Title

Freshwater Ecotoxicity in Mexico: Evaluating the Environmental Impact of Insec6cides of an Agricultural Extension Project



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Publication Date

2024

Peer reviewed|Thesis/dissertation

# Freshwater Ecotoxicity in Mexico:
# Evaluating the Environmental Impact of Insecticides of an Agricultural Extension Project

By

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THESIS

Submitted in partial satisfaction of the requirements for the degree of

MASTER OF SCIENCE

in

International Agricultural Development

in the

OFFICE OF GRADUATE STUDIES

of the

UNIVERSITY OF CALIFORNIA

DAVIS

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2024

**Abstract**

This thesis assesses the environmental impact of insecticides applied during a 10-year extension project conducted across Mexico by the International Maize and Wheat Improvement Center (CIMMYT). Utilizing the internationally recognized USEtox model, we calculated the freshwater ecotoxicity of over 46,000 applications of insecticides from a dataset collected by CIMMYT since 2012. The database not only includes information on active ingredients applied but also on management practices and two extension approaches: traditional extension services and so-called innovation modules, which involve side-by-side comparisons of conventional and recommended applications of insecticides. This study provides a unique opportunity to apply USEtox to real-life data that has been collected over more than a decade, using it as a tool to evaluate an extension project.

Results reveal substantial variability in terms of the ecotoxicity of active ingredients applied, with some active ingredients being substantially toxic even in small doses applied compared to other active ingredients, highlighting the importance of including as much data in impact assessments as possible. Not only did we calculate the most and least toxic active ingredients, but we also plotted trends over time. These revealed partial success in reducing the environmental footprint of the extension effort. Additionally, we could show which management practices and extension modes were associated with lower freshwater ecotoxicity scores. This study not only contributes to advancing the application of USEtox in real-life scenarios but also highlights the importance of field-based data and standardized models to make recommendations for agricultural pest management practices to lower their impact on the environment.

# Acknowledgments

First of all, I want to thank my project partner Simon Fonteyne, alongside all the farmers, extension agents, and staff at CIMMYT who participated in and worked on this project for more than a decade, for all their dedication and efforts, and for showing me the importance of collaboration and perseverance in achieving sustainable agricultural practices. I also want to thank my committee, Louise, Alissa, and Gina, for their guidance, feedback, and support throughout the project. Special thanks go to Cam, who initiated the project and provided his initial guidance. In addition, I want to thank GFAD and UC Davis' Jastro Shields Award for making it possible to travel to Mexico, meet with our project partners, and experience agricultural research for development firsthand. I also feel grateful for the support of Fulbright Austria, which enabled me to step out of my comfort zone and come to California—my time here at UC Davis has been a learning experience full of ups and downs, shaping me both professionally and personally. Lastly, I want to thank my family, friends, and my partner Lukas for their unwavering care and support throughout every step of this journey, making my time here at UC Davis so special. Never in my wildest dreams would I have imagined becoming a part of such an inspiring community and learning so much. ... Go Aggies!

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# 1 Introduction

Agriculture has become one of the main drivers for humanity to transgress the planetary boundaries, defined as different Earth system processes that once crossed could lead to detrimental environmental shifts threatening human development [Campbell et al., 2017, p.1]. Rockström et al. [Campbell et al., 2017, p.1,2] introduced the concept of these planetary boundaries to emphasize that continuous human development is only possible within a narrow'safe operating space', marked by the planetary boundaries [Diamond et al., 2015, p.9]. Some of these planetary boundaries include land use change, freshwater use, or disruption of biochemical flows, such as the nitrogen or phosphorus cycle [Campbell et al., 2017, p.1,2]. Agriculture has, like no other sector, contributed to the loss of biodiversity, another boundary that humanity has already crossed [Campbell et al., 2017, p.4]. This could be partly explained by the high rates of synthetic pesticides applied worldwide, another planetary boundary proposed by Rockström et al. [Diamond et al., 2015, p.13]. Even though these detrimental effects have been known for decades, pesticides still remain widely used in agriculture [Campbell et al., 2017, p.13]. Therefore, substituting pesticides with less toxic substances and promoting the sustainable use of pesticides are the key strategies to preserve Earth's biophysical integrity [Diamond et al., 2015, p.13].

CIMMYT, the International Maize and Wheat Improvement Center, is heavily involved in promoting sustainable agricultural practices to foster rural development while also reducing the environmental footprint of agriculture. This commitment is not only carried out through various research but also through numerous extension projects. This paper will focus on one of these projects addressing the overuse of synthetic insecticides. More than a decade ago, the excessive application of highly toxic insecticides caught CIMMYT's attention, prompting an effort to mitigate the environmental impact of chemical pest control. The goal was to promote less toxic alternatives— synthetic insecticides and bioinsecticides— to lower the environmental footprint of farming communities in Mexico. Two different extension approaches were chosen— the 'classical' extension approach, in which farmers were advised by CIMMYT's extension agents. The other one involved closer collaboration between farmers and extension agents, by assorting plots with two different treatments close to each other— one with the usual pest control management of farmers (*parcela testigo*) and one with CIMMYT's recommendations (*parcela innovation*). This approach is called innovation modules. Even though this project has been carried out for over ten years, with many different farmers involved throughout Mexico, the success of this project remains unclear. Therefore, the primary goal of this paper is a comprehensive evaluation of the described project in terms of its environmental impact.

In order to provide an in-depth assessment, this study addresses the following questions: Which chemicals promoted by CIMMYT inhibit the highest and the lowest toxicity levels? How have toxicity levels of the project evolved over time? Do different modes of action have a tendency to have higher or lower levels of toxicity? Are the different management practices and extension efforts associated with higher or lower toxicity levels? In order to assess toxicity levels, USEtox was selected to calculate the freshwater ecotoxicity of each application recorded by CIMMYT. USEtox is an internationally renowned model that standardizes the calculation of different freshwater ecotoxicity models, providing a consistent approach to quantify the environmental impact of chemicals [Fantke et al., 2015]. USEtox allows the calculation for the environmental impact of chemicals only in freshwater ecosystems–freshwater ecotoxicity. Current efforts include the expansion to other environmental compartments, further increasing its applicability for other impact assessments [Fantke et al., 2015]. In order to assess how different extension approaches and management practices are correlated with freshwater ecotoxicity, a multilinear regression model was developed. This model includes a range of variables, including plot size, production cycle (summer and winter), hydrological regime (irrigation or rainfed), conservation agriculture, intercropping, and the different extension modes, and how they affect ecotoxicity per hectare.

The significance of this paper extends beyond the CIMMYT's project alone. Studies aiming at evaluating the environmental impact of pesticides have been applied to national sales data in a specific country. In contrast, this paper will apply USEtox to data recorded in the field, therefore adding a new dimension of USEtox by providing a more precise toxicity assessment in a practical scenario with real-life data. The collected dataset comprised over 46,000 entries—this level of detail will enable a more nuanced and accurate explanation of toxicity levels compared to aggregated national sales data. Furthermore, no data is available on the types and amounts of specific insecticides used by Mexican farmers. This gap further represents a barrier to fully understanding the environmental impacts of insecticide use and the development of mitigation strategies or recommendations for using specific insecticides.

Another layer of impact assessment with USEtox will be added by also assessing whether management practices and extension approaches are associated with higher or lower levels of freshwater ecotoxicity. By exploring the relationship between management practices, extension strategies, and ecotoxicity, this paper aims to provide a broader application of USEtox. We want to highlight the potential of USEtox as a tool that can guide extension agents to find and promote insecticides that lower the environmental impact of agriculture, as well as finding the extension approach that is most successful in doing so. No study exists comparing CIMMYT's conventional extension approaches and CIMMYT's innovation modules; therefore, we are hoping to contribute to filling this knowledge gap. This will demonstrate the broader applicability of USEtox beyond traditional impact assessment, highlighting that it can be a framework for addressing and solving environmental challenges in agriculture and extension services. It will also underscore the essential role of robust data and standardized impact assessment tools in order to direct agriculture in a way that it is compatible with the planetary boundaries, respecting ecosystems and supporting sustainable development. In the following chapters, we will provide an overview of relevant literature, materials, and methods used. We will present our results, followed by a discussion about their implications.

# 2 Background

The current chapter will provide background information about the maize production in Mexico, important insect pests, and ways to control them. After providing background information about pesticide use in Mexico, we will provide an overview of impact assessment in pesticides, as well as USEtox. Lastly, we will introduce the International Maize and Wheat Improvement Center and their extension approaches.

## 2.1 Maize Production and Significance in Mexico

### 2.1.1 The Origins and Significance of Maize in Mexico

Ever since its domestication over 7,000 years ago, maize (Zea mays) has become one of the most widely grown crops worldwide, tremendously impacting the global agri-food system [Erenstein et al., 2022, p.1295]. Also known as corn, maize has played a major role in feeding humanity, both as a direct source of nourishment and as a feed for livestock [Erenstein et al., 2022, p.1295]. Only a handful of cereals (including wheat, rice, and maize) provide almost 50% of the global food calories, showing the significance of this crop class compared to other food classes [Ranum et al., 2014, p.105]. Maize therefore plays a crucial role in food security worldwide, especially because of global challenges such as a growing world population or climate change [Langner et al., 2019, p.649].

Like other cereals, maize (*Zea mays*) is a grass and belongs to the family *Poaceae* (*Gramineae*), tribe *Maydeae* [García-Lara and Serna-Saldivar, 2019, p.1]. Through archaeological records and genetic studies, it is possible to reconstruct the history of maize [Ranum et al., 2014, p.104]. The most recognized theory of domestication is that maize evolved directly from teosinte [García-Lara and Serna-Saldivar, 2019, p.4]. Three reasons support this theory: first, both maize and teosinte have the exact same number of chromosomes [García-Lara and Serna-Saldivar, 2019, p.4]. Second, both share many morphological and structural similarities, including their pollen [García-Lara and Serna-Saldivar, 2019, p.4]. Lastly, the frequent cross-breeding between maize and teosinte, that also occurs in nature [García-Lara and Serna-Saldivar, 2019, p.4]. Others suggest that maize could be a hybrid between teosinte and another wild grass species [Ranum et al., 2014, p.106].

Its wild ancestor, teosinte, is believed to originate in Southern Mexico, where people started to form a symbiotic relationship with teosinte around 9,000 years ago [Langner et al., 2019, p.649]. Archaeological sites reveal early records of this relationship formed between the people and teosinte in the Mexican states of Puebla, Oaxaca, and Mexico [García-Lara and Serna-Saldivar, 2019, p.4], where small cobs were found in caves, estimated to be around 5,000 years old [Ranum et al., 2014, p.106]. By selecting those varieties that fit best the needs of the people and the environment, people have evolved teosinte to a crop with large cobs only within a few thousand years [Ranum et al., 2014, p.106]. Breeding teosinte into a crop carrying a tiny corn ear with a length of 3 cm took less than 200 years, and through time, cobs grew longer and larger, carrying more kernels in more rows [García-Lara and Serna-Saldivar, 2019, p.4]. Its domestication was carried out only a little later compared to wheat and rice, and spread rapidly throughout the Americas and the Caribbean because of its adaptability to different climates and environmental conditions [Ranum et al., 2014, p.106]. It can grow in tropical, subtropical, and temperate regions, with high and low amounts of precipitation, in high and low altitudes [Ranum et al., 2014, p.106-107].

Kernels could be dried, which made them suitable for storage, and were ground up together with calcium hydroxide (lime and water) in order to make the hard kernels more easily digestible [Ranum et al., 2014, p.106]. This process - called *nixtamalization* - also helped to make the vitamin B3 available to native people in Latin America [Ranum et al., 2014, p.106]. Through human selection, teosinte has evolved into one of the most fundamental sources of food for many peoples in the Americas, such as the Incas, Aztecs, and Mayas [Langner et al., 2019, p.649]. Moreover, people of the Americas and maize co-evolved over time and became dependent on each other - people became dependent on maize as a staple food, and maize became dependent on people for seeding, since its seeds would not shatter on their own from the cobs [Ranum et al., 2014, p.106].

However, almost no country in the world has a higher caloric income per capita and day than the country that is considered the origin of maize - Mexico [Ranum et al., 2014, p.106]. Maize is much more than a staple food for the Mexican people — it is deeply embedded in social, economic, and religious practices due to its long history that is deeply intertwined with the country and its people [CONABIO et al., 2017, p.12]. Maize has shaped the cultural diversity and identity of the Mexican people unlike any other crop, and is even linked to myths of origin by Mexicans [CONABIO et al., 2017, p.12]. It is grown throughout the country, and is a fixed component of the Mexican diet with a tremendous culinary variety [CONABIO et al., 2017, p.12].

### 2.1.2 Production Statistics

As mentioned above, maize is deeply embedded in Mexico's agricultural system. For the past five years (from 2020/2021 to 2024/2025), the average yield per year was around 25 million tons [USDA, s.a.], making it one of the top 8 maize-producing countries worldwide [Erenstein et al., 2022, p.1299]. Mexico is a country with a high yield potential, but belongs to the countries with the highest yield gap, and therefore relies on imports to satisfy its demand for maize [CONABIO et al., 2017, p.45, 145]. The average yield of the same time frame equals 3.9 tons per hectare [USDA, s.a.], which is below the global average yield per hectare. Because of Mexico's diverse environments, soils, and climate, maize can be grown in Mexico all year round, with two main growing seasons [USDA, s.a.]. 30% of the annual maize production is grown during the winter - planting takes place between November and February, the harvest between April and July) [USDA, s.a.]. The majority of the maize - around 70% - is grown during the summer growing season [USDA, s.a.]. Planting usually takes place between April and August, and between October and February is the time of harvest [USDA, s.a.]. A tremendous variety of different races of maize is grown throughout the country, under diverse biophysical conditions, ranging from tropical rain forests, to temperate, and arid conditions [Ibarrola-Rivas et al., 2020, p.2]. This versatility is a major contributor to the significance of maize in the Mexican diet [Ibarrola-Rivas et al., 2020, p.2].

The majority of maize production in terms of absolute numbers, however, is concentrated in a few states - the top producing states of white maize are Sinaloa, Jalisco, México, Michoacán, and Guanajuato, with a production of 5.3, 2.9, 2.0, 1.8, and 1.5 tons, respectively [Zahniser et al., 2019, p.11]. White maize is the predominant phenotype cultivated in Mexico, and plays a crucial role in Mexico's food security [CONABIO et al., 2017, p.146]. One-fourth is produced for self-consumption, and almost 60% of the total white maize produced is used to be processed in the food industry [CONABIO et al., 2017, p.146]. Sinaloa has become the most important state for the production of white maize, reaching yields of over 10 tons per hectare [CONABIO et al., 2017, p.145]. These high yields can be explained by the structure of Sinaloa's agriculture - most maize is produced under irrigation and in large farms for commercial purposes [CONABIO et al., 2017, p.146]. Together with Jalisco, over 30% of Mexico's white maize is produced in these two states [CONABIO et al., 2017, p.146]. Yellow maize, in contrast, makes up only 5% of the annual production [CONABIO et al., 2017, p.146].

### 2.1.3 Production Systems and Their Characteristics

The agricultural landscape in Mexico could not be any more heterogeneous - especially when it comes to the production of maize [Ibarrola-Rivas et al., 2020, p.3]. Multiple different climate zones, differing in terms of temperature, precipitation, seasonality, soil types as well as altitudes and terrain are just a few factors that add layers of complexity in the production of maize. Social and economic factors are also contributing to the heterogeneity of the production system, with small-holder farmers on one end of the extremes, and large-scale farmers on the other [Ibarrola-Rivas et al., 2020, p.3]. Maize is cultivated in a variety of production systems, ranging from traditional to conventional, industrialized systems [CONABIO et al., 2017, p.146]. Today, small subsistence farms coexist with large, market-oriented farms [Ibarrola-Rivas et al., 2020, p.3]. Between these two extremes, medium-scale farmers can be found with both elements of this spectrum [Ibarrola-Rivas et al., 2020, p.4]. However, the boundaries of these categories are fluid, meaning that elements that are usually typical for one group can also be found in other groups [Ibarrola-Rivas et al., 2020, p.4]. The main distinguishing feature often defined by researchers is the area of land cultivated by farmers [Ibarrola-Rivas et al., 2020, p.4].

In their study on the different maize production systems in Mexico, Ibarrola-Rivas et al. [2020, p.4] revealed the complexity and diversity of the farming communities in Mexico that are growing maize. Ibarrola-Rivas et al. [2020, p.4] defined these groups in terms of the land cultivated: small-holders producing on less than 2 hectares, medium-scale farmers on land ranging between 2 and 5 hectares, and large-scale farmers producing on more than 50 hectares. (Out of all the farmers cultivating maize, the authors only looked at these 3 groups, leaving out the farms that range in between these farm sizes, in order to exemplify the differences in the Mexican agricultural system [Ibarrola-Rivas et al., 2020, p.4].) In 2020, farmers growing maize consisted of 40% small-scale, 19% medium-scale, and around 4% large-scale farmers out of all farmers in Mexico, producing 2%, 7%, and 66% of the maize cultivated in Mexico, respectively [Ibarrola-Rivas et al., 2020, p.4].

In their study, Ibarrola-Rivas et al. [2020, p.1] also displays other differences between these groups mentioned above. Small-scale farmers are concentrated in Southern states, where tropical conditions predominate [Ibarrola-Rivas et al., 2020, p.10]. The vast majority of small-scale farmers produce partly on land under social tenure (called "*ejido*"), use native seeds, and produce under rainfed conditions [Ibarrola-Rivas et al., 2020, p.6,7]. In addition, this group relies on unpaid family work the most out of the three [Ibarrola-Rivas et al., 2020, p.6,7]. In the traditional *milpa* system, characterized by intercropping and a system where genetic diversity of maize is preserved, is also common in this group [Ureta et al., 2020, p.2]. Despite the fact that yields are lower in the *milpa* system, it delivers a staple source of food, especially in regions unfit for mechanization [CONABIO et al., 2017, p.145]. In contrast, most of the land cultivated by large-scale farmers is privately owned, cultivated with commercial seeds, and irrigated [Ibarrola-Rivas et al., 2020, p.6,7]. The biggest difference between the groups is the focus on self-sufficiency by small-scale farmers compared to large-scale farmers [Ibarrola-Rivas et al., 2020, p.15]. In small-scale systems, more than half of the maize produced is usually used for consumption by the household or feed for animals [Ibarrola-Rivas et al., 2020, p. 10]. Large-scale farmers produce primarily for domestic and international markets and have therefore primarily commercial interests in mind [Ibarrola-Rivas et al., 2020, p. 15]. Those fundamental principles also correspond with the economic income of the different groups, revealing a huge gap in terms of economic opportunities [Ibarrola-Rivas et al., 2020, p. 2]. These economic disparities highlight the different needs that are represented in the agricultural sector, within and among different farming communities.

One aspect that is prevalent in all groups is the application of agrochemicals throughout the whole spectrum [González, 2018, p.54]. This is not only the case in terms of fertilizers, but also in terms of pesticides [Ibarrola-Rivas et al., 2020, p.7]. In their study, around 90% of the total planted area by large-scale farmers was sprayed with herbicides, around 85% with insecticides [Ibarrola-Rivas et al., 2020, p.7]. Two-thirds of the total area cultivated by medium-scale farmers was sprayed with herbicides, half of it with insecticides [Ibarrola-Rivas et al., 2020, p.7]. Lastly, more than half of the area used by small-scale farmers was sprayed with herbicides, and almost 40% with insecticides [Ibarrola-Rivas et al., 2020, p.7]. This wide application of pesticides throughout Mexico's farming communities can be explained by the fact that maize is susceptible to pests, which can cause significant losses [Hernández-Trejo et al., 2019, p.804]. It is estimated that the country's average yield is almost 40% lower than the global average, with many different factors contributing to this yield gap [Blanco et al., 2014, p.1]. One major factor limiting yields represents animal pests including arthropods, which have the potential to reduce global yields by 10% [Blanco et al., 2014, p.1]. Estimates are even higher in Mexico, making the country even more reliant on pest control and management, with synthetic insecticides being the main method to control pests [Blanco et al., 2014, p.1-2].

## 2.2 Insect Pests and Their Management

### 2.2.1 Common Insect Pests for Maize in Mexico

Insects can cause significant losses before, during, and after production, ranging from damaging seeds and seedlings, feeding on different parts of the plant during growth, to post-harvest losses [de Lange et al., 2014, p.331]. In addition, they can also serve as vectors for many plant diseases caused by bacteria or viruses [de Lange et al., 2014, p.331]. Insect pests attack maize during specific stages during their life cycles and can be grouped according to the major target plant or insect groups they belong to [Ortega, 1987, p.2]

The major pest in Mexico's maize production - in fact, throughout Latin America - is the fall armyworm (*Spodoptera frugiperda*), a polyphagous moth that feeds on leaves during its larvae stage [de Lange et al., 2014, p.331][Ortega, 1987, p.33]. They are specifically hard to control because of their growing resistance to chemical control [de Lange et al., 2014, p.331], and their wide geographical distribution in tropical and subtropical regions worldwide [Ortega, 1987, p.33]. Another common pest for maize in Mexico is the corn earworm (*Helicoverpa zea*), also a polyphagous moth feeding on different parts of maize - mainly leaves, tassels, and ears - during its larvae stage, and also functions as a vector for ear-rot pathogens [de Lange et al., 2014, p.331][Ortega, 1987, p.79]. *H. zea* also poses a threat to maize production worldwide, especially in higher altitudes in mountainous regions [Ortega, 1987, p.79]. Another common pest that both can cause damage itself and damage because of distributing pathogens is the corn leafhopper (*Dalbulus maidis*) [de Lange et al., 2014, p.331]. Black cutworms (*Agrotis ipsilon*) cause damage by feeding on maize seedlings before or shortly after emergence from the ground, as well as on tissues of young plants [Ortega, 1987, p.17]. The feeding on young plants will cause wilting, eventually leading to the death of the plant [Ortega, 1987, p.17]. *A. ipsilon* is mostly active during the night, sheltering during the day, and can also be found globally [Ortega, 1987, p.17]. Soldier worms (*Spodoptera exigua*) are also considered main pests in Meixan maize because their larvae not only attack leaves but also the ears of corn [Hernández-Trejo et al., 2019, p.806].

Other common pests are beetles such as scarab beetles (*Phyllophaga* spp.) or beetles of the genus *Diabrotica*, which can damage plant roots significantly during their larvae stage [de Lange et al., 2014, p.331]. Other common pests that are not considered insects include aphids, weevils, and thrips [de Lange et al., 2014, p.331]. The list of pests is very much longer, and most of these pests do not feed on maize exclusively, making it hard for farmers to control these species [de Lange et al., 2014, p.331].

