.; Eds.; Cambridge University Press: Cambridge and New York; 209-332.

Coors, A.; Frische, T. (2011) Predicting the aquatic toxicity of commercial pesticide mixtures. *Environ. Sci. Eur. 23* (22), 1-18.

Cox, C. (1997) Fungicide factsheet: Chlorothalonil. *Journal of pesticide reform17* (4), 14-20.

Curran, M. A. (2007) Co-product and input allocation approaches for creating life cycle inventory data: A literature review. *Int. J. Life Cycle Assess.12* (1), 65-78.

Daylight Hours Explorer. University of Nebraska-Lincoln, Astronomy Education; http://astro.unl.edu/animationsLinks.html (accessed Oct 20, 2014).

de Baan, L.; Alkemade, R.; Koellner, T. (2013) Land use impacts on biodiversity in LCA: a global approach. *Int. J. Life Cycle Assess. 18* (6), 1216-1230.

de Castro, B. S. (2008) A introdução no Brasil do algodão, milho e soja geneticamentemodificados: coincidências reveladoras. Paper presented at the IX Brazilian Association Studies (BRASA) Congress, Tulane University, New Orleans, Louisiana, March 27-29, 2008; http://sitemason.vanderbilt.edu/files/iD6Qxi/Castro%20Bianca%20Scarpeline.pdf (accessed Dec 12, 2013).

de Snoo G. R.; de Wit, P. J. (1998) Buffer zones for reducing pesticide drift to ditches and risks to aquatic organisms. *Ecotoxicol. Environ. Saf.41* (1), 112-118.

de Sousa, S. A. V. (2007) Availability and use of water in Brazil; irrigation. In *Sugar Cane's Energy: twelve studies on Brazilian sugar cane agribusiness and its sustainability;* Macedo, I. C., Ed.; second edition, São Paulo Sugar Cane Agroindustry Union, UNICA: São Paulo, pp 106-108.

de Vries, S. C.; van de Ven, G. W.; van Ittersum, M. K.; Giller, K. E. (2010) Resource use efficiency and environmental performance of nine major biofuel crops, processed by first-generation conversion techniques. *Biomass Bioenergy34* (5), 588-601.

DeLorenzo, M. E.; Scott, G. I.; Ross, P. E. (2001) Toxicity of pesticides to aquatic microorganisms: A review. *Environ. Toxicol. Chem.20* (1), 84-98.

Derpsch, R.; Friedrich, T. (2009) Development and Current Status of No-till Adoption in the World. Proceedings of the 18th Triennial Conference of the International Soil Tillage Research Organization (ISTRO), Izmir, Turkey, June 15-19, 2009; http://www.fao.org/ag/ca/ca-publications/istro%202009.pdf (accessed Jan 14, 2014).

Dijkman, T. J. Technical University of Denmark, Kgs. Lyngby. Personal communication, 2013-2014.

Dijkman, T. J.; Birkved, M.; Hauschild, M. Z. (2012) PestLCI 2.0: a second generation model for estimating emissions of pesticides from arable land in LCA. *Int. J. Life Cycle Assess. 17* (8), 973-986.

Dreyer, L. C.; Niemann, A. L.; Hauschild, M. Z. (2003) Comparison of three different LCIA methods: EDIP97, CML2001 and Eco-indicator 99. *Int. J. Life Cycle Assess.8*(4), 191-200.

EC (2004) Commission decision 2004/248/EC of 10 March 2004 concerning the non-inclusion of atrazine in Annex I to Council Directive 91/414/EEC and the withdrawal of authorisations for plant protection products containing this active substance.*Official Journal of the European Union, Legislation 78,* 53-55.

EC (2009) Directive 2009/28/EC of the European Parliament and of the Council of 23 April 2009 on the promotion of the use of energy from renewable sources and amending and subsequently repealing Directives 2001/77/EC and 2003/30/EC. *Official Journal of the European Union, Legislation140*, 16-62.

Edwards, C. A. (1993) The impact of pesticides on the environment. In *The pesticide question: environment, economics, and ethics;* Pimentel, D.; Lehman, H.; Eds.; Chapman & Hall: New York and London, pp 13-46.

Ekbom, B. (2002) *Resistens mot insektsbekämpningsmedel;* Faktablad om växtskydd, Jordbruk, 109. Swedish University of Agricultural Sciences (SLU), Uppsala.

Emmenegger, M. F.; Gmünder, S.; Reinhard, J.; Zah, R.; Nemecek, T.; Schnetzer, J.; Bauer, C.; Simons, A.; Doka, A. (2012) *Harmonisation and extension of the bioenergy inventories and assessment;* End Report, EMPA Research Institute: Dübendorf.

Eriksson, J.; Mattsson, L.; Söderström M. (2010) *Current status of Swedish arable soils and cereal crops - data from the period 2001-2007;* Swedish Environmental Protection Agency: Stockholm and Östersund; http://www.naturvardsverket.se/Documents/publikationer/978-91-620-6349-8.pdf (accessed Oct 21, 2014)

Ertl, D. Iowa Corn Promotion Board, Iowa Corn Growers Association, USA. Personal communication, 2013.

Eurostat (2007) *The use of plant protection products in the European Union, data 1992-2003;* Eurostat statistical book, Office for Official Publications of the European Communities: Luxembourg.

FAO (1996) Pesticides as water pollutants. In *Control of water pollution from agriculture - FAO irrigation and drainage paper 55;* Ongley, E. D.; Ed.; Food and Agriculture Organization of the United Nations: Rome.

FAO (2003) *International Code of Conduct on the Distribution and Use of Pesticides adopted by the Hundred and Twenty-third Session of the FAO Council in November 2002;* Food and Agriculture Organisation of the United Nations: Rome.

FAO (2011) *Crops statistics – concepts, definitions and classifications;* The Food and Agriculture Organization of the United Nations;http://www.fao.org/economic/ess/ess-trade/ess-prod-method/en/ (Accessed Nov 10, 2014).

FAOSTAT. The FAO statistical database. Statistics Division of the Food and Agriculture Organization of the United Nations: Rome;http://faostat.fao.org (accessed Aug 20, 2014).

Fazio, S.; Monti, A. (2011) Life cycle assessment of different bioenergy production systems including perennial and annual crops. *Biomass Bioenergy35* (12), 4868-4878.

FEBRAPDP Website. Federação Brasileira de Plantio Direto e Irrigação; http://www.febrapdp.org.br/ (accessed Aug 28, 2013).

Fernandez-Cornejo, J.; Nehring, R.; Osteen, C.; Wechsler, S.; Martin, A.; Vialou, A. (2014) *Pesticide Use in U.S. Agriculture: 21 Selected Crops, 1960-2008*; EIB-124, U.S. Department of Agriculture, Economic Research Service.

Ferreira Fernandes, M.; de Oliveira Procópio, S.; Teles, D. A.; de Sena Filho,J.G.; Filho, A. C.;Machado, T.N.(2012)Toxicidade de inseticidas utilizados na cultura da cana-de-açúcar para a bactéria diazotrófica Herbaspirillum seropedicae. *Revista de Ciências Agrárias55* (4), 318-326.

FRAC Website. Fungicide Resistance Action Committee; http://www.frac.info/ (accessed Aug 20, 2014).

Freemeteo Website. http://freemeteo.com (accessed Oct 20, 2014).

Freire, C.; Koifman, S. (2012) Pesticide exposure and Parkinson's disease: Epidemiological evidence of association. *Neurotoxicology 33* (5), 947-971.

Frisvold, G. B.; Hurley, T. M.; Mitchell, P. D. (2009) Overview: herbicide resistant crops – diffusion, benefits, pricing, and resistance management. *AgBioForum 12* (3-4),244–248.

Galdos, M. Brazilian Bioethanol Science and Technology Laboratory, CTBE, Campinas, Sao Paulo. Personal communication, 2013.

Gassmann, A. J. (2012) Field-evolved resistance to Bt maize by western corn rootworm: predictions from the laboratory and effects in the field. *J. Invertebr. Pathol.110*(3), 287-293.

Gassmann, A. J.; Petzold-Maxwell, J. L.; Clifton, E. H.; Dunbar, M. W.; Hoffmann, A. M.; Ingber, D. A.; Keweshan, R. S. (2014) Field-evolved resistance by western corn rootworm to multiple Bacillus thuringiensis toxins in transgenic maize. *Proc. Natl. Acad. Sci. U. S. A. 111* (14), 5141–5146.

Gatto, M. P.; Fioretti, M.; Fabrizi, G.; Gherardi, M.; Strafella, E.; Santarelli, L. (2014) Effects of potential neurotoxic pesticides on hearing loss: A review. *Neurotoxicology 42*, 24-32.

Geiger, F.; Bengtsson, J.; Berendse, F.; Weisser, W. W.; Emmerson, M.; Morales, M. B.; Ceryngier, P.; Liira, J.; Tscharntke, T.; Winqvist, C.; Eggers, S.; Bommarco, R.; Pärt, T.; Bretagnolle, V.; Plantegenest, M.; Clement, L. W.; Dennis, C.; Palmer, C.; Oñate, J. J.; Guerrero, I.; Hawro, V.; Aavik, T.; Thies, C.; Flohre, A.; Hänke, S.; Fischer, C.; Goedhart, P. W. Inchausti, P. (2010) Persistent negative effects of pesticides on biodiversity and biological control potential on European farmland. *Basic Appl. Ecol. 11*(2), 97-105.

Geller, A. M. (2005) Inert ingredients (in pesticides). In *Encyclopedia of Toxicology*, second edition; Wexler, P., Ed.; Elsevier Science Ltd, New York, pp 605-606.

Gilbert, N. (2013) A hard look at GM crops. *Nature 497*, 24-26.

Gilden, R. C.; Huffling, K.; Sattler, B. (2010) Pesticides and health risks. *Journal of Obstetric, Gynecologic, & Neonatal Nursing39*(1), 103-110.

Gilliom, R. J.; Barbash, J. E.; Crawford, C. G.; Hamilton, P. A.; Martin, J. D.; Nakagaki, N.; Nowell, L. H.; Scott, J. C.; Stackelberg, P. E.; Thelin, G. P.; Wolock, D. M. (2006) *The Quality of Our Nation's Waters—Pesticides in the Nation's Streams and Ground Water, 1992-2001.* U.S. Geological Survey, National Water-Quality Assessment Program, Circular 1291.

Gleser, H. J. Chamber of Agriculture in Schleswig-Holstein, Rendsburg, Germany. Personal communication, 2013.

Glyphosate Website (2013) The economical importance of glyphosate herbicides for European agriculture: Case studies in the UK and Germany; http://www.glyphosate.eu/economical-importance-glyphosate-herbicides-european-agriculture-case-studies-uk-and-germany (accessed Sept 3, 2014).

Goedkoop, M.; Heijungs, R.; Huijbregts, M.; De Schryver, A.; Struijs, J.; van Zelm, R. (2009) *ReCiPe 2008: A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level;* first edition; Report I: Characterisation. Dutch ministry of housing, spatial planning and Environment (VROM): the Hague.

Goedkoop, M.; Spriensma, R. (2001) *The Eco-indicator 99. A damage oriented method for Life Cycle Impact Assessment. Methodology Report*; third edition, Pré Consultants: Amersfoort.

González-Alzaga, B.; Lacasaña, M.; Aguilar-Garduño, C.; Rodríguez-Barranco, M.; Ballester, F.; Rebagliato, M.; Hernández, A. F. (2014) A systematic review of neurodevelopmental effects of prenatal and postnatal organophosphate pesticide exposure. *Toxicol. Lett. 230*(2), 104-121.

González-García, S.; Iribarren, D.; Susmozas, A.; Dufour, J.; Murphy, R. J. (2012b) Life cycle assessment of two alternative bioenergy systems involving Salix spp. biomass: Bioethanol production and power generation. *Appl. Energy 95*, 111-122.

González-García, S.; Mola-Yudego, B.; Dimitriou, I.; Aronsson, P.; Murphy, R.J. (2012a) Environmental assessment of energy production based on long term commercial willow plantations in Sweden. *Sci. Total Environ. 421-422*, 210-219.

Gopalakrishnan, G.; Negri, M. C.; Salas, W. (2012) Modeling biogeochemical impacts of bioenergy buffers with perennial grasses for a row-crop field in Illinois. *GCB Bioenergy 4* (6), 739-750.

Green, J. M. (2012) The benefits of herbicide-resistant crops. *Pest Manage. Sci. 68* (10), 1323-1331.

Guinée, J. B. (2001) *Life Cycle Assessment: An operational guide to the ISO Standards; LCA in Perspective; Guide; Operational Annex to Guide*. Centre for Environmental Science, Leiden University: Leiden.

Guinée, J. B.; Heijungs, R.; Huppes, G.; Zamagni, A.; Masoni, P.; Buonamici, R.; Ekvall, T.; Rydberg, T. (2011) Life cycle assessment: past, present and future. *Environ. Sci. Technol.45* (1), 90-96.

Hallmann, C. A.; Foppen, R. P. B.; van Turnhout, C. A. M.; de Kroon, H.; Jongejans, E. (2014) Declines in insectivorous birds are associated with high neonicotinoid concentrations. *Nature511* (7509), 341-343.

Harrison, P.; Pearce, F. (2000) Population, waste and chemicals. In *AAAS Atlas of Population and Environment* [Online]; Markham, V. D., Ed.; American Association for the Advancement of Science and the University of California Press, pp 107-118; http://atlas.aaas.org/index.php (accessed Aug 20, 2014).

Hauschild, M. Z.; Goedkoop, M.; Guinée, J.; Heijungs, R.; Huijbregts, M. A. J.; Jolliet, O.; Margni, M.; de Schryver, A.; Humbert, S.; Laurent, A.; Sala, S.; Pant, R. (2013) Identifying best existing practice for characterization modeling in life cycle impact assessment. *Int. J. Life Cycle Assess.18* (3), 683-697.

Hauschild, M. Z.; Huijbregts, M.; Jolliet, O.; MacLeod, M.; Margni, M.; van de Meent, D.; Rosenbaum, R.; McKone, T. (2008) Building a model based on scientific consensus for life cycle impact assessment of chemicals: the search for harmony and parsimony. *Environ. Sci. Technol. 42* (19), 7032-7037.

Hauschild M. Z.; Jolliet, O.; Huijbregts, M. A. J. (2011) A bright future for addressing chemical emissions in life cycles assessment. *Int. J. Life Cycle Assess.16* (8), 697 – 700.

Hauschild, M. Z; Wenzel, H.; Damborg, A.; Tørsløv, J. (1998) Ecotoxicity as a criterion in the environmental assessment of products. In *Environmental Assessment of Products: Volume 2: Scientific background;* Hauschild, M.; Wenzel, H., Eds.; London, Chapman & Hall, pp 203–314.

Heap, I. (2014) The International Survey of Herbicide Resistant Weeds; www.weedscience.org (accessed Nov 24, 2013).

