



IMPACTS OF CROP PROTECTION PRODUCT APPLICATIONS ON THE ENVIRONMENT

Currently limited to aquatic organisms

Version 1.3 – Report for 2nd review cycle November, 2021

Disclaimer

This material may contain "forward-looking statements" based on current assumptions and forecasts made by Bayer management. Various known and unknown risks, uncertainties and other factors could lead to material differences between the actual future results, financial situation, development or performance of the company and the estimates given here. These factors include those discussed in Bayer's public reports which are available on the Bayer website at http://www.bayer.com/. The company assumes no liability whatsoever to update these forward-looking statements or to conform them to future events or developments.

Content

1.	Context	t and objectives	7
	1.1.	Context	7
	1.2.	Reducing the environmental impact of crop protection requires a holistic approach at crop system level. A review of main levers.	8
	1.3.	International frameworks considered to define the BCS goal of 30% EIR of CP by 2030	10
	1.4.	The BCS goal in light of the UN Sustainable Development Goals and Planetary Boundaries	11
	1.5.	Objectives of the report	12
	1.6.	Critical review	13
	1.7.	Organization of the study	15
	1.8.	Use of the study and target audience	16
2.	Scope o	of the study	16
	2.1.	System studied	16
	2.2.	Functional unit	19
	2.3.	Scenario elements	19
	2.4.	System boundaries	21
3.	Method	1	22
	3.1.	Compilation of inventory data	23
	3.2.	Compilation of inventory data on global crop protection product consumption based the 'Agrowin' database	23
	3.3.	Impact assessment based on active ingredients emissions and freshwater ecotoxicity impact calculation	27

	3.4. Emission modelling with PestLCI					
	3.5. PestLCI input data					
	3.5.1.	Crop types in PestLCI	30			
	3.5.2.	Fractions of applied pesticide intercepted by crop surface area in PestLCI				
	3.5.3.	Application methods in PestLCI	32			
	3.5.4.	Drift reduction in PestLCI	33			
	3.5.5.	Consideration of buffer zone in PestLCI				
	3.6.	Linking PestLCI with USEtox [®] : Emission compartment allocation				
	3.6.1.	Segmentation/mapping of related emissions				
	3.6.2.	Off-field surface emission fractions				
	3.7.	Ecotoxicity impact modelling with USEtox®	35			
	3.7.1.	USEtox [®] input data				
	3.8.	From application scenarios to global EI	42			
	3.9.	Agrowin CP application scenario data processed in PestLCI / USEtox [®] model approach	lling 43			
	3.10.	Exclusions of CP application scenarios	44			
	3.11.	Combining application scenarios with the models to derive EI scores	45			
	3.12.	Aggregating El scores	48			
4.	Interpre	etation	49			
	4.1.	Results and setting a CP EIR baseline for future progress tracking	49			
	4.2.	Sensitivity analysis: USEtox [®]	51			
	4.3.	Qualitative discussion of uncertainty	54			
	4.4.	Main limitations and how they are addressed	55			
5.	Further	developments of this report	56			
6.	Referen	ices	57			
7.	Append	lix I – External Sources in Agrowin 2019 (all other crop-country combi	nations			
are	based o	n non-panel data)	61			
8.	Append	lix II: Checklist Quality Standards for Panel Providers	68			

List of Figures

Figure 1: BCS' crop protection environmental impact reduction framework9
Figure 2: Primary emissions based on PestLCI and their emission vectors to off-field surfaces 22
Figure 3: Gap between reported data and consumption data in global data sets on crop protection use
Figure 4: Agrowin country-specific data sources overview (2016 status)
Figure 5: PestLCI Consensus primary emission distribution processes and compartments for the example of aerial application of pesticides, which first enter the "air" compartment and from there further distribute to other compartments
Figure 6: Coupling of different state-of-the-art models for assessing emissions and toxicity related impacts in LCIA
Figure 7: Impact pathway for freshwater ecotoxicity impacts in USEtox® 2.x (Fantke, et al., 2018b)
Figure 8: Distribution of substances provided for calculation of the application scenario in USEtox [®] results
Figure 9: Overall approach followed to assess the EI of each application scenario. Emission and potential impact results are compartment-specific as shown in Figure 6
Figure 10: Detailed levels of Crop protection application scenarios captured in Agrowin data
Figure 11: Framework representation considering both PestLCI and USEtox® inputs
Figure 12: Definition of key measurement factors within the methodology
Figure 13: Overview of available BCS CPP levers and their role within the EI scope
Figure 14: Outline of the BCS EIR baseline and the performance tracking concept
Figure 15: Stochastic freshwater aquatic ecotoxicity characterization factors (PAF m ³ d/kg emitted) for methamidophos (CAS RN: 10265-92-6) emitted to continental rural air, freshwater, agricultural and natural soil
Figure 16: Spearman Rank Correlation for model input variables with the largest magnitude of influence on characterization factor variability across four emission scenarios in USEtox [®]

List of Tables

Table 1: Critical review panel composition	. 14
Table 2: Contact information for all parties	. 15
Table 3: Crops categories and sub-categories covered in the data set (at crop main group and crop group level)	16
Table 4: Crop classes implemented in the PestLCI Consensus model	. 30
Table 5: Crop protection product application methods and primary emission fraction to air as available in PestLCI	32
Table 6: Percentages of surface areas represented by freshwater, agricultural soil, and natural soil for continental level parameterizations in USEtox [®]	34
Table 7: Chemical input data in USEtox [®] for organic substances or metal ions that are relevant for application scenario calculations	38
Table 8: Stepwise calculation of EI scores for an individual application scenario	. 47
Table 9: Fate, eco-exposure and ecotoxicity effect relevant input data for USEtox [®] and their modelled variance for the neutral test substance methamidophos (CAS RN: 10265-92-6)	52

Table of Abbreviations

AI	Active Ingredient
BCS	Bayer Crop Science
ввсн	Biologische Bundesanstalt, Bundessortenamt and Chemical Industry
CAS	Chemical Abstracts Service
CF	Characterization Factor per active ingredient (PAF m^3 d/kg emitted: Model output of USEtox $^{\ensuremath{\$}}$)
СР	Crop Protection
СРР	Crop Protection Product
CP EI	Crop Protection Environmental Impact
EC	Effect Concentration
EI	Environmental Impact (freshwater ecotoxicity impact of crop protection applied on a field as determined by the combination of the models PestLCI and USEtox [®])
El/quantity	Environmental Impact per quantity (PAF m3 d/Kg applied)
El/ha	Environmental Impact per hectare (PAF m3 d/treated area)
El/scenario	Environmental Impact per scenario (PAF m3 d/country/year)
	[Note: To facilitate readability and understanding, BCS labels this 'EI/scenario' metric as 'EI'; see also 'EI' above]
EIR	Environmental Impact Reduction
На	Hectare
LCA	Life Cycle Assessment
LCM	Life Cycle Management
PAF	Potentially Affected Fraction of species
PDF	Potentially Disappeared Fraction of species
DTU	Technical University of Denmark
UN SDGs	United Nations' Sustainable Development Goals

1. Context and objectives

1.1. Context

Bayer is a Life Science company with a more than 150-year history and core competencies in the areas of health care and agriculture. Contributing to sustainable development has become a core element of Bayer's corporate strategy. For Bayer Crop Science (BCS) division, sustainability focus areas and goals were developed to fulfill the commitment to shape the future of sustainable agriculture. BCS' sustainability focus areas were developed to address the field-to-field-gate impact of agriculture. These commitments complement Bayer's sustainability objective for its own operations, such as the commitment to become carbon neutral by 2030 (scope 1&2 emissions). The field-to-field-gate scope focuses on the sustainability impacts at the farmer-level (i.e., the product use stage). BCS has committed to enable farmers to reduce field GHG-emissions by 30%, reduce the environmental impact of crop protection¹ (see below the scope of environmental impact in the context of this report) by 30% and BCS strives to improve the livelihoods of 100 million smallholder farmers through access to education and tailored solutions. This report focuses exclusively on one of BCS sustainability focus areas: a transformational commitment on the environmental impact reduction (EIR) of crop protection (CP) by 30% until 2030 (in this report, BCS uses the terms 'crop protection products' (CPPs) and 'pesticides' interchangeably).

In the last few decades, the environmental impact of crop protection has decreased while ensuring yield and helping growers produce more with less (Phillips McDougall, 2018). However, with new tools and innovations BCS has the opportunity, and responsibility, to continue reducing this impact. BCS has committed to reducing its global environmental impact of crop protection by 30% by 2030, compared with a five-year average baseline environmental impact (from 2014 to 2018). BCS is currently using a combined model based on PestLCI and USEtox[®], that can calculate BCS global environmental impact of crop protection. So far, this model has been used to screen the EI of all CPPs applied worldwide, based on scenarios for emission and impact modelling consisting of various types of crops grown in various countries.

In this report, environmental impact of crop protection is defined in accordance with the current scope of PestLCI and USEtox[®]. More specifically, BCS relies on the midpoint USEtox[®] impact unit that expresses freshwater ecosystem toxicity as "potentially affected fraction (PAF)" of freshwater species exposed to a chemical in a freshwater environment. More details on the interpretation and calculation of this unit follow in later sections. In this report, **the combination of emissions according to PestLCI and potentially affected fraction of exposed species according to USEtox[®] is called crop protection environmental impact (EI). BCS decided to use the term EI for internal and external communication to facilitate general understanding among customers (farmers) and within other internal and external stakeholders who might lack the understanding of strict LCA terminology and the differences between environmental impact categories. Therefore, this report will also mainly use the term 'EI'**. By using this impact unit, BCS ultimately aims to reduce the impact of crop protection on environmental non-target species. BCS

¹ The designation "environmental impact of crop protection" has been adopted for the purpose of Bayer corporate communication. Any external communication will disclose the limitation of this designation to freshwater ecotoxicity or any other scope according to further methodological developments in the context of the present study.

additional environmental impact categories, such as soil organisms, once the USEtox[®] consortium integrates these categories in the public consensus model.

BCS is partnering with Prof. Peter Fantke and his team from the Technical University of Denmark (DTU; i.e., the director of the PestLCI and USEtox[®] consortium).

The main objective of this report is to document how BCS is utilizing the combined model based on PestLCI and USEtox[®], that can calculate BCS' global EI of crop protection. BCS emphasizes that it only considers the EI of crop protection during its use phase on the field in this report while excluding further upstream and downstream impacts. Other impact categories relevant for crop protection such as potential human health impacts resulting from the ingestion of pesticide residues in crops, or greenhouse gas emissions and climate change impacts are not in the scope of this specific report but are considered by other sustainability commitments BCS has made.

Besides the CP EIR commitment, BCS has established various separate internal sustainability initiatives and taskforces to set up measurement approaches and improvement levers for greenhouse gases for Bayer's own operation and at the field level, smallholder livelihood, biodiversity and soil health, water conservation and product responsibility (e.g. empty container management, safe use trainings), and other initiatives e.g., to achieve globally harmonized safety standards for our crop protection products focused on operator safety.

In the context of this report, BCS does not conduct a full-fledged LCA according to ISO 14040/44 but intends to use the standard as a framework to document the project in the present report. With a critical review of this report by external experts, BCS aims to verify that it uses the PestLCI and USEtox[®] models in a reasonable approach and that the baselining and performance tracking methodology is adequate. In case of external communication of the present report or any material based on it, BCS intends to publish the external expert's panel feedback with transparency, and it intends to consult the panel regularly in the future.

1.2. Reducing the environmental impact of crop protection requires a holistic approach at crop system level. A review of main levers.

BCS aims to reduce its environmental impact of crop protection. The main drivers of the environmental impact of crop protection have been identified as:

- the amount of all crop protection substances applied per hectare area (ha) per growing seasons in a given crop and country,
- the environmental impact of the crop protection applied on the field itself, and
- factors contributing to emissions of crop protection applied on the field into the environment.