Managing and controlling insect pests is crucial for food security because of their high potential to decrease yield, potentially threatening food security [Zelaya-Molina et al., 2022, p.70]. Because of potential and actual yield losses, multiple ways of controlling insect pests have been developed and adopted by farmers [Zelaya-Molina et al., 2022, p.70]. The control mechanisms can be divided into different categories, based on the strategies or methods used.

### 2.2.2 Biological Control

The first category of biological control measures involves the use of organisms to control insect pest populations [Hernández-Trejo et al., 2019, p.807]. These organisms could involve natural enemies of pests (both predators and parasitoids), as well as pathogenic microorganisms to reduce insect pests in agricultural production [Hernández-Trejo et al., 2019, p. 807]. Another important aspect of biological control is the creation of an environment favorable for natural enemies of insect pests [Zelaya-Molina et al., 2022, p.71]. With this approach, the total elimination of insect pests in maize is not possible - much rather, biological control aims at reaching a level where farmers are not affected economically [Hernández-Trejo et al., 2019, p.807]. Another reason why it is fairly unpopular in farming communities is the high amount of time and effort necessary, compared to chemical control measurements [Hernández-Trejo et al., 2019, p.801].

Because of the diversity of natural enemies of pests in corn, each pest in corn could be controlled with multiple different species [Hernández-Trejo et al., 2019, p.809]. This is due to the fact that these beneficial insects, like their prey, occupy a wide range of different habits, life cycles, and ecological niches, each with distinct strategies of survival and preying [Hernández-Trejo et al., 2019, p.809]. Some pests are preyed on by many different species at the same time, such as wasps of the genus *Trichogramma*, for example, which are widely used in Mexico to control Lepidoptera pests [Hernández-Trejo et al., 2019, p.809]. Recent studies have demonstrated some success in controlling Lepidoptera species with *Trichogramma* wasps, ranging from low to relatively good control, or even dependent on the season of the year [Williams et al., 2013, p.127]. However, no comprehensive evaluation of the effectiveness of *Trichogramma* wasps exists for controlling stalk borer populations [Williams et al., 2013, p.127].

Entomopathogens such as fungi, bacteria, or viruses can also help to reduce the numbers of pests - examples are *Beauveria bassiana*, and *Metarhizium anisopliae* (both fungi), as well as *Bacillus thuringiensis*, and *Bacillus sphericus* (both bacteria) [Zelaya-Molina et al., 2022, p.72]. Even though they are considered safe in terms of human health, their prices are relatively high compared to other controls [Blanco et al., 2014, p.2]. Plant extracts (neem oil, garlic extracts, or lemon extracts, for example) are also successful pest repellents, but scientific studies in Mexico are rare [Zelaya-Molina et al., 2022, p.73]. Recent studies have shown the success and potential of so-called pull-push systems - a system that incorporates plants that attract beneficial insects and repel pests - to control fall armyworms in Mexico, but this technique is mainly adopted in Africa and is fairly unknown to Mexican farmers [Guera et al., 2021, p.2].

### 2.2.3 Cultural Control

By altering methods of production, the aim of cultural management practices is to make the infestation of maize as unattractive to pests as possible, especially when the plant is most vulnerable to pests - the seedling stage [García-Lara and Serna-Saldivar, 2019, p.11][University of North Carolina, s.a.]. Examples include crop rotation (breaking the disease cycles of pests), planting hybrids, planting varieties that germinate and grow fast, or applying starter fertilizers that boost plant growth at an early stage [University of North Carolina, s.a.].

An important practice to reduce insect pest pressure is intercropping, which involves growing more than one crop in the same field [Pierre et al., 2022a, p.8]. Pierre et al. [Pierre et al., 2022a, p.8] could demonstrate that by incorporating legumes with maize, the diversity of parasitoids could be more than doubled compared to maize monocultures in Southern Mexico. According to the natural enemy hypothesis, intercropping increases insect diversity in the fields compared to monocultures, including the numbers of natural enemies and parasitoids of insect pests [Pierre et al., 2022a, p.11]. The intercropped plants provide a habitat for more insect species, including natural enemies, which allows for better control of insect pests [Pierre et al., 2022b, p.7]. Some of the intercropped plant species can also function as repellents of insect pests by releasing scents that are not favored by insect pests [Pierre et al., 2022b, p.7]. However, intercropping can be challenging for farmers, since many informed decisions must be made - for example, choosing crops that are compatible with maize, or planting date [Pierre et al., 2022b, p.10]. In the context of Mexico, little research has been done in terms of which species and their benefits are compatible with maize, but also regarding planting dates, and ideal planting density [Pierre et al., 2022b, p.10]. Furthermore, intercropping systems require more labor and could be hard to manage mechanically [Pierre et al., 2022b, p. 10].

A management strategy heavily promoted by CIMMYT is conservation agriculture, a practice which includes no soil disturbance, keeping the ground covered with organic material, and crop rotations [Rivers et al., 2016, p. 81]. Rivers et al. [Rivers et al., 2016, p. 84] could demonstrate in their study that conservation agriculture has mixed results in terms of pest control potential. Early in the growing season, before planting, treatments with organic covering showed higher damage compared to treatments without organic residues [Rivers et al., 2016, p. 85]. In contrast, maize with both no-till and organic cover treatments revealed less damage by Fall armyworm investigations [Rivers et al., 2016, p. 85]. In terms of insect pests, Lepidopteran larvae tended to be higher in no-till treatments, whereas Acrididae (grasshoppers) trended towards tilled treatments [Rivers et al., 2016, p. 84]. This indicates that certain groups are associated with certain living conditions, such as no soil disturbance or organic material as a living habitat [Rivers et al., 2016, p. 84]. Therefore, no recommendation for conservation agriculture as a way of controlling pests could be given [Rivers et al., 2016, p. 85].

### 2.2.4 Chemical Control

Chemical control— insecticides—is efficient and effective in not only reducing but also preventing the growth of insect pests [García-Lara and Serna-Saldivar, 2019, p.12]. They can be distinguished by their active ingredients and mode of action (the way they impact pest populations) [García-Lara and Serna-Saldivar, 2019, p.12]. Several types of insecticides can be distinguished, based on their chemical structure. such as organophosphates, carbamates, organochlorines, or pyrethroids [García-Lara and Serna-Saldivar, 2019, p.11]. They differ in terms of their chemical basis and persistence in the environment, but all regulate insect pests by attacking their nervous systems [García-Lara and Serna-Saldivar, 2019, p.11].

Insecticides can cause a shift from occasional to primary pests - the reduction of the actual target species can cause another pest species to proliferate [Hernández-Trejo et al., 2019, p.805]. They also pose the threat of giving rise to resistant organisms when applied excessively [Hernández-Trejo et al., 2019, p.805, 806], or can dramatically change ecosystems by harming non-target organisms, therefore reducing insect biodiversity [**?**, p.76]. Integrated pest management (IPM) strategies could be adopted to minimize the use of insecticides and their negative impacts - however, IPM strategies are hardly adopted by Mexican maize farmers due to the great number and diversity of growers [Blanco et al., 2014, p.2]. It is challenging to disseminate knowledge and information to farmers that enable them to adopt IPM strategies - knowledge that is necessary to tailor strategies to the unique environment farmers are operating in [Blanco et al., 2014, p.2]. On top of that, they are less cost-effective than the application of synthetic insecticides [Blanco et al., 2014, p.2]. For example, biological sprays containing *Bacillus thuringiensis* cost almost 100% more on average than a synthetic insecticide [Blanco et al., 2014, p.2]. Furthermore, insecticides are easy to apply and purchase [Blanco et al., 2014, p.2]. Therefore, insecticides offer a cheap and effective solution that requires less time, effort, and inputs, and are oftentimes preferred by farming communities [Blanco et al., 2014, p.2].

### 2.2.5 Pesticide Use in Mexico

Since pests occur in all production systems throughout Mexico, so does the use of insecticides [Blanco et al., 2014, p.2]. Insect pests are mainly managed in commercial, large-scale agricultural production systems, and less in small- or medium-scale production systems [Blanco et al., 2014, p.2]. Given the wide range of different products available, and their advantages over other control methods, insecticides are one of the most popular choices for pest control [Blanco et al., 2014, p.2]. In some cases, such as the fall armyworm, insecticides are the primary control mechanism, with more than 3000 tons of active ingredient applied in fields each year [Blanco et al., 2014, p.1].

Figure 1 above shows the estimated development of total use of agricultural pesticides between 1990 and 2022, alongside the total use of herbicides, insecticides, as well as bactericides and fungicides. The two latter are grouped in the same category and make up around 50% of the total use of pesticides over the period depicted [FAOSTAT, s.a.]. Insecticides and herbicides contribute around 25% to the total use of pesticides [FAOSTAT, s.a.]. Between 1990 and 2000, the use of all of the different pesticides remained stable, with insecticides around 6,000 tons per year [FAOSTAT, s.a.]. This trend changes beginning in the early 2000s, when insecticide use dropped by 60% over just two years, only to rise again steadily

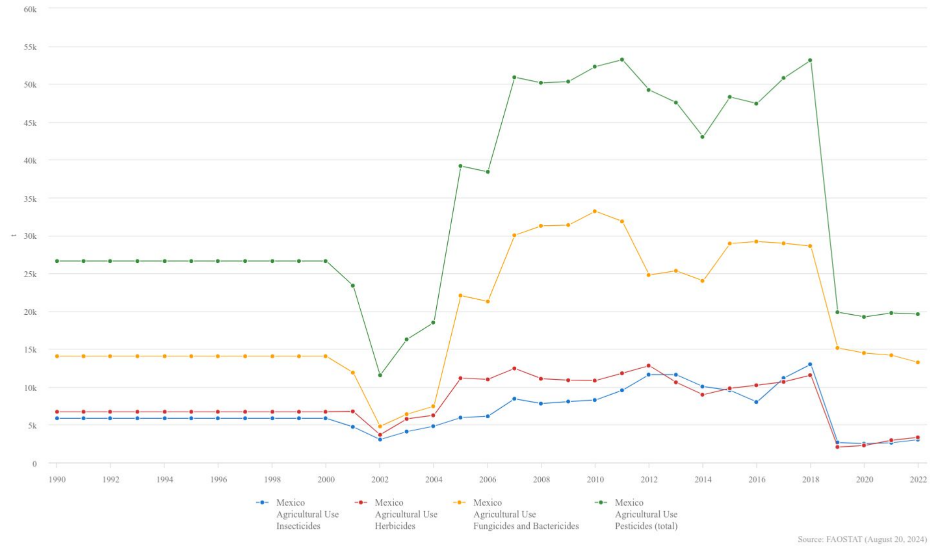



Figure 1: Pesticide Use in Mexico

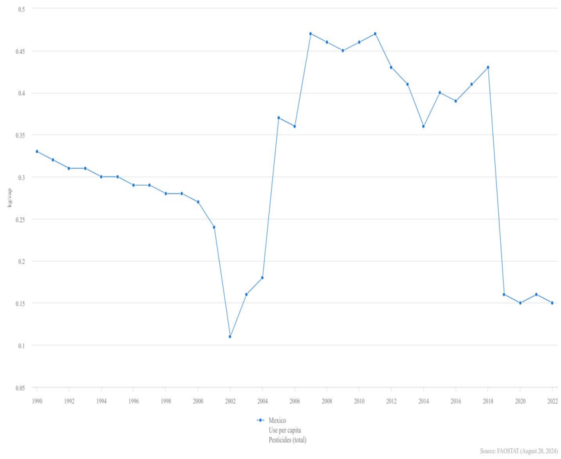
by 200% until 2014, reaching over 12,000 tons per year [FAOSTAT, s.a.]. After a short period in dropping numbers, pesticide use reached its climax during 2018 at 13,000 tons per year [FAOSTAT, s.a.]. After a rapid decline in 2019, insecticide use remains stable at around 3,000 tons per year, which is a lower level than the use during the 1990s [FAOSTAT, s.a.].

Figure 2 below depicts the estimated pesticide use per capita (a) and per area of cropland (b), which follow a similar trend to the total pesticide use in absolute numbers. No data by the FAO was provided for insecticides per capita or per area of cropland, but since insecticide use made up around 25% of the total use, it can be expected that the trends for insecticides are similar to the total pesticide use.

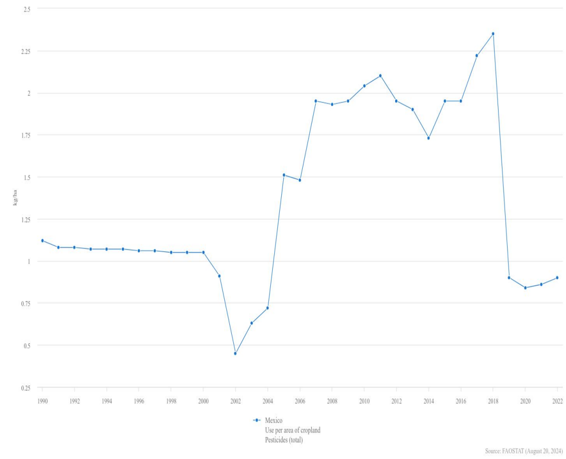
## 2.3 Impact Assessment of Insecticides

### 2.3.1 Significance for Mexico

As mentioned above, no detailed data on which chemicals are applied are available for Mexico. However, an important aspect to mention in this context is the category of highly hazardous pesticides - a category proposed by the United Nations (UN), defined by multiple criteria [González, 2018, p.5]. These pesticides pose a threat to human health by either




(a) Pesticide Use Per Capita




(b) Pesticide Per Area of Cropland

Figure 2: Pesticide Use Trends over the past 40 Years

their high acute toxicity or chronic toxicity in the long term [González, 2018, p.5]; or they are very harmful to the environment, by either causing mortality to aquatic organisms, or pollinators [González, 2018, p.5]. Some registered active ingredients used as insecticides, widely used in Mexico, fall under the category of highly hazardous [González, 2018, p.70]. In 2018, almost 2000 commercial products containing highly hazardous active ingredients were registered in Mexico, making up almost two-thirds of all commercial products registered containing highly hazardous active ingredients [González, 2018, p.70]. Even though total use of insecticides is relatively low compared to other pesticides [FAOSTAT, s.a.], the share of highly hazardous insecticides on the total pesticides containing these substances is significantly higher [González, 2018, p.70]. Numbers about the commercial products registered that contain highly hazardous active ingredients are available, with methyl parathion, chlorpyrifos ethyl, cypermethrin, malathion, and permethrin as a few examples [González, 2018, p.71].

The widespread use of highly hazardous pesticides in Mexico highlights the lack of data available on a national level, which highlights the need for more research, especially in terms of their impact on the environment. Numerous assessment tools and models exist to do so, with USEtox offering a comprehensive approach to quantify and compare impacts of chemicals, including insecticides.

### 2.3.2 Evaluating Insecticide Toxicity Through Impact Assessment

Life Cycle Assessment is a method to calculate the impact of certain products or processes on human health or the environment throughout all stages of their life cycle [Carmichael, 2014, p.13]. Four stages are necessary [Carmichael, 2014, p.13].

(1) The first step is to **define the scope and goals of the assessment** [Carmichael, 2014, p.13]. In our case, the first step is the assessment of the project carried out by CIMMYT, evaluating the top toxic materials as well as the success in reducing the environmental impact and to determine the toxicity of active ingredients used.

(2) The second step is called **Life Cycle Inventory Analysis**, in which the flow and aggregation of relevant materials in relevant compartments of the environment (i.e. air, water) is analyzed and calculated [Carmichael, 2014, p.14]. In our case, the Pest LCI model was used, which will be described in the section below. Pest LCI provides fate factors that allow the calculation of the masses of pesticides applied to different environmental compartments.

(3) The third step involves **Life Cycle Impact Assessments**, which aims to determine the impact of the relevant materials in the relevant compartment [Carmichael, 2014, p.15]. Characterization factors are used to calculate the impact and to make the impact comparable to other substances [Carmichael, 2014, p.15]. Another important aspect to mention here is the fact that two different approaches exist, used by different models: midpoint and endpoint models [Carmichael, 2014, p.17]. The former quantify environmental impacts at various stages, and convert these impacts into specific units, such as CO2 equivalents [Carmichael, 2014, p.17]. Endpoint models translate midpoint results into damage indicators, such as PDF.m2 (Potentially Disappeared Fraction of species on 1m2 in one year) [Carmichael, 2014, p.17]. In our case, USEtox was the model chosen to calculate impact scores at the midpoint level.

(4)The last step is the **interpretation of the results** [Carmichael, 2014, p.21].

### 2.3.3 PestLCI

PestLCI is a model specifically developed to calculate the fate of pesticides entering different environmental compartments [Dijkman et al., 2012, p.974]. Once the pesticide is applied in the field, it enters different surrounding compartments— such as soil, air, and water— immediately but also after a certain period of time [Birkved and Hauschild, 2006, p.435]. Estimated fractions are used and multiplied with the mass or rate of pesticides applied, which allows us to make estimates on how much of the pesticides ends up in which compartment for an average situation [Birkved and Hauschild, 2006, p.15]. The basic formula underlying this model to calculate total emission fraction of pesticide is the sum of the fraction emitted to air, the fraction emitted to groundwater, and the fraction emitted to surface water, using the following formula:

$$f_{em} = \frac{m_{em}}{m_{appl}} = f_{air} + f_{sw} + f_{gw} \tag{1}$$

$f_{em}$ is the total fraction of pesticide released into the environment, which is the fraction of the mass of pesticide emitted into the environment ($m_{em}$) over the mass of pesticide applied ($m_{appl}$) [Birkved and Hauschild, 2006, p.435]. Part of the pesticide is absorbed by plants, which is the reason why the mass applied is lower than the mass entering different compartments [Birkved and Hauschild, 2006, 435]. $f_{air}$, $f_{sw}$, and $f_{gw}$ represent the different compartments, including air, surface water, and groundwater [Birkved and Hauschild, 2006, p.435].

### 2.3.4 USEtox

USEtox is a scientific consensus model, developed to harmonize existing LCI models, making the results of different studies more comparable to each other [Fantke et al., 2017, p. 16]. USEtox calculates characterization factors (CFs) that convert the mass or rates of chemicals emitted into the environment to impact scores [Rosenbaum et al., 2008, p. 702]. Characterization factors of substances represent the potential of these substances to contribute to the environmental impact [Fantke et al., 2017, p. 15]. The impacts USEtox is currently focusing on are human health and freshwater ecotoxicity [Rosenbaum et al., 2008, p. 702].

The approach of USEtox is to follow the cause-and-effect chain to calculate impact scores [Rosenbaum et al., 2008, p.703]. USEtox estimates how much a chemical can harm humans or aquatic species, based on how much is released (mass or rate of chemical released into the environment), which compartment the chemical ends up in, how much a population is exposed to (its bioavailability), and how toxic the substance is [Rosenbaum et al., 2008, p.703]. This cause-and-effect chain is linked by different factors: fate factors (FF), exposure factors (XF), and effect factors (EF) [Fantke et al., 2017, p.21]. Fate factors represent the typical amount of a substance moving into different environmental compartments, and are calculated based on a set of mass balances [Fantke et al., 2017, p.23]. Substances travel through different compartments, remain in the one emitted, or can be physically or chemically transformed, or irreversibly lost [Fantke et al., 2017, p.23]. Exposure factors represent the bioavailability of a substance in the compartment of interest. The effect factors illustrate the effect of substances on species, based on $EC_{50}$ values.

Characterization factors (CF) are the product of these three factors, with the following formula:

$$CF = FF \times XF \times EF \tag{2}$$

Characterization factors are expressed in comparative toxic units (CTUs) - or potentially affected fraction of species (PAF) over time per kg substance emitted [Fantke et al., 2017, p. 22]. USEtox provides a database with over 3,300 substances, where characterization factors can be derived from Fantke et al. [2017].

### 2.3.5 Related Literature

Numerous studies have selected USEtox as part of a Life Cycle Assessment to calculate the impact of pesticides on freshwater ecosystems, some focusing on the environmental impact of pesticides applied in a country, like Erenstein et al. [2021]. Through their work, the authors could demonstrate that the overall freshwater ecotoxicity calculated with USEtox of the top pesticides applied in Finland was declining between 2000 and 2011 because of the outphasing of one active ingredient, demonstrating the drastic impact the substitution of one chemical could potentially have on a national level [Erenstein et al., 2021, p.72]. Other studies focus on the calculation of average impact scores (i.e. for kg pesticide applied, or per kg crop produced). For example, Xue et al. [2015] could identify the most toxic chemicals on average per hectare corn farmland applied, per kg pesticide applied in the Midwest of the United States. The authors could show a tremendous variability in toxicity levels for pesticides, with Chlorpyrifos being the most toxic on average across the nine states included in the study [Xue et al., 2015, p.1125]. A similar study was conducted by Berthoud et al. [2011], where the most toxic pesticides per hectare applied in wheat fields in France were discovered using USEtox. These studies used nationally available data regarding pesticide use and suggested the need to use data collected in the field as a basis to assess toxicity levels of chemicals [Erenstein et al., 2021 & Xue et al., 2015].

One case study that followed this recommendation was conducted in France in 2022 by Renaud-Gentié et al. [2015], where the authors not only calculated specific fate and characterization factors tailored to the conditions in French vineyards but also applied these to three different representative conventional management approaches. The data based on these calculations were obtained in the production season of 2010-2011 [Renaud-Gentié et al., 2015, p.1533]. However, no study with long-term data collected in the field is currently available, which limits the ability to see trends over time and shifts in toxicity. National data also sometimes lacks details, such as the amount of hectares pesticides were applied to or the rates they had been applied to the fields.

Another important factor to further enhance impact assessment is the development of regional characterization factors, as done by Renaud-Gentié et al. Renaud-Gentié et al. [2015]. The need for the development of regional factors was also illustrated by Mankong et al. [2022], who could show the importance of regionally developed characterization factors by contrasting calculations based on the default characterization factors and those specifically calculated to fit the Thai conditions [Mankong et al., 2022, p.10]. However, since calculating characterization factors specifically tailored for the conditions in Mexico, with its diverse climates and soils, would require a highly detailed approach. This level of detail, while beneficial for drawing conclusions, is beyond the scope of this study.