Henderson, A. D.; Hauschild, M. Z.; van de Meent, D.; Huijbregts, M. A. J.; Larsen, H. F.; Margni, M.; McKone, T. E.; Payet, J.; Rosenbaum, R.; Jolliet, O. (2011) USEtox fate and ecotoxicity factors for comparative assessment of toxic emissions in life cycle analysis: sensitivity to key chemical properties. *Int. J. Life Cycle Assess.16* (8), 701-709.

HGCA (2012) *Septoria tritici in winter wheat*; Cereals and oilseeds division (HGCA) of the Agriculture and Horticulture Development Board (AHDB): Warwickshire.

Huijbregts, M. A. J.; Hauschild, M. Z.; Jolliet, O.; Margni, M.; McKone, T.; Rosenbaum, R. K.; van de Meent, D. (2010b) *USEtox^{TM} User manual*. Report version 1.01; http://www.usetox.org/support/tutorials-manuals (accessed Sept 10, 2014).

Huijbregts, M. A. J.; Margni, M.; van de Meent, D.; Jolliet, O.; Rosenbaum, R.; McKone, T.; Hauschild, M. (2010a) *USEtox^{TM} Chemical database: organics*. Report version 1.01; http://www.usetox.org/support/tutorials-manuals (accessed Sept 10, 2014).

Huijbregts, M. A. J.; Thissen, U.; Guinée, J. B.; Jager, T.; Kalf, D.; van de Meent, D.; Ragas, A. M. J.; Wegener Sleeswijk, A.; Reijnders, L. (2000) Priority assessment of toxic substances in life cycle assessment. Part I: Calculation of toxicity potentials for 181 substances with the nested multi-media fate, exposure and effects model USES-LCA. *Chemosphere 41* (4), 541–573.

Huijbregts, M. A. J.; van de Meent, D.; Goedkoop, M.; Spriensma, R. (2002) Ecotoxicological Impacts in Life Cycle Assessment. In *Species Sensitivity Distribution in Ecotoxicology;* Posthuma, L.; Suter II, G. W.; Traas, T. P. Eds.; CRC Press: Lewis, Boca Raton, pp 421–433.

IBGE (2013) *Indicadores IBGE: Estatística da Produção Agrícola: Outubro de 2013;* IBGE, Instituto Brasileiro de Geografia e Estatística; http://www.ibge.gov.br (accessed Dec 18, 2013)

IEA (2009) *Bioenergy - a sustainable and reliable energy source. A review of status and prospects;* Report 2009:06; International Energy Agency Bioenergy: Rotorua.

IEA (2011) *Technology Roadmap, Biofuels for Transport;* International Energy Agency: Paris.

IEA (2012) *Short rotation coppice willow - Best practice guidelines;* Task 43 Technical Report; International Energy Agency Bioenergy: Rotorua.

IEA (2013a) *CO2 Emissions from Fuel Combustion;* International Energy Agency: Paris.

IEA (2013b) *World energy outlook 2013*; International Energy Agency: Paris.

IEA-APTA. The Institute of Agricultural Economics (IEA), São Paulo´s Agency for Agribusiness Technology (APTA): São Paulo. Publications from various years available on: http://www.iea.sp.gov.br/out/trabalhos.php?tipo=avancada&cod Autor=13&buscaBox=&limitStart=20&limitSize=10&total=117 (accessed Aug 20, 2014).

INPE-LABSOLAR (2005) National Institute for Spatial Research (INPE) and Laboratory of Solar Energy, Federal University of Santa Catarina, Brazil (LABSOLAR). Brazil Global Horizontal Solar Radiation Model (40 km). Downloaded from http://en.openei.org/datasets/node/573 (accessed Sept 12, 2013).

Iowa State University Extension and Outreach Website. *Iowa State Soil: Tama Soil Series.* http://www.extension.iastate.edu/soils/iowa-state-soil-tama-soil-series (accessed Sept 9, 2013).

IRAC Website. Insecticide Resistance Action Committee; http://www.irac-online.org/ (accessed Aug 20, 2014).

ISO 14040:2006. *Environmental management - Life cycle assessment – Principles and framework;* International Organization for Standardization: Geneva.

ISO 14044:2006. *Environmental management - Life cycle assessment - Requirements and guidelines;* International Organization for Standardization: Geneva.

Jaeken, P.; Debaer, C. (2005) Risk of water contamination by plant protection products (PPP) during pre-and post treatment operations. *Annual Review of Agricultural Engineering4* (1), 93-114.

Jantalia, C. P.; Resck, D. V.; Alves, B. J.; Zotarelli, L.; Urquiaga, S.; Boddey, R. M. (2007) Tillage effect on C stocks of a clayey Oxisol under a soybean-based crop rotation in the Brazilian Cerrado region. *Soil Tillage Res.95* (1), 97-109.

Jarvis, N.; Larsbo, M. (2012) MACRO (v5.2): Model use, calibration, and validation. *Trans ASABE 55* (4), 1413-1423.

Jarvis, N. J; Larsbo, M.; Roulier, S.; Lindahl, A.; Persson, L. (2007) The role of soil properties in regulating non-equilibrium macropore flow and solute transport in agricultural topsoils. *Eur. J. Soil Sci.58* (1), 282-292.

Joaquim, A. C.; Bertolani, F. C.; Donzelli, J. L.; Boddey, R. M. (2011) *Organic carbon stocks in soils planted to sugarcane in the mid-south region of Brazil: a summary of CTC's data, 1990-2009;* Technical Report, Centro de Technologica Canaviera; Priacicaba, São Paulo, Brazil.

Jolliet, O.; Margni, M.; Charles, R.; Humbert, S.; Payet, J.; Rebitzer, G.; Rosenbaum, R. (2003) IMPACT 2002+: a new life cycle impact assessment methodology. *Int. J. Life Cycle Assess.8* (6), 324-30.

Jolliet, O.; Müller-Wenk, R.; Bare, J.; Brent, A.; Goedkoop, M.; Heijungs, R.; Itsubo, N.; Peña, C.; Pennington, D.; Potting, J.; Rebitzer, G.; Stewart, M.; Udo de Haes, H.; Weidema, B. (2004) The LCIA midpoint-damage framework of the UNEP/SETAC life cycle initiative. *Int. J. Life Cycle Assess. 9* (6), 394-404.

Jørgensen, L. N.; Jahn, M.; Clark, B.; Antichi, D.; Góral, T.; Schepers, H.; Lucas, P.; Gouache, D.; Hornok, L. (2008) *Report on best control practices of diseases in winter wheat in 8 countries in the EU*;Deliverable D 1.2, ENDURE – wheat case study, European Network for Durable Exploitation of Crop Protection Strategies.

JRC (2010) *International Reference Life Cycle Data System (ILCD) Handbook - General guide for Life Cycle Assessment - Detailed guidance;* first edition; Institute for Environment and Sustainability, Joint Research Centre (JRC), European Commission, Publications Office of the European Union: Luxembourg.

JRC (2012) *Assessing GHG default emissions from biofuels in EU legislation. Review of the input database to calculate 'Default GHG emissions', following expert consultation, 22-23 November 2011, Ispra (Italy);* Scientific and Technical Research Report JRC-76057, Institute for Energy and Transport, Joint Research Centre (JRC), European Commission, Publications Office of the European Union: Luxembourg, 2012.

KemI Pesticides Register (Bekämpningsmedelsregistret). The Swedish Chemicals Agency: Sundbyberg. http://webapps.kemi.se/bkmregistret/kemi.spider.web.external/(accessed Oct 20, 2014).

Kim, S.; Dale, B. E. (2005) Life cycle assessment of various cropping systems utilized for producing biofuels: Bioethanol and biodiesel. *Biomass Bioenergy 29* (6), 426-439.

Kim, S.; Dale, B. E. (2008) Life cycle assessment of fuel ethanol derived from corn grain via dry milling. *Bioresour. Technol.99* (12), 5250-5260.

Kim, S.; Dale, B. E. (2009) Regional variations in greenhouse gas emissions of biobased products in the United States – corn-based ethanol and soybean oil. *Int. J. Life Cycle Assess.14* (6), 540-546.

Knudsen, M. T.; Hermansen, J. E.; Dennis, P.; Guerci, M. (2013) Biodiversity - how can we include it in environmental life cycle assessments of products? In *SOLID News*, 3rd issue, pp. 3-4; http://www.solidairy.eu/wp-content/uploads/SOLID_News_APRIL-2013web.pdf (accessed Nov 7, 2014).

Knudsen, M. T.; Dennis, P.; Hermansen, J. E.; Cederberg, C.; Herzog, F.; Vale, J.; Jeanneret, P.; Sarthou, J-P.; Friedel, J.; Balazs, K.; Fjellstad, W.; Kainz, M.; Wolfram, S. Characterization factors from direct measures of plant species in European farmland for land use impacts on biodiversity in life cycle assessment. *In preparation*.

Kós, M. I.; Hoshino, A. C.; Fróes Asmus, C. I.; Mendonca, R.; Meyer, A. (2013) Peripheral and central auditory effects of pesticide exposure: a systematic review. *Cadernos De Saude Publica 29* (8), 1491-1506.

Kounina, A.; Margni, M.; Shaked, S.; Bulle, C.; Jolliet, O. (2014) Spatial analysis of toxic emissions in LCA: A sub-continental nested USEtox model with freshwater archetypes. *Environ. Int. 69*, 67-89.

Länsstyrelsen Skåne (2012) *Grundvattenkvalitet i Skåne län – utvärdering av regional provtagning av grundvatten 2007-2010;* Länsstyrelsen Skåne: Malmö.

Larsen, H. F.; Hauschild, M. Z. (2007a) Evaluation of ecotoxicity effect indicators for use in LCIA. *Int. J. Life Cycle Assess.12* (1), 24-33.

Larsen, H. F.; Hauschild, M. Z. (2007b) GM-Troph - A Low Data Demand Ecotoxicity Effect Indicator for Use in LCIA. *Int. J. Life Cycle Assess.12* (2), 79-91.

Laurent, A.; Olsen, S. I.; Hauschild, M. Z. (2012) Limitations of carbon footprint as indicator of environmental sustainability. *Environ. Sci. Technol. 46* (7), 4100-4108.

Lee, H. L.; Kan, C. D.; Tsai, C. L.; Liou, M. J.; Guo, H. R. (2009) Comparative effects of the formulation of glyphosate-surfactant herbicides on hemodynamics in swine. *Clin. Toxicol. 47* (7), 651-658.

Lehtonen, M.; Goebel, F. R. (2009) *Status report on sugar cane agrochemicals management. Agrochemicals in the sugarcane industries: health and environmental challenges and solutions;* Ethanol & Sugar Impact Analysis (ESIA) and Agricultural Research for Development (CIRAD).

LKSH Website. *Insektizide in Raps im Herbst – Auflagen*; Landwirtschaftskammer Schleswig-Holstein (TheChamber of Agriculture in Schleswig-Holstein); http://www.lksh.de/fileadmin/dokumente/Landwirtschaft/Pflanze/Pflanzenschutz/Insektizide/Raps_I_gesamtAuflagen.pdf(accessed Aug 20, 2014).

LLUR (2006) *Die Böden Schleswig-Holsteins;* Landesamt für Landwirtschaft, Umwelt und ländliche Räume des Landes Schleswig-Holstein (LLUR): Flintbek; http://www.umweltdaten.landsh.de/nuis/upool/gesamt/geologie/boden_sh.pdf (accessed Dec 19, 2013).

Lu, C.; Warchol, K. M.; Callahan, R. A. (2014) Sub-lethal exposure to neonicotinoids impaired honey bees winterization before proceeding to colony collapse disorder. *Bulletin of Insectology 67* (1), 125-130.

Lundgren, J. G.; Gassmann, A. J.; Bernal, J.; Duan, J. J.; Ruberson, J. (2009) Ecological compatibility of GM crops and biological control. *Crop Protection 28* (12), 1017-1030.

McKone, T. E.; Enoch, K. G. (2002) *CalTOX, A multimedia total exposure model spreadsheet User's guide. Version 4.0 (Beta);* Ernest Orlando Lawrence Berkeley National Laboratory.

Meehan, T. D.; Gratton, C.; Diehl, E.; Hunt, N. D.; Mooney, D. F.; Ventura, S. J.; Barham, B. L.; Jackson, R. D. (2013) Ecosystem-Service Tradeoffs Associated with Switching from Annual to Perennial Energy Crops in Riparian Zones of the US Midwest. *PLoS One* 8 (11), e80093.

Meyer, D. Round Table of Responsible Soy. Personal communication, 2013.

Meyer, D.; Cederberg, C. (2010) *Pesticide use and glyphosate resistant weeds – a case study of Brazilian soybean production;* Report 809; SIK, The Swedish Institute for Food and Biotechnology: Göteborg; http://www.sik.se/archive/pdf-filer-katalog/SR809.pdf (accessed Aug 20, 2014).

Milà i Canals, L.; Michelsen, O.; Teixeira, R. F.; Souza, D. M.; Curran, M.; Antón, A. (2014) Building consensus for assessing land use impacts on biodiversity in LCA. Paper presented at the 9th International Conference LCA of Food, San Francisco, USA, October 8-10, 2014; http://lcafood2014.org/papers/128.pdf (accessed Nov 7, 2014).

Milazzo, M. F.; Spina, F.; Vinci, A.; Espro, C.; Bart, J. C. J. (2013) Brassica biodiesels: Past, present and future. *Renewable Sustainable Energy Rev.18,* 350-389.

Mortensen, D. A.; Egan, J. F.; Maxwell, B. D.; Ryan, M. R.; Smith, R. G. (2012) Navigating a critical juncture for sustainable weed management. *BioScience 62* (1), 75-84.

Mostafalou, S.; Abdollahi, M. (2013) Pesticides and human chronic diseases: Evidences, mechanisms, and perspectives. *Toxicol. Appl. Pharmacol. 268* (2), 157-177.

Muñoz-Quezada, M. T.; Lucero, B. A.; Barr, D. B.; Steenland, K.; Levy, K.; Ryan, B.; Iglesias, V.; Alvarado, S.; Concha, C.; Rojas, E.; Vega, C. (2013) Neurodevelopmental effects in children associated with exposure to organophosphate pesticides: A systematic review. *Neurotoxicology 39*, 158-168.

NCDC Website. National Climatic Data Center, National Oceanic & Atmospheric Administration. http://www.ncdc.noaa.gov (accessed Aug 27, 2014).

NCGA (2013) *2013 - World of Corn;* National Corn Growers Association: Chesterfield, Washington; http://www.ncga.com/upload/files/documents /pdf/WOC%202013.pdf (accessed Dec 19, 2013)

Neary, D. G.; Smethurst, P. J.; Baillie, B.; Petrone, K. C. (2011) *Water quality, biodiversity and codes of practice in relation to harvesting forest plantations in streamside management zones;* CSIRO National Research Flagships Sustainable Agriculture: Australia.

Nemecek, T.; Schnetzer, J. (2011) *Methods of assessment of direct field emissions for LCIs of agricultural production systems;* Agroscope Reckenholz-Tänikon Research Station ART & ecoinvent Centre: Zürich.