Thus, the main impact reduction 'levers' can be categorized as follows:

- Optimize crop protection amounts required per hectare through tools like:
 - Precision application: data-driven tools that ensure that the right amount of crop protection is applied in the right place and at the right time.

- Seed treatment: seed-applied crop protection tools can dramatically reduce the volume of chemicals used and potential exposure to wildlife and the environment.
- Seeds and traits: crops bred and designed to better fight the pests and diseases that attack them, ensuring that less chemical crop protection is needed
- Biologics: complement chemical crop protection with biologics to enhance integrated management practices and reduce pest resistance
- Integrated crop management practices such as crop rotations, cover crops, integrated pest management strategies which help to control weeds, pests and diseases and therefore reduce the need for crop protection products.
- Reduce the environmental impact of the crop protection product itself:
 - Better environmental profile of the active ingredient (lower effect on non-target plants and species)
- Reduce the emissions into the environment
 - Mitigation measures such as drift reduction and buffer strips
 - Digitally enabled precision application

BCS's analysis of the major levers starts at the drivers of the environmental impact of crop protection in a given crop and country in terms of specific crop protection products. BCS then assesses its existing portfolio, the innovation pipeline, and alternatives in the market, to understand how CP EI hotspots can be mitigated. In this analysis it became apparent that levers can be categorized further in overarching levers, which are relevant for herbicides, fungicides and insecticides, and levers which are mainly relevant for a specific indication are outlined in Figure 1 below.

Reduce Bayer's crop protection environmental impact by 30% by 2030. Overarching and indication specific improvement levers.



Figure 1: BCS' crop protection environmental impact reduction framework

1.3. International frameworks considered to define the BCS goal of 30% EIR of CP by 2030

We are at a tipping point where both consumers and our planet demand a fundamental change in the agricultural system. With the world population expected to meet the 10 billion mark by 2050, the demand for food and biomass production is steadily increasing (Ray et al., 2013). However, crop cultivation is becoming increasingly challenging for farmers due to changing environmental conditions, raising regulatory requirements and other challenges. Furthermore, the amount of available agricultural land is declining due to increasing urbanization, higher salinity levels and soil erosion. For BCS, all of these factors culminate into a so-called **'agricultural paradox'**: on the one hand, farmers need to produce more food and biomass to meet global demand while on the other hand this need must be met while preserving resources and the environment. Agriculture must strike a balance between the need for tools like crop protection, which enable farmers to keep meeting the world's growing agricultural demands while using less land and resources, and potential trade-offs posed by increasing the use of such tools. With new products and technologies, we aim to ensure that our solutions serve farmers' needs and wellbeing, while also protecting the environment and contributing to food security. Overall, the 'agricultural paradox' is based on the following premises (see also (UNEP, United Nations Environmental Programme, 2021)):

- Development of dietary choices in agricultural system: The world population is growing, and dietary habits are changing. The world population is expected to grow from about 7.8 billion in 2020 to 9.8 billion by 2050. Global income is increasing, and the global middle class is expanding. In spite of the emerging trend towards plant-based meat and other alternative sources of protein, the per capita consumption of meat, refined fats, refined sugars, alcohols, and oils is expected to rise with the increasing wealth along with demand for consumer products that also depend on agriculture. Pesticides are an essential tool in securing higher yields, without which even more land would have to be converted into arable land.
- **Development of output demand in agricultural system**: Demand for food, feed, fibers, fuels, and feedstocks is growing. By 2050 demand for food is projected to grow by 60 percent, meat production by nearly 70 percent, aquaculture production by 90 percent and production of dairy products by 55 percent. Furthermore, cropland is increasingly used for purposes such as production of livestock feed, fibers, biofuels, and feedstocks for the chemical industry.
- Development of agricultural system's vulnerability to climate change: Crop cultivation is becoming increasingly challenging for farmers due to climate change affecting growing conditions. For example, climate change will intensify global water scarcity and change the distributions of pests, which could lead to increased and more widespread use of pesticides.
- **Development of agricultural system's vulnerability to land degradation**: The amount of available agricultural land is declining due to increasing urbanization, higher salinity levels and soil erosion.

To overcome the 'agricultural paradox', BCS decided to set an ambitious goal that is also aiming at attaining the UN Sustainable Development Goals (SDGs) while staying within planetary boundaries (especially, the planetary boundary of 'chemical pollution'; (Rockström, et al., 2009)). Consequently, BCS made the public commitment of reducing the environmental impact of Bayer's crop protection portfolio by 30 percent by 2030. Overall, BCS defined this 30% in the light of established conceptual frameworks and based on internal expert judgement by critically reflecting our technological capability to live up to this commitment. After defining this ambitious goal, BCS decided to use PestLCI and USEtox® as consensus models to assess and verify our progress towards our 30% goal.

1.4. The BCS goal in light of the UN Sustainable Development Goals and Planetary Boundaries

BCS decided to set an ambitious goal that is also aiming at substantial contributions to attaining the United Nations' Sustainable Development Goals (UN SDGs) while staying within planetary boundaries. In light of these internationally established frameworks, BCS made the public commitment of reducing El of Bayer's crop protection portfolio by 30 percent by 2030. BCS's CP EIR goal aims at contributing to attain the **United Nations' Sustainable Development Goals**. The United Nations agreed on 17 SDGs to build a better world for people and our planet by 2030. The 2030 Sustainable Development Agenda emphasizes that development should be compatible with all three dimensions of sustainability: Economic, social, and environmental. Implementing the 2030 Agenda presents an opportunity for collaborative action by many diverse actors, and at all levels, to minimize the adverse environmental impacts of pesticides. Therefore, BCS's CP EIR commitment is at the interface with several goals of the 2030 Agenda to contribute to a sustainable management of pesticides (see also UNEP (2021)).

- SDG 1 No poverty: Increased need for efficient, profitable and sustainable use of pesticides
- SDG 2 Zero hunger: Increased need for effective pest management; Need to increase quality and sustainable use of pesticides in certain parts of the world; Wider adoption of sustainable agricultural production practices
- SDG 3 Good health and well-being: Ensure access to sufficient, safe and nutritious food
- SDG 6 Clean sanitation and water: Minimization of water pollution from pesticides
- SDG 9 Industry, innovation and infrastructure: Development of innovative and sustainable pest management approaches and technologies
- SDG 12 Responsible consumption and production: Wider adoption of sustainable pest management practices; Minimization of impacts of pesticides on natural resources; Further strengthening of sound management of the entire life cycle of pesticides; Further support for and implementation of sustainable pest management technologies by the pesticide industry; Improvement of information provision about the risks of pesticides and ways to minimize these risks
- SDG 13 Climate action: Wider adoption of integrated practices in agriculture that enhance farmers' sustainable productivity as well as climate resilience
- SDG 15 Life on land: Minimization of environmental impacts of pesticide use; Ensuring sustainable control of invasive pest species; Mainstreaming ecosystem and biodiversity values in national and regional pest management policies
- SDG 17 Partnerships for the goals: Improvement of sharing of pesticide management knowledge among relevant stakeholders; Enhancing partnering among UN organizations active in sound management of chemicals

Furthermore, BCS aims at staying within planetary boundaries; especially, within the **planetary boundary of** 'chemical pollution and the release of novel entities' (Rockström J. W., 2009), which is defined as: "Primary types of chemical pollution include radioactive compounds, heavy metals, and a wide range of organic compounds of human origin. Chemical pollution adversely affects human and ecosystem health, which has most clearly been observed at local and regional scales but is now evident at the global scale. Chemical pollution qualifies as a planetary boundary because it can influence Earth System functioning: (1) through a global, ubiquitous impact on the physiological development and demography of humans and other organisms with ultimate impacts on ecosystem functioning and structure and (2) by acting as a slow variable that affects other planetary boundaries. For example, chemical pollution may influence the biodiversity boundary by reducing the abundance of species and potentially increasing organisms' vulnerability to other stresses such as climate change (Jenssen, 2006; Noyes, et al., 2009). Chemical pollution also interacts with the climate-change boundary through the fact that most industrial chemicals are currently produced from petroleum, releasing CO2 when they are degraded or incinerated as waste. There could be even more complex connections between chemical, biodiversity, and climate-change boundaries. For example, climate change will change the distributions of pests, which could lead to increased and more widespread use of pesticides."

The main aim of this report is to assess the environmental impact of crop protection when applied on a field, rather than to directly quantify impacts on biodiversity. BCS acknowledges that a quantification towards the planetary boundary of 'chemical pollution' is currently not possible (Rockström J. W., 2009; Jenssen, 2006; Noyes, et al., 2009).

While being aware that the planetary boundaries framework was published over a decade ago, we argue that it is still a valid scientific framework today with steadily increasing citations every year. However, BCS acknowledges that the planetary boundaries concept has also come under heavy scrutiny and been criticized from both natural and social sciences. For example, Biermann & Kim (2020) provide a recent for critical appraisal:

- The planetary boundaries framework has been influential in generating academic debate and in shaping research projects and policy recommendations worldwide such as setting science-based targets.
- Numerous studies have sought to further refine and implement the planetary boundaries framework by downscaling planetary boundaries or applying the framework to global and national environmental assessments.
- The definition of a safe operating space for humanity has stimulated many social scientists and international lawyers to explore what planetary boundaries thinking could imply for governance and the dominant paradigms of our time.
- Yet the framework has also come under heavy scrutiny and been criticized from both natural and social sciences, humanities scholars, as well as the broader public and policy community.
- The concept of planetary boundaries has shown its limitations in terms of political impact and it seems to lack support from the Global South.

1.5. Objectives of the report

In order to achieve the sustainability goal of reducing the CP EI by 30%, BCS has set the foundations of its performance tracking method. Thus, this report's objective is to:

- Document a method to quantify the BCS' global CP EI in 2018², based on application scenarios from BCS' primary data
- Identify hotspots and improvement potentials in line with the BCS EI reduction target

In 2022, BCS will calculate a five-year average baseline CP EI (from 2014 to 2018³), in order to track performance against the 30 % reduction commitment of the EI by 2030. The 2018 baseline serves to enable BCS to determine its focus areas.

1.6. Critical review

This report is structured in line with the Life Cycle Assessment (LCA) methodology (according to the ISO 14040 and ISO 14044) as a template for documentation of methodological choices, results and interpretations as well as limitations. However, BCS acknowledges that this report only focuses on the field-to-field gate life cycle stage and on pesticide emissions' impacts due to CPP use. Consequently, BCS does not claim that this report complies with ISO 14040/44. As BCS intends to communicate to the public its sustainability commitments and achievements, a critical review has been performed, following a three-step iterative process. This report provides the review panel composition (see Table 1), its conclusions and the details of the comments and final report adaptations.

² The input dataset is currently based on 2018-only data provided via the Agrowin database. The reason for this is that the 2018 data were the most-up-to date data available when BCS started the partnership with the DTU.

³ It is planned to establish a baseline on a 5-year-average (2014 – 2018) to account for the specificities of agriculture such as inter-annual variability, seasonality, or dependence on climatic conditions. BCS and DTU are currently calculating the final baseline based on the 5-year-average (2014 – 2018).