## 2.4 CIMMYT - the International Maize and Wheat Improvement Center

### 2.4.1 CIMMYT's Mission and Efforts

CIMMYT is an international organization and research institute, which aims to empower farmers worldwide through its research [Bentley et al., 2023, p.4]. CIMMYT is part of the Consortium of International Agricultural Research Centers (CGIAR) network, an association of different agricultural research institutes, whose mission it is to elevate poverty, increase food security, and resource use efficiency through their research worldwide [Bentley et al., 2023, p.4]. CIMMYT's mission statement 'Science and innovation for a food and nutrition secure world.' [CIMMYT [a], s.a.] illustrates their over 50-year-long effort to improve livelihoods and food security of rural communities [CIMMYT [a], s.a.]. CIMMYT's research efforts include - and are not limited to - plant breeding for increased yield and resistance to droughts, pests, and diseases, and field experiments for ecological intensification of production systems [CIMMYT [b], s.a.]. Preserving genetic resources, promoting sustainable farming practices, and collaboration with farmers worldwide are also key focus areas pursued by CIMMYT [CIMMYT [a], s.a.].

With a global network of research stations and partners, CIMMYT has impacted thousands of farming communities all over the world [CIMMYT [a], s.a.]. This is especially the case in Mexico, where CIMMYT has been leading many projects in close collaboration with farmers, researchers, and extension agents [CIMMYT, s.a.]. Those projects include, and are not limited to, capacity building, training of farmers, or the promotion of certain management practices. CIMMYT's field trials are not limited to its headquarters in El Batán, but rather, are scattered across the country to encompass different climate zones and growing conditions. Their current research efforts are focused on climate change and the mitigation of the environmental impact of agriculture, but also inclusion (gender and youth issues), and poverty reduction [CIMMYT [a], s.a., p.4].

### 2.4.2 Innovation Modules

A specific extension approach for farmers executed by CIMMYT is called 'innovation modules' [CIMMYT, s.a.]. Innovation modules are plots established on a farmer's land, where new agricultural management practices and technologies are demonstrated through a side-by-side comparison [CIMMYT, s.a.]. On one side, the farmers will continue to carry out their usual management strategies [CIMMYT, s.a.]. On the other side, farmers will adopt new management strategies promoted by CIMMYT [CIMMYT, s.a.]. According to CIMMYT, these innovation modules act as 'living classrooms', making learning and innovations more tangible [CIMMYT, s.a.]. Extension agents and farmers will develop new strategies tailored to local environmental and social conditions [CIMMYT, s.a.]. The idea is that once the farmers have seen the success of the new strategy, and have learned how to adopt it, they will expand this strategy or new technology on other plots of their cultivated land [CIMMYT, s.a.]. Those new practices could include, for example, the right application of fertilizers or, like in our case, the correct application rates of insecticides [CIMMYT, s.a.]. Some of the data collected in the project assessed in this paper has been collected on these plots.

The innovation module approach resembles one very common approach - the so-called 'on-farm demonstration' approach, which allows farmers to see and evaluate new practices and strategies on their own land, guided and designed by extension agents or agronomists [Roo et al., 2019, p.169]. Oftentimes, on-farm demonstrations are also on-farm trials at the same time, where farmers and researchers collaborate with each other in a joint experiment for finding the perfect solution in a specific context [Roo et al., 2019, p.169]. This approach is considered a living classroom, where farmers acquire new skills or learn about new techniques or innovations through learning-by-doing, combined with provided training and support by extension agents [Sseguya et al., 2021, p.2].

Both approaches have limitations in the sense that it is hard to not only quantify the impact of the innovation since the innovation is applied on a small plot, but also to establish a direct causality between the innovation and the expected outcome [Oklahoma State University, 2017]. Since these plots are fairly small and sometimes not close to each other, certain factors like different soil texture or precipitation patterns could make it hard to measure the impact of the innovation [Oklahoma State University, 2017]. In addition, scaling up the innovation to other fields or even other farmers could also be a challenge [Oklahoma State University, 2017].

Some studies suggest that demonstration plots are an effective mode to teach farming communities worldwide about agricultural innovations or best-management practices, while also enhancing the adoption of these innovations and practices [Sseguya et al., 2021, p.14]. In their study surveying 800 farming households in rural Tanzania, [Sseguya et al., 2021, p.13] could demonstrate that farming households that had access to demonstration plots extension services were more likely to buy improved agricultural inputs. [**?**, p.5-6] assessed the success of multi year demonstration plots in terms of improving sugar cane yields and income of farmers and could underscore that farmers that were exposed to this extension mode were more likely to adopt new practices, as well as increase their yields and income. Only a few papers could be found evaluating the success of CIMMYT's innovation module approach. For example, Hauser et al. [2010] could prove that around 40% of farmers that participated in a similar approach (side-by-side, on farm demonstration plots), adopted the innovation (boiling water treatment of plantain suckers), with many farmers expanding the treatment to other plots of their land. However, no papers could be found comparing the success of CIMMYT's innovation module approach with conventional extension services. We want to help fill this gap by comparing the success of the innovation module approach with the traditional extension approach in terms of reducing the environmental footprint of insecticides.

# 3 Material and Methods

## 3.1 CIMMYT's Original Dataset

CIMMYTs has created the database called "BEM-Plaguicidas-Working database-ORIGINAL" as a working database for their extension effort. The purpose of the extension project was to push farmers to use insecticides that are considered less environmentally toxic to reduce the ecological footprint of food production. The data was collected by multiple extension agents and copied into this Microsoft Excel sheet by various staff members.

Two different types of collaboration were carried out: A classic form of extension, where farm advisors advised farmers on their land, and a type of direct comparison: one section called *parcela testigo*, where the normal practices of farmers were carried out, next to a section called *parcela de innovación*, where other active ingredients were applied. The idea of the latter was to have a direct side-by-side comparison of the different active ingredients applied.

Data collection started in 2010 and is still ongoing. The original dataset (July 2023) consists of 69,928 entries, each representing one row. Each of these 69,928 represents one application of a chemical (mainly insecticides). In addition, each row has 71 columns. Their title in Spanish and its English translation can be found in the following table:

Table 1: Summary Table of Spanish and English Titles

| Column | Spanish Title | English Title | Column | Spanish Title | English Title |
|---|---|---|---|---|---|
| A | ID de la bitácora | Log ID | B | ID de tipo de bitácora (clave foránea) | Log type ID (foreign key) |
| C | ID aplicación | Application ID | D | ID tipo de parcela (testigo o innovación) | Plot Type ID (control or innovation) |
| E | Tipo de parcela (testigo o innovación) | Plot Type (control or innovation) | F | ID sección | Section ID |
| G | Nombre de la sección | Section Name | H | ID tipo de bitácora sección (clave foránea) | Section Log Type ID (foreign key) |
| I | ID tipo de aplicación.x | Application Type ID.x | J | ID Parte de la planta dañada por la plaga | Damaged Plant Part by Pest ID |
| K | Parte de la planta dañada por la plaga | Damaged Plant Part by Pest | L | Porcentaje de daño en la planta por la plaga | Percentage of Damage in Plant by Pest |
| M | Cantidad de producto aplicado (unidad/ha) | Amount of product applied (unit/ha) | N | Precio unitario del producto | Unit price of the product |
| O | ID Unidad de medida del producto aplicado | ID of the product's unit of measure applied | P | Unidad de medida del producto aplicado | Unit of measure of the product applied |
| Q | ID del producto aplicado | ID of the applied product | R | Nombre del producto aplicado | Name of the applied product |
| S | Ingrediente activo, análisis (% N-P2O5-K2O) o descripción | Active ingredient, analysis (% N-P2O5-K2O) or description | T | Tipo de producto | Type of product |
| U | ID tipo de aplicación.y | ID of the application type.y | V | Nombre del tipo de aplicación | Name of the application type |
| W | Fecha de la aplicación | Date of the application | X | Nombre de la plaga o enfermedad | Name of the pest or disease |
| Y | Número de plagas que quiere controlar | Number of pests to control | Z | Motivo de aplicación_Plagas | Reason for application_Pests |
| AA | ID del tipo de maleza | ID of the type of weed | AB | Tipo de maleza | Type of weed |
| AC | ID forma de aplicación | ID of the application method | AD | Forma de aplicación | Application method |
| AE | ID lugar de aplicación | ID of the application site | AF | Lugar de aplicación | Application location |
| AG | ID implemento usado | ID of the implement used | AH | Implemento usado | Implement used |

*Continued on next page*

| Column | Spanish Title | English Title | Column | Spanish Title | English Title |
|---|---|---|---|---|---|
| AI | ¿El implemento usado es activo en la base de datos? | Is the implement used active in the database? | AJ | ¿El implemento usado esta aprobado en la base de datos? | Is the implement used approved in the database? |
| AK | Número de productos aplicados | Number of products applied | AL | Costo por la aplicación de los productos ($/ha) | Cost for applying the products ($/ha) |
| AM | Costo por el transporte de los productos empleados ($/ha) | Cost for transporting the products used ($/ha) | AN | Cultivo sembrado | Planted crop |
| AO | Fecha de siembra | Date of planting/sowing | AP | Nombre del principal producto a obtener | Name of the main product to obtain |
| AQ | Tipo de semilla | Type of seed | AR | Nombre de la variedad sembrada | Name of the planted variety |
| AS | ID de la parcela | Plot ID | AT | Año | Year |
| AU | ID de la parcela | Plot ID | AV | Nombre de la institución | Name of the institution |
| AW | Folio único de predio | Unique property folio | AX | ID Tipo de parcela (módulo, área de extensión o área de impacto) | ID of the plot type (module, extension area, or impact area) |
| AY | Tipo de parcela (módulo, área de extensión o área de impacto) | Plot type (module, extension area, or impact area) | AZ | ID estado (INEGI) | State ID (INEGI) |
| BA | Estado | State | BB | ID municipio (INEGI) | Municipality ID (INEGI) |
| BC | Municipio | Municipality | BD | ID localidad (INEGI) | Locality ID (INEGI) |
| BE | Localidad | Locality | BF | Nombre del Hub | Name of the Hub |
| BG | ID formato de las coordenadas | Coordinate format ID | BH | Latitud N | Latitude N |
| BI | Longitud W | Longitude W | BJ | Altitud (m) | Altitude (m) |
| BK | Precipitación media anual (mm) | Average annual precipitation (mm) | BL | tipoProduccion | Production type |
| BM | Ing Act Corregido | Corrected active ingredient | BN | MAP | MAP |
| BO | Tipo_control | Control type | BP | Clases MAP | MAP classes |
| BQ | Mezcla | Mix | BR | WHO | WHO |
| BS | ID Tipo de producto | Product type ID | | | |

As described above, the data have been collected over multiple years, by multiple extension agents and field workers. In addition, the data collected were added to the dataset by different people. Therefore, the data is reported not in a consistent way. Below are some examples of the limitations of the dataset, with a focus on those relevant to the objectives and goals of this thesis. The columns associated with the limitations are also included. These limitations have been mitigated by having taken several steps, which include adding details or information, or deleting data that are not assignable.

- **Data Inconsistency in Commercial Names** (Column R: Nombre del producto aplicado): The commercial names of the same product are reported in multiple different ways. For example, sometimes containing the active ingredient in brackets, sometimes without mentioning the active ingredient in brackets. Another inconsistency in the title represented the fact that if the active ingredient was mentioned in brackets, they themselves would also be reported in a non-consistent way - sometimes, different active ingredients for the same product, or different concentrations of active ingredient with the same product. Therefore, we do not know exactly how many different products were applied in total. In total, 2767 different notations for commercial names of products applied are reported.

- **Data Inconsistency in Active Ingredients** (Column R: Nombre del producto aplicado; Column S: Ingrediente activo): The names of active ingredients used were also named in different ways - both in brackets following the commercial names, as well as in the rows only containing the active ingredients (Column R & S). In addition, if a commercial product was containing two different active ingredients, different notions of these two further increased the inconsistency in the data, sometimes only mentioning one instead of two, for example.

- **Data Inconsistency - Same Commercial Product with Different Concentrations of Active Ingredient**: Sometimes, a commercial product is available with different concentrations of active ingredient. For those products, the concentration of active ingredient is not always included in the dataset, which makes it impossible to calculate the actual rate of active ingredient applied per hectare.

- **Spelling Mistakes**: In addition, some inconsistencies were related to spelling mistakes, and not to different notations. The spelling mistakes can be associated with any column in the dataset, and are not limited to the commercial names or the active ingredient applied.

- **Data Inconsistencies in Different Types of Products** (Column T: Tipo de producto) Different types of inputs were added to the dataset, not only insecticides, but also fungicides, or herbicides. The product types were also used inconsistently, with different terms for the same type of product, especially associated with insecticides. The following table includes all the different types of products used in the original dataset.

| Product Type | Percentage of Product Type | Count of Product Type |
|---|---|---|
| Fungicide | 0.01% | 8 |
| Herbicide | 0.09% | 62 |
| Biological insecticide | 0.61% | 424 |
| Synthetic insecticide | 2.60% | 1818 |
| Insecticide | 96.69% | 67616 |
| **Grand Total** | **100.00%** | **69928** |

- **Data Inconsistencies in Different Control Types** ((Column BO: Tipo_control) The same as above applies here. The following table illustrates the different notations:

- **Classifying inputs as insecticides that are not insecticides** (Row T: Tip de product; row BO: Tipo_control): According to the dataset, over 99% of the entries are classified as insecticides. However, a lot of different products were classified as insecticides, while in reality, they are not insecticides. These products can range from homemade inputs (water and soap, milk, mixtures of garlic and onion extracts, etc.), to

| Control Type | Count of Control Type | Percentage of Control Type | Cumulative Percentage of Control Type |
|---|---|---|---|
| Químico | 60,954 | 89.82% | 89.82% |
| Etológico | 2,527 | 3.72% | 93.54% |
| Biológico | 2,237 | 3.30% | 96.84% |
| Coadyuvante | 716 | 1.06% | 97.89% |
| Unknown | 516 | 0.76% | 98.65% |
| Mineral | 489 | 0.72% | 99.38% |
| Extractos Vegetales | 324 | 0.48% | 99.85% |
| F | 56 | 0.08% | 99.94% |
| Etiológico | 16 | 0.02% | 99.96% |
| Extracto | 12 | 0.02% | 99.98% |
| Químico (Typo) | 9 | 0.01% | 99.99% |
| Trampa | 2 | 0.00% | 99.99% |
| Físico | 2 | 0.00% | 100.00% |
| Hormona | 1 | 0.00% | 100.00% |
| Fertilizante | 1 | 0.00% | 100.00% |
| **Grand Total** | **67,863** | **100.00%** | **100.00%** |

adjuvants, coadjuvants, or fertilizers. Therefore, we do not know how many insecticides were actually applied.

- **Unit of application rate** (Column P: Undid de media del product aplicado): Another inconsistency is the different use of units for the commercial products applied. For example, paquete (pack) of a commercial product is used as a unit, and it is unclear how much of the product one package was containing (Oftentimes, different sizes exist).

- **Time Gap Between Application and Reporting**: The data has been collected sometimes after a couple of months after the actual application, which makes it hard for farming communities to recollect how much they have actually applied.

- **Data Variability - Number of Entries per Year**

- **Data Variability - Number of Entries per State**

## 3.2 Data Preparation

### 3.2.1 Rationale and Objectives

The main focus of this thesis is to assess the Plagucidas project in terms of the most common active ingredients, the most and least toxic active ingredients, and trends. Because the exact application rate of active ingredient is needed to calculate freshwater ecotoxicity, the cleaning-up process was focused on the column R (**name of commercial product applied**). The technical sheet (ficha tecnica) / ficha de la seguridad) of each commercial product can be found online, which provided information about the percentage or concentration of active ingredient per liter/kg of commercial product. Therefore, we can calculate the exact rate of active ingredient applied for each entry.

The first objective for cleaning up the dataset was to eliminate the inconsistencies as much as possible, especially in terms of the names of commercial products and active ingredients. Another important goal was to add information to be able to calculate the exact rate of active ingredient applied. This includes the name of the commercial product applied, its concentration of active ingredient, the unit of concentration, and the name and CAS number of the active ingredient. The last goal was to delete any information that is not relevant for the scope and aim of this thesis.

### 3.2.2 Reducing Inconsistencies & Enhancing Information

As described above, the main focus here was the name of the commercial product applied. The dataset was sorted alphabetically according to the names of commercial products applied. As a next step, the frequency of application of each of the 2767 different notations was calculated in a separate column. If the frequency was over 50 times (over 50 times applied), the name of the commercial product was Googled online, and in case of a match, corrected. The screenshot below shows an example of the correction of the commercial name.

After having looked up the technical sheet online, information was added, including type

| Nombre del producto aplicado | Frequency | Name |
|---|---|---|
| BALAZO 25 (I) [Diazinon] | 89 | Balazo 25 |
| BALAZO 4G (I) [Diazinon] | 28 | Balazo 4G |
| BALAZO 5G (I) [Diazinon] | 52 | Balazo 5G |
| BALAZO T 5% (S/C) [TERBUFOS 5%] | 2 | Balazo 5G |
| BALAZO T 5% (S/C) [TERBUFOS] | 2 | Balazo 5G |

Figure 3: Correcting names of commercial products applied

of substance (insecticide or not), concentration of active ingredient, unit of concentration of the active ingredient, name of active ingredient, and CAS number. This information was then copied to every application with the same notation in the original data set. For example, each 89 rows containing the notation 'BALAZO 25 (I) [Diazinon]', the new information about 'Balazo 25' was added in new columns.

### 3.2.3 Reducing Redundant Information

The following steps were conducted to delete entries with uncertainties:

- Rows containing notations of commercial products that were not assignable - either because their frequency was below 50, or the name did not exist. This step reduced the data sheet from 69,928 to 53,630 entries, which represents approximately 78.48% of the original dataset.

- Applications of insecticides with two active ingredients: In order to expedite the analysis, each of these (1237) were treated as a separate application, adding an additional row for each, which caused total entries to rise to 54,867 entries.

- Rows containing unclear units of application (such as 'Paquete/ha' or 'piezas_ha'. This reduced the data sheet from 54,867 entries to 52,209 entries, which represents approximately 74.68% of the original dataset.

- Because only four entries were made in the year 2010, those were deleted. This reduced the data sheet from 52,209 entries to 52,205 entries.

- Deleting applications that were not carried out in maize: This reduced the data sheet from 52,205 entries to 47,367 entries.

- For the year 2021, no data was available in terms of plot size. Therefore, these were excluded from the analysis.

- Deleting outliers in terms of application rate: In R, we calculated the interquartile range of the application rates in order to determine outliers. Those outliers were deleted, except if they were below the maximum recommended dosis of the commercial product, or if the application was done in a *parcela testigo*. This reduced the dataset from 46,747 entries to 46,419 entries, which represent approximately 66.38% of the original dataset.

## 3.3 CIMMYT's Dataset After Processing

Because of the tremendous amount of data available, this section aims to provide an overview of the extension project by looking at different parameters.

### 3.3.1 Temporal Distribution of the Data

In 5 out of 10 years, entries per year range around 7,000, accounting for around 80% of the total entries. A significant drop in entries was reported in 2014, with only around 2,000 entries per year, with almost the same number in the following year. Those two years account for around 5% each of the total entries. Only 2020 and 2021 account for less than 1% of the total entries, with both representing around 2% of the total entries. The figure below illustrates this variability in entries per year:

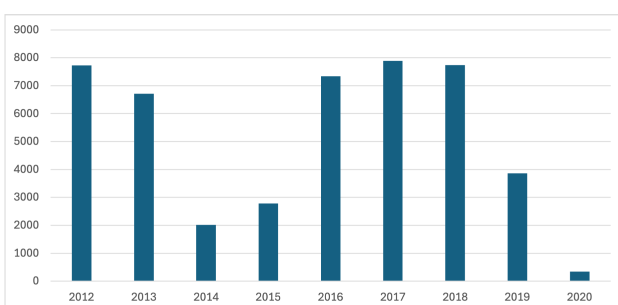



Figure 4: Number of Applications Each Year

### 3.3.2 Geographical Distribution of the Data

The distribution of the entries revealed significant geographic variations, as seen in the table below. The top 5 states - Guerrero, Guanajuato, Chiapas, Morelos, and Jalisco - accounted for almost 70% of the total entries, with 23.61%, 15.39%, 12.12%, 9.27%, and 9.15%, respectively. The table below shows how the entries are allocated to each state:

| **State** | **Number of Entries** | **Percentage of Total** |
|---|---:|---:|
| Guerrero | 11,179 | 23.61% |
| Guanajuato | 7,289 | 15.39% |
| Chiapas | 5,742 | 12.12% |
| Morelos | 4,391 | 9.27% |
| Jalisco | 4,331 | 9.15% |
| Michoacán de Ocampo | 1,731 | 3.66% |
| Veracruz de Ignacio de la Llave | 1,522 | 3.21% |
| México | 1,389 | 2.93% |
| Oaxaca | 1,339 | 2.83% |
| Sinaloa | 1,180 | 2.49% |
| Durango | 1,177 | 2.49% |
| Hidalgo | 959 | 2.03% |
| San Luis Potosí | 660 | 1.39% |
| Querétaro | 624 | 1.32% |
| Campeche | 556 | 1.17% |
| Puebla | 521 | 1.10% |
| Chihuahua | 518 | 1.09% |
| Colima | 350 | 0.74% |
| Yucatán | 343 | 0.72% |
| Tabasco | 292 | 0.62% |
| Tlaxcala | 281 | 0.59% |
| Aguascalientes | 233 | 0.49% |
| Coahuila de Zaragoza | 224 | 0.47% |
| Quintana Roo | 129 | 0.27% |
| Sonora | 105 | 0.22% |
| Zacatecas | 93 | 0.20% |
| Nayarit | 80 | 0.17% |
| Tamaulipas | 75 | 0.16% |
| Nuevo León | 30 | 0.06% |
| Baja California Sur | 14 | 0.03% |

Table 2: Distribution of Entries by State

### 3.3.3 Management Practices

In total, 2,008 different maize varieties had been reported to be sprayed with insecticides between 2012 and 2021. P4082W, DK-357, IMPACTO, CIMARRON, and ANTILOPE had the highest entries, with 5.70%, 3.88%, 3.33%, 3.03%, and 2.76% of the total entries, respectively. All other varieties had less than 1% of the total entries. In addition, not much information was provided about the seeds themselves - only about one-third of the entries provided information about whether the seeds used to grow maize were hybrid (26%) or *creoilla* (6%), which could be translated to native seeds.