Nordborg, M.; Cederberg, C.; Berndes, G. (2014) Modeling potential freshwater ecotoxicity impacts due to pesticide use in biofuel feedstock production: the cases of maize, rapeseed, *Salix*, soybean, sugarcane and wheat. *Environ. Sci. Technol. 48* (19), 11379-11388.

Ometto, A. R.; Hauschild, M. Z.; Roma, W. N. L. (2009) Lifecycle assessment of fuel ethanol from sugarcane in Brazil. *Int. J. Life Cycle Assess. 14* (3), 236-247.

Owen, M. D. K.; Hartzler, R. (2011) *2012 Herbicide guide for Iowa corn and soybean production;* Iowa State University Extension Weed Management: Ames.

Owen, M. D. K.; Hartzler, R. (2012) *2013 Herbicide guide for Iowa corn and soybean production;* Iowa State University Extension Weed Management: Ames.

Owen, M. D. K.; Hartzler, R. (2013) *2014 Herbicide guide for Iowa corn and soybean production;* Iowa State University Extension Weed Management: Ames.

Parish, E. S.; Hilliard, M. R.; Baskaran, L. M.; Dale, V. H.; Griffiths, N. A.; Mulholland, P. J.; Sorokine, A.; Thomas, N. A.; Downing, M. E.; Middleton, R. S. (2012) Multimetric spatial optimization of switchgrass plantings across a watershed. *Biofuels, Bioprod. Biorefin. 6* (1), 58-72.

Payet, J. (2004) *Assessing toxic impacts on aquatic ecosystems in life cycle assessment (LCA);* Ph.D. Thesis. Ecole Polytechnique Fédérale de Lausanne.

Pennington, D. W.; Margni, M.; Payet, J.; Jolliet, O. (2006) Risk and regulatory hazard-based toxicological effect indicators in life-cycle assessment (LCA). *Hum. Ecol. Risk Assess. 12* (3), 450-475.

Pennington, D. W.; Payet, J.; Hauschild, M. (2004) Aquatic ecotoxicological indicators in life-cycle assessment. *Environ. Toxicol. Chem. 23* (7), 1796-807

Phipps, R.; Park, J. (2002) Environmental benefits of genetically modified crops: global and European perspectives on their ability to reduce pesticide use. *Journal of Animal and Feed Sciences 11* (1), 1-18.

PHYSPROP. The Physical Properties Database, Syracuse Research Centre. http://www.srcinc.com/what-we-do/product.aspx?id=133 (accessed May 3, 2013).

Pimentel, D.; Acquay, H.; Biltonen, M.; Rice, P.; Silva, M.; Nelson, J.; Lipner, V.; Giordano, S.; Horowitz A.; D'amore, M. (1993) Assessment of environmental and economic impacts of pesticide use. In *The pesticide question: environment, economics, and ethics;* Pimentel, D.; Lehman, H.; Eds.; Chapman & Hall: New York and London, pp 47-84.

Pimentel, D.; Levitan, L. (1986) Pesticides: amounts applied and amounts reaching pests. *Bioscience 36*, 86–91.

POPS (2001) *Stockholm Convention on Persistent Organic Pollutants*;

http://chm.pops.int/Portals/0/Repository/convention_text/UNEP-POPS-COP-CONVTEXT-FULL.English.PDF (accessed Sept 12, 2014).

Posthuma, L.; Suter II, G. W.; Traas, T. P. (2002) *Species Sensitivity Distribution in Ecotoxicology*; CRC Press: Lewis, Boca Raton, USA.

Potting, J.; Hauschild, M. (2006) Spatial differentiation in life cycle impact assessment: a decade of method development to increase the environmental realism of LCIA. *Int. J. Life Cycle Assess. 11*, 11-13.

PPDB (2014) *The University of Hertfordshire Agricultural Substances Database Background and Support Information*; Agriculture & Environment Research Unit, University of

Hertfordshire: Herts; http://sitem.herts.ac.uk/aeru/ppdb/en/docs/Background_and_Support.pdf (accessed Oct 20, 2014).

PPDB. The Pesticide Properties DataBase. Agriculture & Environment Research Unit, University of Hertfordshire: Herts. http://sitem.herts.ac.uk/aeru/footprint/index2.htm (accessed Sept 10, 2014).

PVGIS. Photovoltaic Geographical Information System. European Communities, 2001-2012; http://re.jrc.ec.europa.eu/pvgis/ (accessed Sept 12, 2013).

PVWatts 40 km Grid Data Calculator v. 2. National Renewable Energy Laboratory, U.S Department of Energy. http://www.nrel.gov/rredc/pvwatts/grid.html (accessed Aug 27, 2014).

Reichenberger, S.; Bach, M.; Skitschak, A.; Frede, H. G. (2007) Mitigation strategies to reduce pesticide inputs into ground- and surface water and their effectiveness; A review. *Sci. Total Environ. 384* (1-3), 1-35.

Renewable Energy Directive (RED) 2009/28/EC of the European Parliament and of the Council of 23 April 2009 on the promotion of the use of energy from renewable sources and amending and subsequently repealing Directives 2001/77/EC and 2003/30/EC. *Official Journal of the European Union, Legislation140*, 16-62.

Repetto, R.; Baliga, S. S. (1996) *Pesticides and the immune system: the public health risks;* World Resources Institute: Washington; http://www.wri.org/publication/

pesticides-and-immune-system (accessed Aug 20, 2014).

Ricci, A. Jr. (2007) Pesticides: herbicides. In *Sugar Cane's Energy: twelve studies on Brazilian sugar cane agribusiness and its sustainability;* Macedo, I. C., Ed.; second edition, São Paulo Sugar Cane Agroindustry Union, UNICA: São Paulo, pp 157-161.

Roeleveld, N.; Bretveld, R. (2008) The impact of pesticides on male fertility. *Current Opinion in Obstetrics & Gynecology 20* (3), 229-233.

Rosenbaum, R. K.; Anton, A.; Bengoa, X.; Bjørn, A.; Brain, R.; Bulle, C.; Cosme, N.; Dijkman, T. J.; Fantke, P.; Felix, M.; Geoghegan, T. S.; Gottesbüren, B.; Hammer, C.; Humbert, S.; Jolliet, O.; Juraske, R.; Lewis, F.; Maxime, D.; Nemecek, T.; Payet, J.; Räsänen, K.; Roux, P.; Schau, E. M.; Sourisseau, S.; van Zelm, R.; von Streit, B.; Wallman, M. (2015) The Glasgow consensus on the delineation between pesticide emission inventory and impact assessment for LCA. *Int. J. Life Cycle Assess. In press.*

Rosenbaum, R. K.; Bachmann, T. M.; Gold, L. S.; Huijbregts, M. A. J.; Jolliet, O.; Juraske, R.; Koehler, A.; Larsen, H. F.; MacLeod, M.; Margni, M.; McKone, T. E.; Payet, J.; Schumacher, M.; van de Meent, D.; Hauschild, M. Z. (2008) USEtox – the UNEP-SETAC toxicity model: recommended characterization factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. *Int. J. Life Cycle Assess.13* (7), 532-546.

Rossberg, D. (2013) Erhebungen zur Anwendung von Pflanzenschutzmitteln in der Praxis im Jahr 2011. *Journal für Kulturpflanzen 65* (4), 141-151.

SCB (2013) *Yearbook of agricultural statistics 2013 including food statistics;* Statistics Sweden: Örebro; http://www.scb.se/en_/Finding-statistics/Publishing-calendar/Show-detailed-information/?publobjid=20457+ (accessed Nov 7, 2014).

Schäfer, R. B.; Caquet, T.; Siimes, K.; Mueller, R.; Lagadic, L.; Liess, M. (2007) Effects of pesticides on community structure and ecosystem functions in agricultural streams of three biogeographical regions in Europe. *Sci. Total Environ. 382* (2-3), 272-285.

Scheffler, R.; Neill, C.; Krusche, A.V.; Elsenbeer, H. (2011) Soil hydraulic response to land-use change associated with the recent soybean expansion at the Amazon agricultural frontier. *Agric., Ecosyst. Environ.144* (1), 281-289.

Schiesari, L.; Waichman, A.; Brock, T.; Adams, C.; Grillitsch, B. (2013) Pesticide use and biodiversity conservation in the Amazonian agricultural frontier. *Philos. Trans. R. Soc., B. 368* (1619), 20120378.

Schmidt-Walter, P.; Lamersdorf, N. P. (2012) Biomass Production with Willow and Poplar Short Rotation Coppices on Sensitive Areas—the Impact on Nitrate Leaching and Groundwater Recharge in a Drinking Water Catchment near Hanover, Germany. *BioEnergy Res. 5* (3), 546-562.

Seabra, J. E.; Macedo, I. C.; Chum, H. L.; Faroni, C. E.; Sarto, C. A. (2011) Life cycle assessment of Brazilian sugarcane products: GHG emissions and energy use. *Biofuels, Bioprod. Biorefin. 5* (5), 519-532.

Sharma, S. D.; Singh, M.(2001)Surfactants increase toxicity of glyphosate and 2,4-D to Brazil Pusley. *HortScience36* (4), 726-728.

SIDRA-IBGE. Sistema IBGE de Recuperação Automática, SIDRA. IBGE, Instituto Brasileiro de Geografia e Estatística. Tabela 99; http://www.sidra.ibge.gov.br (accessed Aug 20, 2014).

Skenhall, S. A.; Berndes, G.; Woods, J. (2013) Integration of bioenergy systems into UK agriculture - new options for management of nitrogen flows. *Biomass Bioenergy54*, 219-226.

Smith, D. T.; Richard, E. P. Jr.; Santo, L. T. (2008) Weed control in sugarcane and the role of triazine herbicides. In *The triazine herbicides: 50 years Revolutionizing Agriculture;* LeBaron, H. M.; McFarland, J. E.; Burnside, O. C., Eds.; Elsevier: San Diego, Amsterdam and Oxford, pp 185-198.

Soy Stats Website. International: *Adoption of Biotech Enhanced Seedstock.* http://soystats.com (accessed Jan 15, 2014).

Sparovek, G. University of São Paulo, USP, Brazilian Bioethanol Science and Technology Laboratory, CTBE, Brazil. Personal communication, 2013.

Sparovek, G.; Berndes, G.; Klug, I. L. F.; Barretto, A. G. O. P. (2010) Brazilian agriculture and environmental legislation: status and future challenges. *Environ. Sci. Technol.* 44 (16), 6046-6053.

Statistikamt Nord (2013) *Bodennutzung und Ernte in Schleswig-Holstein 2012;* Statistikamt Nord - Statistical Office of Hamburg and Schleswig-Holstein: Hamburg; https://www.statistik -nord.de/uploads/tx_standocuments/C_I_C_II_j12_SH.pdf (accessed Aug 20, 2014).

Tessum, C. W.; Marshall, J. D.; Hill, J. D. (2012) A Spatially and Temporally Explicit Life Cycle Inventory of Air Pollutants from Gasoline and Ethanol in the United States. *Environ. Sci. Technol. 46* (20), 11408-11417.

Thornthwaite, C. W. (1948) An Approach toward a Rational Classification of Climate. *Geogr. Rev. 38* (1), 55-94.

Tiktak, A.; Hendriks, R. F. A.; Boesten, J. J. T. I.; van der Linden, A. M. A. (2012) A spatially distributed model of pesticide movement in Dutch macroporous soils. *J. Hydrol.* 470-471, 316-327.

TOXNET. Toxicology data network, US National Library of Medicine: Rockville Pike; http://toxnet.nlm.nih.gov/ (accessed Sept 3, 2014).

Traas, T. P.; van de Meent, D.; Posthuma, L.; Hamers, T.; Kater, B.J.; de Zwart, D.; Aldenberg, T. (2002) The Potentially Affected Fraction as a Measure of Ecological Risk. In *Species Sensitivity Distribution in Ecotoxicology;* Posthuma, L.; Suter II, G. W.; Traas, T. P. Eds.; CRC Press: Lewis, Boca Raton, pp 315–344.

Udo de Haes, H. A.; Sleeswijk, A. W.; Heijungs, R. (2006) Similarities, differences and synergisms between HERA and LCA—an analysis at three levels. *Hum. Ecol. Risk Assess.12* (3), 431-49.

USDA (2009) *Pesticide Data Program - Annual Summary, Calendar Year 2008*. Agricultural Marketing Service, United States Department of Agriculture: Washington

USDA NASS (2011) *Agricultural chemical use: Corn, upland cotton and fall potatoes 2010,* United States Department of Agriculture, National Agricultural Statistics Service:Washington; http://www.nass.usda.gov/Surveys/Guide_to_NASS_Surveys/Chemical_Use/FieldCropChemicalUseFactSheet06.09.11.pdf (accessed Oct 21, 2014).

USDA NASS Quick Stats Database. United States Department of Agriculture, National Agricultural Statistics Service. http://quickstats.nass.usda.gov/ (accessed Aug 20, 2014).

USDA Soil Texture Calculator. United States Department of Agriculture, Natural Resources Conservation Service; http://soils.usda.gov/technical/aids/ investigations/texture/ (accessed Sept 9, 2013).

US-EPA (1997) *Pesticides Industry Sales and Usage - 1994 and 1995 Market Estimates;* EPA-733-R-97-002; Office of Prevention, Pesticides and Toxic Substances, United States Environmental Protection Agency: Washington.

US-EPA (1999) *Pesticides Industry Sales and Usage - 1996 and 1997 Market Estimates;* EPA-733-R-99-001; Office of Prevention, Pesticides and Toxic Substances, United States Environmental Protection Agency: Washington.

US-EPA (2002) *Pesticides Industry Sales and Usage - 1998 and 1999 Market Estimates;* EPA-733-R-02-001; Office of Prevention, Pesticides and Toxic Substances, United States Environmental Protection Agency: Washington.

US-EPA (2004) *Pesticides Industry Sales and Usage - 2000 and 2001 Market Estimates;* EPA-733-R-04-001; Office of Prevention, Pesticides and Toxic Substances, United States Environmental Protection Agency: Washington.

US-EPA (2011) *Pesticides Industry Sales and Usage - 2006 and 2007 Market Estimates;* EPA-733-R-11-001; Office of Chemical Safety and Pollution Prevention, United States Environmental Protection Agency: Washington.

US-EPA (2012) Estimation Programs Interface EPISuite^{TM}, US Environmental Protection Agency: Washington. Download setup file available at: http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm. (accessed Sept 11, 2014).

US-EPA ECOTOXicology (ECOTOX) Database Version 4.0, United States Environmental Protection Agency: Washington http://cfpub.epa.gov/ecotox(accessed Sept 3, 2014).

US-EPA OPP Pesticide Ecotoxicity Database. Office of Pesticide Programs, United States Environmental Protection Agency; http://www.ipmcenters.org/Ecotox/ (accessed Sept 3, 2014).

USEtox Website. http://www.usetox.org/ (accessed 7 Jan, 2014).