Table 1: Critical review panel composition

Members	Country	Area of expertise
Thomas Nemecek	Switzerland	Deputy Lead Life Cycle Assessment Research Group Agroscope. Worldwide known researcher on Life Cycle Assessment, specifically in its applications on agriculture.
Jeffrey Jenkins	U.S.A.	Professor at Oregon State University. Expertise in environmental analytical chemistry, ecological risk assessment, and agronomically- based ecohydrologic modeling to characterize watershed scale pesticide use and the potential impact on water quality.
Valery Forbes	U.S.A.	Dean and Professor at University of Minnesota. Broad expertise in mechanistic effect modeling and ecological risk assessment of pesticides and other chemicals.
Assumpció Anton	Spain	Researcher at Food and Agricultural Research Institute, IRTA. Expertise in the development and application of LCA methodology in agriculture.
Tiago Rocha	Brazil	Consultant Partner at ACV Brasil and PhD in Environmental Technology. Extensive experience in life cycle assessment, specifically in the area of carbon footprint.
Lorie Hamelin	France	Researcher at the Federal University of Toulouse (France), studying the environmental impacts related to large-scale transitions towards low fossil carbon use
Anne-Marie Boulay	Canada	Assistant Professor in Chemical Engineering at Polytechnique Montreal and CIRAIG. Expertise on water footprint methodologies and impact assessment associated with plastic litter in LCA. She is the Canadian chair of ISO sub-committee on Life Cycle Assessment (TC207/SC5).
Jessica Hanafi	Indonesia	PhD in Life Cycle Engineering. Established the Indonesian Association of Life Cycle Assessment and Sustainability Professional. ISO Technical Committee on Life Cycle Assessment (TC 207/SC5), environmental labelling (SC3), Greenhouse Gas (SC7) and project leader for ISO/TS 14074 LCA normalization and weighting. Applied LCA based on ISO 14040/44 to various industrial sectors, including agriculture.
Laura Golsteijn (Chair of the panel)	Netherlands	Senior LCA Consultant at PRé. PhD in Toxic Impact Modelling. Supporting clients to understand, develop and embed environmental metrics to improve the sustainability of supply chains and products.

1.7. Organization of the study

The overall impact assessment calculation process can be summarized as follows (see also Table 2): For the compilation of inventory data, BCS provided the underlying crop protection application data to DTU. For the subsequent impact assessment, DTU used the crop protection application data to calculate primary distribution fractions of pesticide emissions in PestLCI and calculated the characterization factors for the active ingredients in USEtox[®]. Finally, DTU combined the primary distribution fractions from PestLCI with the characterization factors from USEtox[®] to calculate the CP EI scores (More details on the compilation of inventory data, impact assessment, and interpretation follow in later sections of this report).

Organization	Contact	Role	Tasks
Bayer Crop Science	Daniel Glas, daniel.glas@bayer.com	Project lead Bayer	 Apply global CP EI baseline Bayer internally to identify Bayer hotspots. Develop roadmap to deliver against Bayer's commitment. Assess how to integrate learning into CP product development (R&D
			 Create IT tools to enable Bayer organization to work with EI data.
Technical University of Denmark	Peter Fantke, pefan@dtu.dk	Project lead DTU	 Apply PestLCI and USEtox[®] model to generate global CP EI baseline. Advance models further (both on emissions and impact side).

Table 2: Contact information for all parties

1.8. Use of the study and target audience

The results of this study are intended to transparently and publicly describe the baseline, performance tracking and CP EI calculation method. BCS aims to publish the expert panel's feedback as well to ensure transparency and strive for credibility. Therefore, the main target audience are investors, press, academic partners, and the general public. Potentially, this report might also be used in the future for auditing processes, and as background-information material for peer-reviewed publications in scientific journals.

This report is not BCS's main vehicle for informing external stakeholders. BCS is currently developing other internal and external training and communication materials and channels that will be specifically tailored to the information-needs of the respective stakeholder group.

2. Scope of the study

2.1. System studied

As shown in Table 3 below, the system of this study includes BCS entire CP portfolio applied on BCS customers' fields globally in 2018. According to the inventory data, this covers 270 active ingredients which are used in 2,056 CPP in 82 countries and 54 crops (at crop group level, see Table 3)

Table 3: Crops	categories a	and sub-categories	covered in the	data set (at	crop main grou	up and crop group
level)						

Crop Main Group	Crop Group
BEETS	BEETS
CEREALS	BARLEY
	CEREALS-OTHER
	OATS
	RYE
	WHEAT
CORN/MAIZE	CORN-TRADITIONAL
	CORN-TRANSGENIC
COTTON	COTTON TRADITIONAL

	COTTON TRANSGENIC		
ENVIRONMENTAL MARKETS	TREES		
(only covering farm level)	TURF+GROUND-MANAGEMENT		
FRUITS & NUTS	BANANAS		
	BERRIES & SMALL-FRUITS		
	CITRUS		
	FRUITS: OTHER		
	FRUITS: TROPICAL&SUBTROPICAL		
	POME-FRUITS		
	STONE-FRUITS		
	TREE NUTS		
GRAPES/VINES	GRAPES/VINES		
OILSEED-RAPE/CANOLA	OILSEED RAPE TRADIT.		
OTHER CROPS	FALLOW-LAND/SET-ASID		
	FIBER CROPS: OTHER		
	FORAGE CROPS		
	GROUNDNUTS/PEANUTS		
	OILSEEDS: OTHER		
	OTHER-CROPS UNSPEC.		
	SORGHUM & MILLET		
	SPICES		
	SPICES		
PLANTATION	SPICES SUNFLOWER CACAO		
PLANTATION	SPICES SUNFLOWER CACAO COFFEE		
PLANTATION	SPICES SUNFLOWER CACAO COFFEE OIL PLANTATIONS		

	TEA
	ТОВАССО
POTATOES	POTATOES
RICE	RICE
SOYBEANS	SOYBEANS TRADITIONAL
	SOYBEANS TRANSGENIC
SUGAR CANE	SUGAR CANE
VEGETABLES & FLOWERS	FLOWERS+ORNAMENTALS
	VEG: BRASSICAS
	VEG: BULB
	VEG: FRUIT-CUCURBITS
	VEG: FRUIT-OTHERS
	VEG: FRUIT-SOLANACEAE
	VEG: LEAFY&FRESH-HERBS
	VEG: LEGUMES
	VEG: ROOT&TUBER
	VEG: STALK&STEM
	VEGETABLES-OTHER

2.2. Functional unit

The function of the studied system in this report is the environmental impact of all Bayer CPPs applied per ha per crop and country (EI/ha crop,country), such as fungicides, insecticides, herbicides, and seed treatments. Therefore, BCS defines the functional unit (FU) as follows:

• Functional unit: per hectare and growing season

BCS has decided to define the FU per ha as opposed to considering the yield (environmental impact of crop protection per kg crop produced) to reflect societal, political and shareholder expectations, to reduce the environmental impact of the BCS crop protection portfolio irrespective of yield.

2.3. Scenario elements

The specific elements embedded in the specific global CP application scenarios will be explained in the following (elements for each individual scenario):

AgroWin⁴ data input:

General scenario information:

- Scenario ID: running number
- Country: China
- Region: Asia/Pacific
- Crop: e.g., Apple
- Crop group: e.g., Pome fruits
- Crop main group: e.g., Fruits & nuts
- Crop growth stage: according to BBCH classification⁵
- Active ingredient name: e.g., Beta-Cyfluthrin. *Note:* The term 'active ingredient' (or active substance) refers to the chemically active part of a manufactured pesticide which is majorly responsible for the targeted action; i.e., defeating pest and suppressing weed.
- Indication: e.g., Insecticide

⁴ AgroWin is a database-software by Lexagri which generates a complete view of the entire crop protection market by harmonizing multiple data sources (for further details c.f. section 3.2).

⁵ BBCH - Biologische Bundesanstalt, Bundessortenamt and Chemical Industry. The BBCH scale provides a framework to develop scales for individual crops wherein similar growth stages of each plant species are allocated within the same BBCH code.

• CAS registration number of active ingredient: e.g., 1820573-27-0

Market/product information:

- Name of Distributor Group and specific (sub) distributor: e.g., BCS
- Product Name: e.g., BULDOCK
- Active ready mix: names of active ingredients if multiple active ingredients are contained in a product

Application data:

- Treated area (ha per year): 'Treated area' refers to the hectares or size of farmland on which CP was applied during the cultivation of a crop.
- Applied mass (kg of active ingredient applied per year)
- Applied dose (kg of active ingredient applied per ha)
- Application Method (translated into application methods included in PestLCI): e.g., Boom-sprayerconventional-nozzle

PestLCI output values (PestLCI input parameters not listed here. See section 3.4):

Primary distribution fractions [kg emitted/kg applied] for environmental compartments:

- Air
- Field Soil
- Field Crop
- Off-field surface

Area fraction for off-field surfaces [m² compartment/m² total] for:

- Off-field agricultural soil
- Off-field natural soil (*Note*: Natural soil means non-agricultural soil)
- Off-field water

USEtox[®] output value per active ingredient (USEtox[®] input parameters not listed here. See section 3.7):

Freshwater characterization factors (CF) [PAF m³ d/kg emitted] for the environmental compartments:

- Air emission
- Agricultural soil emission

- Natural soil emission
- Freshwater emission

El output score combining PestLCI primary distribution fractions, USEtox[®] CFs and AgroWin information:

Final freshwater impact scores per environmental compartments and in total (CP EI score):

- PAF m³ d/kg applied (BCS label = EI / quantity)
- PAF m³ d/ha (BCS label = EI / ha)
- PAF m³ d/country/year (BCS label = EI)

2.4. System boundaries

The system boundaries comprise the off-field surface area. The assessment builds upon currently available consensus models, combining PestLCI Consensus as emission assessment model and USEtox[®] as impact assessment model. Consensus models are defined as models that were developed not only on state-of-theart science, but additionally on broad agreement among scientific and user communities regarding aspects that cannot be entirely addressed through science alone, but that require choices, such as the delineation of the technological and environmental system under study (see e.g. Hauschild et al. (2008) and Rosenbaum et al. (2015)). PestLCI is a model that was developed to simulate initial pesticide distribution directly after field application until different pesticide fractions reach the environmental distribution after emission, subsequent exposure to humans, and ecosystem and toxicity-related effects. Both models reflect state-of-the-science in environmental impact assessment of pesticides.

Figure 2 illustrates that the system under consideration is divided into two parts: The Technosphere (i.e. the space that is directly affected by agricultural intervention, which consists of the field to the field-edge, an air column above, and the soil below) and the environment. The environment is further divided into different emission compartments namely, air, field soil surface (agricultural soil), off-field surfaces, groundwater, and deposition on crops. Chemicals leaving the Technosphere into the environment are considered as emissions. The active ingredient mass reaching the environment as emissions within minutes after application, following primary partitioning are defined by the PestLCI consensus model as primary emission distribution fractions. These are then linked to USEtox[®] for impact assessment. See Section 3.3 for more information

The transfer of data from PestLCI into the USEtox[®] model:



Figure 2: Primary emissions based on PestLCI and their emission vectors to off-field surfaces

3. Method

The overall impact assessment calculation process can be summarized as follows:

- 1. For the compilation of inventory data, BCS provided the underlying crop protection application data (based on the Agrowin database by Lexagri) to DTU.
- 2. For the subsequent impact assessment, DTU used the crop protection application data to calculate primary distribution fractions of pesticide emissions in PestLCI per application scenario, and calculated the characterization factors (CFs) for the active ingredients in USEtox[®]. Some pesticides that are used in the current approach have not originally been available in PestLCI or USEtox[®]. In these cases, common LCA practice has been followed by introducing the missing substances or substance data based on available public databases.
- 3. Finally, DTU combined the primary distribution fractions from PestLCI with the characterization factors from USEtox[®] to calculate the final (midpoint) freshwater ecotoxicity impacts.

In the following, we provide more details on the compilation of inventory data, impact assessment, and interpretation.

3.1. Compilation of inventory data

The data inventory includes relevant input data from each application scenario (e.g. amount applied per ha as Reference flow) as well as data from widely used state-of-the-art consensus models for environmental evaluation (using LCA) of agricultural pesticides as well as for quantifying freshwater ecotoxicity from chemical emissions.