Most of the entries represent applications to maize that is grown during the main growing season - summer. These entries consistently accounted for around 15% of the total entries in 5 years (2012, 2013, 2016, 2017, 2018). In total, applications on summer maize represented over 69% of the total entries, whereas applications to winter wheat accounted for less than 5%. The numbers of entries for summer maize follow the same trend as the total number of entries. The figure below shows how many entries per year are applied to summer maize and winter maize.

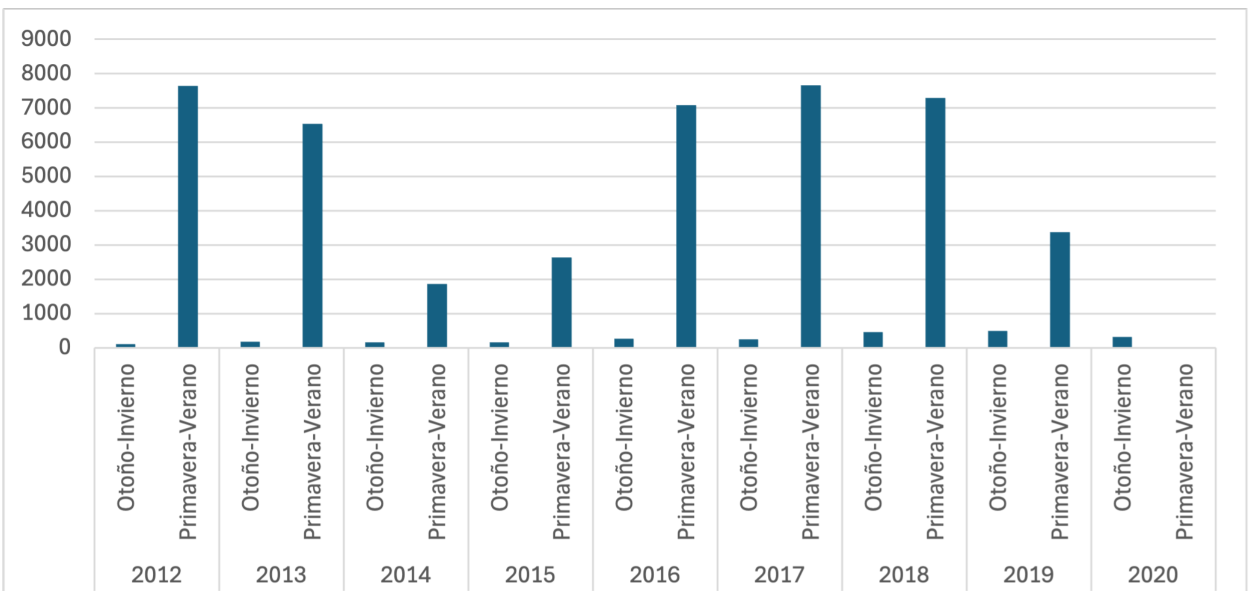



Figure 5: Production Cycles: Temporal Distribution of Plots per Year – Wintercycle (*Otoño-Invierno*) & Summercycle (*Primavera-Verano*)

25% of the entries represent insecticide applications on irrigated maize - the vast majority (75%) of the entries are applications on rain-fed maize fields. The figure below shows the yearly distribution of this data.

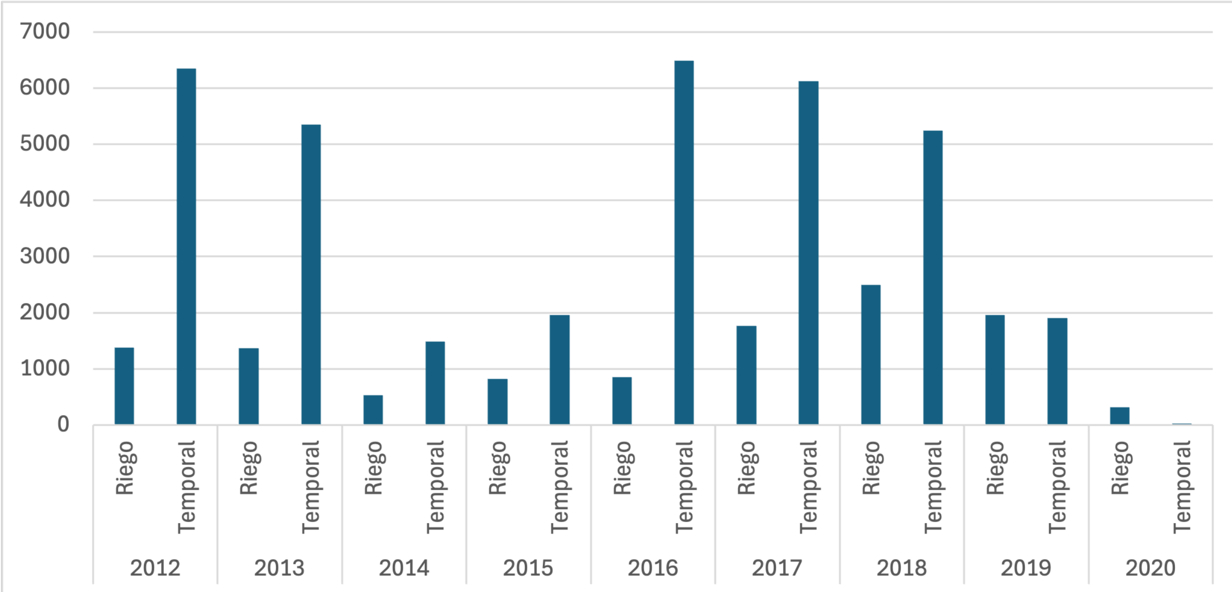



Figure 6: Hydrological Regime: Number of Irrigated Plots (*Riego*) Vs. Rainfed Plots (*Temporal*)

The vast majority of the applications were carried out on fields where solely maize was planted. This portion represented over 96% of the total entries. The rest is divided by sorghum (2.7% of the total entries), and maize cultivated with other crops in the same field (0.7% of the total entries). Here, maize was grown with either beans, soybeans, sunflower, peas, zucchinis, squash, coffee, and others.

### 3.3.4 Plot Sizes

The following table provides an overview of the distribution of plot sizes in the dataset:

Table 3: Distribution of Plot Sizes (in hectare) in the Dataset

| **Statistic** | **Value** |
|---|---|
| Minimum | 0.01 |
| 1st Quartile | 1.00 |
| Median | 2.00 |
| Mean | 3.54 |
| 3rd Quartile | 4.00 |
| Maximum | 97.00 |

Plot sizes range from 0.01 hectare to 97 hectares, with the medium plot size of 3.54 hectares. The majority of the plots captured in the dataset (75

#### 3.3.5 Extension Approaches

The vast majority of the applications were carried out under the conventional extension approach (*parcela extension*), around 32854, which represents 70.78% of the data. In addition, *parcela innovación* and *parcela testigo* represent 14.10% (6544) and 15.12% (7020) of the total applications, respectively.

### 3.4 Calculating Mass of Active Ingredients Applied

The dataset provided information about the rate of commercial product applied, as well as the area of the fields (in hectares) where commercial products were applied. In order to calculate the mass of active ingredient applied to each field, the concentration of active ingredient in the commercial products applied was researched online. The mass of active ingredient applied for each application was then calculated using the following formula:

$$m_{\mathrm{j,\,k}} = r_{\mathrm{i}} \times c_{\mathrm{i,j}} \times a_k \tag{3}$$

Where:

- $m_{\mathrm{j,k}}$ represents the mass of active ingredient $j$ from commercial product $i$ on field $k$, expressed in kilograms (kg).
- $r_{\mathrm{i}}$ denotes the application rate of commercial product $i$ to the field, expressed in kilograms per hectare (kg/ha).
- $c_{\mathrm{i,j}}$ refers to the concentration of active ingredient $j$ within commercial product $i$, expressed as a fraction of the total product mass (e.g., 0.5 for 50% concentration).
- $a_k$ refers to the area of the field $k$, expressed in hectares (ha).

This formula accounts for the different concentrations of active ingredients across different commercial products, as well as the different areas of fields.

## 3.5 Life Cycle Inventory Analysis Using PestLCI

PestLCI is implemented in a Microsoft Excel file, and allows the user to choose specific parameters, such as location, type of crops, etc. It then provides fate factors (FF) that calculate the fate of pesticides applied to surface water, agricultural soils, natural soils, air, and crops. These fate factors are constants. The table below displays the different fate factors provided by PestLCI for the specific conditions in Mexico:

| **Compartment** | **Fate Factor** |
|---|---|
| Freshwater | 0.000211 |
| Agricultural Soil | 0.227 |
| Natural Soil | 0.00611 |
| Air | 0.1 |

Table 4: Fate factors for calculating the mass of pesticides entering different environmental compartments.

The fate factors were then used to calculate the mass of the active ingredientj for each application to the fieldk, entering the following compartments (1) fresh water, (2) agricultural soil, (3) natural soil, (4) air.

The following equations were used:

$$m_{\text{fresh water},j,k} = m_{\text{j,k}} \times FF_{\text{fresh water}} \tag{4}$$

$$m_{\text{agricultural soil},j,k} = m_{\text{j,k}} \times FF_{\text{agricultural soil}} \tag{5}$$

$$m_{\text{natural soil},j,k} = m_{\text{j,k}} \times FF_{\text{natural soil}} \tag{6}$$

$$m_{\text{air},j,k} = m_{\text{j,k}} \times FF_{\text{air}} \tag{7}$$

Where:

- $m_{\mathrm{j,k}}$: represents the mass of active ingredient $j$ applied to field $k$.
- $m_{\text{fresh water},j,k}$: represents the mass of active ingredient $j$ applied to field $k$ that enters the freshwater compartment (in kg).
- $FF_{\text{fresh water}}$: The fate factor for freshwater, which quantifies how much of the applied substance typically reaches freshwater environments.
- $m_{\text{agricultural soil},j,k}$: represents the mass of active ingredient $j$ applied to field $k$ that enters the agricultural soil compartment (in kg).
- $FF_{\text{agricultural soils}}$: The fate factor for freshwater, which quantifies how much of the applied substance typically reaches agricultural soils.
- $m_{\text{natural soil},j,k}$: represents the mass of active ingredient $j$ applied to field $k$ that enters the natural soil compartment (in kg).
- $FF_{\text{agricultural soils}}$: The fate factor for natural soils, which quantifies how much of the applied substance typically reaches natural soils.
- $m_{\text{air},j,k}$: represents the mass of active ingredient $j$ applied to field $k$ that enters the air compartment (in kg).
- $FF_{\text{air}}$: The fate factor for air, which quantifies how much of the applied substance typically reaches the air compartment.

Before we can make all the calculations, we first need to derive characterization factors for all the substances that are missing in the database of USEtox.

## 3.6 Calculation of Characterization Factors for Unavailable Substances in USEtox Database

However, not all the substances used in the project are included in this database. In fact, 13 of the substances applied in the extension project were not included in the dataset.

The documentation [Fantke et al., 2017] and the manual *Usetox 2.0 Manual: Organic Substances* [Fantke et al., 2015, p.9-13] provide a methodology on how to calculate CFs for substances missing in the dataset.

### 3.6.1 Deriving Physio-Chemical Properties of Missing Chemicals

The following table provides a summary of the physio-chemical data needed for USEtox to calculate CFs for pesticides:

| **Notation as in USEtox model** | **Unit** | **Explanation** | **Source** |
|---|---|---|---|
| MW | g mole$^{-1}$ | Molecular weight | EPISuite |
| pKa | - | Dissociation constants | SPARC |
| $K_{ow}$ | - | Octanol – water partition coefficient | EPISuite |
| $K_{oc}$ | l kg$^{-1}$ | Organic carbon - water partition coefficient | EPISuite |
| $P_{vap25}$ | Pa | Vapor pressure at 25°C | EPISuite |
| $Sol_{25}$ | mg l$^{-1}$ | Water solubility at 25°C | EPISuite |
| $K_{H25C}$ | Pa·m$^3$ mole$^{-1}$ | Henry's law constant | EPISuite, USEtox manual |
| $K_{DOC}$ | l kg$^{-1}$ | Dissolved organic carbon – water partition coefficient | USEtox manual |
| $k_{degA}$ | s$^{-1}$ | Degradation rate in air | EPISuite |
| $k_{degW}$ | s$^{-1}$ | Degradation rate in water | EPISuite |
| $k_{degSd}$ | s$^{-1}$ | Degradation rate in sediment | EPISuite |
| $k_{degSl}$ | s$^{-1}$ | Degradation rate in soil | PPDP |
| avlog$EC_{50}$ | log mg l$^{-1}$ | Measure of ecotoxic effect based on acute and chronic $EC_{50}$ data | PPDB, EFAS, ECOTOX, & papers |

Table 5: Inputs needed to calculate CFs in USEtox, including units, explanations, and sources

Most of the physico-chemical data were derived from EPISuite - the Estimation Program Interface Suite™, a program running on Windows. EPISuite contains different estimation programs, a database for different substances, including an experimental database. If the active ingredient was not included in the database, SMILES numbers (Simplified Molecular Input Line Entry System) were the only input necessary to calculate the input data. In line with the recommendation provided in the USEtox manual [Fantke et al., 2015, p.9-13], experimental data was prioritized. The following data was derived from EPISuite and its programs:

- MW: MWs were collected from the 'all results tab' in EPISuite;
- pKa: Since SPARC was not able to calculate the values for the substances, the default assumption in accordance with the manual was chosen;
- $K_{ow}$: If experimental data was not available, the KOWWIN program was used to calculate Log $K_{ow}$, to further calculate $K_{ow}$;
- $K_{oc}$: If experimental data was not available, the KOCWIN program was used to derive $K_{oc}$ estimates, based on MCI;
- $P_{vap25}$: If experimental data was lacking, the estimates from the MPBPVP program were used, depending on whether the substance is solid or liquid. If the former was the case, estimates based on the modified Grain method were used. If the substance was liquid, the average from the modified Grain method and Antoine method was calculated.
- $Sol_{25}$: Estimates could be found using the WSKOWWIn program.
- $K_{H25C}$: If estimates from the HENRIWIN program were lacking, the formula KH25C = MW * Pvap25 $Sol25^{-1}$ was used to calculate $K_{H25C}$.
- $k_{degA}$: The APOWIN provided estimates of the overall OH rate constant, which was multiplied by [OH], the hydroxyl radical concentration per 12 hours of daylight (in OH

radicals or molecules $cm^3$). The default value of $1.5*10^6$ was used, as recommended by the manual [Fantke et al., 2015, p.10].

- $k_{degW}$: BIOWIN3 - a separate model included in EPISuite - was used to derive $k_{degW}$, based on the length of the ultimate bio-degradation timeframe of the substance.

The following calculations were carried out to derive the following data, in accordance with the manual [Fantke et al., 2015, p.9-10]:

- $K_{H25C}$: If estimates from the EPISuite program were lacking, the formula KH25C = MW * Pvap25 $Sol25^{-1}$ was used to calculate $K_{H25C}$.

- $k_{degSd} = k_{degW} / 9$

To derive $k_{degSl}$, the following calculation was carried out: $k_{degSl} = \ln(2) / (DT50 * 86400$ seconds per day), where DT50 is the degradation data in soil based on experimental data, derived from the Pesticide Properties Database ( PPDP). If experimental data was missing, the equation $k_{degSl} = k_{degW} / 2$ was carried out, in accordance with the manual [Fantke et al., 2015, p.10].

### 3.6.2 Deriving Average log$EC_{50}$ Values

To derive avlog$EC_{50}$ values,the following databases were used to collect chronic and acute $EC_{50}$ values:

- PPDP - Pesticide Property Database [PPDP],

- EFSA - European Food Safety Authority Chemical Hazards database [EFS],

- ECOTOX - Ecotoxicology Database [ECOTOX, 2022],

- Various scientific papers.

If numerous chronic $EC_{50}$ values were reported for the same species $i$ and same active ingredient $j$, the geometric mean of these values was calculated with the following equation [Fantke et al., 2015, p.14]:

$$\text{Geometric mean EC}_{50,ij} = \sqrt[n]{\text{EC}_{50,ij,1} \times \text{EC}_{50,ij,2} \times \cdots \times \text{EC}_{50,ij,n}} \tag{8}$$

To calculate *avlogchronicEC₅₀* for each substance $j$, chronic $EC_{50}$ values are needed. However, sometimes acute $EC_{50}$ values are provided. To convert acute to chronic $EC_{50}$ values, the following equation was used, according to the manual [Fantke et al., 2015, p.14]:

$$\text{Chronic EC}_{50} = \frac{\text{Acute EC}_{50}}{2} \tag{9}$$

To calculate avlogchronic$EC_{50}$ values for each substance, the following equation was used:

$$\text{avlogEC}_{50,j} = \frac{\sum_{i=1}^{N} \log(chronicEC_{50i,j})}{N} \tag{10}$$

Where $avlogchronicEC_{50}$ is the average of chronic $EC_{50}$ values of $N$ number of species $_{\mathrm{i}}$ for substance $j$.

The following table provides an overview of the acute and chronic $EC_{50}$ values, as well as the reference and log transformation for each active ingredient:

| **Trophic Level** | **Species** | **Days** | **Acute $EC_{50}$ (mg/L)** | **Chronic $EC_{50}$ (mg/L)** | **Reference** | **Log (Chronic $EC_{50}$)** |
|---|---|---|---|---|---|---|
| **Abamectin (71751-41-2): avlog $EC_{50}$= -1.619513124** | | | | | | |
| Green Algae | Scenedesmus obliqnus | 4 | 9.8882 | 4.9441 | ECOTOX | 0.694087246 |
| Green Algae | Scenedesmus obliqnus | 4 | 7.3096 | 3.6548 | ECOTOX | 0.562863616 |
| Invertebrate | Daphnia similis | 2 | 0.0000051 | 0.00000255 | ECOTOX | -5.59345982 |
| Insect | Chironomus xanthus | 4 | 0.00267 | 0.001335 | ECOTOX | -2.874518734 |
| Insect | Scenedesmus subspicatus | 3 | 4.4 | 2.2 | Lumaret et al. [2012] | 0.342422681 |
| Fish | Danio rerio | 2 | 0.033 | 0.0165 | ECOTOX | -1.782516056 |
| Bacteria | V. fischeri | 30 min | 0.69 | 0.345 | ECOTOX | -0.462180905 |
| Invertebrate | Daphnia magna | | | 0.000143614 | geo mean | -3.842803021 |
| Invertebrate | Daphnia magna | 1 | 0.00033 | 0.000165 | Lumaret et al. [2012] | |
| Invertebrate | Daphnia magna | 2 | 0.00025 | 0.000125 | Lumaret et al. [2012] | |
| **Beta-Cyfluthrin (1820573-27-0)): avlog $EC_{50}$= -0.873220343** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 0.00029 | 0.000145 | PPDP | -3.838631998 |
| Aquatic Plant | Lemna gibba | 7 | 0.00084 | 0.00042 | PPDP | -3.37675071 |
| Algae | Scenedesmus subspicatus | 3 | 0.002 | 0.001 | PPDP | -3 |
| Cyanobacteria | A. flos-aquae | 4 | 62.3364 | 31.1682 | Ma [2005] | 1.493711722 |
| Cyanobacteria | M. aeruginosa | 4 | 87.0454 | 43.5227 | Ma [2005] | 1.63871583 |
| Cyanobacteria | M. flos-aquae | 4 | 34.6256 | 17.3128 | Ma [2005] | 1.238367312 |
| Green Algae | S. capricornutun | 4 | 3.5152 | 1.7576 | Ma [2005] | 0.244920044 |
| Green Algae | S. quadricauda | 4 | 2.3663 | 1.18315 | Ma [2005] | 0.073039808 |
| Green Algae | S. obliqnus | 4 | 97.0396 | 48.5198 | Ma [2005] | 1.685919002 |
| Green Algae | C. vulgaris | 4 | 4.4095 | 2.20475 | Ma [2005] | 0.343359351 |

| Trophic Level | Species | Days | Acute $EC_{50}$ (mg/L) | Chronic $EC_{50}$ (mg/L) | Reference | Log (Chronic $EC_{50}$) |
|---|---|---|---|---|---|---|
| Green Algae | C. pyrenoidosa | 4 | 885.2353 | 442.61765 | Ma [2005] | 2.646028728 |
| Hemiptera, Notonectidae | Anisops sardeus | 1 | 0.00001 | 0.000005 | ECOTOX | |
| Hemiptera, Notonectidae | Anisops sardeus | 2 | 0.000004 | 0.000002 | ECOTOX | |
| Hemiptera, Notonectidae | Anisops sardeus | | | 3.16228E-06 | geo mean | -5.5 |
| Branchiopoda, Anostraca | Streptocephalus sudanicus | 1 | 0.000021 | 0.0000105 | ECOTOX | |
| Branchiopoda, Anostraca | Streptocephalus sudanicus | 2 | 0.000019 | 0.0000095 | ECOTOX | |
| Branchiopoda, Anostraca | Streptocephalus sudanicus | | | 9.98749E-06 | geo mean | -5.000543548 |
| **Chlorantraniliprole (500008-45-7): avlog $EC_{50}$= -0.825644711** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 0.0116 | 0.0058 | PPDP | -2.236572006 |
| Aquatic Plant | Lemna gibba | 7 | 2 | 1 | PPDP | 0 |
| Algae | Pseudokirchneriella subcapitata | 3 | 4 | 2 | PPDP | 0.301029996 |
| Midge | Chironomus riparius | 2 | 0.0859 | 0.04295 | Barbee et al. [2010] | -1.367036832 |
| **Emamectin benzoate (155569-91-8): avlog $EC_{50}$= -2.197221531** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 0.001 | 0.0005 | PPDP | -3.301029996 |
| Aquatic Plant | Lemna gibba | 7 | 0.094 | 0.047 | PPDP | -1.327902142 |
| Fish | Pimephales promelas | 4 | 0.194 | 0.097 | PPDP | -1.013228266 |