Uzogara, S. G. (2000) The impact of genetic modification of human foods in the 21st century: A review. *Biotechnol. Adv. 18* (3), 179-206.

van der Sluijs, J. P.; Simon-Delso, N.; Goulson, D.; Maxim, L.; Bonmatin, J. M. Belzunces, L. P. (2013) Neonicotinoids, bee disorders and the sustainability of pollinator services. *Current Opinion in Environmental Sustainability 5* (3–4), 293-305.

Van Hoof, G.; Schowanek, D.; Franceschini, H.; Muñoz, I. (2011) Ecotoxicity impact assessment of laundry products: a comparison of USEtox and critical dilution volume approaches. *Int. J. Life Cycle Assess. 16* (8), 803-818.

Van Maele-Fabry, G.; Hoet, P.; Lison, D. (2013) Parental occupational exposure to pesticides as risk factor for brain tumors in children and young adults: A systematic review and meta-analysis. *Environ. Int. 56*, 19-31.

Van Maele-Fabry, G.; Hoet, P.; Vilain, F.; Lison, D. (2012) Occupational exposure to pesticides and Parkinson's disease: A systematic review and meta-analysis of cohort studies. *Environ. Int. 46*, 30-43.

Van Maele-Fabry, G.; Libotte, V.; Willems, J.; Lison, D. (2006) Review and meta-analysis of risk estimates for prostate cancer in pesticide manufacturing workers. *Cancer Causes & Control 17* (4), 353-373.

van Zelm, R.; Huijbregts, M. A. J.; van de Meent, D. (2009) USES-LCA 2.0—a global nested multi-media fate, exposure, and effects model. *Int. J. Life Cycle Assess. 14* (3), 282-284.

van Zelm, R.; Huijbregts, M. A. J.; van de Meent, D. (2010) Transformation products in the life cycle impact assessment of chemicals. *Environ. Sci. Technol.44* (3), 1004-1009.

van Zelm, R; Larrey-Lassalle, P; Roux P. (2014) Bridging the gap between life cycle inventory and impact assessment for toxicological assessments of pesticides used in crop production. *Chemosphere 100*, 175-181.

Vinson, F.; Merhi, M.; Baldi, I.; Raynal, H.; Gamet-Payrastre, L. (2011) Exposure to pesticides and risk of childhood cancer: a meta-analysis of recent epidemiological studies. *J. Occup. Environ. Med. 68* (9), 694-702.

von Blottnitz, H.; Curran, M. A. (2007) A review of assessments conducted on bio-ethanol as a transportation fuel from a net energy, greenhouse gas and environmental life cycle perspective. *J. Cleaner Prod.15* (7), 607-619.

Wegener Sleeswijk, A. (2011) Regional LCA in a global perspective. A basis for spatially differentiated environmental life cycle assessment. *Int. J. Life Cycle Assess. 16* (2), 106-112.

Wegener Sleeswijk, A.; Heijungs, R. (2010) GLOBOX: A spatially differentiated global fate, intake and effect model for toxicity assessment in LCA. *Sci. Total Environ.408* (14), 2817-2832.

Weltklima Database. Deutscher Wetterdienst. (2007) Downloadable from http://www.dwd.de (accessed Sept 12, 2013).

Wenzel, H.; Hauschild, M.; Alting, L. (1997) *Environmental Assessment of Products. Vol. 1: Methodology, tools and case studies in product development;* first edition; Chapman & Hall, United Kingdom, Kluwer Academic Publishers, Hingham, MA.

WHO (1990) *Public health impact of pesticides used in agriculture;* World Health Organization: Geneva.

WHO (2010) *The WHO recommended classification of pesticides by hazard and guidelines to classification 2009;* World Health Organization: Geneva.

Williams, I. H. (2010) The Major Insect Pests of Oilseed Rape in Europe and Their Management: An Overview. In *Biocontrol-Based Integrated Management of Oilseed Rape Pests*;Williams I. H., Ed.;Springer: Dordrecht, Heidelberg, London and New York, pp. 1- 43.

Wiloso, E. I.; Heijungs, R.; de Snoo, G. R. (2012) LCA of second generation bioethanol: A review and some issues to be resolved for good LCA practice. *Renewable Sustainable Energy Rev. 16*(7), 5295-5308.

World Weather Online Website; http://www.worldweatheronline.com (accessed Sept 12, 2013).

Yang, Y. (2013) Life cycle freshwater ecotoxicity, human health cancer, and noncancer impacts of corn ethanol and gasoline in the US. *J. Cleaner Prod.53*, 149-157.

Yang, Y.; Bae, J.; Kim, J.; Suh, S. (2012) Replacing gasoline with corn ethanol results in significant environmental problem shifting. *Environ. Sci. Technol.46* (7), 3671-3678.

Yngveson, N. Swedish Rural Economy and Agricultural Societies Malmöhus, Borgeby.Personal communication, 2014.

APPENDIX 1. PESTICIDE ACTIVE SUBSTANCES AND CHARACTERIZATION FACTORS

Table A1 lists pesticide ASs included in this study along with their Chemical Abstracts Service Registry Numbers (CAS-RN), characterization factors (CF) and CF classification.

Pesticides classified as interim are either dissociating (i.e., ionize in water) or have ecotoxic effect data covering less than three different trophic levels. CFs calculated in this study are based on ecotoxic effect data for algae, crustacean and fish species, according to Larsen and Hauschild (2007b), see further in Appendix 5. All calculated CFs, except lactofen, have effect data that satisfy the minimum requirement. The dissociation of pesticides with calculated CFs was not determined and they could therefore not be classified as recommended or interim.

Table A1. Pesticide ASs included in this study with CAS-RNs, CFs and CF classification (H = herbicide, F = fungicide, I = insecticide, N = nematicide, PGR = plant growth regulator). Pesticide ASs that were not originally present in the database of PestLCI v.2.0, but that we added, are marked with †. Pesticide ASs that did not originally have USEtox CFs, but that we calculated, are marked with *.

CAS-RN	**Pesticide active substance common name**	**CF for emission to air (CTUe kg^{-1})**	**CF for emission to freshwater (CTUe kg^{-1})**	**CF classification**
34256-82-1	Acetochlor (H)	1367	67 801	recommended
67375-30-8	Alpha-cypermethrin (I)	254 034	35 089 624	interim
834-12-8	Ametryn (H) †	1804	76 179	recommended
1912-24-9	Atrazine (H)	3288	87,654	recommended
25057-89-0	Bentazone (H)	7	201	recommended
68359-37-5	Beta-cyfluthrin (I) †	7 861 577	490 012 232	recommended
188425-85-6	Boscalid (F) †*	352	13 597	
1563-66-2	Carbofuran (N)	5898	112 462	recommended
999-81-5	Chlormequat-chloride (PGR)	25	177	interim
1897-45-6	Chlorothalonil (F)	76 270	1 152 875	recommended
2921-88-2	Chlorpyrifos (I)	9535	6 206 819	recommended
90982-32-4	Chlorimuron-ethyl (H) †*	2806	17 642	
500008-45-7	Chlorantraniliprole (I) †*	11 339	88 704	
99129-21-2	Clethodim (H) †	11	3291	interim
83164-33-4	Diflufenican (H)	30	1247	interim
149961-52-4	Dimoxystrobin (F) †*	5229	728 310	
163515-14-8	Dimethenamid-P (H) †*	2384	110 876	
330-54-1	Diuron (H)	2537	60 117	recommended
133855-98-8	Epoxiconazole (F) †*	2171	112 489	
16672-87-0	Ethephon (PGR)	445	1364	interim
80844-07-1	Etofenprox (I) †	<1	619	interim
67564-91-4	Fenpropimorph (F)	7	7380	interim
120068-37-3	Fipronil (I) †	11 724	2 012 897	recommended
145701-23-1	Florasulam (H) †*	1651	10 650	
81406-37-3	Fluroxypyr 1-methylheptyl ester (H) †	905	77 290	recommended
96525-23-4	Flurtamone (H) †*	1230	60 205	
142459-58-3	Flufenacet (H) †	3771	168 237	recommended
907204-31-3	Fluxapyroxad (Xemium) (F) †*	442	28 730	
38641-94-0	Glyphosate isopropylamine salt (H) †	23	546	interim

51235-04-2	Hexazinone (H) †	3495	118 374	recommended
104098-48-8	Imazapic (H) †*	843	6891	
144550-36-7	Iodosulfuron methyl sodium (H) *	1662	11 090	
77501-63-4	Lactofen (H) †*	2012	80 421	
91465-08-6	Lambda-cyhalothrin (I)	576 370	138 991 256	recommended
2039-46-5	MCPA dimethylamine salt (H) †	45	857	interim
24307-26-4	Mepiquat-chloride (PGR)	8	798	recommended
208465-21-8	Mesosulfuron-methyl (H) †*	5390	16 934	
67129-08-2	Metazachlor (H)	70	7364	recommended
125116-23-6	Metconazole (F) †*	264	16 380	
16752-77-5	Methomyl (I)	3163	28 979	recommended
220899-03-6	Metrafenone (F) †*	74	29 536	
4685-14-7	Paraquat (H) †	1334	118 762	interim
23950-58-5	Propyzamide (H)	232	4308	recommended
178928-70-6	Prothioconazole (F) †*	3300	70 791	
175013-18-0	Pyraclostrobin (F) †*	1510	497 696	
90717-03-6	Quinmerac (H) †	24	505	interim
100646-51-3	Quizalofop-P-ethyl (H) †*	258	27 257	
107534-96-3	Tebuconazole (F)	1771	68 297	recommended
34014-18-1	Tebuthiuron (H) †	1638	12 728	recommended
83121-18-0	Teflubenzuron (I) †	50 982	971 086	interim
111988-49-9	Thiacloprid (I) *	45	6256	
153719-23-4	Thiamethoxam (I) *	25	3441	
95266-40-3	Trinexapac-ethyl (PGR)	3	1304	interim

APPENDIX 2. COLLECTION OF PHYSICO-CHEMICAL DATA FROM EPISUITE

In calculation of new USEtox CFs, we derived the required physico-chemical data from the Estimation Program Interface Suite^{TM} (EPISuite) for Windows v. 4.11 (US-EPA, 2012), in line with the recommendation in Huijbregts et al. (2010a).

EPISuite is a "toolbox" of thirteen different estimation programs for physico-chemical properties of chemicals, developed by the US Environmental Protection Agency's (EPA) office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). The only input required for running EPISuite is the chemical's SMILES (see Table 4.2). Besides estimation models, several of the programs have built-in databases with experimentally determined data. We prioritized experimental data and used estimated values only when experimentally determined data were not available, in line with the recommendation.

All thirteen programs are either be run simultaneously by entering SMILES on the main screen, selecting "Full" under "Output" and pressing the "Calculate" button. Alternatively, programs can be run one at a time, in "single-program" mode, by selecting program from the left-hand menu on the main screen. The single-program mode was found to have the advantage of always displaying experimental data, when available.

Molecular weight are available at the "All results" tab in the EPISuite Results window.

KOWWIN estimates the logarithmic octanol-water partition coefficient (Log Kow) of organic compounds and contains an experimental database (US-EPA, 2012). Experimental data for Log Kow, also denoted Log P in EPISuite, were found under the "All results" tab in the Result window or under the KOWWIN tab, and raised to the power of ten to get the required Kow-value (Note that "Exp. Log" refers to experimental log). In case experimental data were lacking, the KOWWIN estimate for Log Kow was used.

KOCWIN estimates the organic carbon – water partition coefficient (Koc) of organic compounds. The Koc is defined as "*the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium*" (US-EPA, 2012). KOCWIN has two estimation routes for Koc: Molecular Connectivity Index (MCI) and Log Kow estimation method, as well as an experimental database. First priority was given to experimental data, found by entering the KOCWIN program in single program mode or under the "All results" tab in the Results window. Note that experimental data are not shown under the KOCWIN tab in the Results window. The Log Koc was raised to the power of ten to get the Koc value. If experimental data were lacking, we used the KOCWIN estimate from MCI, according to the recommended procedure (Huijbregts et al. 2010a). If the MCI-estimate was lacking, we used the USEtox built-in estimation $Koc = 1.26 \cdot Kow^{0.81}$, applied automatically when the corresponding Excel-box was left blank (Huijbregts et al. 2010a).

HENRYWIN estimates the Henry's Law Constant of organic compounds at 25°C and contains an experimental database (US-EPA, 2012). Experimental data for K_H25C were found by entering the EPISuite HENRYWIN program in single program mode or under the "All results" tab in the Results window. Note that experimental data are not shown under the HENRYWIN tab in the Results window. If experimental data were not available, we used the USEtox built-in estimation $K_H25C = MW \cdot Pvap25\, Sol25^{-1}$, applied automatically when the corresponding Excel-box was left blank (Huijbregts et al. 2010a). EPISuite estimates for K_H25C were thus not used.

MPBPVP estimates melting point, boiling point, and vapor pressure, and was used for retrieval of vapor pressure at 25°C. MPBPVP contains an experimental database and three estimation methods for vapor pressure: the Antoine, the modified Grain and the Mackay methods (US-EPA, 2012). The physical state of a chemical determines which method is most appropriate (Huijbregts et al. 2010a). Experimental data for vapor pressure at 25°C were found under the MPBPVP “General” tab in the Results window or under the “All results” tab in the Results window and converted to Pa, if given in mm Hg (1 mm Hg = 133.32 Pa). If experimental data were lacking, we used the Modified Grain method estimate for solids, or the average of the Antoine and Modified Grain estimate for liquids and gases, in line with the recommended procedure (Huijbregts et al. 2010a). The physical state of pesticides was found in the PPDB. The Modified Grain and Antoine method estimates are available under the MPBPVP “Vapour pressure” tab in the Results window.

WSKOWWIN estimates the water solubility of organic compounds using the log octanol-water partition coefficient (Log Kow) and contains an experimental database (US-EPA, 2012). Experimental data for Sol25 were found under the “Water Solubility” tab in the Results window. If experimental data were lacking the EPISuite WSKOW estimate from Log Kow was used, also available under the “Water Solubility” tab in the Results window.

Neither experimental nor estimated K_{DOC} values are available in EPISuite. Instead the USEtox built-in estimation $K_{DOC} = 0.08 \cdot Kow$ for chemicals with Log Kow < 7.5 was used for all pesticides, applied automatically when the corresponding Excel-box was left blank (Huijbregts et al. 2010a).

Neither experimental nor estimated degradation rates in air, water, sediment and soil are available in EPISuite. Instead, we used Equation A1 to estimate the degradation rate in air, $kdeg_A$, in line with the recommended procedure (Huijbregts et al. 2010a).

$$kdeg_A = \frac{K_{OH} \cdot [OH]}{2}$$

Equation A1

where K_{OH} denotes the overall hydroxyl radical rate constant (in units of cm^3 $molecules^{-1}$ sec^{-1}) and [OH] denote the hydroxyl radical concentration per 12 hours of daylight (in units of molecules or radicals cm^{-3}). A default value of $[OH] = 1.5 \cdot 10^6$ was used, according to Huijbregts et al. (2010a).