Substance characteristics like environmental degradation half-lives, solubility and ecotoxicological data are necessary for product registration and can be pulled from public databases, such as the <u>Pesticides Properties</u> <u>DataBase (PPDB)</u>, the <u>Bio-Pesticides Database</u> and <u>FooDB</u>. Climate, field and soil data inputs are based on pre-defined regional data sets of the PestLCI and USEtox[®] models. The climate, field and soil data are set for default (sub)continental and global systems in the USEtox[®] model (incl. land area with the fraction of freshwater, natural and agricultural soil, sea area, the temperature, wind speed, rain rate, freshwater depth, fraction of freshwater discharge from the continental to the global system, fractions of the rain rate that run off and respectively infiltrate the soil, soil erosion and irrigation). USEtox[®] also includes urban landscape data containing the urban area and the fractions of non-paved and paved area, and in addition for 8 continental landscapes and 16 sub-continental landscapes. Amongst others, the windspeed has been calculated based on GEOSChem wind speeds for IMPACT World and rain rates are based on GIS computation for IMPACT World. Further information of the model climate, soil and field data can be found in Rosenbaum et al. (2008) and Kounina et al. (2014). A consistent set made up respectively of emission fraction and mass balance equations are at the core of the two models and were applied by DTU as further described in Gentil-Sergent et al. (2020) (for PestLCI) and Rosenbaum et al. (2008) (for USEtox[®]).

3.2. Compilation of inventory data on global crop protection product consumption based the 'Agrowin' database

BCS complements these inventory data parameters with the AgroWin[®] database and software, which delivers crucial parts of application data for crop protection programs. AgroWin is a database-software by Lexagri (2021) which generates a complete view of the entire crop protection market by harmonizing multiple data sources. This software is used within BCS to access a detailed historic consumption market data overview (starting 1996) and reflects how farmers use products/seeds in the field. Overall, the database covers 90% of global crop protection products market value. Focusing on BCS, the database covered about 85-95% of the BCS market value in the past depending on the year. The data in AgroWin represents so-called consumption data, in other words: what have farmers actually planted and applied on their fields as opposed to sales data (what has been sold by crop protection manufacturers into the market).

The gap between consumption data and reported data from crop protection manufacturers can be attributed to several factors such as intercompany sales, channel inventories or royalties. Figure 3 below illustrates the different factors that cause an unquantifiable gap between reported data and consumption data. BCS relies on AgroWin for consumption data.



> Reported Data: Data as published in business reports (e.g. stock-market communication)

- > Intercompany Sales: Sales between companies who then either process the product further before selling or sell the product directly
- > Channel Inventories: Products already sold to the distributor, but not yet to the farmer
- Royalties: Payment made by one party to another for the right to ongoing use of that asset
- > Crop Year: A Crop Year is the period of time between two harvests and does not reflect Fiscal Year
- > Consumption Data: Reflects the amount of product or the treated area farmers use during a certain period (e.g. crop year)

Figure 3: Gap between reported data and consumption data in global data sets on crop protection use

The AgroWin database is built on two sets of data: panel data and non-panel data. Panel data are first-hand information from farmers through interviews after crop season. Collecting such information is based on interviewing global panels of farmers on how farmers use products in the field. These panel data are externally sourced from agricultural market research companies (e.g., Kynetec, SPARK, Kleffman Group,etc) which conduct global interview-based panel studies for monitoring market trends. At the end of a crop cultivation season, farmers are interviewed and asked about which crop protection products and practices the applied. For example, farmers are asked:

- Which crop protection products they used?
- How many hectares they treated (treated area)?
- How many kilograms of a product they used (volume applied)?
- At which crop growth stage they applied a product?
- Which application methods they applied?
- What was the reason for application? (Pest, Disease, etc.)

Panel data is freely available to purchase and the data is typically licensed to the purchaser for a specific use case. In each crop cultivation season, the purchasers of panel data decide if and to which extent interview panel data need to be collected depending on the commercial relevance of a market. This means that the comprehensiveness and frequency of data collection is higher in relatively big and commercially relevant markets such as the US-corn market (typically panel data are collected once per year). In other markets with a lower commercial relevance, the frequency of panel data collection can be lower and irregular (e.g. only every 2-3 years in the Belgium-potato market). Once market research companies such as Kynetec have collected the farmer interview panel data, these data are automatically moved to the company Lexagri which compiles and harmonizes these panel data about the use of crop protection products and seeds in their Agrowin database. That means Lexagri does not conduct interview panels itself, but only compiles and harmonizes the data from the original sources (e.g., Kynetec panel data) to Agrowin.

Panels are not conducted in every country for many reasons such as low commercial relevance in the market. BCS does not buy all available panel data for cost reasons. Countries where panel data are used in Agrowin are shown in Figure 4. Non-panel data are based on different sources such as industry sales

statistics published by governments, sales statistics made available from market research companies or in some countries BCS's own assumptions. Non-panel data is typically made available as sales data which is then translated to consumption data.



Own internal estimates

Figure 4: Agrowin country-specific data sources overview (2016 status)

Data quality and data quality assurance of Agrowin

Panel data are BCS preferred option to use in the Agrowin database, however panels use different methodologies (e.g. for sampling) and approaches (e.g. mathematical approaches to project sample data to overall market). Therefore, the quality of the panel data still needs to be continuously verified for each data set as BCS strives for quality accuracy of 95 %.

The quality accuracy of 95% relates to the stratification of the interview sampling. The number of interviews and the distribution throughout the country is very important for the quality of the study. When defining the stratification method, different criteria such as soil, climate, farmer age, farmer education, etc. need to be considered. In general, stratified sampling is a method of sampling from a population which can be partitioned into subpopulations. In statistical surveys, when subpopulations within an overall population vary, it could be advantageous to sample each subpopulation (stratum) independently. Stratification is the process of dividing members of the population. That is, it should be collectively exhaustive and mutually exclusive. Every element in the population must be assigned to one and only one stratum. The objective is to improve the accuracy of the sample by reducing sampling error. Stratification gives a smaller error in estimation and greater accuracy than the simple random sampling method.

BCS has defined Quality Standards for Panel Providers with more than 30 criteria to ensure the panel data quality (see Appendix II). For example, criteria like age and educational level of the farmer, climate and spatial distribution of soil type within a country are used to ensure a representative selection and

distribution of farmers in the sample of interview participants. BCS acknowledges that data quality also depends on the education, training, and experience of the interviewers.

Once data are collected, incorporated and harmonized in Agrowin, through excel files which include multiple cross-checks, data is confirmed by country planners with the help of a check file to review. This is an important step, as the system reflects the countries' official view on their respective market. Despite those precautions, non-panel data quality depends strongly on internal education level and expertise of the country planner and Business Intelligence manager as they decide on method for data collection. Data then often needs to be transferred from sales information to consumption data. BCS is also aware that inputs from excel files have potential for human errors. However, internal data checks and corrections are mainly related to prices or product allocation to reflect the correct distributer to a given Product. The Product usage itself (including dose rates and other usage attributes) is usually not changed from the original source.

Data quality assurance of Agrowin

Panel data quality is assured by selecting representative farmers as interview participants. A representative selection and distribution of farmers in a panel is mainly based on the following criteria: Age of the farmer, educational level of the farmer, and spatial distribution of soil types cultivated within a country. For example: a panel on the German-Wheat market is based on approximately 3000 interviews. Data quality also depends on the education, training, and experience of the interviewers, for example: interviewers need to adequately utilize showcards in interviews to ensure that farmers with a low education level understand interview questions.

Data limitations of non-panel data and how they are addressed

The frequency and comprehensiveness of the purchased interview panel data varies with regards to crops covered. In big and commercially relevant markets, Bayer (together with other data purchasers) typically buys panel data on a yearly basis. In markets with a lower commercial relevance, the frequency of panel data collection can be lower and irregular (e.g. only every 2-3 years in the Belgium-potato market). As of 2020, BCS plans to purchase all available panel data globally on an annual basis.

However, the purchasers might even decide to not purchase a panel study on a certain market at all because the commercial relevance of that market is too low. For countries and markets where no panel data are available, data gaps are filled by using national statistics (e.g., import and export data). If there are no national statistics, dedicated Bayer market analysis and business intelligence colleagues fill the data gaps based on their expert knowledge of the respective markets (e.g., based on sales information).

Furthermore, potential Agrowin data gaps can be filled by using market growth rates from the Bayer forecasting tool 'Optimas'⁶ (including e.g., planted acreage, area treated and value per hectare). These

⁶ OPTIMAS is used for short-term and long-term market planning): Short term planning in OPTIMAS is an annual process with quarterly updates. It provides a market overview by fiscal year and reflects the crop protection (CP) and seeds & traits (S&T) market value at (net) ex-manufacturer level for the previous year, running year as well as a 3-year forecast. The data for row crops is derived from the "driver tree logic" including planted acreage, area treated and value per hectare. Furthermore, country planners are asked to lay down key driver assumptions (qualitative descriptions). The accountability for short term market data lies in the countries/regions. This means that dedicated business intelligence (BI) colleagues in the countries

future-oriented growth rates are then back-casted to fill gaps in the past-oriented Agrowin panel data. As an additional verification, these backwards extrapolations are shown to the dedicated market analysis and business intelligence colleagues for the respective countries and markets to validate and confirm (or disapprove) these proxy data for Agrowin.

Overall, the hierarchy of data is based on 1) using panel data, 2) using national statistics, 3) using expert market knowledge of dedicated market analysis and business intelligence colleagues, 4) backwards extrapolation of future oriented market growth data from Optimas as proxy data for Agrowin. As mentioned above, as of 2021 BCS plans to primarily rely on panel data globally, being the most reliable and representative market information available.

3.3. Impact assessment based on active ingredients emissions and freshwater ecotoxicity impact calculation

3.4. Emission modelling with PestLCI

To estimate emission fractions for CPPs applied to agricultural fields for each application scenario, PestLCI Consensus version 1.0 was used as implemented in the web-based tool⁷. This tool builds on a mass-balance model developed initially by Birkved and Hauschild (PestLCI - A model for estimating field emissions of pesticides in agricultural LCA, 2006) and further advanced by Dijkman et al. (2012) and by Gentil (2020) and Gentil et al. (2021).

PestLCI Consensus provides 'primary emission distribution fractions' (i.e., active ingredient mass reaching the environment as emissions within minutes after application, following primary partitioning) for compartments air, field crop surface, field soil surface, and off-field surfaces. Primary emission fractions are mainly influenced by growth stage and morphology of treated field crops defining the fraction of applied mass that is intercepted by crop surfaces, and by the drift deposition function for a given crop protection product application method defining the fraction reaching off-field surfaces. Primary emission fractions have been applied for each application scenario and can then be transferred into the USEtox® model. The primary

are entering the data, which needs to be aligned with the regional Business Intelligence function and approved by the local management. The long-term planning process in OPTIMAS is an annual process, which each year starts directly after the budget planning and ends around mid of February. The 3-year short term CP and S&T market planning of the countries always forms the basis for the long-term planning process. Long-term market planning covers a time period of 20 years and is generated (from year 4 onwards) by the Crop Strategy & Portfolio Management (CSPM) Teams from the global Crop Science headquarter in Monheim, Germany. As a pre-step, the 20-year area planning for row crops needs to be reviewed and corrected by the country Business Intelligence planners in selected key markets over July and August.

⁷ Available at <u>https://pestlciweb.man.dtu.dk</u>

distribution processes considered in PestLCI Consensus are presented in Figure 5, and are further detailed in Dijkman et al. (2012) and Gentil (2020) and Gentil et al. (2021).

PestLCI Consensus furthermore provides 'secondary emission fractions' (i.e. pesticide mass reaching the environment within a given timeframe, typically 1 day) for compartments air, field crop surface, field crop leaf uptake, field soil, groundwater below field, and off-field surfaces, also considering degradation in field crop and soil. Secondary emission fractions are likewise a function of crop characteristics and application method, but depend on additional aspects, such as climate and field characteristics, application month, and active ingredient physicochemical properties. Secondary distribution was excluded from the environmental impact assessment because the level of detail required to model secondary distribution processes are not readily available in the present screening-level assessment, which would introduce large additional uncertainties related to collecting and defining e.g., field-level characteristics at the global scale. BCS is considering including secondary distribution in future EIR reports.