| Trophic Level | Species | Days | Acute $EC_{50}$ (mg/L) | Chronic $EC_{50}$ (mg/L) | Reference | Log (Chronic $EC_{50}$) |
|---|---|---|---|---|---|---|
| Algae | Pseudokirchneriella subcapitata | 3 | 0.0072 | 0.0036 | PPDP | -2.443697499 |
| Fish | Zebrafish | N/A | 0.00215 | 0.001075 | Gu et al. [2023] | |
| Fish | Zebrafish | N/A | 0.00354 | 0.00177 | Gu et al. [2023] | |
| Fish | Zebrafish | N/A | 0.02172 | 0.01086 | Gu et al. [2023] | |
| Fish | Zebrafish | N/A | 0.00172 | 0.00086 | Gu et al. [2023] | |
| Fish | Zebrafish | N/A | 0.00094 | 0.00047 | Gu et al. [2023] | |
| Fish | Zebrafish | N/A | 0.00095 | 0.000475 | Gu et al. [2023] | |
| Fish | Zebrafish | | | 0.001258202 | geo mean | -2.900249754 |
| **Flubendiamide (272451-65-7): avlog $EC_{50}$= -1.064339525** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 0.06 | 0.03 | PPDP | |
| Invertebrate | Daphnia magna | 2 | 0.0026 | 0.0013 | EFSA | |
| Invertebrate | Daphnia magna | | | 0.006244998 | geo mean | -2.204467696 |
| Aquatic Plant | Lemna gibba | 7 | 0.0546 | 0.0273 | PPDP | -1.563837353 |
| Algae | Pseudokirchneriella subcapitata | 3 | 0.069 | 0.0345 | PPDP | -1.462180905 |
| Insect | Chironomus riparius | N/A | 18.8 | 9.4 | Authority [2013] | 0.973127854 |
| **Flupyradifurone (951659-40-8): avlog $EC_{50}$= 0.325787082** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 77.6 | 38.8 | PPDA | 1.588831726 |
| Aquatic Plant | Lemna gibba | 7 | 67.7 | 33.85 | PPDA | 1.529558673 |
| Algae | Pseudokirchneriella subcapitata | 3 | 100 | 50 | PPDA | 1.698970004 |
| Amphipod | Hyalella azteca | 28 | | 0.016 | ECOTOX | -1.795880017 |

| Trophic Level | Species | Days | Acute $EC_{50}$ (mg/L) | Chronic $EC_{50}$ (mg/L) | Reference | Log (Chronic $EC_{50}$) |
|---|---|---|---|---|---|---|
| Invertebrate | Hexagenia spp. | 4 | 0.081 | 0.0405 | EXOTOX | -1.392544977 |
| **Gamma-Cyhalothrin (76703-62-3): avlog $EC_{50}$=-4.215904542** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 0.000045 | 0.0000225 | PPDA | -4.647817482 |
| Algae | Pseudokirchneriella subcapitata | 3 | 2.85 | 1.425 | PPDA | 0.153814864 |
| Amphipod | Gammarus pseudolimnaeus | 4 | 0.000000446 | 0.000000223 | EFSA | -6.651695137 |
| Amphipod | Hyalella azteca | 3 | 0.0000028 | 0.0000014 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000017 | 0.00000085 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000024 | 0.0000012 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000104 | 0.0000052 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000015 | 0.00000075 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000074 | 0.0000037 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000039 | 0.00000195 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000014 | 0.0000007 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000036 | 0.0000018 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000022 | 0.0000011 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000111 | 0.00000555 | EFSA | |
| Amphipod | Hyalella azteca | 3 | 0.0000157 | 0.00000785 | EFSA | |
| Amphipod | Hyalella azteca | | | 1.91461E-06 | geo mean | -5.717920415 |
| **Novaluron (116714-46-6): avlog $EC_{50}$=-2.051710841** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 0.058 | 0.029 | PPDA | -1.537602002 |

| Trophic Level | Species | Days | Acute $EC_{50}$ (mg/L) | Chronic $EC_{50}$ (mg/L) | Reference | Log (Chronic $EC_{50}$) |
|---|---|---|---|---|---|---|
| Aquatic Plants | Lemna gibba | 7 | 0.075 | 0.0375 | PPDA | -1.425968732 |
| Algae | Pseudokirchneriella subcapitata | 3 | 9.68 | 4.84 | PPDA | 0.684845362 |
| Insect | Culex quinquefasciatus | N/A | 0.00000236 | 0.00000118 | Ahmed and Vogel [2020] | -5.928117993 |
| **Spinetoram (935545-74-7): avlog $EC_{50}$=-1.062412612** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 0.228 | 0.114 | PPDA | -0.943095149 |
| Aquatic Plants | Lemna gibba | 7 | 14.2 | 7.1 | PPDA | 0.851258349 |
| Algae | Pseudokirchneriella subcapitata | 3 | 0.0779 | 0.03895 | PPDA | -1.409492538 |
| Algae | Navicula pelliculosa | 3 | 0.0779 | 0.03895 | EFSA | -1.409492538 |
| Invertebrate | Daphnia pulex | 1 | 0.01976 | 0.00988 | Shen et al. [2022] | |
| Invertebrate | Daphnia pulex | 2 | 0.00319 | 0.001595 | Shen et al. [2022] | |
| Invertebrate | Daphnia pulex | | | 0.00396971 | geo mean | -2.401241184 |
| Mollusca | Oyster | N/A | 0.393 | 0.1965 | NIAID Data Discovery Portal | -0.706637445 |
| **Spinosad (168316-95-8): avlog $EC_{50}$= 0.302114408** | | | | | | |
| Invertebrate | Daphnia magna | 2 | 1 | 0.5 | Lumaret et al. [2012] | |
| Invertebrate | Daphnia magna | 2 | 9.1 | 4.55 | Lumaret et al. [2012] | |
| Invertebrate | Daphnia magna | | | 1.508310313 | geo mean | 0.1784907 |
| Algae | Navicula pelliculosa | 5 | 0.079 | 0.0395 | Guston [2010] | |
| Algae | Navicula pelliculosa | 5 | 0.35 | 0.175 | Guston [2010] | |
| Algae | | | 0.083141446 | | geo mean | -1.080182428 |

| Trophic Level | Species | Days | Acute $EC_{50}$ (mg/L) | Chronic $EC_{50}$ (mg/L) | Reference | Log (Chronic $EC_{50}$) |
|---|---|---|---|---|---|---|
| Algae | Anabaena flosaquae | 5 | 6.1 | 3.05 | Guston [2010] | 0.484299839 |
| Algae | Selenastrum capricornutum | 7 | 105.5 | 52.75 | | 1.722222464 |
| Algae | Skeletonema costatum | 5 | 0.23 | 0.115 | Guston [2010] | -0.93930216 |
| Aquatic Plant | Lemna gibba | 14 | | 6.6 | Guston [2010] | |
| **Sulfaxflor (946578-00-3): avlog $EC_{50}$= -0.264906249** | | | | | | |
| Algae | Navicula pelliculosa | 4 | 101 | 50.5 | PPDA | 1.703291378 |
| Insect | Chironomus kiinensis | N/A | 0.0352 | 0.0176 | Liu et al. [2021] | -1.754487332 |
| Invertebrate | Daphnia magna | N/A | 0.361 | 0.1805 | Gauthier and Mabury [2021] | -0.743522794 |
| **Thiamethoxam (153719-23-4): avlog $EC_{50}$= 0.908758844** | | | | | | |
| Amphipod Crustacean | Hyalella azteca | 28 | | 0.2 | ECOTOX | -0.698970004 |
| Invertebrate | Hexagenia spp. | 4 | 0.63 | 0.315 | ECOTOX | -0.501689446 |
| Invertebrate | Daphnia magna | 2 | 100 | 50 | PPDA | 1.698970004 |
| Invertebrate | Ceriodaphnia dubia | 2 | 80 | 40 | PPDA | 1.602059991 |
| Aquatic Plant | Lemna gibba | 7 | 90 | 45 | PPDA | 1.653212514 |
| Algae | Pseudokirchneriella subcapitata | 3 | 100 | 50 | PPDA | 1.698970004 |
| **Zeta Cypermetrhin (97955-44-7): avlog $EC_{50}$= -3.547672866** | | | | | | |
| Invertebrate | Ceriodaphnia dubia | 2 | 0.00014 | 0.00007 | PPDA | -4.15490196 |
| Algae | Pseudokirchneriella subcapitata | 3 | 1 | 0.5 | PPDA | -0.301029996 |

| Trophic Level | Species | Days | Acute $EC_{50}$ (mg/L) | Chronic $EC_{50}$ (mg/L) | Reference | Log (Chronic $EC_{50}$) |
|---|---|---|---|---|---|---|
| Amphid | Gammarus pulex | 4 | 0.0000013 | 0.00000065 | Yılmaz and Taş [2021] | -6.187086643 |

All the values as shown in the figure above were then copied into the USEtox data file, and CFs could be calculated.

## 3.7 Characterization Factors Used for Calculations

The following characterization factors were used to calculate impact scores:

Table 7: Midpoint Ecotoxicological Characterization Factors for Various Compounds

| Name | CAS RN | Midpoint Ecotox. Charact. factor [PAF.$m^3$.day/$kg_{emitted}$] | | | |
|---|---|---|---|---|---|
| | | Air | Fr Water | Nat Soil | Agr. Soil |
| Abamectin* | 71751-41-2 | 2,38E+03 | 5,30E+05 | 4,67E+02 | 4,67E+02 |
| Acephate | 30560-19-1 | 7,32E+01 | 7,45E+02 | 1,61E+02 | 1,61E+02 |
| Alpha-Cypermethrin | 67375-30-8 | 1,35E+06 | 1,09E+08 | 4,77E+04 | 4,77E+04 |
| Beta-Cyfluthrin* | 1820573-27-0 | 1,10E+03 | 1,66E+05 | 1,63E+02 | 1,63E+02 |
| Bifenthrin | 82657-04-3 | 1,85E+05 | 1,35E+07 | 7,38E+03 | 7,38E+03 |
| Carbofuran | 1563-66-2 | 7,99E+03 | 1,34E+05 | 2,32E+04 | 2,32E+04 |
| Chlorantraniliprole* | 500008-45-7 | 8,23E+04 | 4,87E+05 | 1,26E+05 | 1,26E+05 |
| Chlorpyrifos | 2921-88-2 | 4,00E+04 | 1,34E+07 | 6,27E+04 | 6,27E+04 |
| Cypermethrin | 52315-07-8 | 1,65E+06 | 1,29E+08 | 1,11E+05 | 1,11E+05 |
| Deltamethrin | 52918-63-5 | 4,88E+04 | 6,25E+06 | 5,46E+03 | 5,46E+03 |
| Diazinon | 333-41-5 | 2,28E+03 | 2,24E+05 | 7,90E+03 | 7,68E+03 |
| Dimethoate | 60-51-5 | 9,41E+02 | 1,94E+04 | 4,21E+03 | 4,21E+03 |
| Emamectin benzoate* | 155569-91-8 | 3,08E+03 | 7,01E+05 | 1,22E+00 | 1,22E+00 |
| Fenpropathrin | 39515-41-8 | 2,33E+06 | 2,30E+08 | 3,89E+05 | 3,89E+05 |
| Fenvalerate | 51630-58-1 | 8,05E+05 | 4,36E+07 | 3,55E+05 | 3,55E+05 |
| Fipronil | 120068-37-3 | 4,95E+04 | 3,58E+06 | 1,13E+05 | 1,13E+05 |
| Flubendiamide* | 272451-65-7 | 2,77E+04 | 7,75E+05 | 1,90E+04 | 1,90E+04 |
| Flupyradifurone* | 951659-40-8 | 5,00E+02 | 1,65E+04 | 1,69E+03 | 1,69E+03 |
| Gamma-Cyhalothrin* | 76703-62-3 | 6,25E+04 | 9,17E+07 | 1,21E+04 | 1,21E+04 |
| Imidacloprid | 138261-41-3 | 1,08E+03 | 4,09E+03 | 2,20E+03 | 2,20E+03 |
| Lambda-cyhalothrin | 91465-08-6 | 2,80E+06 | 3,51E+08 | 6,55E+04 | 6,55E+04 |
| Malathion | 121-75-5 | 6,55E+02 | 6,76E+04 | 3,20E+02 | 3,20E+02 |
| Methamidophos | 10265-92-6 | 7,16E+02 | 1,08E+04 | 2,38E+03 | 2,38E+03 |

*Continued on next page*

| Name | CAS RN | Midpoint Ecotox. Charact. factor [PAF.m$^3$.day/kg$_{\text{emitted}}$] | | | |
|---|---|---|---|---|---|
| | | Air | Fr Water | Nat Soil | Agr. Soil |
| Metomil | 16752-77-5 | 3,28E+03 | 3,14E+04 | 6,02E+03 | 6,02E+03 |
| Novaluron* | 116714-46-6 | 1,56E+05 | 7,45E+06 | 2,05E+05 | 2,05E+05 |
| Permethrin | 52645-53-1 | 2,10E+04 | 2,18E+06 | 1,77E+03 | 1,77E+03 |
| Pirimicarb | 23103-98-2 | 2,56E+01 | 2,11E+03 | 5,04E+01 | 1,93E+02 |
| Spinetoram* | 935545-74-7 | 1,24E+04 | 5,75E+05 | 3,73E+01 | 3,73E+01 |
| Spinosad* | 168316-95-8 | 3,56E+02 | 1,58E+04 | 3,68E+01 | 3,68E+01 |
| Sulfoxaflor* | 946578-00-3 | 9,49E+02 | 6,45E+04 | 6,38E+02 | 6,38E+02 |
| Tebupirimfos | 96182-53-5 | 4,24E+03 | 1,06E+06 | 1,33E+05 | 1,33E+05 |
| Tefluthrin | 79538-32-2 | 1,99E+04 | 2,95E+07 | 5,56E+03 | 5,56E+03 |
| Terbufos | 13071-79-9 | 4,29E+03 | 4,57E+06 | 8,47E+04 | 8,47E+04 |
| Thiamethoxam* | 153719-23-4 | 7,28E+01 | 2,92E+03 | 3,68E+02 | 3,68E+02 |
| Thiodicarb | 59669-26-0 | 2,63E+03 | 1,15E+05 | 5,90E+03 | 5,90E+03 |
| Zeta-Cypermethrin* | 1315501-18-8 | 1,51E+05 | 4,38E+07 | 7,50E+03 | 7,50E+03 |

*Note: * indicates that the values are based on our own calculations.*

## 3.8 Impact Assessment Using USEtox

### 3.8.1 Calculating Impact Scores for Each Application

To calculate the Impact Score IS (in PAF.m$^3$.day/kg$_{\text{emitted}}$) on freshwater ecosystems of applicationn of active ingredientj to fieldk, the masses of active ingredientj entered into different environmental compartments were multiplied with the corresponding Characterization Factors (CFs). Those were either provided by USEtox in its database, or calculated following the methodology in the USEtox manual. The following formula was used:

$$\begin{aligned} \textit{Impact Score}_n = {} & m_{\text{fresh water},j,k} \times CF_{\text{fresh water,j}} \\ & + m_{\text{agricultural soil},j,k} \times CF_{\text{agricultural soil,j}} \\ & + m_{\text{natural soil},j,k} \times CF_{\text{natural soil,j}} \\ & + m_{\text{air},j,k} \times CF_{\text{air,j}} \end{aligned} \tag{11}$$

Where:

- $\textit{Impact Score}_n$ is the Impact Score of application $n$ of active ingredient $j$, expressed in PAF.m$^3$.day/kg$_{\text{emitted}}$.

- $m_{\text{freshwater},j,k}$, $m_{\text{air},j,k}$, $m_{\text{agricultural soil},j,k}$, $m_{\text{natural soil},j,k}$ represent the masses of the active ingredient $j$ in the compartments freshwater, air, agricultural soil, and natural soil, respectively, for each pesticide application $n$.

- $CF_{\text{freshwater,j}}$, $CF_{\text{air,j}}$, $CF_{\text{ag soil,j}}$, and $CF_{\text{nat soil,j}}$ represent the corresponding characterization factors for active ingredient $j$ and the corresponding compartment.

Combining PestLCI models and their fate factors with Characterization factors derived from USEtox is the state of the art for assessing the freshwater ecotoxicity of pesticides. Pesticides - once applied in the fields - can reach the freshwater compartment through different compartments and by different means, such as transportation or transformation. USEtox takes this into account and calculates the potential impact of pesticides that move to different compartments. Therefore, by looking at different compartments - others than freshwater - USEtox provides a more realistic and holistic picture of the freshwater ecotoxicity of pesticides. This approach takes into account the whole life cycle of a chemical, and how it eventually impacts freshwater, reaching this compartment through indirect pathways or transformations over time.

### 3.8.2 Calculating Total Impact Scores per Active Ingredient

To calculate the total impact score of active ingredientj (in PAF.m$^3$.day/kg$_{\text{emitted}}$), all applications of active ingredientj were summed up:

$$\begin{aligned} \textit{Total Impact Score}_j = \sum_{n=1}^{N} \Big( & m_{\text{fresh water},j,n} \times CF_{\text{fresh water,j}} \\ & + m_{\text{agricultural soil},j,n} \times CF_{\text{agricultural soil,j}} \\ & + m_{\text{natural soil},j,n} \times CF_{\text{natural soil,j}} \\ & + m_{\text{air},j,n} \times CF_{\text{air,j}} \Big) \end{aligned} \tag{12}$$

### 3.8.3 Calculating Average Impact Scores

To calculate the impact score of active ingredientj per hectare ($\mathrm{IS}_{\mathrm{hectar,j}}$) (in PAF.$\mathrm{m}^3$.day/$\mathrm{kg}_{\mathrm{emitted}}$ $\mathrm{hectar}^{-1}$), the total impact score of active ingredientj was divided by the total areaa of fields, wherej was applied:

$$avIS_{hectar,j} = \frac{\text{Total Impact Score}_\text{j}}{\text{a}_\text{j}} \tag{13}$$

To calculate the average impact score of active ingredientj per application, Total Impact $\text{Score}_\text{j}$ was divided by the number of applications ofj:

$$avIS_{application,j} = \frac{\text{Total Impact Score}_\text{j}}{\text{n}_\text{j}} \tag{14}$$

## 3.9 Statistical Analysis

The purpose of this impact assessment is also to find out what management practices are drivers for freshwater ecotoxicity. In order to estimate the effect of different management practices on freshwater ecotoxicity (impact scores in PAF $\mathrm{m}^3$ $\mathrm{day}^{-1}$)–or, the response variable–, a linear regression model was developed. For each of the over 46,000 applications, the impact score was calculated following the steps described above. The effect of management variables on freshwater ecotoxicity was tested using RStudio.

As a first step, we assessed whether our response variable (impact scores) followed a normal distribution. Because of the sheer size of the dataset, we could not perform the

Shapiro-Wilk test, which can only handle datasets below 5000 entries. Instead, we examined Q-Q plots and concluded that our response variable was not normally distributed and exhibited significant skewness.

We tested several transformations to address this skewness, including square root transformation, inverse transformation, and log transformation, to give examples. Based on the Q-Q plots, we determined that the log transformation provided the most suitable normalization of our response variable.

As a second step, we assessed whether predictor variables of interest were correlated with each other. To do so, we calculated a correlation matrix using the cor() function in R, which revealed that none of the numeric variables were correlated with each other (all values were below the threshold of 0.7). To extend this analysis to non-numeric, categorical variables, we created dummy variables for each categorical predictor variable using the model.matrix() function. After combining them with the numeric predictor variables, we visualized the correlation matrices using the corrplot() function in the corrplot package. Again, no variable was correlated with another one.

Among the predictor variables, 'plot size' was the only numeric variable with a wide range of different values. After using the summary() function in R, this wide range of values was illustrated with a minimum value of 0.01 hectare to a maximum of 97 hectares, with a median of 2 hectares and a mean of 3.537 hectares. In order to reduce skewness, we applied the log() function in R to this predictor variable, normalizing the data.

Initially, we tried to fit the data using a linear mixed-effects model (lm and lmer) with the log-transformed response variable 'impact score'. Since the log transformation of the response variable itself did not resolve convergence issues, likely due to the extreme skewness of the data, we selected a generalized linear model (glm). These can provide more flexibility and are better adapted to handle skewed data. We also tested a generalized linear mixed-effects model (glmer) which included 'years' as a random effect variable. Diagnostic results revealed that 'years' had no significant effect on the model. At the same time, we also tried different transformations of the response variable, like the box-cox transformation, alongside different models, like a generalized additive model, or a polymodel, none of these were good to fit our data. Because of this, we proceeded with a glm model with a 'Gamma' family, not including 'years' as a random variable. The reason for choosing the 'Gamma' family was the capability of the model of handling extremely skewed data, while also performing a log transformation of the response variable.

The following model was chosen: We used a Gamma generalized linear model (GLM) with a log link function to model the response variable, `is_total`, as a function of the following variables:

- `is_hectare`: Response variable impact score for each application per hectare. We chose a normalized measure of environmental impact to account for variations in plot size, allowing us to interpret the results as impact intensity per unit area.
- `log(plot_size + 1)`: Log-transformed plot size values.
- `intercropping`: Indicator variable for intercropping (if another crop besides maize was grown in the field).
- `conservation_agriculture`: Indicator variable for conservation agriculture (if conservation agriculture was practiced or not).
- `as.factor(hydrological_regime)`: Factor variable indicating whether the field was irrigated or raindfed.
- `as.factor(production_cycle)`: Factor variable indicating whether the crop was grown during the summer or winter growing season.
- `as.factor(education)`: Factor variable for different extension approaches.

The model formula is given by:

```
glm( is_hectare ~
     log(plot_size + 1)+
     intercropping+
     conservation_agriculture+
     as.factor(hydrological_regime)+
     as.factor(production_cycle)+
     as.factor(education) )
```

with the following family and link function:

Family: Gamma, Link: Log

To ensure that the model was a good fit for our data, we performed some tests. As a first step, we performed visual diagnostics, using the glm.diag() and glm.diag.plot() function in R, which are specifically tailored for glm models.

Figure X displays visualized diagnostics for our generalized linear model, revealing that our model is in general a good fit for our observations.

- Residuals vs. Linear Predictor (Top Left): This plot displays the residuals plotted against the linear predictor. Ideally, residuals are randomly distributed in the plot, without any clear pattern (i.e. a funnel-shape). In our model, there might be some clustering around certain values, but we cannot depict any clear pattern or trend.

- Cook's Distance vs. Leverage (Bottom Left): This plot illustrates Cook's distance as a function of leverage, revealing the influence of each entry on our model. In our model, only a few entries have a high Cook's distance, while most values display a low Cook's value.