AOPWIN (the Atmospheric Oxidation Program) estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals (US-EPA, 2012), and was used here to retrieve the overall hydroxyl radical rate constants, K_{OH}. Experimental data for K_{OH} were available by entering AOPWIN in single program mode or under the “All results” tab in the Results window. If experimental data were lacking the “overall OH rate constant” estimate available under the AOPWIN ”Hydroxyl Radicals Page 2” (or for some pesticides only by entering the program in single program mode) was used.

BIOWIN is a collection of seven separate models that estimate the probability of rapid aerobic and anaerobic biodegradation of an organic compound in the presence of mixed populations of environmental microorganisms (US-EPA, 2012). We used Biowin3, “expert survey ultimate biodegradation model”, for derivation of biodegradation rates in water, soil and sediment in line with the recommended procedure (Huijbregts et al. 2010a). First, Table A2 was consulted to determine the biodegradation rate in water, $kdeg_W$, based on the Biowin 3 “Ultimate biodegradation timeframe” output, found under the BIOWIN “General” tab in the Results window.

Table A2. Relationship between EPISuite Biowin3 output and biodegradation rate in water (table adopted from Huijbregts et al. 2010a).

EPISuite BIOWIN Biowin3 output (available under the BIOWIN “General” tab in the Results window)	**Biodegradation rate in water, $kdeg_{W}$, s^{-1}**
Hours	4.7E-05
Hours to Days	6.4E-06
Days	3.4E-06
Days to Weeks	9.3E-07
Weeks	5.3E-07
Weeks to Months	2.1E-07
Months	1.3E-07
Recalcitrant	4.5E-08

Biodegradation rates in sediment and soil, $kdeg_{Sd}$ and $kdeg_{Sl}$, were then estimated based on the degradation rate in water, according to Equations A2 and A3, in line with the recommended procedure (Huijbregts et al. 2010a).

$$kdeg_{Sd} = \frac{kdeg_{W}}{9}$$

Equation A2

$$kdeg_{Sl} = \frac{kdeg_{W}}{2}$$

Equation A3

where $kdeg_{Sd}$ denote the biodegradation rates in sediment; $kdeg_{Sl}$ denote the biodegradation rates in soil and $kdeg_{W}$ denote the biodegradation rates in water.

APPENDIX 3. PHYSICO-CHEMICAL DATA USED IN PESTLCI

Table A3. Full set of physico-chemical data used in PestLCI. † marks pesticide ASs that were not originally included in PestLCI v.2.0, but that we added. * marks pesticide ASs that did not originally have USEtox CFs, but that we calculated.Note that reference temperatures for solubility andvapor pressure is 20and 25˚C for all ASs.

Pesticide active substance	**Molecular weight, g mole^{-1}**	**Molecular volume, cm^3 mole^{-1}**	**Solubility in water, g l^{-1}**	**Vapor pressure, Pa**
Acetochlor (H)	269.8	240.9	2.82E-01	2.20E-05
Alpha-cypermethrin (I)	416.3	313.1	4.00E-06	3.40E-07
Ametryn (H) †	227.1	192.5	2.00E-01	3.65E-04
Atrazine (H)	215.7	169.8	3.50E-02	3.90E-05
Bentazone (H)	240.3	178.5	5.70E-01	1.70E-04
Beta-cyfluthrin (I) †	434.3	317.3	1.20E-06	5.60E-08
Boscalid (F) †*	343.2	194.4	4.60E-03	7.20E-07
Carbofuran (N)	221.6	194.4	3.22E-01	8.00E-05
Chlormequat-chloride (PGR)	158.1	'N/A'	8.86E+02	1.00E-06
Chlorothalonil (F)	265.9	154.6	8.10E-04	7.60E-05
Chlorpyrifos (I)	350.6	236.7	1.05E-03	1.43E-03
Chlorimuron-ethyl (H) †*	414.8	277.7	1.20E+00	4.90E-10
Chlorantraniliprole (I) †*	483.2	320.0	8.80E-04	6.30E-12
Clethodim (H) †	359.9	312.4	5.45E+00	2.08E-06
Diflufenican (H)	394.3	274.0	5.00E-05	4.25E-06
Dimoxystrobin (F) †*	326.4	263.2	4.30E-03	6.00E-09
Dimethenamid-P (H) †*	275.8	229.8	1.45E+00	2.50E-03
Diuron (H)	233.1	170.1	3.56E-02	1.15E-06
Epoxiconazole (F) †*	329.8	236.4	7.10E-03	1.00E-05
Ethephon (PGR)	144.5	92.0	1.00E+03	1.00E-03
Etofenprox (I) †	376.5	321.8	2.25E-05	8.13E-07
Fenpropimorph (F)	303.5	326.8	4.32E-03	3.90E-03
Fipronil (I) †	437.2	233.6	3.78E-03	2.00E-06
Florasulam (H) †*	359.3	204.5	6.36E+00	1.00E-05
Fluroxypyr 1-methylheptyl ester (H) †	367.2	289.4	1.36E-04	1.00E-05
Flurtamone (H) †*	333.3	249.2	1.07E-02	4.50E-07
Flufenacet (H) †	363.3	250.6	5.60E-02	9.00E-05
Fluxapyroxad (Xemium) (F) †*	381.3	'N/A'	3.44E-03	2.70E-09
Glyphosate isopropylamine salt (H) †	228.2	'N/A'	1.16E+01	2.10E-06
Hexazinone (H) †	252.3	201.8	3.30E+01	3.00E-05
Imazapic (H) †*	275.3	210.2	2.23E+00	1.00E-05
Iodosulfuron methyl sodium (H) *	529.3	300.7	2.50E+01	6.70E-09
Lactofen (H) †*	461.8	341.6	5.00E-04	9.30E-06
Lambda-cyhalothrin (I)	449.9	334.6	5.00E-06	2.00E-07
MCPA dimethylamine salt (H) †	245.7	'N/A'	5.84E+03	4.95E-07
Mepiquat-chloride (PGR)	149.7	129.0	5.00E+02	1.00E-08
Mesosulfuron-methyl (H) †*	503.5	340.2	4.83E-01	1.10E-08
Metazachlor (H)	277.8	232.1	4.50E-01	9.30E-05
Metconazole (F) †*	319.8	280.6	3.04E-02	2.10E-08
Methomyl (I)	162.2	137.9	5.50E+01	7.20E-04
Metrafenone (F) †*	409.0	282.3	4.92E-04	1.53E-04
Paraquat (H) †	186.3	124.2	6.20E+02	1.00E-05
Propyzamide (H)	256.1	203.5	9.00E-03	2.67E-05

Prothioconazole (F) †*	344.3	228.0	3.00E-01	4.00E-07
Pyraclostrobin (F) †*	387.8	303.4	1.90E-03	2.60E-08
Quinmerac (H) †	221.6	157.5	1.07E+02	1.00E-10
Quizalofop-P-ethyl (H) †*	373.0	274.1	6.10E-04	1.10E-07
Tebuconazole (F)	307.8	268.1	3.60E-02	1.30E-06
Tebuthiuron (H) †	228.0	191.9	2.50E+00	2.70E-04
Teflubenzuron (I) †	381.1	231.4	1.00E-05	9.16E-07
Thiacloprid (I) *	252.7	177.4	1.84E-01	3.00E-10
Thiamethoxam (I) *	291.7	170.2	4.10E+00	6.60E-09
Trinexapac-ethyl (PGR)	252.3	185.7	1.02E+01	2.16E-03

Table A3. Continued. Note that reference temperature for biodegradation is 20˚C for all ASs.

Pesticide active substance	**pKa (first), -**	**Log Kow, -**	**Koc $l\ kg^{-1}$**	**Soil t½ Lab 20˚ C, days**	**Atmospheric OH rate(days) at 25˚ C, $cm^3\ molecule^{-1}\ s^{-1}$**
Acetochlor (H)	'N/A'	4.14	1.56E+02	10.6	4.960E-11
Alpha-cypermethrin (I)	5.00	5.50	5.79E+04	100.0	2.140E-11
Ametryn (H) †	10.07	2.63	3.16E+02	60.0	2.854E-11
Atrazine (H)	1.70	2.70	1.00E+02	66.0	2.730E-11
Bentazone (H)	3.28	-0.46	5.30E+00	45.0	6.220E-11
Beta-cyfluthrin (I) †	'N/A'	5.90	6.43E+04	27.8	1.250E-11
Boscalid (F) †*	'N/A'	2.96	1.23E+03	246.0	2.601E-11
Carbofuran (N)	'N/A'	1.80	8.65E+01	12.8	2.600E-11
Chlormequat-chloride (PGR)	'N/A'	-3.47	1.68E+02	23.2	7.360E-12
Chlorothalonil (F)	'N/A'	2.94	8.50E+02	15.7	6.180E-15
Chlorpyrifos (I)	'N/A'	4.70	8.15E+03	76.0	9.170E-11
Chlorimuron-ethyl (H) †*	4.20	0.11	1.06E+02	40.0	4.270E-11
Chlorantraniliprole (I) †*	10.88	2.86	3.62E+02	597.0	1.670E-11
Clethodim (H) †	4.47	4.14	1.50E+05	0.6	1.550E-10
Diflufenican (H)	'N/A'	4.20	2.00E+03	141.8	3.200E-12
Dimoxystrobin (F) †*	'N/A'	3.59	4.86E+02	210.0	8.668E-11
Dimethenamid-P (H) †*	'N/A'	1.89	1.70E+02	23.0	5.234E-11
Diuron (H)	'N/A'	2.87	8.13E+02	75.5	5.040E-10
Epoxiconazole (F) †*	'N/A'	3.30	1.07E+03	226.0	8.780E-12
Ethephon (PGR)	2.82	-1.89	2.54E+03	16.5	1.050E-12
Etofenprox (I) †	'N/A'	6.90	1.78E+04	16.0	6.220E-11
Fenpropimorph (F)	6.98	4.50	4.38E+03	19.6	1.380E-10
Fipronil (I) †	'N/A'	3.75	8.38E+02	142.0	9.610E-11
Florasulam (H) †*	4.54	-1.22	2.20E+01	1.6	6.271E-12
Fluroxypyr 1-methylheptyl ester (H) †	'N/A'	5.04	2.46E+04	1.0	3.680E-10
Flurtamone (H) †*	'N/A'	3.20	4.47E+03	130.0	8.920E-11
Flufenacet (H) †	'N/A'	3.20	4.01E+02	32.0	1.745E-11
Fluxapyroxad (Xemium) (F) †*	12.58	3.13	3.43E+04	183.0	1.540E-11
Glyphosate isopropylamine salt (H) †	2.30	-3.87	6.92E+03	47.0	1.458E-10
Hexazinone (H) †	2.20	1.17	5.40E+01	90.0	9.019E-11
Imazapic (H) †*	2.00	2.47	1.37E+02	120.0	1.490E-11
Iodosulfuron methyl sodium (H) *	3.22	1.59	7.68E+01	2.0	2.530E-12
Lactofen (H) †*	'N/A'	4.81	1.00E+04	4.0	3.210E-12
Lambda-cyhalothrin (I)	'N/A'	6.90	1.57E+05	70.7	3.150E-11
MCPA dimethylamine salt (H) †	'N/A'	0.74	6.21E+01	24.0	1.210E-11
Mepiquat-chloride (PGR)	'N/A'	-3.55	8.90E+02	18.4	2.810E-11

Mesosulfuron-methyl (H) †*	4.35	-0.48	1.07E+01	45.0	2.130E-10
Metazachlor (H)	'N/A'	2.49	5.40E+01	15.6	5.900E-11
Metconazole (F) †*	11.38	3.85	3.18E+03	84.0	1.590E-11
Methomyl (I)	'N/A'	0.09	7.20E+01	7.0	6.650E-12
Metrafenone (F) †*	'N/A'	4.30	7.06E+03	250.6	2.040E-10
Paraquat (H) †	'N/A'	-4.50	1.00E+06	5000.0	2.156E-11
Propyzamide (H)	'N/A'	3.30	8.40E+02	47.0	1.320E-11
Prothioconazole (F) †*	6.90	3.82	1.77E+03	0.5	1.130E-10
Pyraclostrobin (F) †*	'N/A'	3.99	9.30E+03	62.0	2.060E-10
Quinmerac (H) †	4.31	-1.41	8.60E+01	17.4	4.370E-12
Quizalofop-P-ethyl (H) †*	'N/A'	4.61	7.74E+03	0.4	2.840E-11
Tebuconazole (F)	'N/A'	3.70	7.69E+02	365.0	1.150E-11
Tebuthiuron (H) †	1.20	1.79	8.00E+01	360.0	3.320E-12
Teflubenzuron (I) †	9.20	4.30	2.61E+04	92.1	6.190E-12
Thiacloprid (I) *	'N/A'	1.26	6.15E+02	15.5	8.930E-11
Thiamethoxam (I) *	'N/A'	-0.13	5.62E+01	121.0	2.490E-10
Trinexapac-ethyl (PGR)	4.57	-0.29	2.80E+02	0.3	9.510E-11

APPENDIX 4. PHYSICO-CHEMICAL DATA USED IN USETOX

Table A4. Full set of physico-chemical data used in USEtox. † marks pesticide ASs that were not originally included in PestLCI v.2.0, but that we added. * marks pesticide ASs that did not originally have USEtox CFs, but that we calculated. For more information (on e.g. notations), refer to Chapter 4.4.