Figure 5: PestLCI Consensus primary emission distribution processes and compartments for the example of aerial application of pesticides, which first enter the "air" compartment and from there further distribute to other compartments.

When using the PestLCI model, the following main assumptions were established: Only primary emission distribution was calculated for the present study as all long-term processes are already covered in USEtox[®] and because currently, the uncertainty related to some of the processes included in the secondary distributions are higher than the rather small additional accuracy gained for a low-tier screening assessment. Initial distributions cover initial processes within a few minutes after crop protection product application. Four relevant compartments for initial primary distribution are described below:

• Field soil surface: initial primary distribution on soil is the fraction of crop protection product deposited on soil when applying the crop protection product. The fraction deposited on soil is

calculated as the remainder of all CPPs involved in the initial (primary) distribution: i.e. it is the remaining fraction of crop protection product that is (a) not volatilized during application, (b) not deposited off-field due to wind drift, and (c) not intercepted by the leaves in the selected growth stage of the crop.

- Air: initial primary distribution to air consists of the fraction remaining airborne during crop
 protection product application. This fraction is a fixed value, depending on the primary drift of the
 application method and the drift reduction.
- Field crop leaf surfaces: Initial fraction to field crop leaf surface is the fraction of crop protection product deposited on crop leaf when applying the crop protection product.
- Off-field surfaces: Initial fraction to off-field surfaces are emissions to off-field agricultural soil, natural soil or surface water that arise as a consequence of wind drift deposition during crop protection product application.

Primary emission fractions are derived based on distributing applied pesticide mass according to mass balance principles. As a starting point, within few minutes after pesticide application, a mass fraction of pesticides is deposited to off-field surfaces (f_{dep}). It is derived from drift deposition functions specific to each application method. Drift deposition functions were collected for various crop-application method combinations and implemented into PestLCI (see Gentil-Sergent et al. (2021)). Another mass fraction goes to the air by wind drift (f_{air}) as a default fraction per application method and crop, and the remaining mass fraction reaches the field surface via direct deposition (f_{field}), which is typically the intended target area for applied pesticides. With that, the governing emission equations reads according to Gentil-Sergent et al. (2021):

 $1 = f_{field} + f_{air} + f_{dep}$

Equation 1

The fraction reaching the field surface area (f_{field}) is partially deposited on crop leaves ($f_{\text{field}\rightarrow\text{crop}}$) according to crop intercepted mass fraction $f_{\text{intercept,crop}}$ and calculated as:

 $f_{\text{field} \rightarrow \text{crop}} = f_{\text{field}} \times f_{\text{intercept, crop}}$

Equation 2

Then, the fraction left on the field after crop interception ($f_{\text{field}\rightarrow\text{soil}}$) will reach field soil surfaces and is calculated as:

 $f_{\text{field} \rightarrow \text{soil}} = f_{\text{field}} \times (1 - f_{\text{intercept, crop}})$

Equation 3

3.5. PestLCI input data

To run the PestLCI Consensus model, some input data are mandatory, and some are optional. For the primary emissions, the mandatory data are crop type, applied pesticide fraction intercepted by field crop surfaces, and application method. The optional input data are drift reduction methods during application, presence (or not) of a buffer zone, width of the buffer zone and field width perpendicular to the wind direction. The following model inputs have been used in this study relevant for primary emissions: Crop type

derived from associating reported crop to PestLCI crop type (indirect influence; in particular, it influences the available options for the next two parameters)

- Fraction of applied pesticide intercepted by field crop surface area, derived from reported BBCH range
- Application methods

Due to the lack of data the following model inputs relevant for primary emissions have not been used in this study:

- Buffer zone (in the present screening-level assessment, buffer zones were not considered)
- Drift reduction methods have only been used in a limited number of application scenarios where information on the applied drift reduction method has been available. If no such information was available in the AgroWin data set, no assumption has been made.

Other model inputs, such as crop protection product characteristics relevant for secondary emissions, climate, month of applications and soil, have no influence in the calculation of primary emissions, and are hence not relevant for application scenarios. The listed main model inputs influencing primary emissions are described in the following.

Crop types in PestLCI

3.5.1. Crop types in PestLCI

There are sixteen representative crop classes available in the PestLCI Consensus model that were selected from more than 172 crops based on the FAO and Central Product Classification (CPC) Version 2.1. The crop type Agrowin data that BCS provided to DTU were assigned by DTU to one of these 16 available crop classes, which are listed in Table 4. For example, the Pooideae crop class are subfamily of the grass family Poaceae which in turn includes cereals such as wheat, barley, oat, rye and pasture grasses. Panicoideae is also a subfamily of the grasses, and it comprises agricultural crops such as sugarcane, maize (or corn), and sorghum. The selected crop type in PestLCI will define the range of available application methods and with that will influence the selection of the available off-field drift deposition functions that are relevant.

Table 4: Crop classes implemented in the PestLCI Consensus model

ID	Crop class	ID	Crop class
1	Pooideae	9	Fruits tropical
2	Panicoideae	10	Fruits temperate
3	Paddy rice	11	Citrus fruits
4	Pulses	12	Grapes/vines
5	Roots, tubers and bulbs	13	Berries

6	Oil-bearing crops	14	Nuts
7	Vegetables leafy	15	Oil-bearing trees
8	Vegetables fruit	16	Other permanent crops

3.5.2. Fractions of applied pesticide intercepted by crop surface area in PestLCI

In the following section, different underlying cases for deriving fractions intercepted by crop surfaces from crop growth stages are described, along with the various challenges for the different cases, including difficulties to allocate specific crops to crop classes for which interception fractions are available.

For application scenario calculations, foliar interception fractions were assigned to the different crop growth stage (i.e. "BBCH") ranges and then applied to each related scenario. For that, BCS crops were mapped to crops from Linders et al. (2000), where crop and growth phase-specific (BBCH) interception fractions have been proposed for different crops/crop classes using the growth stages with BBCH-scale (Meier, 2018). Where a direct match was possible, BCS crops were mapped to their respective crop or crop family (e.g. Apple was directly linked to 'Pomme Fruit' or Apricots to 'Stone fruit').

When this was not possible, the crop with the closest looking leaves and maximum soil coverage from Linders et al. (2000) was chosen as a proxy. For instance, Amaranth was approximated with cereals and burdock root with sugar beets. If neither a direct link nor an approximation was possible, assigning an interception fraction was done based on the BBCH alone. Here, for each BBCH indicated, the smallest interception fraction of all crops/crop classes in Linders et al. (2000) that corresponds to this BBCH was assumed. For example, the BCS crop 'Agave' remained unclassified into any given crop class and was associated with a crop growth stage (BBCH) of 10 at the time of crop protection product application. There is a total of 27 crops in Linders et al. (2000) (e.g. Bulbs I, Beans I, Carrots I) which have a BBCH code of 10. The smallest related interception fraction is 0.1 for Onions I, indicating a very early crop stage for these crops that leads to only a small fraction intercepted by the crops. This interception fraction was used for Agave at a BBCH of 10 and any other BCS crop that remained unclassified and had an entry (application scenario) associated with a BBCH of 10. The main BBCH codes (not a linear numerical scale but numeric codes between '00' and '99' assigned to different crop life cycle stages) are described in Meier (2018). Crop interception fractions, instead, range from 0 (no crop interception) to 1 (100% crop interception) as described in Linders et al. (2000).

After BCS crops had been mapped to the respective crop/crop class, the reported BBCH at time of crop protection product application was compared with the BBCH ranges for a given crop/crop class from Linders et al. (2000) to extract the related interception fraction. For example, the BCS crop 'Barley-spring' had one application scenario associated with a BBCH of 70 (A7090H-POST-FLOWERING-AUT-CER). For the crop class 'Cereals' a BBCH of 70 means booting/senescence (BBCH range 40-99) and corresponds to an interception fraction of 0.9 (Linders, Mensink, Stephenson, Wauchope, & Racke, 2000). If BCS's (or the farmer's) reported BBCH for any given crop exceeded the largest BBCH value available for the corresponding crop/crop class, the maximum available interception fraction for that crop/ crop class was taken.

Finally, if the reported BBCH did not fall into any of the BCCH ranges indicated for a given crop/crop class, the closest lower BBCH range was taken as reference point. For example, Broccoli is sprayed at a BBCH of 21 (crop growth stage: S2129-SIDE-SHOTS-SPR-LEG). The related crop 'Cabbage' has interception fraction values indicated for the BBCH ranges 10-19 and 40-49. The closest lower BBCH range to 21 is thus 10-19 with an interception fraction of 0.25.

Two additional assumptions were made in the derivation of the fraction intercepted for different crops and application scenarios. Any BCS crop allocated to "bare-soil" (e.g. NON-CROP-LAND) was assigned an interception fraction value of zero as no crop coverage is assumed in these scenarios. Finally, whenever the crop growth stage was indicated by BCS to be '9900H-POSTHARVEST', we assumed the pesticide to be no longer applied on the field. In this case, no BBCH or interception fraction was assigned to the respective crop and application scenario; hence, these scenarios have been excluded from the analysis that is restricted to scenarios implying emissions from pesticide applications to agricultural fields.

3.5.3. Application methods in PestLCI

From the 31 application methods available in the PestLCI Consensus, 12 representative application methods were selected and manually associated with the data provided by BCS. These representative application methods are listed in Table 5. For each application method, DTU used a fixed value for primary emission fractions to air⁸.

Table 5: Crop protection product application methods and primary emission fraction to air as available inPestLCI

ID	Application method	Primary emission to air (%)
5	Boom sprayer - conventional nozzle – other crops	10
6	Boom sprayer - conventional nozzle - roots/tubers	10
13	Air blast sprayer - early stages (leafless)	20
14	Air blast sprayer - late stages (in leaf)	8
17	Air blast sprayer - grapes/vines	12.5
18	Air blast sprayer - other crops	10
19	Hand operated sprayer - crops that are < 50 cm	6
20	Hand operated sprayer - crops that are > 50 cm	10
22	Aerial application (N/A, EPPO)	25
23	Soil incorporation (N/A, N/A)	0
24	Recycling tunnel - Air induction Flat spray nozzles	1.25*
28	Air-assisted sprayer side by side - flat fan nozzles	7.5*

*Emission reduction included

⁸ An overview is also given at https://pestlciweb.man.dtu.dk/images/Application_Method_CropV3.png.

3.5.4. Drift reduction in PestLCI

Additional drift reduction was not included in application scenario calculations. This means that drift reduction was only taken into account if already included in the application method (indicated with '*' in Table 5) as reported by AgroWin[®] data.

3.5.5. Consideration of buffer zone in PestLCI

No buffer zone was assumed for the current calculations of primary emissions due to lack of data in AgroWin[®]. A buffer zone is the distance between the point of direct pesticide application and the nearest downwind boundary of a sensitive habitat. In pesticide application, it is required to maintain a distance between the site of spray application and environmentally sensitive areas. The current calculations, with regards to the effect of possible mitigation measures on emissions into different environmental compartments, therefore, represent a worst case.

3.6. Linking PestLCI with USEtox®: Emission compartment allocation

Emission results from PestLCI Consensus are associated with specific environmental compartments. These compartments, priori, do not match the emission compartments in the impact assessment model USEtox[®]. Hence, the different compartments in both models were assigned in a way to allow combining both emission results and ecotoxicity impact results. Figure 6 illustrates how application scenario emission compartments from the primary emission distribution in PestLCI Consensus are matched to the emission compartments of USEtox[®] (boxes relevant for application scenario are the initial distribution fractions within PestLCI Consensus (upper left) and USEtox[®] (right).