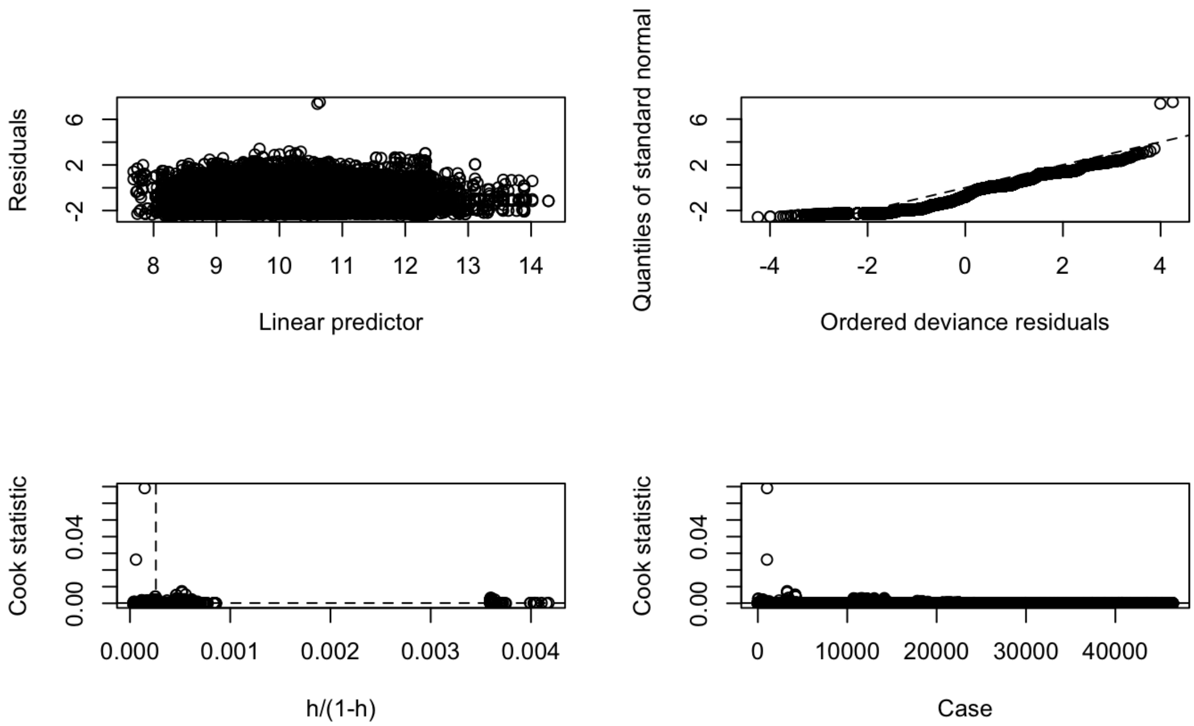



Figure 7: Model Diagnostics

- Q-Q Plot of Deviance Residuals (Top Right): This plot shows the distribution of the deviance residuals compared to a standard distribution. Ideally, the plotted values should follow the line, which is generally the case with our model, with some deviations. The Gamma family can handle these deviations. The points significantly deviating from the crossed line are outliers, but these are expected in a dataset of over 46,000 entries.

- Cook's Distance vs. Case (Bottom Right): This plot displays Cook's distance across the observations. Again, the vast majority of our observations display a low Cook's value.

Furthermore, we performed a multicollinearity check among predictor variables, using the vif() function in R. This function calculates the Generalized Variance Inflation Factor (GVIF) for each variable in the model. All predictor variables showed a low GVIF value close to 1, not exceeding a GVIF value of 1.3, suggesting that there are no multicollinearity issues with our models. The typical threshold to be exceeded is considered to be a GVIF value of 5.

After the model was run, we used the emmeans() and contras() 'pairwise' functions in R for those variables displaying a significant p value of below 0.05. In addition, we used the Tukey correction for the p-values. After that, we used the exp() function to back-transform our log-transformed data, making the results more easily interpretable.

In order to evaluate the relationship between modes of action and impact scores, we performed an analysis of variance (ANOVA) in R. We used the log-transformed impact scores as the dependent variable (`log (is_total) + 1`) to model it as a function of the categorical variable `mode_of_action`. The log transformation was applied to stabilize variance and meet the assumptions of the ANOVA. Tukey's Honestly Significant Difference (HSD) test was carried out to identify which pairs of mean log-transformed impact scores of different modes of actions differ from each other. To further investigate the relationships between management practices and the mode of actions, multiple generalized linear models were developed. Each model used a binary response variable (including conservation agriculture, hydrological regime, production cycle, intercropping), with mode of action as the predictor. Additionally, a multinomial logistic regression model was developed to evaluate the association between mode of action and the different modes of extension. The results provide an insight into which modes of actions are associated with which management practice and extension treatment.

# 4 Results

The following section will provide information about the total applications of each active ingredient, as well as the total amount of active ingredients applied (in kg) in the fields. In addition, the total impact scores in PAF $m^3$ $day^{-1}$ for each active ingredient , as well as the average impact scores per hectare and per application for each active ingredient. Furthermore, trends over the years will be presented for total impact scores and the average impact score per hectare and per application.

## 4.1 Numbers of Application of Each Active Ingredient

The following table (table 8) provides an overview of how often each active ingredient was applied between 2012 and 2020, ordered from the top (most often applied active ingredient) to the least applied:

Table 8: Numbers of Application of Each Active Ingredient

| Active Ingredient | Applications | % of Applications | Active Ingredient | Applications | % of Applications |
|---|---|---|---|---|---|
| Cypermethrin | 10,185 | 21.28% | Bifenthrin | 276 | 0.58% |
| Chlorpyrifos | 9,457 | 19.76% | Abamectin | 265 | 0.55% |
| Spinetoram | 6,525 | 13.63% | Diazinon | 249 | 0.52% |
| Permethrin | 4,058 | 8.48% | Malathion | 215 | 0.45% |
| Emamectin Benzoate | 3,933 | 8.22% | Tefluthrin | 215 | 0.45% |
| Lambda-cyhalothrin | 3,555 | 7.43% | Thiamethoxam | 214 | 0.45% |
| Chlorantraniliprole | 2,244 | 4.69% | Sulfoxaflor | 179 | 0.37% |
| Deltamethrin | 783 | 1.64% | Thiodicarb | 132 | 0.28% |
| Carbofuran | 696 | 1.45% | Fipronil | 137 | 0.29% |
| Imidacloprid | 646 | 1.35% | Methamidophos | 122 | 0.25% |
| Terbufos | 562 | 1.17% | Fenpropathrin | 100 | 0.21% |
| Metomil | 478 | 1.00% | Flupyradifurone | 94 | 0.20% |
| Zeta-Cypermethrin | 460 | 0.96% | Spinosad | 73 | 0.15% |
| Dimethoate | 426 | 0.89% | Alpha-Cypermethrin | 68 | 0.14% |
| Flubendiamide | 421 | 0.88% | Tebupirimfos | 67 | 0.14% |
| Beta-Cyfluthrin | 366 | 0.76% | Gamma-Cyhalothrin | 60 | 0.13% |
| Fenvalerate | 283 | 0.59% | Acephate | 31 | 0.06% |
| Novaluron | 279 | 0.58% | Pirimicarb | 5 | 0.01% |
| **Grand Total** | **46,417** | **100.00%** | | | |

The most frequently applied active ingredients are cypermethrin, chlorpyrifos, and spinetoram, with 10,185, 9,457, and 6,525 applications. Combined together, these three represent over 50% of the dataset. Other, less frequently used active ingredients are permethrin, emamectin benzoate, lambda-cyhalothrin, and chlorantraniliprole, each representing between 5 and 10% of the dataset. Other active ingredients (around 30) represent less than 2% of the dataset.

## 4.2 Amount (kg) of Each Active Ingredient Applied

The following table provides an overview of how much each active ingredient was applied in total between 2012 and 2021, ordered from the top to the least amount applied:

Table 9: Numbers of Application of Each Active Ingredient

| **Active Ingredient** | **Amount applied (kg)** | **Amount applied (%)** | **Active Ingredient** | **Total AI applied (kg)** | **Total AI applied (%)** |
|---|---|---|---|---|---|
| Chlorpyrifos | 24,596.55 | 52.16% | Imidacloprid | 194.63 | 0.41% |
| Malathion | 5,520.60 | 11.71% | Deltamethrin | 143.41 | 0.30% |
| Cypermethrin | 4,481.16 | 9.50% | Emamectin Benzoate | 139.01 | 0.29% |
| Permethrin | 2,899.93 | 6.15% | Novaluron | 101.80 | 0.22% |
| Terbufos | 2,173.37 | 4.61% | Tebupirimfos | 91.52 | 0.19% |
| Metomil | 1,656.14 | 3.51% | Thiamethoxam | 89.86 | 0.19% |
| Diazinon | 696.96 | 1.48% | Acephate | 60.43 | 0.13% |
| Carbofuran | 683.21 | 1.45% | Thiodicarb | 53.30 | 0.11% |
| Dimethoate | 491.54 | 1.04% | Zeta-Cypermethrin | 45.83 | 0.10% |
| Fenpropathrin | 470.28 | 1.00% | Bifenthrin | 45.29 | 0.10% |
| Spinetoram | 460.46 | 0.98% | Abamectin | 21.46 | 0.05% |
| Tefluthrin | 348.44 | 0.74% | Spinosad | 20.41 | 0.04% |
| Methamidophos | 329.97 | 0.70% | Beta-Cyfluthrin | 20.24 | 0.04% |
| Lambda-cyhalothrin | 314.30 | 0.67% | Sulfoxaflor | 18.72 | 0.04% |
| Chlorantraniliprole | 266.83 | 0.57% | Flupyradifurone | 15.83 | 0.03% |
| Fenvalerate | 242.65 | 0.51% | Alpha-Cypermethrin | 15.63 | 0.03% |
| Flubendiamide | 238.71 | 0.51% | Pirimicarb | 3.62 | 0.01% |
| Fipronil | 201.24 | 0.43% | Gamma-Cyhalothrin | 1.63 | 0.00% |

As in the previous section, we can see a concentration in total kg of active ingredients applied in only a handful of substances. Chlorpyrifs, malathion, cypermethrin, and permethrin represent almost 80% of the total mass applied, with 24595.55, 5530.60, 4481.16 and 2899.93 kg, respectively. Only a few others - such as permethrin, terbufos, and metomil - make up around 5% of the total mass of active ingredients applied. The majority of the other active ingredients, on the other hand, make up less than 2% of the total dataset.

### 4.3 Total Impact Scores of Each Active Ingredient

The following table summarizes the total impact scores (in in PAF $m^3$ $day^{-1}$) of each active ingredient, ordered from the highest to the lowest.

Table 10: Summary of Impact Score (IS) in PAF and Corresponding Percentages

| Active Ingredient | Sum of IS | % of total IS | Active Ingredient | Sum of IS | % of total IS |
|---|---:|---:|---|---:|---:|
| Cypermethrin | 977315024.80 | 50.38% | Deltamethrin | 1071465.01 | 0.06% |
| Chlorpyrifos | 527433623.00 | 27.19% | Malathion | 852153.19 | 0.04% |
| Fenpropathrin | 175042471.10 | 9.02% | Spinetoram | 630842.29 | 0.03% |
| Lambda-cyhalothrin | 116081776.30 | 5.98% | Dimethoate | 530658.82 | 0.03% |
| Terbufos | 45939973.58 | 2.37% | Beta-Cyfluthrin | 303849.08 | 0.02% |
| Fenvalerate | 41846673.18 | 2.16% | Bifenthrin | 211904.27 | 0.01% |
| Chlorantraniliprole | 10060742.94 | 0.52% | Methamidophos | 207447.62 | 0.01% |
| Permethrin | 8620286.11 | 0.44% | Imidacloprid | 121004.30 | 0.01% |
| Novaluron | 6612728.99 | 0.34% | Thiodicarb | 88623.66 | 0.00% |
| Fipronil | 6449055.44 | 0.33% | Emamectin Benzoate | 63417.02 | 0.00% |
| Carbofuran | 4260117.18 | 0.22% | Gamma-Cyhalothrin | 46399.04 | 0.00% |
| Tefluthrin | 3313889.56 | 0.17% | Abamectin | 9844.60 | 0.00% |
| Tebupirimfos | 2896738.72 | 0.15% | Thiamethoxam | 8417.68 | 0.00% |
| Metomil | 2878286.95 | 0.15% | Flupyradifurone | 7084.41 | 0.00% |
| Alpha-Cypermethrin | 2643362.04 | 0.14% | Sulfoxaflor | 4814.64 | 0.00% |
| Flubendiamide | 1757515.69 | 0.09% | Acephate | 2720.00 | 0.00% |
| Diazinon | 1440540.56 | 0.07% | Spinosad | 969.83 | 0.00% |
| Zeta-Cypermethrin | 1195807.47 | 0.06% | Pirimicarb | 170.59 | 0.00% |
| **Grand Total** | **1939950407** | **100.00%** | | | |

Just like in the table above, the total impact scores of all the active ingredients throughout the whole Pesticidal project were caused by only a handful of active ingredients. The highest impact scores were caused by cypermethrin, chlorpyrifos, and fenopropathrin, representing 50.38%, 27.19%, and 9.02% of the total impact score of the project, respectively. Again, only a handful of other active ingredients stand out by making up between 2 and 6% of the total impact score, namely lambda-cyhalothrin, terbufos, and fenvalerate.

## 4.4 Average Impact Score per Hectare & per Application

The following table provides an overview of the impact scores (in PAF.$m^3$.day/$kg_{emitted}$) per hectare as well as per hectare and application, starting with the highest average impact score:

Table 11: Summary of IS $ha^{-1}$ and IS $application^{-1}$

| Active Ingredient | IS $ha^{-1}$ | Active Ingredient | IS $application^{-1}$ |
|---|---|---|---|
| Fenpropathrin | 105997.05 | Fenpropathrin | 1750424.71 |
| Cypermethrin | 34886.80 | Fenvalerate | 142888.62 |
| Fenvalerate | 32273.91 | Cypermethrin | 72049.44 |
| Terbufos | 22824.25 | Terbufos | 60615.75 |
| Chlorpyrifos | 16052.76 | Alpha-Cypermethrin | 38872.97 |
| Lambda-cyhalothrin | 9259.18 | Fipronil | 38655.24 |
| Fipronil | 7577.59 | Chlorpyrifos | 33489.92 |
| Tebupirimfos | 7433.63 | Lambda-cyhalothrin | 28815.05 |
| Alpha-Cypermethrin | 5253.84 | Tefluthrin | 15393.85 |
| Tefluthrin | 2881.32 | Novaluron | 13271.77 |
| Novaluron | 2729.33 | Metomil | 5492.29 |
| Carbofuran | 2440.80 | Chlorantraniliprole | 4361.32 |
| Diazinon | 2048.00 | Carbofuran | 4026.06 |
| Malathion | 1211.55 | Flubendiamide | 2693.31 |
| Flubendiamide | 1085.24 | Zeta-Cypermethrin | 2586.66 |
| Metomil | 955.12 | Tebupirimfos | 2532.10 |
| Chlorantraniliprole | 826.47 | Diazinon | 1378.48 |
| Permethrin | 736.73 | Dimethoate | 1216.91 |
| Zeta-Cypermethrin | 662.71 | Methamidophos | 1090.96 |
| Deltamethrin | 575.15 | Beta-Cyfluthrin | 830.19 |
| Methamidophos | 568.30 | Permethrin | 778.89 |
| Dimethoate | 403.10 | Gamma-Cyhalothrin | 773.32 |
| Beta-Cyfluthrin | 392.47 | Thiodicarb | 671.39 |
| Thiodicarb | 366.82 | Bifenthrin | 601.70 |
| Bifenthrin | 274.00 | Deltamethrin | 530.86 |
| Gamma-Cyhalothrin | 128.96 | Malathion | 364.54 |
| Imidacloprid | 73.60 | Imidacloprid | 137.35 |
| Spinetoram | 23.01 | Acephate | 87.74 |
| Acephate | 23.00 | Spinetoram | 85.56 |
| Flupyradifurone | 18.81 | Flupyradifurone | 75.37 |
| Pirimicarb | 14.63 | Abamectin | 36.67 |
| Sulfoxaflor | 8.02 | Pirimicarb | 34.12 |
| Thiamethoxam | 6.94 | Sulfoxaflor | 26.90 |
| Abamectin | 6.46 | Thiamethoxam | 24.85 |
| Emamectin Benzoate | 4.84 | Emamectin Benzoate | 6.87 |
| Spinosad | 1.20 | Spinosad | 5.55 |

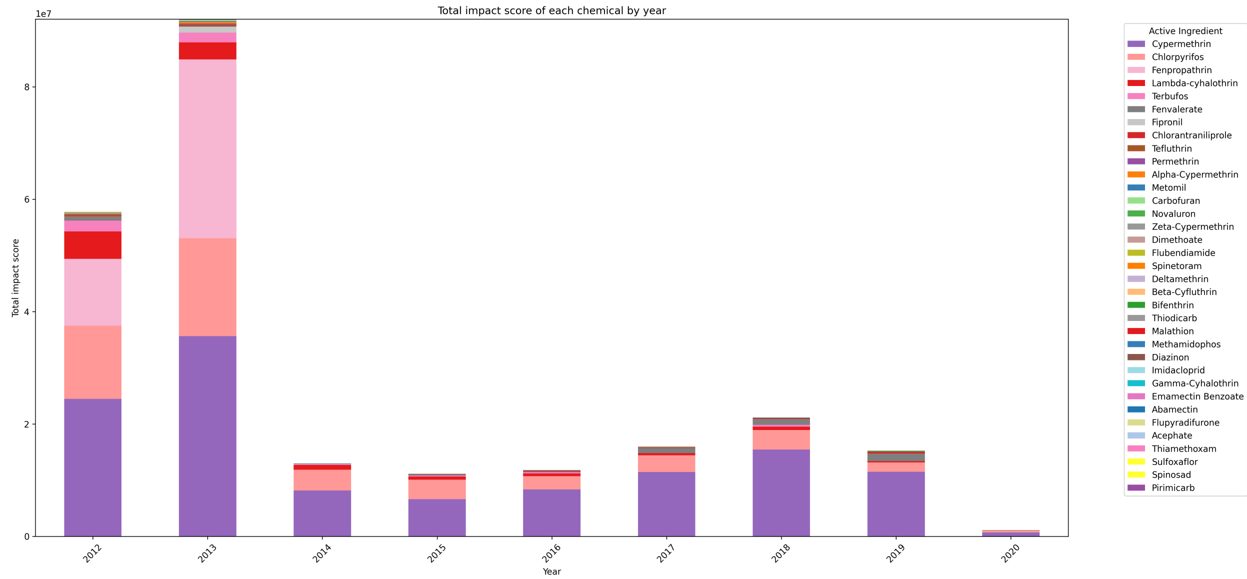
We can observe a high variability in average impact scores, both in terms of per hectare applied and per application. Fenpropathrin stands out with the highest scores in both categories (IS $ha^{-1}$and IS $application^{-1}$), which is higher than any other active ingredient. Other active ingredients with high scores in both categories are fenvalerate and cypermethrin, which together with fenpropathrin represent the top three active ingredients in terms of their environmental impact on freshwater ecosystems. Chlorpyrifos, an active ingredient heavily applied during the project, also ranges relatively high on average. In contrast, spinosad and emamectin benzonate are both scoring very low in both categories.

## 4.5 Trends

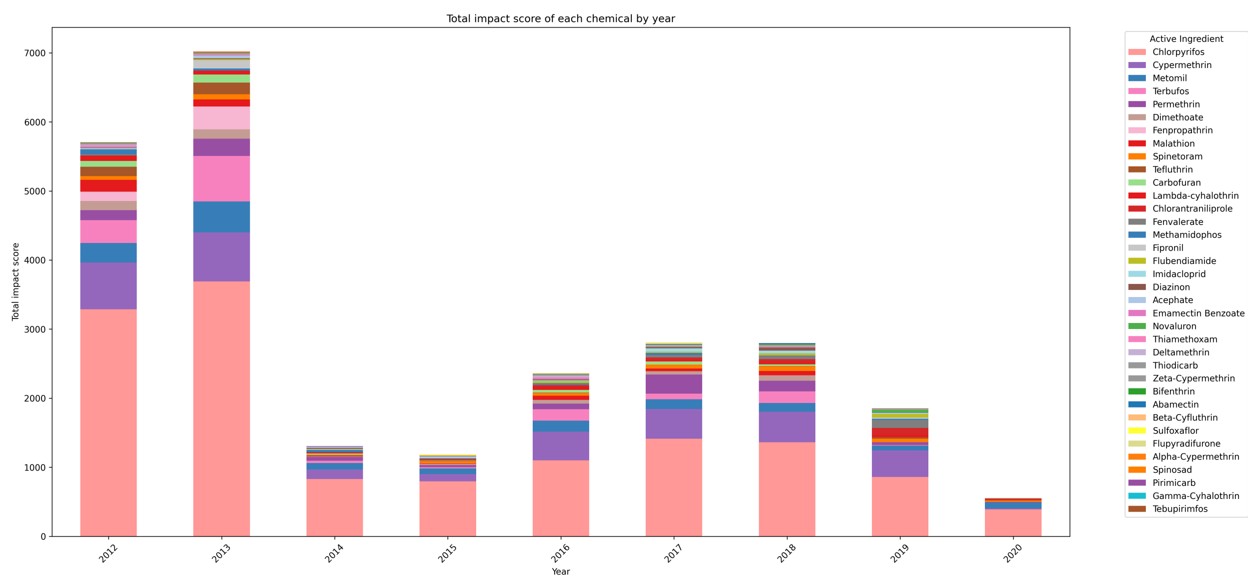
The following three figures contrast the total impact score (in PAF.m$^3$.day/kg$_{\text{emitted}}$) and the impact score (PAF.m$^3$.day/kg$_{\text{emitted}}$) per hectare, as well as per application over the course of the project.

Figure 8 compares the development of the total impact score per active ingredient and year (Figure a) with the total application of each active ingredient. The stacked bar charts display the continuous impact of each of the 36 active ingredients used in the project (Figure a), as well as the total amount applied (Figure b). Each active ingredient is represented by a different color. High bar charts suggest a high impact on freshwater ecosystems, or high amounts of active ingredients applied. Remarkably, we can see an overall high impact in the years 2012 and 2013, with a sudden drop in the following year. Over time, the total impact score per year fluctuates around 20,000,000 PAF.m$^3$.day/kg$_{\text{emitted}}$, with another sharp drop in 2020. Notably, only three active ingredients are responsible for the overall environmental impact: Cypermethrin, chlorpyrifos, and fenpropathrin, the latter one being specifically toxic in the first two years. Most of the other active ingredients cannot be detected in the bar charts of Figure a because of their little contribution to the overall freshwater ecotoxicity. On the other hand, Figure b illustrates that a limited subset of insecticides accounts for the majority of the total application volume, with chlorpyrifos, cypermethrin, metomyl, and terbufos being the major ones. Even though chlorpyrifos makes up around 50% of the total application volume per year, its overall impact is lower than other active ingredients, such as cypermethrin and fenpropathrin.