Pesticide active substance	**MW, g mole^{-1}**	**Kow, -**	**Koc, l kg^{-1}**	**K_H25C, Pa·m^3 mole^{-1}**	**Pvap25, Pa**
Acetochlor (H)	269.8	1.07E+03	2.09E+02	4.52E-03	3.73E-03
Alpha-cypermethrin (I)	416.3	1.15E+06	1.00E+05	4.24E-02	1.73E-01
Ametryn (H) †	227.3	9.55E+02	3.89E+02	2.45E-04	3.65E-04
Atrazine (H)	215.7	4.07E+02	1.74E+02	2.38E-04	3.85E-05
Bentazone (H)	240.3	2.19E+02	3.31E+01	2.20E-04	4.60E-04
Beta-cyfluthrin (I) †	434.3	8.91E+05	1.00E+05	2.93E-03	2.00E-08
Boscalid (F) †*	343.2	9.12E+02	9.46E+03		9.19E-09
Carbofuran (N)	221.3	2.09E+02	5.62E+01	3.12E-04	6.47E-04
Chlormequat-chloride (PGR)	158.1	1.58E-04	2.99E+01	1.62E-09	1.00E-05
Chlorothalonil (F)	265.9	1.12E+03	1.82E+03	2.02E-01	7.60E-05
Chlorpyrifos (I)	350.6	9.12E+04	5.01E+03	2.96E-01	2.71E-03
Chlorimuron-ethyl (H) †*	414.8	3.16E+02	1.10E+02	1.84E-10	5.33E-10
Chlorantraniliprole (I) †*	483.2	9.55E+03	4.90E+02		1.47E-13
Clethodim (H) †	359.9	1.62E+04	7.97E+03	9.39E-05	3.55E-07
Diflufenican (H)	394.3	7.94E+04	2.43E+04	3.28E-02	4.24E-06
Dimoxystrobin (F) †*	326.4	2.29E+05	5.10E+04		1.01E-07
Dimethenamid-P (H) †*	275.8	1.41E+02	1.41E+02	8.31E-03	3.67E-02
Diuron (H)	233.1	4.79E+02	2.51E+02	5.09E-05	9.20E-06
Epoxiconazole (F) †*	329.8	2.75E+03	2.27E+04		3.75E-05
Ethephon (PGR)	144.5	6.03E-01	1.00E+00	1.89E-09	1.31E-05
Etofenprox (I) †	376.5	1.12E+07	2.76E+05	1.05E+01	2.79E-05
Fenpropimorph (F)	303.5	8.51E+04	2.67E+04	2.46E-01	3.51E-03
Fipronil (I) †	437.2	1.00E+04	5.92E+03	8.50E-05	3.71E-07
Florasulam (H) †*	359.3	1.35E+02	1.61E+02		5.77E-07
Fluroxypyr 1-methylheptyl ester (H) †	367.3	3.39E+04	2.86E+03	5.47E-03	1.35E-06
Flurtamone (H) †*	333.3	5.75E+03	4.47E+03		5.05E-05
Flufenacet (H) †	363.3	1.58E+03	2.45E+03	5.82E-04	9.00E-05
Fluxapyroxad (Xemium) (F) †*	381.3	2.95E+03	3.43E+04		1.21E-07
Glyphosate isopropylamine salt (H) †	228.2	3.98E-04	1.00E+00	2.12E-07	2.11E-06
Hexazinone (H) †	252.3	7.08E+01	5.37E+01	2.28E-07	3.00E-05
Imazapic (H) †*	275.3	2.95E+02	1.78E+02		1.03E-09
Iodosulfuron methyl sodium (H) *	529.2	6.76E+01	1.23E+02		3.55E-19
Lactofen (H) †*	461.8	6.46E+04	1.00E+04	4.78E-02	9.33E-06
Lambda-cyhalothrin (I)	449.9	1.00E+07	1.82E+05	1.49E-01	2.00E-07
MCPA dimethylamine salt (H) †	200.6	1.78E+03	5.37E+01	1.34E-04	7.87E-04
Mepiquat-chloride (PGR)	149.7	1.51E-03	1.00E+06	1.48E-08	4.95E-05
Mesosulfuron-methyl (H) †*	503.5	6.31E+00	1.07E+01		2.26E-14
Metazachlor (H)	277.8	1.35E+02	1.00E+03	5.73E-05	1.53E-04
Metconazole (F) †*	319.8	7.08E+03	3.18E+03	2.62E-04	1.23E-05
Methomyl (I)	162.2	3.98E+00	2.00E+01	1.99E-06	7.20E-04
Metrafenone (F) †*	409.3	5.25E+04	2.08E+04		9.83E-07
Paraquat (H) †	257.2	1.95E-03	1.62E+04	5.59E-09	1.35E-05
Propyzamide (H)	256.1	2.69E+03	2.04E+02	9.87E-04	5.80E-05
Prothioconazole (F) †*	344.3	4.07E+03	2.92E+03		4.45E-12

Pyraclostrobin (F) †*	387.8	9.77E+03	4.79E+04		1.10E-07
Quinmerac (H) †	221.6	7.41E+02	4.70E+02	1.82E-05	1.83E-05
Quizalofop-P-ethyl (H) †*	372.8	1.91E+04	7.74E+03	1.07E-03	8.65E-07
Tebuconazole (F)	307.8	5.01E+03	1.54E+03	1.46E-05	1.71E-06
Tebuthiuron (H) †	228.3	6.17E+01	6.76E+01	1.21E-05	2.67E-04
Teflubenzuron (I) †	381.1	3.63E+04	2.07E+03	1.60E-05	8.00E-10
Thiacloprid (I) *	252.7	2.14E+02	1.12E+03		1.51E-04
Thiamethoxam (I) *	291.7	6.27E+00	2.66E+02		5.43E-05
Trinexapac-ethyl (PGR)	252.3	3.98E+01	3.00E+01	1.94E-01	2.16E-03

Table A4. Continued.

Pesticide active substance	**Sol25, mg l^{-1}**	**kdeg$_{A}$,s^{-1}**	**kdeg$_{W}$, s^{-1}**	**kdeg$_{Sd}$,s^{-1}**	**kdeg$_{Sl}$,s^{-1}**
Acetochlor (H)	2.23E+02	3.72E-05	1.34E-07	1.49E-08	6.69E-08
Alpha-cypermethrin (I)	1.00E-02	1.61E-05	4.46E-08	4.95E-09	2.23E-08
Ametryn (H) †	2.09E+02	2.14E-05	1.34E-07	1.49E-08	6.69E-08
Atrazine (H)	3.47E+01	2.05E-05	1.34E-07	1.49E-08	6.69E-08
Bentazone (H)	5.00E+02	4.66E-05	2.14E-07	2.38E-08	1.07E-07
Beta-cyfluthrin (I) †	3.00E-03	9.38E-06	4.46E-08	4.95E-09	2.23E-08
Boscalid (F) †*	2.02E+01	6.78E-06	1.30E-07	1.44E-08	6.50E-08
Carbofuran (N)	3.20E+02	1.95E-05	2.14E-07	2.38E-08	1.07E-07
Chlormequat-chloride (PGR)	9.96E+05	5.52E-06	2.14E-07	2.38E-08	1.07E-07
Chlorothalonil (F)	8.10E-01	4.64E-09	4.46E-08	4.95E-09	2.23E-08
Chlorpyrifos (I)	1.12E+00	6.88E-05	4.46E-08	4.95E-09	2.23E-08
Chlorimuron-ethyl (H) †*	1.20E+03	3.20E-05	1.30E-07	1.44E-08	6.50E-08
Chlorantraniliprole (I) †*	3.68E-01	1.25E-05	4.50E-08	5.00E-09	2.25E-08
Clethodim (H) †	1.36E+00	1.16E-04	2.14E-07	2.38E-08	1.07E-07
Diflufenican (H)	5.00E-02	2.40E-06	4.46E-08	4.95E-09	2.23E-08
Dimoxystrobin (F) †*	2.28E-01	6.50E-05	1.30E-07	1.44E-08	6.50E-08
Dimethenamid-P (H) †*	1.20E+03	3.93E-05	1.30E-07	1.44E-08	6.50E-08
Diuron (H)	4.20E+01	8.16E-06	2.14E-07	2.38E-08	1.07E-07
Epoxiconazole (F) †*	6.63E+00	6.58E-06	4.50E-08	5.00E-09	2.25E-08
Ethephon (PGR)	1.00E+06	7.90E-07	2.14E-07	2.38E-08	1.07E-07
Etofenprox (I) †	1.00E-03	4.66E-05	1.34E-07	1.49E-08	6.69E-08
Fenpropimorph (F)	4.30E+00	1.04E-04	1.34E-07	1.49E-08	6.69E-08
Fipronil (I) †	1.90E+00	7.21E-05	4.46E-08	4.95E-09	2.23E-08
Florasulam (H) †*	8.24E+01	4.70E-06	4.50E-08	5.00E-09	2.25E-08
Fluroxypyr 1-methylheptyl ester (H) †	9.00E-02	2.76E-05	4.46E-08	4.95E-09	2.23E-08
Flurtamone (H) †*	4.87E+01	6.77E-06	1.30E-07	1.44E-08	6.50E-08
Flufenacet (H) †	5.60E+01	1.31E-05	4.46E-08	4.95E-09	2.23E-08
Fluxapyroxad (Xemium) (F) †*	4.35E+00	1.16E-05	4.50E-08	5.00E-09	2.25E-08
Glyphosate isopropylamine salt (H) †	1.05E+06	5.93E-05	5.35E-07	5.94E-08	2.67E-07
Hexazinone (H) †	3.30E+04	6.76E-05	2.14E-07	2.38E-08	1.07E-07
Imazapic (H) †*	2.23E+03	1.12E-05	1.30E-07	1.44E-08	6.50E-08
Iodosulfuron methyl sodium (H) *	1.26E+01	1.90E-06	1.30E-07	1.44E-08	6.50E-08
Lactofen (H) †*	1.00E-01	2.40E-06	4.50E-08	5.00E-09	2.25E-08
Lambda-cyhalothrin (I)	5.00E-03	2.36E-05	4.46E-08	4.95E-09	2.23E-08
MCPA dimethylamine salt (H) †	6.30E+02	9.47E-06	5.35E-07	5.94E-08	2.67E-07
Mepiquat-chloride (PGR)	5.00E+05	2.11E-05	5.35E-07	5.94E-08	2.67E-07
Mesosulfuron-methyl (H) †*	1.42E+02	1.59E-04	1.30E-07	1.44E-08	6.50E-08
Metazachlor (H)	4.30E+02	4.43E-05	1.34E-07	1.49E-08	6.69E-08

Metconazole (F) †*	1.50E+01	1.19E-05	1.30E-07	1.44E-08	6.50E-08
Methomyl (I)	5.80E+04	4.99E-06	5.35E-07	5.94E-08	2.67E-07
Metrafenone (F) †*	2.48E-01	1.53E-04	1.30E-07	1.44E-08	6.50E-08
Paraquat (H) †	6.20E+05	1.59E-05	2.14E-07	2.38E-08	1.07E-07
Propyzamide (H)	1.50E+01	9.93E-06	1.34E-07	1.49E-08	6.69E-08
Prothioconazole (F) †*	5.53E+00	8.47E-05	4.50E-08	5.00E-09	2.25E-08
Pyraclostrobin (F) †*	1.43E+00	1.55E-04	1.30E-07	1.44E-08	6.50E-08
Quinmerac (H) †	2.23E+02	2.73E-06	2.14E-07	2.38E-08	1.07E-07
Quizalofop-P-ethyl (H) †*	4.00E-01	2.13E-05	1.30E-07	1.44E-08	6.50E-08
Tebuconazole (F)	3.60E+01	8.61E-06	1.34E-07	1.49E-08	6.69E-08
Tebuthiuron (H) †	2.50E+03	2.49E-06	2.14E-07	2.38E-08	1.07E-07
Teflubenzuron (I) †	1.90E-02	4.65E-06	4.46E-08	4.95E-09	2.23E-08
Thiacloprid (I) *	2.32E+02	6.70E-05	1.30E-07	1.44E-08	6.50E-08
Thiamethoxam (I) *	2.86E+03	1.87E-04	2.10E-07	2.33E-08	1.05E-07
Trinexapac-ethyl (PGR)	2.80E+00	7.13E-05	5.35E-07	5.94E-08	2.67E-07

APPENDIX 5. ECOTOXIC EFFECT DATA USED IN USETOX

Table A5. Full set of avlogEC50-parameters used in USEtox. For further details, refer to Chapter 4.4. Pesticide ASs that were not originally present in the database of PestLCI v.2.0, but that we added, are marked with †. Pesticide ASs that did not originally have USEtox CFs, but that we calculated, are marked with *.

Pesticide active substance	**avlogEC50**
Acetochlor (H)	-0.405
Alpha-cypermethrin (I)	-3.478
Ametryn (H) †	-0.455
Atrazine (H)	-0.514
Bentazone (H)	1.990
Beta-cyfluthrin (I) †	-4.603
Boscalid (F) †*	0.227
Carbofuran (N)	-0.759
Chlormequat-chloride (PGR)	2.045
Chlorothalonil (F)	-1.566
Chlorpyrifos (I)	-2.376
Chlorimuron-ethyl (H) †*	0.218
Chlorantraniliprole (I) †*	-0.291
Clethodim (H) †	0.715
Diflufenican (H)	1.345
Dimoxystrobin (F) †*	-1.758
Dimethenamid-P (H) †*	-0.613
Diuron (H)	-0.489
Epoxiconazole (F) †*	-0.576
Ethephon (PGR)	1.158
Etofenprox (I) †	0.432
Fenpropimorph (F)	0.284
Fipronil (I) †	-1.695
Florasulam (H) †*	0.634
Fluroxypyr 1-methylheptyl ester (H) †	-0.259
Flurtamone (H) †*	-0.381
Flufenacet (H) †	-0.584
Fluxapyroxad (Xemium) (F) †*	-0.055
Glyphosate isopropylamine salt (H) †	1.236
Hexazinone (H) †	-0.781
Imazapic (H) †*	0.599
Iodosulfuron methyl sodium (H) *	0.392
Lactofen (H) †*	-0.373
Lambda-cyhalothrin (I)	-4.465
MCPA dimethylamine salt (H) †	1.039
Mepiquat-chloride (PGR)	0.023
Mesosulfuron-methyl (H) †*	0.210
Metazachlor (H)	0.554
Metconazole (F) †*	0.194
Methomyl (I)	-0.489
Metrafenone (F) †*	-0.195
Paraquat (H) †	-0.890
Propyzamide (H)	0.794
Prothioconazole (F) †*	-0.214

Pyraclostrobin (F) †*	-1.558
Quinmerac (H) †	1.585
Quizalofop-P-ethyl (H) †*	-0.066
Tebuconazole (F)	-0.419
Tebuthiuron (H) †	0.187
Teflubenzuron (I) †	-1.347
Thiacloprid (I) *	0.632
Thiamethoxam (I) *	0.759
Trinexapac-ethyl (PGR)	0.818

Table A6. Full set of ecotoxic effect data used for calculation of new CFs in USEtox (ASs marked with * in Table A1). For further details, refer to Chapter 4.4. Additional sources in {} below table.