Figure 6: Coupling of different state-of-the-art models for assessing emissions and toxicity related impacts in LCIA

When doing the compartment allocation from PestLCI to USEtox[®], the following main assumptions were established:

3.6.1. Segmentation/mapping of related emissions

Air emissions were assigned to continental rural air in USEtox[®], field soil emissions were assigned to continental agricultural soil in USEtox[®], and field crop surface emissions were not assigned to any emission compartment in USEtox[®]. The latter introduces the assumption that these emissions do not contribute to ecotoxicity impacts, which will, however, be negligible, since only marginal parts of what reaches field crops might in some cases volatilize back into air, while another part could reach the soil via e.g. wash-off or flow through the crop compartments. However, the largest fraction by far either ends up inside the crop as residues or degrades. Introducing these aspects presents an additional complexity which are not relevant for a screening-level assessment (Fantke, Charles, de Alencastro, Friedrich , & Jolliet, 2011).

3.6.2. Off-field surface emission fractions

Finally, emission fractions reaching off-field surface areas were distributed according to the percentages of surface areas represented by freshwater, agricultural soil, and natural soil for continental level parameterizations in USEtox[®] (for each considered scenario; via country-continent associations; from Kounina et al. (2014). The off-field surface area fractions (percentages) for the different continental parameterizations are shown in Table 6 below.

Continent	Freshwater	Natural soil	Agricultural soil
North America	3.44%	86.56%	10%
Latin America	1.76%	88.24%	10%
Europe	1.57%	88.43%	10%
Africa + Middle East	1.97%	88.03%	10%
Central Asia	1.66%	88.34%	10%
Southeast Asia	4.09%	85.91%	10%

Table 6: Percentages of surface areas represented by freshwater, agricultural soil, and natural soil for continental level parameterizations in USEtox[®].⁹

⁹ These fractions are based on consistently parameterized fate parameters in USEtox (Kounina, Margni, Shaked, & Bulle, 2014) and are only relevant for the marginal emission fraction that reaches off-field areas. Since characterization factors for both agricultural and natural soil are in almost all cases virtually the same, this approximation is appropriate for a screening-level approach and consistent with USEtox.

Northern regions	4.93%	85.07%	10%
Oceania	1.03%	88.97%	10%

While the area of most countries falls 100% within a single parameterized continent, some countries are distributed over more than one continental region. For these cases, allocation is based on population distribution taking as reference the continent with higher within-country population share, and climate distribution taking as reference the continent with higher suitability for within-country share used for agriculture (e.g. Russian Federation's Tundra region denoted part of region W12 in USEtox[®] is less suitable than other regions for agricultural production, and Russian Federation's Taiga and temperate regions denoted W1 in USEtox[®] have been used to represent the entire Russian Federation). USEtox[®] continental regions (incl. W12 and W1) along with the parameterization of continents including influence of climate, water versus land surface distribution and other aspects are fully detailed in Kounina et al. (2014).

3.7. Ecotoxicity impact modelling with USEtox®

The overall scope of the assessment is limited to freshwater ecotoxicity impacts, which was considered the only scientifically mature indicator at the time of USEtox® release in 2008 (Rosenbaum, Bachmann, Gold, & Huijbregts, 2008)¹⁰. In a current global guidance effort under UN Environment, this recommendation has been revisited, and additional indicators (i.e., soil terrestrial ecotoxicity) are currently being evaluated for possible inclusion into a future update of USEtox® (Fantke, et al., 2018a). Since its release, USEtox® has been widely used by LCA practitioners. The European Commission recommends it as a reference model to characterize human toxicity and freshwater aquatic ecotoxicity impacts from life cycle chemical emissions for the International Reference Life Cycle Data System Handbook and the Product Environmental Footprint context (Saouter, et al., 2020). Despite the consensus on USEtox®, stakeholders still debate appropriate methods for characterizing ecotoxicity in life cycle impact assessment (LCIA). Since the release of USEtox® in 2008, practitioners and stakeholders have requested an extension of ecotoxicity characterization beyond freshwater environments. Several efforts have explored the possibility of including other compartments and have resulted in emerging models supporting the assessment of fate, exposure, and ecotoxicological effects for marine, terrestrial, pollinators, and birds' toxicity. Despite the clear recommendations to continue with efforts of integrating these topics (and other topics such as adding characterization factors for metal/inorganic/biological/natural active substances; adding groundwater, sediment and plant compartments) into LCIA, the respective models and their underlying data are yet to become mature enough for inclusion into LCIA (Crenna, Sala, Polce, & Collina, 2017; Fantke, et al., 2018a; Gentil, Fantke, Mottes, & Basset-Mens, 2019).

Therefore, for this report, only freshwater ecotoxicity impacts have been considered since this is the best understood biosphere and a major share of emissions will end up in freshwater (Henderson, et al., 2011). A

¹⁰ Further developments of those models are in progress, in order to extend to other environmental compartments, but are not yet finished nor have reached any consensus at the date of production of the present report.

full description of the environmental mechanism for freshwater ecotoxicity impacts is provided in Henderson et al. (2011). BCS plans to enlarge the scope by integrating the impacts on terrestrial organisms like earthworms or pollinators in the near future, when the models are mature enough.

To estimate ecotoxicity impacts per unit emission into a given environmental compartment for pesticides applied to agricultural fields, the USEtox[®] model version 2.12 was used as available at <u>https://usetox.org/</u>. This tool is a global scientific consensus model (Hauschild M., et al., 2008; Rosenbaum, Bachmann, Gold, & Huijbregts, 2008) developed under the auspices of and formally endorsed by the UNEP-SETAC Life Cycle Initiative (Westh, et al., 2015). USEtox[®] calculates characterization factors for freshwater ecotoxicity by combining a multimedia box model and an impact assessment model:

"Assessing ecotoxicological effects of a chemical emitted into the environment implies the analysis of a cause-effect chain that links chemical emissions to impacts on freshwater ecosystems through four assessment steps: environmental fate, (freshwater ecosystem) exposure, (freshwater ecotoxicological) effects, and damages on ecosystem quality" (Fantke, et al., 2017a).

"USEtox[®] follows the whole impact pathway from a chemical emission to the final impact on humans and ecosystems. This includes modelling the environmental distribution and fate, human and ecosystem population exposure, and toxicity-related effects associated with the exposure." (Fantke, et al., 2017a). For ecotoxicity impacts, USEtox[®] currently only includes freshwater ecosystems, since data and processes are available and best understood for freshwater ecosystems as compared to e.g. marine and terrestrial soil ecosystems in an LCIA context, of which the latter are currently difficult to characterize (see e.g. Hendersen et al. (2011)).

Combining fate, exposure and effects yields characterization factors (CFs) for ecotoxicity. These freshwater ecotoxicity characterization factors are expressed in "Potentially Affected Fraction" (PAF) of freshwater species, integrated over exposure water volume and chemical residence time in water per unit mass emitted. These characterization factors provide information on the sensitivity of different tested species to different concentration levels of the dissolved substance in freshwater (ecotoxicity effect). For example, most species start being affected within a specific range of the concentration level, whereas the most sensitive species are affected at lower level of concentration. These combined effect concentrations are used to express the potential impact on the overall exposed ecosystem.

These CFs serve as characterization results at the midpoint global level in LCA. They can be combined with a damage factor translating ecotoxicity impacts into damages on ecosystem quality, to arrive at a damage (endpoint) level in LCA. However, damage factors are not applied in the present study, which only provides results at midpoint level in line with the goal and scope of the present assessment. This report only focuses on the characterization factor for aquatic ecotoxicity impacts at midpoint level providing an estimate of the potentially affected fraction of species (PAF). This report does not cover the CF at endpoint level which would be associated with the potentially disappeared fraction of species (PDF) integrated over time and volume per unit mass of a chemical emitted. Further details about the general LCA midpoint-damage characterization framework are given in Hauschild and Huijbregts (2015). Uncertainty in all steps is explicitly taken into account in USEtox[®], allowing for a comparative assessment of the environmental impacts of chemicals to provide insights on "best in class" products in product comparisons regarding the environmental performance of products in terms of ecotoxicity related to chemical emissions.

The main steps in characterizing the impact pathway for freshwater ecotoxicity in USEtox[®] 2.x are illustrated in Figure 7, with further details provided elsewhere (Rosenbaum, Bachmann, Gold, & Huijbregts, 2008; Henderson, et al., 2011; Fantke, et al., 2018b).


Figure 7: Impact pathway for freshwater ecotoxicity impacts in USEtox[®] 2.x (Fantke, et al., 2018b)

The freshwater ecotoxicity characterization factor, CF [PAF m³ d/kg emitted], representing the potentially affected fraction (PAF) of species integrated over the considered freshwater compartment volume and time per kg of chemical emitted to an environmental compartment, is derived as follows:

 $CF = FF \times XF \times EF$

Equation 4

where FF [kg in freshwater/(kg emitted/d)] is the fate factor relating the chemical mass in the freshwater compartment to the chemical mass emitted per day into the same or another environmental compartment, XF [kg bioavailable/kg in freshwater] is the ecosystem exposure factor representing the bioavailability of chemicals to organisms in the freshwater compartments considered for ecotoxicity, EF [PAF m³ freshwater/kg bioavailable] is the ecotoxicity effect factor relating the potential of the bioavailable fraction of a chemical to cause toxic effects to an exposed ecosystem expressed as potentially affected fraction of species in the exposed ecosystem integrated over the considered freshwater volume to the bioavailable chemical mass in freshwater. When the emission compartment is different from the compartment of the exposed ecosystem, the fate factor is interpreted as product of the residence time of a chemical in the receiving exposure compartment, FFi2 [day], and the overall time-integrated chemical mass fraction transferred from the emission compartment i_1 to the exposure compartment i_2 , $f_{i_2 \leftarrow i_1}$ [kg in compartment/kg emitted], i.e. $FF = f_{i2 \leftarrow i1} \times FFi_2$. For better interpretation, the CF unit can be understood as an equivalent water volume with a potentially affected fraction of freshwater species of 100% over one day. Describing the full units of all factors is important to understand these factors. More specifically, fate factor units can only be reduced to "day" where emission and receiving compartment are the same, whereas for cases where emission and receiving compartment are not the same, fate factors denote mass received for a given emission rate. Exposure factors are dimensionless but refer effectively to a chemical mass fraction. Finally, effect factors are interpreted as inverse of a chemical water concentration leading to a certain fraction of species that shows a potential effect. Further details are found elsewhere (Rosenbaum, Bachmann, Gold, & Huijbregts, 2008; Henderson, et al., 2011; Fantke, et al., 2017a).

One of the main assumptions in USEtox® is that solutions are provided for steady-state conditions for environmental fate processes, which assumes constant, continuous emission inputs into the different environmental compartments. This assumption, however, is mostly relevant for industrial chemicals emitted continuously over time, where emission pattern might vary e.g. with season. For pesticides, this assumption is not relevant as fate factors in this case are interpreted as time-integrated mass due to a given pesticide amount applied at a given point in time (see Rosenbaum et al. (2007)). With that, this assumption does not influence the accuracy of results for pesticides applied to agricultural fields. Another assumption is that all environmental compartments are homogeneously mixed, assuming that regardless of where within the same continent an emission occurs, it will yield the same ecotoxicity impact magnitude and compartmental distribution. Emissions to different continental regions will however be different as a function of differences in compartment properties (e.g. volume). This assumption is in line with box model principles that are commonly applied in screening level assessment within and outside LCA (MacLeod, Scheringer, McKone, & Hungerbuhler, 2010). With that, the nested compartment model USEtox[®] is most applicable to situations where emission locations are unknown, to estimate the relative magnitude of toxicity potency across various chemicals and emission scenarios, as compared to estimating local and absolute risks, for which more sophisticated and localized models have to be applied. In the context of BCS' application scenarios, it is mainly applicable to screen many scenarios for dominating combinations of crop, country and active ingredient, as well as of active ingredient within a given crop-country combination.

3.7.1. USEtox® input data

The most important inputs that drive ecotoxicity characterization results are physicochemical substance data. An overview of required inputs in USEtox[®] are provided in Table 7.