The next figure (Figure 9), compares the average impact score of each active ingredient per hectare and year (Figure a), with the average amount of active ingredient applied per hectare and year (Figure b). Each active ingredient is represented with a different color.



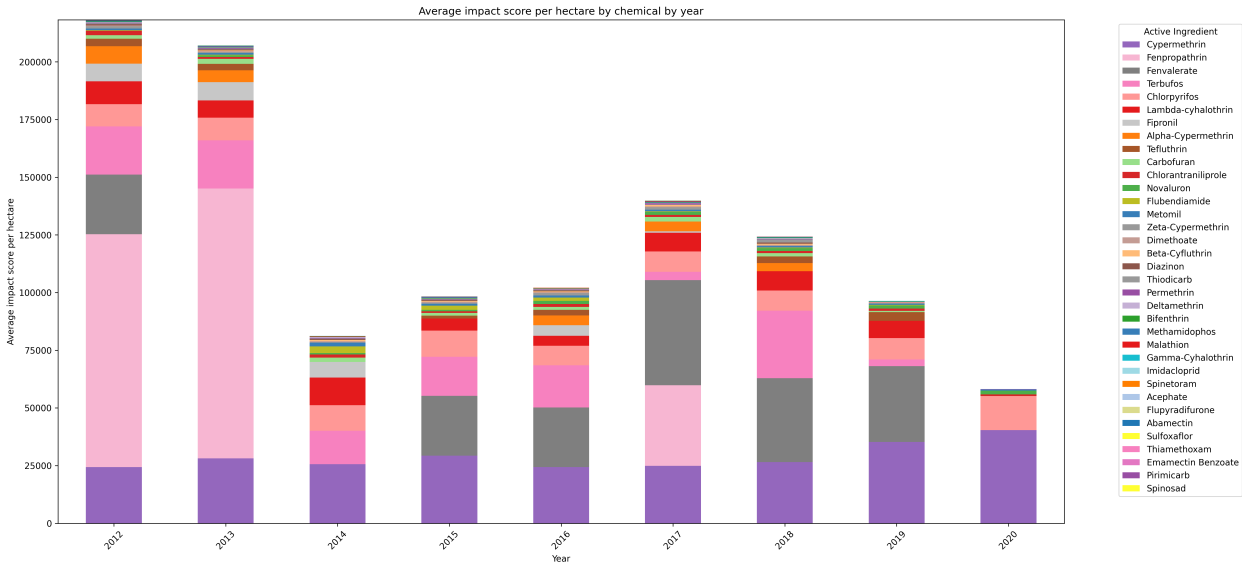

(a) Total Impact Score per Active Ingredient and Year



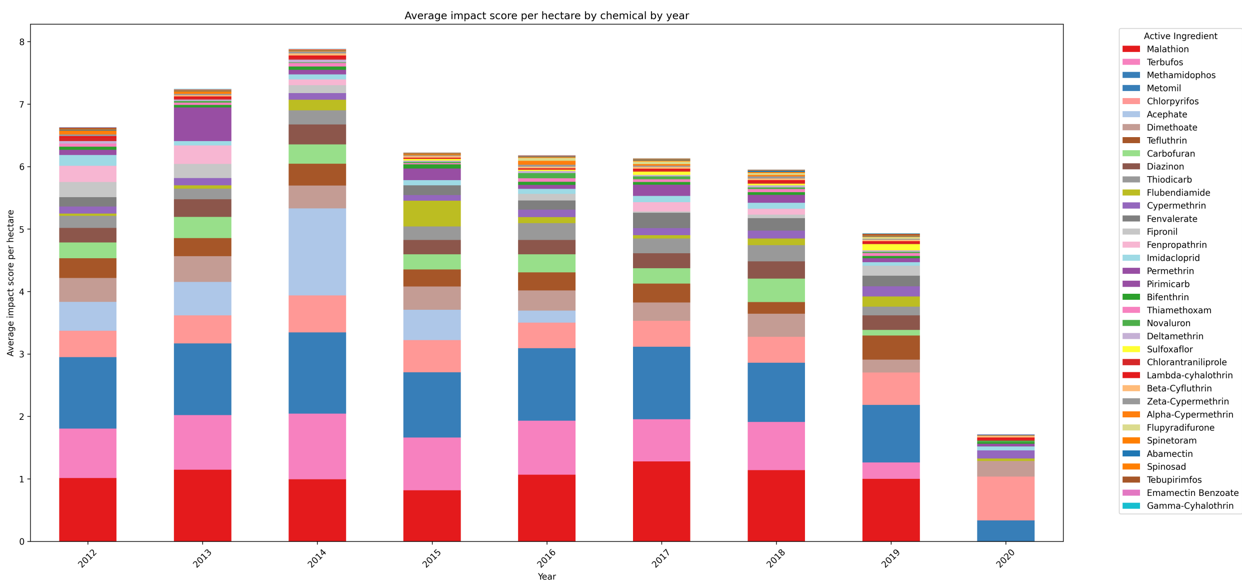

(b) Total Amount of Active Ingredient and Year

Figure 8: Comparison of Impact Score and Total Amount per Active Ingredient and Year

In Figure a, we can also see a high average impact score per hectare applied in the first two years of the project. In contrast to the total impact score, we can see a steady decline each year on average after the sharp decline in 2014. In addition, Figure a also displays a steady decline in impact score per hectare and year. Furthermore, the graph highlights that, like in the figure described above, only a few active ingredients are the drivers of




(a) Average Impact Score per Active Ingredient Applied per Hectare and Year

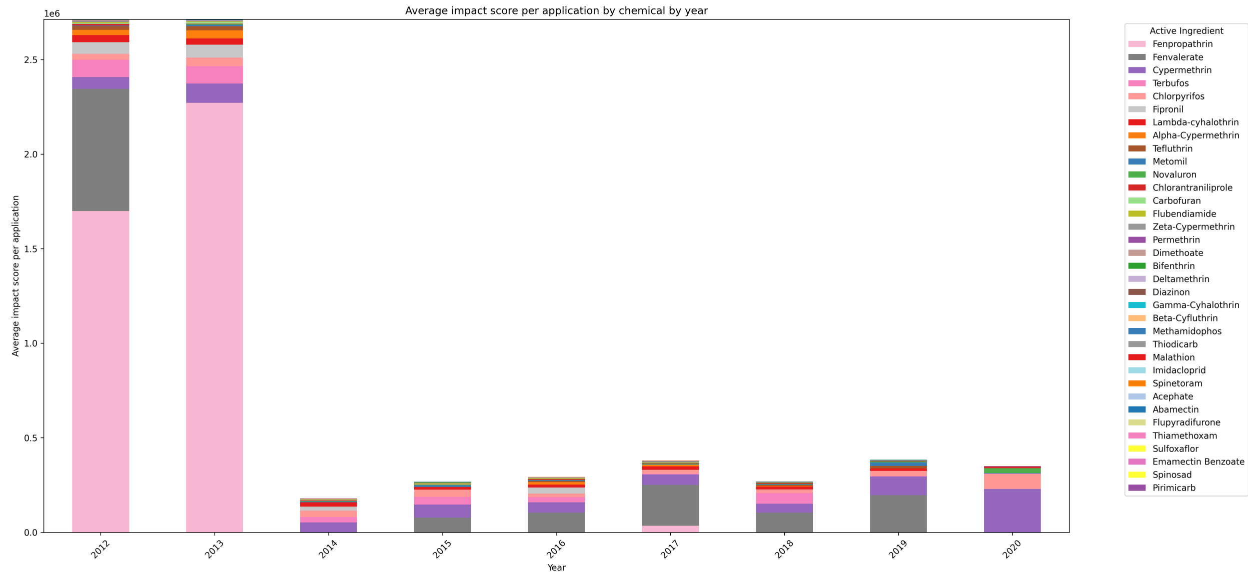



(b) Average Amount of Active Ingredient Applied per Hectare and Year

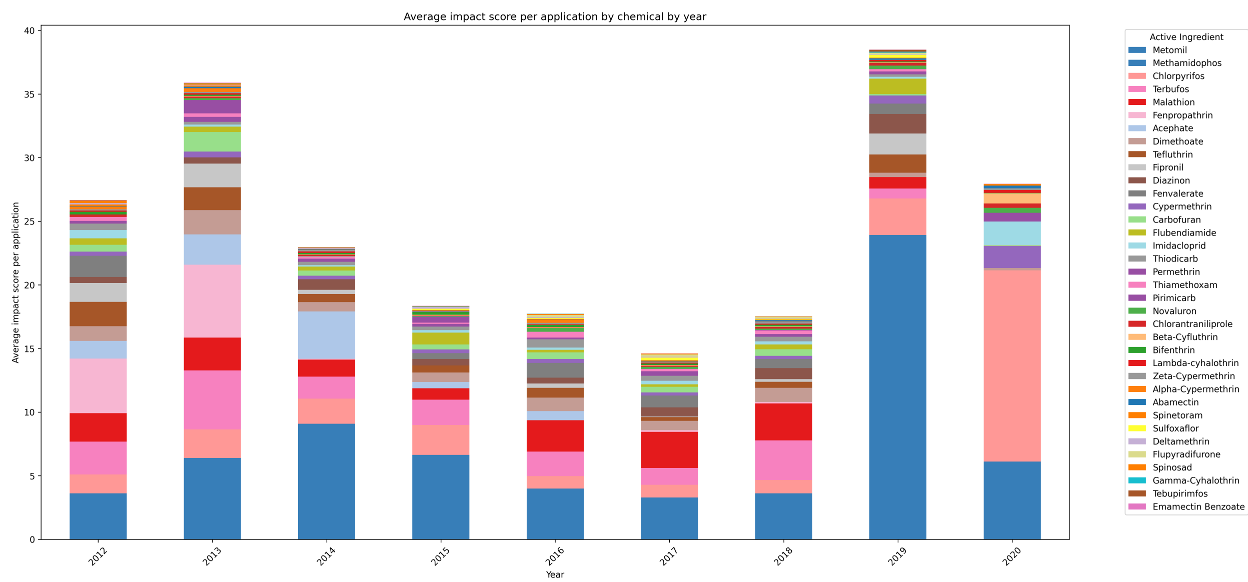
Figure 9: Comparison of Impact Score and Amount per Active Ingredient per Hectare and Year

freshwater ecotoxicity per hectare. Like in the absolute numbers, cypermethrin (throughout the project), chlorpyrifos, and fenpropathrin (in the first two years) demonstrate how much they contribute to freshwater ecotoxicity. In addition, fenvalerate, terbufos, and lambda cyhalothrin are also drivers of ecotoxicity. In contrast, not all of these are under the top active ingredients applied on average per hectare and year–only terbufos and chlorpyrifos. On the other hand, metomil, metamidophos, and malathion were among the top active ingredients applied on average per hectare and year, but their impact compared to others was rather low. Furthermore, we can see a decline in average active ingredients applied per hectare and year, starting in time 2015.

The next figure (Figure 10), compares the average impact score of each active ingredient per application and year (Figure a), with the average amount of active ingredient applied per application and year (Figure b). Figure a does not display a clear trend over time. After a sharp drop of average impact score per application in the first two years, numbers fluctuate without any pattern. In addition, fenpropathrin was again responsible for high impact score numbers in the first two years. The graph also provides insights on which active ingredients were contributing, on average per application, the most to freshwater ecotoxicity. In this case, fenvalerate, cypermethrin, terbufos, as well as chlorpyrifos must be mentioned in this context. On the contrary, not all of these belong to the top active ingredients per application, only chlorpyrifos and terbufos. Once again, metomil and methamidophos were under the top active ingredients per application, but displayed a low impact score comparatively.




(a) Average Impact Score per Active Ingredient per Application and Year




(b) Average Amount of Active Ingredient per Application and Year

Figure 10: Comparison of Impact Score and Amount per Active Ingredient per Application and Year

## 4.6 Mode of Actions

Table 12 classifies each active ingredient utilized in the project according to its corresponding mode of action.

Table 13 provides an overview of the different modes of action used in the project, together

Table 12: Active Ingredients by Mode of Action

| **Mode of Action** | **Active Ingredients** |
|---|---|
| Pyrethroid | Bifenthrin, Cypermethrin, Permethrin, Tefluthrin, Zeta-Cypermethrin, Deltamethrin, Lambda-cyhalothrin |
| Organophosphate | Chlorpyrifos, Terbufos, Thiodicarb, Diazinon, Acephate, Carbofuran, Dimethoate, Malathion, Methamidophos |
| Spinosyn | Spinetoram, Spinosad |
| Avermectin | Abamectin, Emamectin Benzoate |
| Diamede | Chlorantraniliprole, Flubendiamide |
| Neonicotinoid | Imidacloprid, Thiamethoxam, Sulfoxaflor, Flupyradifurone |
| Pyrazole | Novaluron |
| Phenylpyrazole | Fipronil |

with their application numbers, total amount of hectares applied, and total amount in kg applied. Pyrethroid is the top mode of action in the two former categories, accounting for 35% of the total applications and hectares applied, followed by organophosphates and spinosyns. Organophosphates, however, were applied much more in terms of kg than other modes of action, followed by pyrethroids.

Table 13: Number of Applications and Total Plot Size Applied

| **Mode of Action** | **Number of Applications** | | **Plot Size Applied (ha)** | | **Amount Applied (kg)** | |
|---|---|---|---|---|---|---|
| | Count | % | Size | % | kg | % |
| Pyrethroid | 20,107 | 38.57 | 61,330.33 | 37.76 | 5,843.20 | 22.83 |
| Organophosphate | 11,371 | 21.80 | 39,324.92 | 24.22 | 18,394.21 | 71.87 |
| Spinosyn | 6,576 | 12.61 | 28,169.53 | 17.34 | 414.62 | 1.62 |
| Avermectin | 4,169 | 8.00 | 14,555.56 | 8.96 | 79.51 | 0.31 |
| Diamede | 2,660 | 5.10 | 13,769.68 | 8.47 | 412.24 | 1.61 |
| Neonicotinoid | 1,122 | 2.15 | 3,788.98 | 2.33 | 231.57 | 0.90 |
| Pyrazole | 278 | 0.53 | 2,392.84 | 1.47 | 56.80 | 0.22 |
| Phenylpyrazole | 135 | 0.26 | 847.07 | 0.52 | 162.84 | 0.64 |

The following table (Table 14) presents a summary of the total impact scores in PAF.$m^3$.day/$kg_{emitted}$ for each mode of action, as well as the average impact score per application and per hectare on which each mode of action was applied. As above, pyrethroids are responsible for most of the total impact scores (around 74%), but also exhibit high scores for average impact scores per application and hectare. Organophosphates also score high in both these categories, together with phenylpyrazoles and pyrazoles. Spinosyns, neonicotinoids, and avermectins score low both in total as well as in average categories.

Table 14: Total & Average Impact Scores (IS) in PAF.m$^3$.day/kg$_{\text{emitted}}$ per Mode of Action

| **Mode of Action** | **IS** | | **Average IS** | **Average IS** |
|---|---|---|---|---|
| | Total | Percentage (%) | **per Application** | **per Hectare** |
| Pyrethroid | 1,051,299,869.7 | 73.95 | 52,285.27 | 17,141.60 |
| Organophosphate | 331,005,920.9 | 23.28 | 29,109.66 | 8,417.21 |
| Diamede | 10,903,874.7 | 0.77 | 4,099.20 | 791.88 |
| Phenylpyrazole | 5,218,457.9 | 0.37 | 38,655.24 | 6,160.60 |
| Pyrazole | 3,689,551.5 | 0.26 | 13,271.77 | 1,541.91 |
| Spinosyn | 55,6910.3 | 0.04 | 84.69 | 19.77 |
| Neonicotinoid | 10,4547.3 | 0.01 | 93.18 | 27.59 |
| Avermectin | 36,323.3 | <0.01 | 8.71 | 2.50 |

The ANOVA table below highlights the significant influence of mode of action on our response variable, freshwater ecotoxicity (expressed in PAF.m$^3$.day/kg$_{\text{emitted}}$). The significant effect ($p < 0.001$) highlights the importance of mode of action on freshwater ecotoxicity.

Table 15: ANOVA Summary Table for Mode of Action on log(is_total + 1)

| **Source** | **Df** | **Sum Sq** | **Mean Sq** | **F value** | **Pr()** | **Eta² (95% CI)** |
|---|---|---|---|---|---|---|
| as.factor(mode_of_action) | 7 | 338,158 | 48,308 | 12,841.22 | < 0.001 *** | 0.66 [0.66, 1.00] |
| Residuals | 46,410 | 174,593 | 4 | | | |

The following table summarizes the results of the Tukey post-hoc comparisons for different modes of action on our response variable, freshwater ecotoxicity, including both log-based and log-transformed differences, alongside Tukey-adjusted p-values for significance. The exponentiated values (Exp(Diff), Exp(lower CI), and Exp(Upper CI)) represent a multiplicative change in freshwater ecotoxicity associated with each comparison. Only 4 comparisons did not show any significant differences, with p-values above 0.05.

Table 16: Tukey Post-Hoc Comparison of Means for Different Modes of Action

| Comparison | Difference (log) | Lower CI (log) | Upper CI (log) | p adj | Exp(Diff) | Exp(Lower CI) | Exp(Upper CI) |
|---|---|---|---|---|---|---|---|
| avermectin-organophosphate | -7.6430 | -7.7495 | -7.5366 | <0.001 | 0.0005 | 0.0004 | 0.0005 |
| avermectin-pyrethroid | -7.2659 | -7.3660 | -7.1659 | <0.001 | 0.001 | 0.001 | 0.001 |
| avermectin-spinosyn | -1.8743 | -1.9907 | -1.7579 | <0.001 | 0.15 | 0.14 | 0.17 |
| diamede-avermectin | 5.9219 | 5.7760 | 6.0678 | <0.001 | 232.35 | 151.77 | 315.87 |
| diamede-organophosphate | -1.7211 | -1.8477 | -1.5945 | <0.001 | 0.18 | 0.16 | 0.20 |
| diamede-pyrethroid | -1.3440 | -1.4653 | -1.2227 | <0.001 | 0.26 | 0.23 | 0.29 |
| diamede-spinosyn | 4.0476 | 3.9125 | 4.1827 | <0.001 | 57.16 | 50.07 | 65.53 |
| neonicotinoid-avermectin | 2.2915 | 2.0938 | 2.4892 | <0.001 | 9.90 | 7.78 | 10.56 |
| neonicotinoid-diamede | -3.6304 | -3.8397 | -3.4212 | <0.001 | 0.03 | 0.02 | 0.04 |
| neonicotinoid-organophosphate | -5.3515 | -5.5355 | -5.1676 | <0.001 | 0.005 | 0.004 | 0.006 |
| neonicotinoid-pyrethroid | -4.9744 | -5.1548 | -4.7941 | <0.001 | 0.007 | 0.006 | 0.008 |
| neonicotinoid-spinosyn | 0.4172 | 0.2273 | 0.6071 | <0.001 | 1.52 | 1.26 | 1.84 |
| organophosphate-pyrethroid | 0.3771 | 0.3081 | 0.4461 | <0.001 | 1.46 | 1.36 | 1.56 |
| phenylpyrazole-avermectin | 7.7035 | 7.1895 | 8.2176 | <0.001 | 1571.25 | 918.13 | 2025.63 |
| phenylpyrazole-diamede | 1.7816 | 1.2630 | 2.3003 | <0.001 | 5.94 | 3.53 | 10.98 |
| phenylpyrazole-neonicotinoid | 5.4121 | 4.8765 | 5.9476 | <0.001 | 222.18 | 157.13 | 276.32 |
| phenylpyrazole-organophosphate | 0.0605 | -0.4484 | 0.5695 | >0.05 | 1.06 | 0.64 | 1.77 |
| phenylpyrazole-pyrethroid | 0.4376 | -0.0700 | 0.9453 | >0.05 | 1.55 | 0.93 | 2.57 |
| phenylpyrazole-spinosyn | 5.8293 | 5.3181 | 6.3404 | <0.001 | 341.19 | 206.73 | 453.90 |
| phenylpyrazole-pyrazole | 0.5173 | -0.0994 | 1.1340 | >0.05 | 1.68 | 0.91 | 3.10 |
| pyrazole-avermectin | 7.1863 | 6.8221 | 7.5504 | <0.001 | 1321.50 | 918.02 | 1452.13 |
| pyrazole-diamede | 1.2643 | 0.8938 | 1.6349 | <0.001 | 3.54 | 2.54 | 5.13 |
| pyrazole-neonicotinoid | 4.8948 | 4.5009 | 5.2886 | <0.001 | 102.63 | 89.47 | 114.34 |
| pyrazole-organophosphate | -0.4568 | -0.8136 | -0.0999 | <0.05 | 0.63 | 0.44 | 0.90 |
| pyrazole-pyrethroid | -0.0797 | -0.4347 | 0.2753 | >0.05 | 0.92 | 0.65 | 1.32 |
| pyrazole-spinosyn | 5.3120 | 4.9520 | 5.6719 | <0.001 | 202.84 | 141.47 | 214.67 |
| spinosyn-organophosphate | -5.7687 | -5.8598 | -5.6777 | <0.001 | 0.003 | 0.003 | 0.003 |
| spinosyn-pyrethroid | -5.3916 | -5.4751 | -5.3081 | <0.001 | 0.005 | 0.004 | 0.005 |

## 4.7 Management Practices and Extension Approaches

As described above, we fitted a generalized linear model with a Gamma distribution and log link to examine if our predictor variables are associated with our response variable (freshwater ecotoxicity). Table 15 below illustrates the results, including estimates (based on log-transformed data), their exponentiated estimates, the standard error, t-values, and significance levels of each of the predictor variables. The estimates were back-transformed from the log transformation, making it easier to interpret on the original scale of the response variable. After estimates have been back-transformed, they become multiplicative effects (factors) for the different treatments of each predictor - for example, an exponentiated estimate of 0.80 implies that on average, the treatment is associated with a decrease in freshwater ecotoxicity of 20

The model revealed that freshwater ecotoxicity per hectare does not increase with plot size, since the p-value is above 0.05. Among the categorical variables, `intercropping` did show a significant difference, with a p-value below 0.05. `hydrological_regime Riego–`

| Variable | Estimate | Std. Error | t value | Pr(<\|t\|) | Exponentiated Estimate |
|---|---|---|---|---|---|
| (Intercept) | 9.03629 | 0.01947 | 464.180 | *** | 8410.96 |
| intercropping | 0.24974 | 0.10784 | 2.316 | * | 1.28 |
| log(plot_size + 1) | 0.01987 | 0.01356 | 1.465 | | 1.02 |
| as.factor(hydrological_regime)Riego | -0.07915 | 0.02102 | -3.765 | *** | 0.92 |
| conservation_agriculture1 | -0.10957 | 0.01837 | -5.964 | *** | 0.90 |
| as.factor(production_cycle)Otoño-Invierno | -0.40696 | 0.04020 | -10.124 | *** | 0.67 |
| as.factor(education)Parcela innovación | 0.06349 | 0.02444 | 2.598 | ** | 1.07 |
| as.factor(education)Parcela testigo | 0.16889 | 0.02371 | 7.122 | *** | 1.18 |

*Note.* Significance levels: *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

Table 17: GLM Coefficients with Exponentiated Estimates, t values, and p values

irrigation–, `conservation_agriculture`, and `production_cycle Otoño-Invierno`–Winter– showed a significant negative effect, with estimates of -0.07915, -0.10957, and -0.40696, respectively, and p < 0.001. Different extension treatments also showed significant differences, `education Parcela innovación` p < 0.01, and `education Parcela testigo` p < 0.001). The results of the model are summarized in Table 17.