Trophic level	**Species**	**Days**	**EC(L)50, mg l^{-1}**		**Source**	**Log**
			chronic	**acute**		
Boscalid (F)						
Algae	*Pseudokirchneriella subcapitata, 2 tests*	3.4	1.12	2.24	{1}	0.05
Aquatic invertebrate	*Daphnia magna*	2	2.67	5.33	AGRITOX	0.43
Fish	*Oncorhynchus mykiss*	4	1.35	2.70	AGRITOX	0.13
Fish	*Lepomis macrochirus*	4	2.0	4.0	AGRITOX	0.30
Chlorimuron-ethyl (H)						
Aquatic plant	*Lemna gibba*	7	0.00023	0.00045	PPDB	-3.65
Aquatic invertebrate	*Daphnia magna, 2 tests*	2	50	100	PPDB, ECOTOX	1.70
Algae	*Chlorella pyrenoidosa*	4	15.31		ECOTOX	1.18
Algae	*Scenedesmus acutus*	4	11.83		ECOTOX	1.07
Algae	*Scenedesmus quadricauda*	4	0.10		ECOTOX	-1.00
Algae	*Chlorella vulgaris*	4	19.24		ECOTOX	1.28
Algae	*Pseudokirchneriella subcapitata*	4	5.53		ECOTOX	0.74
Fish	*Lepomis macrochirus*	4	1.0	2.0	TOXNET	0
Fish	*Oncorhynchus mykiss*	4	4.20	8.40	TOXNET	0.62
Chlorantraniliprole (I)						
Fish	Oncorhynchus mykiss	4	6.90	13.8	TOXNET	0.84
Aquatic invertebrate	*Daphnia magna, 5 tests*	2	0.003	0.007	AGRITOX, ECOTOX, OPP	-2.47
Aquatic plant	*Lemna Gibba*	14	2.00		AGRITOX	0.30
Algae	*Pseudokirchneriella subcapitata, 4 tests*	5	2.31		AGRITOX. ECOTOX	0.36
Aquatic invertebrate	*Centroptilum triangulifer*	2	0.01	0.01	AGRITOX	-2.24
Algae	*Anabaena flos-aquae*	N/A	1.00	2.00	OPP	0
Algae	*Navicula pelliculosa*	N/A	7.55	15.1	OPP	0.88
Algae	*Selenastrum capricornutum*	N/A	1.00	2.00	OPP	0
Dimoxystrobin (F)						
Algae	*Pseudokirchneriella subcapitata*	4	0.0085	0.017	AGRITOX	-2.07
Aquatic invertebrate	*Daphnia magna*	2	0.0197	0.0394	AGRITOX	-1.71
Fish	*Lepomis macrochirus*	4	0.0256	0.0512	AGRITOX	-1.59

Fish	*Oncorhynchus mykiss*	4	0.0217	0.0434	AGRITOX	-1.66
Dimethenamid-P						
Fish	*Oncorhynchus mykiss*	4	5	10	AGRITOX	0.70
Fish	*Lepomis macrochirus*	4	3.150	6.3	AGRITOX	0.50
Algae	*Raphidocelis subcapitata*	5	0.009	0.02	PPDB	-2.07
Aquatic invertebrate	*Daphnia magna*	2	6	12	AGRITOX, ECOTOX	0.78
Algae	*Anabaena flos-aquae, 2 tests*	5	0.304		AGRITOX, ECOTOX	-0.52
Aquatic plant	*Lemna gibba*	14	0.009		AGRITOX	-2.05
Algae	*Navicula pelliculosa*	5	0.340		AGRITOX	-0.47
Algae	*Pseudokirchneriella subcapitata*	5	0.017		AGRITOX	-1.77
Epoxiconazole (F)						
Aquatic plant	*Lemna gibba, 3 tests*	7	0.0047	0.0094	AGRITOX, PPDB	-2.33
Aquatic invertebrate	*Daphnia magna*	2.21	1.65	8.69	PPDB, AGRITOX	0.22
Algae	*Pseudokirchneriella subcapitata,* *2 tests*	3	1.72	3.45	AGRITOX, PPDB	0.24
Freshwater Insect	*Chironomus riparius*	28	0.06		AGRITOX	-1.20
Fish	*Oncorhynchus mykiss*	4	1.57	3.14	AGRITOX	0.20
Florasulam (H)						
Aquatic plant	*Lemna Gibba*	14	0.0012		AGRITOX	-2.93
Algae	*Navicula pelliculosa*	5	1.4		AGRITOX	0.14
Algae	*Pseudokirchneriella subcapitata*	3	0.0089		AGRITOX	-2.05
Algae	*Anabaena flos-aquae*	5	0.4		AGRITOX	-0.44
Aquatic invertebrate	*Daphnia magna*	2	146.0	292.0	AGRITOX	2.16
Aquatic invertebrate	*Palaemonetes pugio*	4	60.0	120	AGRITOX	1.78
Aquatic invertebrate	*Crassostrea virginica*	4	62.5	125	AGRITOX	1.80
Algae	*Selenastrum capricornutum*	4	21.6		OPP	1.33
Fish	*Oncorhynchus mykiss*	4	50.0	100.0	AGRITOX	1.70
Fish	*Lepomis macrochirus*	4	61.0	122	AGRITOX	1.79
Fish	*Menidia beryllina*	4	50.0	100	AGRITOX	1.70
Flurtamone (H)						
Aquatic plant	*Lemna gibba*	14	0.01		AGRITOX	-2.00
Algae	*Raphidocelis subcapitata*	3	0.01	0.02	AGRITOX, PPDB	-2.00
Aquatic invertebrate	*Daphnia magna*	2	6.5	13.0	AGRITOX	0.81
Fish	*Lepomis macrochirus*	4	5.5	11.0	AGRITOX	0.74
Fish	*Oncorhynchus mykiss*	4	3.50	7.00	AGRITOX	0.54
Fluxapyroxad (Xemium) (F)						
Aquatic invertebrate	*Daphnia magna, 2 tests*	2	13.28	26.55	AGRITOX, ECOTOX	1.12
Aquatic invertebrate	*Crassostrea virginica*	4	0.55	1.10	AGRITOX	-0.26
Algae	*Pseudokirchneriella subcapitata,* *2 tests*	3	1.04		AGRITOX, ECOTOX	0.02

Algae	*Anabaena flos-aquae*	3	1.38		AGRITOX	0.14
Algae	*Navicula pelliculosa*	3	2.31		AGRITOX	0.36
Aquatic plant	*Lemna gibba*	7	2.19		AGRITOX	0.34
Fish	*Cyprinus carpio*	4	0.15	0.29	AGRITOX	-0.84
Fish	*Lepomis macrochirus*	4	0.58	1.15	AGRITOX	-0.24
Fish	*Oncorhynchus mykiss*	4	0.27	0.55	AGRITOX	-0.56
Fish	*Pimephales promelas*	4	0.23	0.47	AGRITOX	-0.63
Imazapic (H)						
Aquatic invertebrate	*Daphnia magna, 2 tests*	2	48.99	97.98	{2}	1.69
Algae	*Pseudokirchneriella subcapitata*	3	0.03	0.05	PPDB	-1.59
Fish	*Oncorhynchus mykiss*	4	50	100	PPDB	1.70
Iodosulfuron methyl sodium (H)						
Aquatic invertebrate	*Daphnia magna, 2 tests*	2	46.61	93.22	AGRITOX, ECOTOX	1.67
Algae	*Navicula pelliculosa, 2 tests*	3.4	90.28		AGRITOX, ECOTOX	1.96
Algae	*Pseudokirchneriella subcapitata,* *2 test*	3.4	0.0536		AGRITOX, ECOTOX	-1.27
Aquatic plant	*Lemna sp.*	14	0.000762		AGRITOX, ECOTOX	-3.12
Algae	*Anabaena flosaquae*	4	1.30		ECOTOX	0.11
Fish	*Lepomis macrochirus*	4	50	100	AGRITOX	1.70
Fish	*Oncorhynchus mykiss*	4	50	100	AGRITOX	1.70
Lactofen (H)						
Aquatic invertebrate	*Daphnia magna, 7 tests*	2	1.09	2.18	{3}	0.04
Fish	*Lepomis macrochirus, 3 tests*	4	0.23	0.46	{4}	-0.64
Fish	*Oncorhynchus mykiss, 2 tests*	4	0.30	0.61	OPP, TOXNET	-0.52
Mesosulfuron-methyl (H)						
Aquatic invertebrate	*Daphnia magna, 2 tests*	2	47.49	94.97	AGRITOX, ECOTOX	1.68
Algae	*Pseudokirchneriella subcapitata*	3.4	0.14	0.20	{5}	-0.84
Aquatic plant	*Lemna gibba*	7	0.00031	0.00062	{6}	-3.51
Algae	*Navicula pelliculosa*	4	70.80		ECOTOX	1.85
Algae	*Anabaena flosaquae*	4	2.40		ECOTOX	0.38
Fish	*Oncorhynchus mykiss*	4	50	100	AGRITOX	1.70
Metconazole (F)						
Aquatic invertebrate	*Daphnia magna*	2	2.1	4.2	AGRITOX	0.32
Algae	*Pseudokirchneriella subcapitata*	3	1.7		AGRITOX	0.23
Insecta (invertebrate)	*Chironomus riparius*	28	1.6		OPP	0.20
Fish	*Oncorhynchus mykiss*	4	1.05	2.1	AGRITOX	0.02
Metrafenone (F)						
Aquatic invertebrate	*Daphnia magna*	2	0.46	0.92	AGRITOX	-0.34
Algae	*Pseudokirchneriella subcapitata*	3	0.71		AGRITOX	-0.15

Algae	*Navicula pelliculosa*	4	0.914		ECOTOX	-0.04
Algae	*Anabaena flosaquae*	4	0.862		ECOTOX	-0.06
Fish	*Oncorhynchus mykiss*	4	0.41	0.82	AGRITOX	-0.39
Prothioconazole (F)						
Aquatic plant	*Lemna gibba*	7	0.04	0.07	PPDB	-1.43
Algae	*Pseudokirchneriella subcapitata,* *2 tests*	3	0.77	1.55	{7}	-0.11
Aquatic invertebrate	*Daphnia magna*	2	0.65	1.30	AGRITOX	-0.19
Algae	*Selenastrurn capricornutum*	4	0.88		OPP	-0.06
Algae	*Navicula pelliculosa*	4	0.16		OPP	-0.79
Fish	*Cyprinus carpio*	4	3.46	6.91	AGRITOX	0.54
Fish	*Lepomis macrochirus*	4	2.30	4.59	AGRITOX	0.36
Fish	*Oncorhynchus mykiss*	4	0.92	1.83	AGRITOX	-0.04
Pyraclostrobin (F)						
Aquatic plant	*Lemna gibba*	7	0.860	1.720	PPDB	-0.07
Aquatic invertebrate	*Daphnia magna*	2	0.008	0.016	AGRITOX	-2.11
Algae	*Pseudokirchneriella subcapitata*	3	0.253	0.843	PPDB, AGRITOX	-0.60
Freshwater Molluscs	*Lampsilis siliquoidea, 3 tests*	4.1.2	0.052	0.105	ECOTOX	-1.28
Fish	*Lepomis macrochirus, 2 tests*	4	0.007	0.015	OPP, AGRITOX	-2.13
Fish	*Cyprinus carpio*	4	0.006	0.012	AGRITOX	-2.22
Fish	*Oncorhynchus mykiss*	4	0.003	0.006	AGRITOX	-2.51
Quizalofop-P-ethyl (H)						
Aquatic invertebrate	*Daphnia magna, 4 tests*	2	1.08	2.17	AGRITOX, PPDB, OPP ECOTOX	0.04
Algae	*Pseudokirchneriella subcapitata,* *4 tests*	3.5	0.57		AGRITOX, ECOTOX	-0.24
Algae	*Navicula pelliculosa, 3 tests*	3.5	0.42		AGRITOX, ECOTOX	-0.37
Aquatic plant	*Lemna gibba, 3 tests*	7. 14	0.17		AGRITOX, ECOTOX, OPP	-0.76
Algae	*Raphidocelis subcapitata*	3	0.85	1.70	PPDB	-0.07
Algae	*Scenedesmus acutus*	4	66.19		ECOTOX	1.82
Algae	*Chlorella vulgaris*	4	1.10		ECOTOX	0.04
Fish	*Lepomis macrochirus*	4	0.11	0.21	AGRITOX	-0.98
Thiacloprid (I)						
Aquatic plant	*Lemna gibba*	15	95.40		AGRITOX	1.98
Algae	*Scenedesmus subspicatus*	3	44.70		AGRITOX	1.65
Algae	*Pseudokirchneriella subcapitata*	5	60.60		AGRITOX	1.78
Aquatic invertebrate	*Daphnia magna*	2	42.55	85.10	AGRITOX	1.63
Aquatic invertebrate	*Hyalella azteca*	4	0.02	0.04	AGRITOX	-1.69
Freshwater Insect	*Cheumatopsyche brevilineata*	2	0.0026	0.0053	ECOTOX	-2.58
Fish	*Lepomis macrochirus*	4	12.60	25.20	AGRITOX	1.10
Fish	*Oncorhynchus mykiss*	4	15.25	30.50	AGRITOX	1.18

Thiamethoxam (I)						
Algae	*Pseudokirchneriella subcapitata*	3	82		AGRITOX	1.91
Algae	*Pseudokirchneriella subcapitata*	4	100		AGRITOX	2.00
Aquatic plant	*Lemna gibba*	7	45	90	PPDB	1.65
Aquatic invertebrate	*Crassostrea virginica*	4	60	119	AGRITOX	1.77
Aquatic invertebrate	*Daphnia magna*	2	50	100	AGRITOX	1.70
Aquatic invertebrate	*Daphnia pulex*	1	50	100	AGRITOX	1.70
Aquatic invertebrate	*Thamnocephalus platyurus*	1	50	100	AGRITOX	1.70
Aquatic invertebrate	*Mysidopsis bahia*	4	3	7	AGRITOX	0.54
Aquatic invertebrate	*Gammarus sp*	2	1	3	AGRITOX	0.15
Aquatic invertebrate	*Asellus aquaticus*	2	0	0	AGRITOX	-0.80
Aquatic invertebrate	*Ostracoda*	2	0	0	AGRITOX	-1.05
Aquatic invertebrate	*Lymnea stagnalis*	2	50	100	AGRITOX	1.70
Aquatic invertebrate	*Radix peregra*	2	50	100	AGRITOX	1.70
Aquatic invertebrate	*Chaoborus crystallinus*	2	4	7	AGRITOX	0.56
Aquatic invertebrate	*Crangonyx pseudogracillis, 2 tests*	2	0	1	AGRITOX	-0.40
Aquatic invertebrate	*Lymnea stagnalis*	2	50	100	AGRITOX	1.70
Freshwater insect	*Chironomus riparius, 3 tests*	2	0.02	0.05	AGRITOX, ECOTOX	-1.62
Aquatic invertebrate	*Dyticidae, 2 tests*	2	0.03	0.06	AGRITOX	-1.55
Aquatic invertebrate	*Cloeon dipterum, 2 tests*	2	0.02	0.03	AGRITOX	-1.82
Aquatic invertebrate	*Brachionus calyciflorus*	1	50	100	AGRITOX	1.70
Fish	*Lepomis macrochirus*	4	57	114	TOXNET	1.76
Fish	*Oncorhynchus mykiss*	4	50	100	TOXNET	1.70

{1} PPDB, AGRITOX & http://ec.europa.eu/food/plant/protection/evaluation/newactive/boscalid.pdf
{2} PPDB & http://efw.bpa.gov/environmental_services/Document_Library/Vegetation_Management/sheets/Imazapic.pdf
{3} OPP, PPDB, ECOTOX & http://www.epa.gov/oppsrrd1/registration_review/lactofen/lactofen_summary.pdf
{4} OPP, TOXNET & http://www.epa.gov/oppsrrd1/registration_review/lactofen/lactofen_summary.pdf
{5} ECOTOX & http://ec.europa.eu/food/plant/protection/evaluation/newactive/mesosulfuron_en.pdf
{6} http://ec.europa.eu/food/plant/protection/evaluation/newactive/mesosulfuron_en.pdf
{7} PPDB and http://www.bayercropscience.co.uk/assets/Uploads/Redigo_Twin.pdf

APPENDIX 6. REGIONALIZATION OF PESTLCI: CLIMATE DATA

Table A7. The full climate data sets for the five studied regions. Refer to Chapter 4.3 for further details.