Parameter	Unit	Subst	ances
		Organics	Metals
Chemical abstract service registry number CAS RN		х	Х
Chemical common name		Х	Х
Molar weight MW	g/mol	Х	Х
pKa chemical class		Х	
pKa base reaction pKa.gain		х	
pKa acid reaction pKa.loss		Х	
Partitioning coefficient between n-octanol and water Kow	1/1	х	
Partitioning coefficient between organic carbon and water Koc	l/kg	х	

Table 7: Chemical input data in USEtox[®] for organic substances or metal ions that are relevant for application scenario calculations

Henry's law constant (at 25°C) Кн	Pa∙m³/mol	Х	
Vapor pressure (at 25°C) Pvap	Ра	х	х
Solubility (at 25°C) Sol	mg/l	х	
Partitioning coefficient between dissolved organic carbon and water Kdoc	l/kg		х
Partitioning coefficient between suspended solids and water Kpss	l/kg		х
Partitioning coefficient between sediment particles and water Kp _{sd}	l/kg		х
Partitioning coefficient between soil particles and water Kpsi	l/kg		х
Degradation half-life in air to derive degradation rate constant HLair	d	х	
Degradation half-life in water to derive degradation rate constant HLwater	d	х	
Degradation half-life in sediment to derive degradation rate constant HLsediment	d	х	
Degradation half-life in soil to derive degradation rate constant HLsoil	d	х	
Dissipation half-life in above-ground plant tissues to derive dissipation rate constant HLplant	d	х	
Bioaccumulation factor in plant roots BAFroot	kgveg/kgsoil	х	х
Bioaccumulation factor in plant leaves BAFleaf	kgveg/kgsoil	х	х
Bioaccumulation factor in fish BAFfish	l/kgfish	х	х
Species-specific EC50 (effect concentrations at which 50% of individuals for a single species show an effect) combined to derive hazard concentration HC50 as the concentration at which 50% of the exposed species exceed their EC50. HC50 itself is never reported in underlying databases, but instead calculated from the various available EC50 data across species per chemical.	Mg/l	X	х

The substance data describe the physical-chemical characteristics, degradation rates, toxicity, ecotoxicity, bioaccumulation factors and biotransfer factors of a substance. The bioaccumulation, biotransfer and ecotoxicity are three different substance data that are used to understand the behavior of a chemical in relation to biological organisms. Biotransfer is the process by which a chemical substance is absorbed from

one organism by another mostly through ingestion. The biotransfer factors from USEtox[®] into meat and milk are not relevant for freshwater ecotoxicity impact pathway of USEtox[®] and have thus not been considered. Bioaccumulation is the overtime accumulation of a chemical in an organism (e.g., Fish) while ecotoxicity is the potential adverse effects that a chemical substance causes to an aquatic organism.

The degradation rate constants are used to determine the environmental fate of the substance or active ingredient. Majorly this consists of the substance transformation processes which includes substance degradation in air, water, sediments, and soil. The Partition coefficient is used to describe how a chemical solute is distributed between two immiscible solvents. They are used as a measure of a solute's hydrophobicity and a proxy for its membrane permeability. Hydrophobicity is the physical property of a molecule that is seemingly repelled from a mass of water (known as a hydrophobic). Partition coefficients (sometimes referred to as partition ratios) are widely used in environmental science to relate the concentration of a chemical solute in one phase to that in a second phase between which equilibrium applies or is approached. The solutes include organic and inorganic substances and the phases of interest include air, water, soils, sediments, and aerosols.

Ecotoxicity test results are reported as Effect Concentrations ECx, where the effect may be mortality, immobilization, reproduction or other endpoints and 'x' refers to the fraction of the tested organisms or organism groups showing the effect. EC50 results are determined from statistical evaluation of the concentration-effect values in experiments. The middle of the derived concentration effect curve is considered to be more robust than lower ends. Therefore, EC50 values are used for determination of the ecotoxicological effect factor to minimize uncertainties in the effect factor.

After the EC50 test results from different species are collated, the distribution of the test results for the chemical (or active ingredient) across different test organisms is shown in the Species Sensitivity Distribution (SSD) curve (Postshuma, Suter II, & Traas, 2002). An SSD of chronic EC50s depicts the fraction of species in the ecosystem which are affected above their chronic EC50 value as a function of the bioavailable concentration (X) of the chemical. The SSD-midpoint has been named the HC50, which is the Hazardous Concentration for 50% of the species. This USEtox® HC50-value of the chemical indicates the concentration corresponding to 50% of the species being exposed above their EC50 value. In a series of chemicals, it holds that the lower the HC50-value of a chemical, the higher the relative ecotoxicity of a compound. This principle is the basis for quantifying expected aquatic ecosystem impacts in USEtox®.

A selection is made from the available toxicity data, which may represent acute or chronic exposures. To reveal the possible chronic effects of a substance on the ecosystem, preference is given to results from chronic or sub-chronic tests at the EC50-level in the LCIA step (Jolliet, et al., 2006; Larsen & Hauschild, 2007). The motives for this are, amongst others, the statistical robustness of deriving the 50%-response level, and – not the least – the ecological interpretation of the EC50-endpoint in terms of impacts that are meaningful and can be observed in field-exposed ecosystems. Chronic EC50 exposure data were given priority. However, when chronic data is not available, acute EC50-data are used to derive the chronic-equivalent EC50 per species by dividing by an acute-to-chronic ratio (ACR) (Rosenbaum, Bachmann, Gold, & Huijbregts, 2008).

Among the listed substance parameters, degradation rate constants, ecotoxicity effect data, and partitioning coefficients (mainly Kaw, and Kow via its influence on Koc) are the factors that are most influential on variability of characterization results across substances. Based on the available information for each parameter, different sources have been used to derive a value for each parameter per substance in order to calculate characterization results.

The different sources have been used in the following hierarchy:

• First priority – USEtox[®]: Whenever data were available for a given substance in the official USEtox[®] substances databases (Rosenbaum, Bachmann, Gold, & Huijbregts, 2008) this source was used.

- Second priority Solutions: For ecotoxicity effect information only, results from the Solutions project (Posthuma, van Gils, van de Meent, & de Zwart, 2019) were applied whenever USEtox[®] data were not available.
- Third priority PPDB: Whenever USEtox[®] data were not available for any given substance parameter nor data from the Solutions project for effect information, data from the Pesticide Property Database (Footprint, 2020) have been applied.
- Fourth priority CompTox: Whenever no other source provided data for a given parameter, substance data from the U.S. Environmental Protection Agency's CompTox Chemistry Dashboard database (Williams, et al., 2017) were applied, based on the OPERA prediction models suite (Mansouri, Williams, Grulke, & Judson, 2018).

Based on the available substance property data and based on the general applicability of USEtox[®] to characterize organic substances and metal ions, a total of 892 substances could be characterized. Among these, there are 801 organic substances, 47 additional organic compounds that contain a metal ion, but are treated as organic substances, and 39 metal-based compounds that were treated based on their containing metal ions. And 5 organometals that were treated based on their containing metal ions. And 5 organic compounds containing a metal ion could not be characterized due to missing relevant substance data. All other substances that were not characterized in USEtox[®] belong to chemical groups for which USEtox[®] is not applicable, including biological agents, complex mixtures, inorganic compounds (other than metal ions), and metal-based compounds for which the relevant metal ion is not included in USEtox[®]. Since results of both organic and metal-based substances are expressed in the same metrics, they can be aggregated and discussed together. However, when aggregated results of these two substance groups are predominated by one of the substance groups, results can also be discussed separately.

An overview of the substances included and excluded from USEtox[®] calculations for application scenarios are provided in Figure 8.



Figure 8: Distribution of substances provided for calculation of the application scenario in USEtox® results

The 'not characterized' compounds are substances for which minimum input data requirements could not be fulfilled after considering all the four substance property data input sources (i.e. USEtox[®], Solutions, PPDB, and CompTox database) or substances which currently cannot be characterized by USEtox[®]

3.8. From application scenarios to global EI

When PestLCI and USEtox[®] are combined into one model, the output is a CP EI score per application scenario. Figure 9 shows the overall approach followed to assess the environmental score of each application scenario. Results of both models have been evaluated in various other studies, with uncertainty ranges provided that are dominated by effect factors in USEtox[®], and overall ranging from 1 to 3 orders of magnitude for ecotoxicity impacts (see e.g. Dijkman et al. (2012), Rosenbaum et al., (2008).

As described above, the PestLCI Consensus model was used for evaluating emissions of agricultural CPPs. Output of the PestLCI Consensus model are emission fractions (i.e. emitted mass into a given environmental compartment per mass applied for a given scenario). For application scenario calculations, emission fractions considering initial partitioning and drift within minutes after crop protection product application have been adopted, so-called primary distribution fractions.

For quantifying ecotoxicity impacts from chemical emissions, the USEtox[®] model, version 2.12, was then used. These results have been adopted for application scenario calculations, following the recommended procedure for deriving characterization factors in USEtox[®] as described in the official USEtox[®] documentation (Fantke, et al., 2017a). USEtox[®] is based on models that have for each process and parameter been extensively evaluated, peer-reviewed and widely applied in scientific and practical application studies. USEtox[®] itself is the most widely applied, evaluated and accepted LCIA toxicity characterization model in LCA (see e.g. the >1000 peer-reviewed articles, reports and books referencing Rosenbaum et al., (2008).



Figure 9: Overall approach followed to assess the EI of each application scenario¹¹. Emission and potential impact results are compartment-specific as shown in Figure 6.

As outlined in section 1, BCS considers the combined modelling output of emissions according to PestLCI and characterization factor according to USEtox[®] as crop protection environmental impact (EI).

3.9. Agrowin CP application scenario data processed in PestLCI / USEtox® modelling approach

Information for 500,873 crop protection product application scenarios (for the whole CP market) for the year 2018 have been provided to DTU by BCS as a starting point for calculating related environmental impact. Each application scenario represents an active ingredient contained in a crop protection product applied in a given crop and country, with a given treated area per active ingredient and a given volume per active ingredient. The application method and application timing in terms of the crop growth stage is available in the data set.

Scenarios cover 96 distinct countries, 55 crop groups, 1082 active ingredients, and 108 distinct application methods. The data set covers both active ingredients and crop protection products sold by BCS and the rest of the crop protection market. For BCS (without the rest of the CP market competitors), the study relies on a data set covering 54,204 crop protection application scenarios, 82 countries, 55 crop groups, 340 active ingredients and 2,291 crop protection products containing the beforementioned 340 active ingredients. Certain scenarios had to be excluded from the study. The reasons are outlined below in section 3.10.

The crop protection application scenarios are captured in AgroWin in the structure shown in Figure 10 below:

¹¹ *Note:* the reference unit can vary depending on the objective; here it refers to one hectare.

Crop Protection:



Figure 10: Detailed levels of Crop protection application scenarios captured in Agrowin data

3.10. Exclusions of CP application scenarios

Out of the assessed crop protection product application scenarios, 54,185 scenarios (10.8 % of all scenarios) have been excluded from the analysis. The main reasons for excluding scenarios or not providing impact results are as follows:

- ~1000 data points excluded due to negative or null reported area treated and/or mass applied. In Agrowin, this can happen when the data on treated area or mass applied are either not available or when farmers have given back a certain amount of product before using it.
- ~2000 data points excluded due to application method or crop stage not valid/not in PestLCI Consensus
- >50,000 data points excluded due to missing Chemical Abstracts Service (CAS) number¹², not characterizable in USEtox[®] or missing chemical/ecotoxicity data to derive characterization factors or ecotoxicity.