Table 18 describes the estimated marginal means (Emmean) for each level of factors analyzed, including hydrological regime, conservation agriculture, production cycle, and education. Table 19 presents the results of the pairwise contrasts between levels of each factor, together with exponentiated estimates. The contrasts were adjusted using Tukey's Honest Significant Difference test. As above, the exponentiated estimates are multiplicative factors, revealing the difference between levels of each factor. Table 19 includes the pairwise comparisons based on exponentiated values. Impact scores are lower by a factor of 0.78 in intercropped systems and higher in rainfed systems, plots not under conservation agriculture, and during summer.

| Factor | Level | Emmean | SE | df | Lower CI | Upper CI |
|---|---|---|---|---|---|---|
| **Intercropping** | Practiced | 8.846 | 0.020 | 46407 | 8.807 | 8.885 |
| | Not Practiced | 9.096 | 0.109 | 46407 | 8.882 | 9.309 |
| **Hydrological Regime** | Temporal | 9.01 | 0.0574 | 46407 | 8.90 | 9.12 |
| | Riego | 8.93 | 0.0579 | 46407 | 8.82 | 9.04 |
| **Conservation Agriculture** | Practiced | 8.92 | 0.0573 | 46407 | 8.80 | 9.03 |
| | Not Practiced | 9.03 | 0.0575 | 46407 | 8.91 | 9.14 |
| **Production Cycle** | Primavera-Verano | 9.17 | 0.0550 | 46407 | 9.07 | 9.28 |
| | Otoño-Invierno | 8.77 | 0.0649 | 46407 | 8.64 | 8.89 |
| **Education** | Parcela Área de extensión | 8.89 | 0.0569 | 46407 | 8.78 | 9.00 |
| | Parcela innovación | 8.96 | 0.0594 | 46407 | 8.84 | 9.07 |
| | Parcela testigo | 9.06 | 0.0598 | 46407 | 8.95 | 9.18 |

Table 18: Estimated Marginal Means for Each Factor (log scale)

| Factor | Contrast | Estimate | SE | df | t-ratio | p-value | Exp. Estimate |
|---|---|---|---|---|---|---|---|
| **Intercropping** | Not Practiced - Practiced | -0.25 | 0.108 | 46407 | -2.316 | * | 0.78 |
| **Hydrological Regime** | Temporal - Riego | 0.0791 | 0.021 | 46407 | 3.765 | *** | 1.08 |
| **Conservation Agriculture** | Not Practiced - Practiced | 0.11 | 0.0184 | 46407 | 5.964 | *** | 1.12 |
| **Production Cycle** | Primavera-Verano - Otoño-Invierno | 0.407 | 0.0402 | 46407 | 10.124 | *** | 1.50 |
| **Education** | Área de extensión - Parcela innovación | -0.0635 | 0.0244 | 46407 | -2.598 | ** | 0.94 |
| | Área de extensión - Parcela testigo | -0.1689 | 0.0237 | 46407 | -7.122 | *** | 0.84 |
| | Parcela innovación - Parcela testigo | -0.1054 | 0.0309 | 46407 | -3.412 | ** | 0.90 |

*Note.* Significance levels: *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

Table 19: Contrasts for Factor Levels with Exponentiated Estimates

To further explore the associations between management practices and freshwater ecotoxicity, we created logistic regression models for each management practice. Each model used a binary response variable (conservation agriculture, hydrological regime, production cycle, intercropping), with mode of action as the predictor. Additionally, a multinomial logistic regression model was developed to evaluate the association between mode of action and the different modes of extension. The results are presented in tables 20 to 23. The odds ratio describes how likely a mode of action is associated with the management practice or extension treatment. Positive coefficients suggest a higher likelihood, negative a lower likelihood. Table 20 describes the odds coefficient of conservation agriculture being practiced vs. not practiced for each mode of action. Table 21 describes the odds coefficient of hydrological regime being rainfed vs. irrigated for each mode of action. Table 22 describes the odds coefficient of production cycle being summer vs. winter for each mode of action.

| Mode of Action | Estimate | Odds Ratio | Std. Error | Significance |
|---|---|---|---|---|
| Intercept | -0.876 | 0.416 | 0.015 | *** |
| Organophosphate | -0.094 | 0.910 | 0.026 | *** |
| Spinosyn | 0.498 | 1.645 | 0.029 | *** |
| Avermectin | -0.109 | 0.896 | 0.038 | ** |
| Diamede | -0.033 | 0.968 | 0.046 | |
| Neonicotinoid | 0.607 | 1.835 | 0.062 | *** |
| Pyrazole | -0.352 | 0.703 | 0.144 | * |
| Phenylpyrazole | 0.532 | 1.703 | 0.175 | ** |

*Note.* Significance levels: *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

Table 20: GLM Results for Conservation Agriculture (Practiced vs. Not Practiced) by Mode of Action, Including Odds Ratios

| Mode of Action | Estimate | Odds Ratio | Std. Error | Significance |
|---|---|---|---|---|
| Intercept | -1.415 | 0.243 | 0.018 | *** |
| Organophosphate | 0.155 | 1.168 | 0.029 | *** |
| Spinosyn | 0.536 | 1.709 | 0.032 | *** |
| Avermectin | 0.245 | 1.278 | 0.041 | *** |
| Diamede | 1.364 | 3.911 | 0.043 | *** |
| Neonicotinoid | 1.666 | 5.290 | 0.063 | *** |
| Pyrazole | 2.023 | 7.559 | 0.127 | *** |
| Phenylpyrazole | -0.824 | 0.439 | 0.292 | ** |

*Note.* Significance levels: *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

Table 21: GLM Results for Hydrological Regime (Rainfed vs. Irrigated) by Mode of Action, Including Odds Ratios

| Mode of Action | Estimate | Odds Ratio | Std. Error | Significance |
|---|---|---|---|---|
| Intercept | -3.309 | 0.036 | 0.038 | *** |
| Organophosphate | 0.108 | 1.114 | 0.062 | . |
| Spinosyn | 1.016 | 2.761 | 0.057 | *** |
| Avermectin | 0.311 | 1.364 | 0.082 | *** |
| Diamede | 1.128 | 3.090 | 0.075 | *** |
| Neonicotinoid | 0.833 | 2.301 | 0.118 | *** |
| Pyrazole | 1.691 | 5.427 | 0.166 | *** |
| Phenylpyrazole | -1.589 | 0.204 | 1.004 | |

*Note.* Significance levels: *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

Table 22: GLM Results for Production Cycle by Mode of Action (Summer vs. Winter), Including Odds Ratios

| Predictor | Estimate | Odds Ratio | Std. Error | Significance |
|---|---|---|---|---|
| Intercept | -4.91793 | 0.0073 | 0.08306 | *** |
| Organophosphate | -0.46480 | 0.6284 | 0.16192 | ** |
| Spinosyn | -0.03759 | 0.9631 | 0.16968 | |
| Avermectin | -0.27648 | 0.7584 | 0.22499 | |
| Diamede | -1.86841 | 0.1545 | 0.58362 | ** |
| Neonicotinoid | 0.30281 | 1.3536 | 0.31418 | |
| Pyrazole | -12.64814 | 0.0000 | 237.27594 | |
| Phenylpyrazole | -12.64814 | 0.0000 | 340.49380 | |

*Note.* Significance levels: *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

Table 23: Logistic Regression Results: Intercropping as Response Variable

| Education Level | Intercept | Organophosphate | Spinosyn | Avermectin |
|---|---|---|---|---|
| **Parcela Innovación** | | | | |
| Estimate | -1.613 | 0.028 | 0.136 | 0.095 |
| Std. Error | 0.021 | 0.034 | 0.040 | 0.048 |
| Odds Ratio | 0.199 | 1.028 | 1.146 | 1.099 |
| Significance | *** | | *** | * |
| **Parcela Testigo** | | | | |
| Estimate | -1.495 | 0.077 | -0.069 | -0.137 |
| Std. Error | 0.020 | 0.032 | 0.041 | 0.050 |
| Odds Ratio | 0.224 | 1.080 | 0.933 | 0.872 |
| Significance | *** | * | | ** |
| | **Diamede** | **Neonicotinoid** | **Pyrazole** | **Phenylpyrazole** |
| **Parcela Innovación** | | | | |
| Estimate | -0.646 | -0.286 | 0.148 | 0.215 |
| Std. Error | 0.072 | 0.096 | 0.170 | 0.239 |
| Odds Ratio | 0.524 | 0.751 | 1.159 | 1.240 |
| Significance | *** | ** | | |
| **Parcela Testigo** | | | | |
| Estimate | -0.773 | -0.516 | 0.161 | 0.184 |
| Std. Error | 0.072 | 0.100 | 0.162 | 0.231 |
| Odds Ratio | 0.462 | 0.597 | 1.175 | 1.202 |
| Significance | *** | *** | | |

*Note.* Significance levels: *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$

Table 24: Multinomial Logistic Regression Results for Education Levels (Traditional Extension vs. Innovation or Testigo) with Mode of Action Predictors (Including Odds Ratios)

# 5 Discussion

## 5.1 Active Ingredients and Trends

The purpose of this paper was to find out the top active ingredients applied in the CIMMYT's extension project, as well as the most and least toxic active ingredients used. Through this study, we found out that the most applied active ingredients used in the project were only a handful of different chemicals, with Cypermethrin, spinetoram, and chlorpyrifos, and spinetoram as the leading substances in terms of the number of applications. Permethrin, emamectin benzoate, and lambda-cyhalothrin were overall also widely used compared to the other 28 chemicals in the database. In contrast, the different application rates of these substances led to a different picture in terms of the amount of active ingredients in kg applied. Over 52% of the total active ingredients applied consisted of chlorpyrifos. Malathion, cypermethrin, and permethrin accounted for 11.71%, 9.50%, and 6.16%, respectively. These findings offer insights into the current state of insecticide use and agricultural practices in Mexico, alongside the role of extension services in promoting specific insecticides. The concentration of specific active ingredients could indicate that only a certain handful of chemicals are used by farming communities partnering with extension services, at least in the states of Guerrero, Guanajuato, Chiapas, Morales, and Jalisco, since those were states with the most data entries. Similar results could be found when looking at the modes of action, where we can also see a concentration in pyrethroids, organophosphates, and spinosyns. Relying only on a few active ingredients could potentially have negative implications for future production, for example, by the development of pest resistance. The dominance of certain products could also have harmful effects for certain species, especially non-target organisms. To calculate the effects of those chemicals, we used USEtox in order to calculate the impact of the active ingredients used in the project on freshwater ecosystems, expressed in Potentially Affected Species ($PAF.m^3.day/kg_{emitted}$).

It is no surprise that cypermethrin and chlorpyrifos account for almost 75% of the total impact scores, since they were also applied at a high rate. However, when looking at the average impact scores per hectare or per application, we can see a different picture. Cypermethrin and chlorpyrifos still rank high, but fenpropathrin accounts for the highest impact scores per hectare and per application. In the former category, it is three times more toxic than cypermethrin. In the latter, it is even more than 12 times more toxic per application than the second most toxic active ingredient per application, fenvalerate. Both fenpropathrin and fenvalerate score high in average impact scores, even though they only account for 1% and 0.51% of the total amount of active ingredients applied during the project. At the same time, spinetoram, which accounts for almost 14% of all applications, and only 0.98% of total active ingredients applied, scores also relatively low in both average categories. Permethrin and terbufos, both accounting around 5% of the total active ingredients applied, rank differently in terms of average impact scores–terbufos ranks high in both average categories, while permethrin scores relatively low in both average categories compared to fenpropathrin.

These results highlight not only the huge variability of different impact scores in terms of their freshwater ecotoxicity, especially when looking at average impact score per hectare applied. These results highlight the importance of context in impact assessments. Some active ingredients are so toxic that even if they account for a small percentage of the total active ingredients applied, they can account for a big portion of overall toxicity, as we have seen with fenpropathrin. Many studies assessing the freshwater ecotoxicity are based on national sales data, focusing on the top active ingredients applied on a national level, and lacking information on how much active ingredients were applied per hectare. This means that by looking at top active ingredients sold by year, we could potentially only see a partial picture of the actual impact on freshwater ecosystems, because some very highly toxic active ingredients had not been included in the study. At the same time, some very toxic active ingredients that were applied at a high rate could be comparatively less toxic because they were applied on more hectares, lowering their average impact per hectare.

These different pictures could also be seen in the plots for the trends–chlorpyrifos, for example, accounted for a major part of total active ingredients applied per year, followed by cypermethrin. In terms of total impact score per year, cypermethrin accounted for a major part of total impact score per year, followed by chlorpyrifos, except in the first two years. Here, fenpropathrin caused total impact scores to be very high, even though it was applied at lower amounts compared to other active ingredients, such as metomil, terbufos, and permethrin. When looking at average impact score per active ingredient applied per hectare and year, we can see that cypermethrin, fenpropathrin, fenvalerate, terbufos, chlorpyrifos, and lambda-cyhalothrin accounted for more than 75% of the yearly impact scores per hectare. In contrast, malathion, terbufos , mathamidofos, metomil, and chlorpyrifos were the top active ingredients applied per hectare and year, accounting for almost 50% of the average amount of active ingredients applied per hectare and year, combined. Here we can see again how even though some active ingredients were applied at a higher rate per hectare and year, they do not account for a high impact score per hectare and year, or vice versa. We can make similar observations in terms of average impact score per application and year, where some active ingredients account for a high impact score per application and year, while being applied at a relatively lower rate.

In addition, we can see that oftentimes a spike in total or average impact scores per year is caused by only a handful–sometimes one, or two– active ingredients. This is the case, for example, for fenpropathrin, causing a wide increase in average impact scores per application and year, as well as per hectare and year during 2012 and 2013. Another example that is more consistent over time would be cypermethrin and chlorpyrifos. Both are responsible for the fluctuations in total impact score per year as a function of their application amount. This highlights the fact that even at a small rate, active ingredients can have significant impacts on freshwater ecotoxicity, and that only a handful of active ingredients actually influence overall and average toxicity compared to others. Therefore, substituting active ingredients such as fenpropathrin, cypermethrin, and chlorpyrifos could have a tremendous impact on the environmental footprint of farming communities. The overall environmental impact can be easily targeted by targeting those active ingredients with a high impact score but a low application rate. Another strategy would be to diversify and substitute those active ingredients that account for high impact scores at high application amounts, which is more challenging.

It is important to mention that this study was only focusing on freshwater ecotoxicity, not other environmental factors such as $CO_2$ equivalents (because of production), pollinators or other species outside freshwater, or human health indicators. Future research for these potential impacts is necessary, in order to find the best trade-offs between environmental and human health. Another important fact to consider is that both fate and characterization factors are based on a continental scale, and are not very precise in terms of environmental context. The magnitude of change when developing specific fate and characterization factors could be demonstrated by Berthoud et al. [2011], who could demonstrate the magnitude in difference between locally developed, site-specific factors and their results with results that were based on the default continental factors. Similar conclusions were drawn by Mankong et al. [2022], who also calculated factors specifically for the country of their study.

Overall, substituting insecticides with other measures could also be an important strategy to lower the environmental footprint of agriculture and pest management. Blanco et al. [2014] could demonstrate in their study that only a few percentage of Mexico's Maize production areas are under Integrated Pest Management, with a lot of potential of expanding this strategy to diversify pest management regimes in Mexico. By enhancing Integrated Pest Management strategies, Mexico's Maize production could potentially decrease the use of synthetic insecticides, lowering its reliance on chemical inputs and the chance of pests developing pesticide resistances. highlighting a significant opportunity to expand IPM adoption. This transition could also lower the environmental impact of agriculture overall, cutting back its influence on humanity's planetary boundaries.

## 5.2 Mode of Action, Management Practices and Extension Approaches

Even though freshwater ecotoxicity is primarily dependent on chemical and physical properties, we could see that most of the modes of action used in CIMMYT's extension project differed significantly from each other in terms of their impact scores. Only four comparisons did not display such a significant difference. This could also have important implications in terms of recommendations for substituting different active ingredients with each other–

active ingredients with high impact scores should be substituted with active ingredients with a mode of action that has, in general, lower impact scores.

We added another layer of impact assessment using USEtox by further exploring how management practices such as conservation agriculture and extension treatments are associated with freshwater ecotoxicity. Interestingly, our analysis could also demonstrate that cultural practices were associated with higher or lower impact scores. Conservation agriculture, irrigation, intercropping, as well as growing maize during the fall-winter production cycle, are associated with lower impact scores per hectare. This could be because of several active ingredients or modes of action being more or less used within these practices. Our study could also demonstrate that impact scores per hectares were not associated with the size of the field. Since Ibarrola-Rivas et al. [2020] found out in their study that farmers were using agrochemicals at a higher rate in smaller fields, potentially leading to higher impact scores, we could demonstrate that under extension services, plot size did not affect the average impact score of insecticides in terms of their freshwater ecotoxicity when extension services were involved. This highlights the importance of extension systems for not only raising crop productivity but also for ameliorating the environmental footprint of agriculture.

We could also demonstrate that certain management practices are associated with higher or lower impact scores, which can be explained due to the dominance of certain modes of action. For example, plots not under conservation agriculture exhibited on average a lower impact score by 12%. This could be explained by the higher chance of spinosyns and neonicotinoids in this production system - both modes of action with a significantly low impact score compared to the other modes of action applied in the project. A similar conclusion could be drawn with intercropping, which leads to a lower impact score of 22%, which could also be explained by the lower chances of applying organophosphates, which exhibit higher impact scores in general. At the same time, the higher diversity in both of these management practices could also have an impact on pest pressure, as indicated by Pierre et al. [2022a] and Rivers et al. [2016]. Another important factor for lesser pest pressure could be because of the timing of growing maize - hence, the production cycle. With lesser pest pressure, it could be the case that other modes of action are more dominant, or less amounts of insecticides are necessary to be applied in the fields.

Our study could also provide insights into the success of two different extension modes promoted by CIMMYT. With the traditional extension approach leading to a significant reduction both compared to *Parcela innovación* and *Parcela testigo*, with a reduction of 10% and 16%, respectively. This could also be explained by the different modes of action dominating these treatments. In both *Parcela innovación* and *Parcela testigo*, less neonicotinoids, diamedes, (which are associated with lower impact scores) and more organophosphates were applied (which are associated with higher impact scores). These findings underscore the essential role of selecting appropriate modes of action for reducing the environmental impact in extension projects. In addition, these results also underscore the importance of impact assessment in order to promote the right practices. Lastly, they also highlight the importance of finding the right extension mode when promoting different management practices. In our case, the traditional extension approach showed the highest reduction in environmental footprint, compared to the more time- and resource-intensive approach comparing *Parcela innovación* and *Parcela testigo*. These results are based on average impact score per hectare, suggesting that instead of focusing extension efforts on comparisons between two demonstration plots (*Parcela innovación* and *Parcela testigo*), extension efforts achieve faster and better results when directly guiding farmers.

# 6 Conclusion

Because of their high potential of causing substantial damage to maize yields - the staple food of Mexico - maize farmers throughout Mexico are relying heavily on chemical control mechanisms. The high reliance on insecticides to control pests could have tremendous effects on the environment, especially non-target organisms. This study was an assessment of an extension project, conducted over 10 years by CIMMYT, the International Maize and Wheat Improvement Center. The project was carried out throughout Mexico, with special emphasis on the states Guerrero, Guanajuato, Chiapas, and Morelos. Over ten years (between 2012 and 2021), extension agents collaborated with local maize farmers to promote the sustainable use of insecticides, trying to eliminate the environmental footprint of chemical control.

We calculated the freshwater ecotoxicity of the active ingredient applied throughout the extension project, after we calculated the mass applied per active ingredient. To calculate impact scores, we used PestLCI and USEtox, both internationally standardized and widely-used models to calculate the impact of chemicals on the environment. We found that throughout the extension project, only a few active ingredients dominated in terms of mass applied, such as cypermethrin and chlorpyrifos. Even though we could determine the relative low toxicity of cypermethrin and chlorpyrifos, these two active ingredients contributed substantially to the overall freshwater ecotoxicity because of their high numbers of applications. In addition, we could also show that even a low number of a substance with high toxicity could have tremendous effects on freshwater species, such as fenpropathrin. These two findings highlight the importance of life cycle assessments, that enable us to determine the impact of certain chemicals released into the environment, which allows us to find substitutions for extremely toxic chemicals. We also found out that some management practices were associated with higher or lower toxicity scores, because of the mode of action that were used in these practices.

At the same time, it is important to note that we only looked at freshwater ecotoxicity, not the effect on humans or other species, as well as the huge potential of integrated pest management strategies in maize production. However, the application of USEtox for the assessment of an extension project with real-life data collected, offered a new, and detailed impact assessment. This new level of detail underscores the importance to include as many data as possible in the impact assessment to see nuanced variations and trends over time, which is not possible with national datasets. It showed how much potential very few chemicals could have to harm freshwater ecosystems because of their high toxicity levels, and how using different active ingredients and modes of action can lower the environmental footprint of insecticides. Therefore, USEtox can provide valuable insides which pesticides to use to lower toxicity levels in freshwater ecosystems in farming systems that rely on chemical inputs. By providing these recommendations - which chemicals to use and which ones to avoid - USEtox can provide a basis for informed decisions, such as which extension appraoch is the most effective, or which mode of action or active ingredient to promote when necessary. USEtox has the potential to inform decision-making and developing strategies to lower the environmental impact of agriculture.

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