	Sao Paulo, Brazil	**Mato Grosso, Brazil**	**South Central Sweden**	**Northern Germany**	**Iowa, USA**
Latitude (degrees)	21.29 S	14.24 S	58.2	53.38 N	42.55 N
Longitude (degrees, E+ W-)	47.33 W	56.27 W	15.3	10.0 E	92.4 W
Elevation (m)	620	400	80	15	300
TG jan (degC)	23.8	24	-1.8	0.5	-7.5
TG feb (degC)	24	27	-2.3	1.1	-4.78
TG mar (degC)	23.5	24.3	0.5	3.7	2.11
TG apr (degC)	22.1	27.7	6.2	7.3	9.39
TG may (degC)	19.6	24.4	11.1	12.2	15.8
TG jun (degC)	17.6	25.4	14.5	15.5	21.1
TG jul (degC)	17.8	24.5	17.3	16.8	23.1
TG aug (degC)	20.1	24.7	16.3	16.6	21.78
TG sept (degC)	21.5	25.3	11.9	13.5	17.2
TG oct (degC)	23.1	24.5	6.8	9.7	10.1
TG nov (degC)	23.6	25	2.7	5.1	2.38
TG dec (degC)	23.6	25.5	-0.8	1.9	-5.4
TG average (degC)	21.7	25.2	6.9	8.7	8.8
TMIN jan (degC)	19.7	20.4	-4.8	-2.2	-12.5
TMIN feb (degC)	19.7	21.2	-5.4	-1.8	-9.6
TMIN mar (degC)	18.7	20.4	-3.8	0.4	-3.3
TMIN apr (degC)	17.3	20.4	0.6	3.0	2.89
TMIN may (degC)	14.3	19.1	5.1	7.2	9.4
TMIN jun (degC)	11.6	15.1	8.6	10.4	14.9
TMIN jul (degC)	11.4	16.4	11.9	12.2	17.1
TMIN aug (degC)	13.2	19.1	11.4	11.9	15.67
TMIN sept (degC)	15.6	19.5	7.3	9.4	10.38
TMIN oct (degC)	17.4	20.8	3.2	6.3	3.72
TMIN nov (degC)	18.6	21.8	-0.1	2.5	-2.8
TMIN dec (degC)	19.4	19.9	-3.6	-0.7	-10.27
TMIN average (degC)	16.4	19.5	2.6	4.9	3.0
TMAX jan (degC)	29.8	32.3	0.8	2.7	-2.5
TMAX feb (degC)	30.6	31.6	0.9	3.8	0.11
TMAX mar (degC)	30.3	31.4	4.6	7.2	7.5
TMAX apr (degC)	29.0	33.6	11.7	11.9	15.8
TMAX may (degC)	27.0	31.5	16.6	17.0	22.2
TMAX jun (degC)	25.9	32.1	20.2	20.2	27.33
TMAX jul (degC)	26.3	32.8	22.5	21.4	29.11
TMAX aug (degC)	28.4	34.9	21.3	21.6	27.8
TMAX sept (degC)	29.0	32.5	16.7	18.0	24.1
TMAX oct (degC)	30.5	32.2	10.3	13.3	16.6
TMAX nov (degC)	30.3	32.9	5.2	7.6	7.72
TMAX dec (degC)	29.4	32.9	1.7	4.0	-0.67
TMAX average (degC)	28.86	32.56	11.10	12.44	14.66
Rainfall Jan (mm)	245.5	268.1	34.0	61.0	21.1
Rainfall Feb (mm)	172.6	235.5	30.8	41.0	25.2
Rainfall Mar (mm)	155.4	203.4	22.7	56.0	52.3

Rainfall Apr (mm)	84.3	137.8	37.8	51.0	94.2
Rainfall May (mm)	77.1	55.5	41.9	57.0	115.1
Rainfall Jun (mm)	31.1	9.5	57.8	74.0	126.5
Rainfall Jul (mm)	27.6	6.9	73.1	82.0	124.7
Rainfall Aug (mm)	28.2	27.3	47.1	70.0	108.5
Rainfall Sep (mm)	69.3	72.2	60.9	70.0	66.8
Rainfall Oct (mm)	127.9	151.1	44.4	63.0	63.0
Rainfall Nov (mm)	182.9	204.5	43.6	71.0	51.1
Rainfall Dec (mm)	264.5	248.0	41.4	72.0	30.5
Total rainfall year (mm)	1466	1620	536	768	879
Rain days (>1mm) Jan	20	24	8	12	11
Rain days (>1mm) Feb	16	20	7	9	10
Rain days (>1mm) Mar	15	22	6	11	13
Rain days (>1mm) Apr	9	16	7	10	16
Rain days (>1mm) May (mm)	7	8	7	10	18
Rain days (>1mm) Jun (mm)	3	3	11	11	15
Rain days (>1mm) Jul (mm)	3	2	9	12	14
Rain days (>1mm) Aug (mm)	4	3	9	11	16
Rain days (>1mm) Sep (mm)	8	7	9	11	13
Rain days (>1mm) Oct (mm)	11	16	8	10	12
Rain days (>1mm) Nov (mm)	15	20	10	12	11
Rain days (>1mm) Dec (mm)	19	23	9	12	11
Rain days (>1mm) Average (mm)	10.81	13.63	8.36	10.93	13.35
Average rainfall on rainy day Jan (mm)	12.3	11.2	4.3	5.1	1.9
Average rainfall on rainy day Feb (mm)	10.8	11.8	4.3	4.6	2.5
Average rainfall on rainy day Mar (mm)	10.4	9.2	3.6	5.1	4.0
Average rainfall on rainy day Apr (mm)	9.4	8.6	5.3	5.1	5.9
Average rainfall on rainy day May (mm)	11.0	6.9	6.1	5.7	6.4
Average rainfall on rainy day Jun (mm)	10.4	3.2	5.4	6.7	8.4
Average rainfall on rainy day Jul (mm)	9.2	3.5	8.6	6.8	8.9
Average rainfall on rainy day Aug (mm)	7.1	9.1	5.1	6.4	6.8
Average rainfall on rainy day Sep (mm)	8.7	10.3	6.8	6.4	5.1
Average rainfall on rainy day Oct (mm)	11.6	9.4	5.3	6.3	5.2
Average rainfall on rainy day Nov (mm)	12.2	10.2	4.3	5.9	4.6
Average rainfall on rainy day Dec (mm)	13.9	10.8	4.7	6.0	2.8
Average rainfall on rainy day Average (mm)	10.6	8.7	5.3	5.8	5.2
Rain frequency Jan (day-1)	1.6	1.3	3.9	2.6	2.8
Rain frequency Feb (day-1)	1.8	1.4	3.9	3.1	2.8
Rain frequency Mar (day-1)	2.1	1.4	4.9	2.8	2.4
Rain frequency Apr (day-1)	3.3	1.9	4.2	3.0	1.9
Rain frequency May (day-1)	4.4	3.9	4.5	3.1	1.7
Rain frequency Jun (day-1)	10.0	10.0	2.8	2.7	2.0
Rain frequency Jul (day-1)	10.3	15.5	3.6	2.6	2.2
Rain frequency Aug (day-1)	7.8	10.3	3.3	2.8	1.9
Rain frequency Sep (day-1)	3.8	4.3	3.3	2.7	2.3
Rain frequency Oct (day-1)	2.8	1.9	3.7	3.1	2.6
Rain frequency Nov (day-1)	2.0	1.5	3.0	2.5	2.7
Rain frequency Dec (day-1)	1.6	1.3	3.5	2.6	2.8
Rain frequency Average (day-1)	4.299	4.59	3.736	2.802	2.346
Annual potential evaporation (mm)	1065	1426	593	618	686
Solar irradiation Jan (Wh m-2 day-1)	7077	5920	313	568	1930

Solar irradiation Feb (Wh m-2 day-1)	5882	5175	910	1190	2800
Solar irradiation Mar (Wh m-2 day-1)	5496	5140	1880	2480	3620
Solar irradiation Apr (Wh m-2 day-1)	5433	5340	3360	4270	5000
Solar irradiation May (Wh m-2 day-1)	4369	5039	5080	5180	5800
Solar irradiation Jun (Wh m-2 day-1)	3617	3969	5240	5410	6440
Solar irradiation Jul (Wh m-2 day-1)	3342	4441	5050	5100	6380
Solar irradiation Aug (Wh m-2 day-1)	4941	5351	4165	4240	5490
Solar irradiation Sep (Wh m-2 day-1)	5796	5807	2490	3030	4280
Solar irradiation Oct (Wh m-2 day-1)	6728	6003	1210	1690	3050
Solar irradiation Nov (Wh m-2 day-1)	6564	5820	198	719	1870
Solar irradiation Dec (Wh m-2 day-1)	6255	5484	231	578	1610
Solar irradiation Average (Wh m-2 day-1)	5456	5292	2520	2880	4028

APPENDIX 7. REGIONALIZATION OF PESTLCI: SOIL DATA

Table A8. The full soil data sets for the five studied regions. Refer to Chapter 4.3 for further details.

	São Paulo, Brazil	**Mato Grosso, Brazil**	**Iowa, USA**	**Northern Germany**	**South Central Sweden**
start layer 1 (m)	0	0	0	0	0
start layer 2 (m)	0.25	0.20	0.20	0.14	0.20
start layer 3 (m)	0.50	0.40	0.33	0.47	0.30
start layer 4 (m)	1	0.60	0.53	0.91	0.50
start layer 5 (m)		1	0.76	1	0.70
start layer 6 (m)			1		1
start layer 7 (m)					
pH layer 1	6	6	6.10	6	6.40
pH layer 2	5.50	5.30	6.40	5.60	6.80
pH layer 3	5.30	5.60	6.20	5.30	7
pH layer 4		5.70	6	5	7.40
pH layer 5			6.10		7.60
pH layer 6					
pH layer 7					
f(clay) layer 1	0.33	0.43	0.31	0.16	0.41
f(silt) layer 1	0.15	0.02	0.66	0.37	0.36
f(sand) layer 1	0.52	0.55	0.03	0.47	0.23
f(clay) layer 2	0.36	0.49	0.34	0.25	0.48
f(silt) layer 2	0.13	0.10	0.63	0.33	0.35
f(sand) layer 2	0.52	0.41	0.03	0.42	0.17
f(clay) layer 3	0.36	0.54	0.33	0.29	0.41
f(silt) layer 3	0.10	0.07	0.63	0.31	0.43
f(sand) layer 3	0.54	0.39	0.04	0.40	0.16
f(clay) layer 4		0.53	0.31	0.27	0.37
f(silt) layer 4		0.08	0.65	0.31	0.39
f(sand) layer 4		0.39	0.04	0.42	0.24
f(clay) layer 5			0.27		0.30
f(silt) layer 5			0.67		0.33
f(sand) layer 5			0.06		0.37
f(clay) layer 6					
f(silt) layer 6					
f(sand) layer 6					
f(OC) layer 1 %	1.14	2.70	2.32	2.10	2.32
f(OC) layer 2 %	0.84	1	1.32	0.60	1.50
f(OC) layer 3 %	1.16	0.70	0.79	0.30	0.50
f(OC) layer 4 %		0.50	0.40	0.20	0.40
f(OC) layer 5 %			0.23		0.40
f(OC) layer 6 %					
Soil bulk density	1450	1350	1500	1577	1400
Name layer 1	N/A	N/A	Ap	Au	N/A
Name layer 2	N/A	AB	Bt1	E	N/A
Name layer 3	BA	Bo1	Bt2	Btw	N/A
Name layer 4		Bo2	Bt3	Cbt	N/A
Name layer 5			Bt4		N/A

APPENDIX 8. SENSITIVITY ANALYSIS - DEFAULT SOIL

Table A9. Default soil used in the soil sensitivity analysis (see Chapter 6.4).

Soil property	**Value**
No of horizons modeled	4
Uniform horizon depth (cm)	25
pH-H_2O top layer / average	5.3 / 6.4
Sand (%) top layer / average (particles > 50 µm)	46 / 44.5
Silt (%) top layer / average (particles 2-50 µm)	36 / 32
Clay (%) top layer / average (particles < 2 µm)	18 / 23.5
Organic carbon (%) top layer / average	2.8 / 2.4
Soil bulk density (kg m^{-3})	1490

ACKNOWLEDGEMENTS

We would like to thank the following persons and organizations for data provision and consultation: R.Barizon, Brazilian Agricultural Research Corporation, EMBRAPA; O. Cavelett and M. Galdos, theBrazilian Bioethanol Science and Technology Laboratory (CTBE);H. J. Gleser, theChamber of Agriculture in Schleswig-Holstein; S.Azevedo, The Mato Grosso State Soy and Corn Producers Association (APROSOJA); D. Meyer, Round Table of Responsible Soy; N. Yngveson, Swedish Rural Economy and Agricultural Societies Malmöhus, Sweden; G. Sparovek,University of São Paulo and CTBE, andManoel Regis Lima Verde Leal, CTBE.A special thanks to T. J. Dijkman,Technical University of Denmark,for support with modeling in PestLCI, and to Natalie Hunt and Jason Hill for their review and feedback that helped us to improve the report.Financial support from IEA Bioenergy Task 43 is gratefully acknowledged.

IEA Bioenergy

IEA Bioenergy is an international collaboration set up in 1978 by the IEA to improve international co-operation and information exchange between national RD&D bioenergy programmes. IEA Bioenergy's vision is to achieve a substantial bioenergy contribution to future global energy demands by accelerating the production and use of environmentally sound, socially accepted and cost-competitive bioenergy on a sustainable basis, thus providing increased security of supply whilst reducing greenhouse gas emissions from energy use. Currently IEA Bioenergy has 22 Members and is operating on the basis of 13 Tasks covering all aspects of the bioenergy chain, from resource to the supply of energy services to the consumer.

IEA Bioenergy Task 43 – Biomass Feedstock for Energy Markets – seeks to promote sound bioenergy development that is driven by well-informed decisions in business, governments and elsewhere. This will be achieved by providing to relevant actors timely and topical analyses, syntheses and conclusions on all fields related to biomass feedstock, including biomass markets and the socioeconomic and environmental consequences of feedstock production. Task 43 currently (2013-2015) has 13 participating countries: Australia, Canada, Croatia, Denmark, European Commission - Joint Research Centre, Finland, Germany, Ireland, Netherlands, Norway, Sweden, UK, USA.

Further Information

Task 43
Website www.ieabioenergytask43.org
Göran Berndes – Task leader
Email: goran.berndes@chalmers.se
Tat Smith – Associate Task Leader
Email: tat.smith@utoronto.ca

IEA Bioenergy Secretariat
Website: www.ieabioenergy.com
Pearse Buckley – Secretary
Email: pbuckley@odbtbioenergy.com
Arthur Wellinger – Technical Coordinator
Email: wellinger@triple-e-und-m.ch

iea Energy Technology Network