The excluded scenarios refer to the entire data set covering the whole CP market. For BCS-specific product related application scenarios only 2,813 application scenarios (5.2% of the BCS application scenarios) had to

¹² The CAS number is a unique identifier assigned to every chemical substance described in open scientific literature (link: CAS registry description Archived 25 July 2008 at the Wayback Machine, by Chemical Abstracts Service)

be excluded. 2,273 out of 2,813 application scenarios (80%) due to USEtox[®] limitations. The remaining 20% mainly due to limitations of PestLCI and to a minor degree due to data issues from AgroWin. Therefore, most application scenarios had to be excluded due to current limitations of the USEtox[®] model.

Translating the application scenario exclusions for BCS into excluded active ingredients and crop protection products for the reasons outlined above:

- Entire data set covering BCS and other manufacturers: 1082 active ingredients out of which 892 active ingredients could be characterized in USEtox[®] and are therefore part of the study
- BCS: 54 crop groups are part of the BCS assessment. The crop group "environmental markets" was excluded. "Environmental markets" contains crop protection uses on e.g. turf or forest. BCS's EIR commitment refers only to field applications.
- BCS: 340 active ingredients out of which 270 active ingredients could be characterized in USEtox[®]. Most of the excluded active ingredients relate to BCS's biological portfolio.
- BCS: 2,291 crop protection products out of which 2,056 are part of the study

For BCS most of the excluded active ingredients are BCS biological portfolio. Therefore, BCS's CP EI based on the current study might be conservative.

Despite these exclusions, BCS and DTU argue that this is the largest high-quality CP application data set ever used to our knowledge. In a second iteration, BCS and DTU want to fill the data gaps where possible (e.g. by filling in missing application methods). If there is no data in certain cases (e.g., CP applications in Africa), BCS can fill the gaps (transparently) based on reasonable market intelligence assumptions because official statistics such as FAO do not offer such comprehensive, harmonized, and high-quality application data sets.

The majority of the excluded scenarios relates to 139 out of 1082 substances not commonly included in assessment models or chemical and ecotoxicity databases (e.g. microorganisms). With that, these chemicals are likely not leading to a relevant contribution to overall global impacts at a screening-level, whereas they might become relevant in refined, more local assessments.

3.11. Combining application scenarios with the models to derive EI scores

The following general approach has been applied to assess the environmental impact of each application scenarios which is shown in a simplified version in Figure 11, Table 8, and Figure 12 below:

- Mass applied of crop protection product has been combined with area treated to derive an applied dose [kg applied/ha treated] for each scenario.
- An area split for the emission fraction reaching off-field surfaces has been assigned to each combination based on mapping the reported country to a continent available in USEtox® 2.x, parameterized based on Kounina et al. (2014), namely we assigned a certain fraction of the off-field area to USEtox'® freshwater, agricultural soil and natural soil compartments. For countries that belong to more than one parameterized continent (e.g. Russian Federation), the continent in which the largest area fraction of the given country falls was selected. This was considered sufficient for a screening-level approach as this only affected a handful of countries that have a major share in one and only a very minor share in another continent.

- For each emission compartment defined in the PestLCI Consensus model, application-scenariospecific emission results from the PestLCI Consensus model have been derived based on mapping reported crops to crop types, reported crop stages to crop surface interception area fractions for field crops, and reported application methods to drift functions for a pre-defined set of application methods available in PestLCI Consensus. Details on the mapping and assumptions made to derive emission results are presented in sections 3.4 and 3.5.
- For each emission compartment defined in the USEtox[®] model, active-ingredient-specific ecotoxicity impact results from the USEtox[®] model have been derived for a global average model setup (default model settings), based on implementing all reported active ingredients into the substance databases of USEtox[®] that can be characterized and that have all required physicochemical property data available and accessible. Details on the substance input data collection and assumptions made to derive ecotoxicity impact results are presented in section 3.7.
- Emission results (kg emitted into a given emission compartment defined in the PestLCI Consensus model per kg applied for a given application scenario) have been combined with ecotoxicity impact characterization results (PAF m³ d/kg emitted into an emission compartment defined in the USEtox® model), based on matching emission compartments between both models following the approach described in Fantke (2019) and in Gentil et al. (2020), as well as based on assigning the area split for off-field surfaces to respective emission compartments in the USEtox® model, as shown in Figure *6*, and detailed out in Table 6.



Figure 11: Framework representation considering both PestLCI and USEtox® inputs

	= Mass of emission x Characterization factor	
El / Quantity	$= \frac{\overline{Kgemitted}}{Kgapplied} \times \frac{PAF m^{3} d}{\overline{Kgemitted}}$ $= PAF m^{3} d / Kg applied$	The combination of emissions from PestLCI and characterization factors from USEtox [®] yields potential ecotoxicity impacts per kg applied in a given application scenario (PAF m ³ d/kg applied). BCS calls this value El/quantity .
	= (EI/ Quantity) x (Applied dose)	
El / ha	$= \frac{PAF \ m^{3} \ d}{Kg \ applied} \times \frac{Kg \ applied}{treated \ hectares}$ $= PAF \ m^{3} \ d \ / \ hectare$	Further, the El/quantity score in a given application scenario is multiplied with the applied dose (kg applied/ha treated) to arrive at 'impact per ha treated' [PAF m ³ d/ha treated]. BCS calls this value El/ha].
	= (EI / ha) x (Treated hectares/ Country)	
El / Scenario [labelled as 'El' by BCS]	$=\frac{PAF \ m^3 \ d}{Treated \ hectares} \times \frac{Treated \ hectares}{Country}$	Finally, the EI/ha score is multiplied with treated area [ha/country] to arrive at a 'cumulative impact per scenario' in a given country [PAF m ³ d/country. BCS calls this value EI]
	= PAF m ³ d / Country	

 Table 8: Stepwise calculation of EI scores for an individual application scenario

Note. The crossed-out elements show how different the different parameters cancel out each other in the stepwise calculation of EI scores for each individual application scenario



Figure 12: Definition of key measurement factors within the methodology

3.12. Aggregating El scores

Aggregation of EI across application scenarios will enable calculation of cumulative impacts at different aggregation levels. In general, the aggregation can be described as follows. For each application scenario (see again section 2.3. for all elements of an individual scenario), the environmental impact scores are computed. The following equation shows that the aggregation is based on the sum of the total EI scores across the scenarios of interest (e.g., at the level of a crop, country, indication, application method etc. or even combinations of these).

$$EI = \sum (EI/kg)_i \cdot dose_i \cdot ha_i$$

Equation 5

Where (*i*) indexes the scenarios for the CP application (consisting of the scenario elements described in section 2.3). Thus, in a scenario, $(El/kg)_i$ is the environmental impact per quantity of applied active ingredient, with a specific *dose*_i, on a certain number of treated hectares (*ha*_i). For example, we can sum the EI for:

- all active ingredients used to treat cabbage crops (i.e., at the aggregation level of a single crop).
- all vegetables cultivated in Vietnam (i.e., at the aggregation level of a crop-country-combination).
- all active ingredients used in all crop classes cultivated in Vietnam (i.e., at the aggregation level of a country).
- various other potential aggregation levels, such as crop, country, active ingredient, indication, crop growth stage, application method, etc. (and any combinations of these).

4. Interpretation

4.1. Results and setting a CP EIR baseline for future progress tracking

To achieve a 30% reduction of CP EI by 2030, BCS takes a 2-step approach: determination of focus areas based on a 2018 data set and establishment of a final baseline on a 5-year-average (2014-2018). The 2018 CP EI calculated for all application scenarios at the crop class level will be used to determine BCS' focus areas to achieve a 30% reduction by 2030. The input dataset is currently based on 2018-only data provided via the Agrowin database. The reason for this is that the 2018 data were the most-up-to date data available when BCS started the partnership with the DTU. Because it is the first time for BCS to work with the models PestLCI and USEtox[®], and the first time for the DTU with such a comprehensive global data set of the whole crop protection market, the partners decided to focus first on 2018 data exclusively and to finetune the impact calculation process.

However, it is planned to establish a baseline on a 5-year-average (2014 - 2018) to account for the specificities of agriculture, such as inter-annual variability, seasonality or dependence on climatic conditions. BCS and DTU are currently calculating the final baseline based on the 5-year-average (2014 - 2018).

The baseline will always be calculated at product level consisting of all Bayer crop protection products applied globally, according to AgroWin data. BCS will regularly assess the overall adoption of impact-reducing levers they bring to the market to track their progress against the baseline — and against the 30 percent reduction commitment of BCS' environmental impact by 2030.

As described above, each application scenario has its own environmental impact score which is dependent on, inter alia, substance characteristics of the active ingredients contained in the crop protection products applied on field, dose rates of active ingredient per ha, application method, application timing, the crop and country where the product has been applied. BCS first aimed to identify which scenarios had the strongest contribution on the global environmental impact. There are many aggregation methods of the different metrics available. BCS is currently working with a *'treated-area-weighted El/ha'* as the measure of environmental impact. From this, focus areas can be determined, e.g., in terms of combinations of crops, countries, and active ingredients. The treated-area-weighted El/ha represents how efficiently, from an environmental impact perspective, the crop protection portfolio is meeting the needs of the growers. It is calculated as the ratio of the cumulative environmental impact and the total treated area:

'Treatedarea weighted EI/ha' =
$$\frac{EI}{ha} = \frac{\sum (EI/kg)_i \cdot dose_i \cdot ha_i}{\sum ha_i} = \frac{\sum EI_i}{\sum ha_i}$$

Equation 6

If the treated area is not used to scale the cumulative environmental impact, some increases in the metric could be encountered due to a greater need for crop protection by growers even if the leveraged products show a lower individual environmental impact. In addition, weighing for treated area across the entire BCS CP portfolio ensures that both CP intensive crops, such as fruits, with relatively small treated areas and CP

extensive crops, such as soybeans, with large treated areas, are adequately reflected in the BCS impact assessment.

BCS is currently evaluating its levers to achieve the 30% commitment. BCS intends to publish a target delivery roadmap at a later point in time. Generally, there are indication specific (i.e. herbicides, fungicides, insecticides) and overarching levers available if we consider BCS's technological capabilities (see Figure 13).

Reduce Bayer's crop protection environmental impact by 30% by 2030. Overarching and indication specific improvement levers.



Figure 13: Overview of available BCS CPP levers and their role within the EI scope.

Future scenarios will be calculated by using the same calculation approach as for the baseline. The underlying market research input data will be provided annually (approximately, in June) by the data provider 'Lexagri' via the 'Agrowin' database which covers 90% of the global crop protection market. Therefore, the envisioned scope of the data will be the same as for the baseline data. That encompasses data on: CP applications per crop and country; CP applications differentiated per trait system (for some countries where data are available); application method; dose; total ha treated per product; and application timing (crop growth stage). Based on these annual input data updates, the impact calculation will be done automatically based on the same PestLCI and USEtox® modelling framework as used for the baseline calculation. This automated impact calculation will be critically examined and verified externally by the Technical University of Denmark. Finally, the calculated impact scores of the future scenarios will be compared against the baseline impact to track progress against the 30% objective.

If additional input data become available in the future, BCS will evaluate with the Technical University of Denmark how to best integrate these data. Such potential data might encompass: Environmental mitigation measures as practically applied on field; Seeds & Traits specific collected CP application data in additional countries; Field information (if we choose to measure at field-level) such as field size, slope, off-field surfaces, drainage depth, etc.; Agronomic practices relevant for CP program/doses such as tillage, cover crops, crop rotation (see Figure 14). Potential data sources for these future data might be product labels for mitigation measure data, or field information and agronomic practices based on future market research data collected by Kynetec and provided to Bayer by Lexagri via the Agrowin database. BCS intends to consult external expert panel if and when such additional data is available to evaluate whether and how to adjust the baseline and performance tracking.

BAYER

Baseline and performance tracking concept

Scope determined by: 1) scope of the models 2) Bayer improvement levers 3) availability of baseline data 4) availability of performance tracking data



Figure 14: Outline of the BCS EIR baseline and the performance tracking concept.

4.2. Sensitivity analysis: USEtox®

A full sensitivity analysis, starting from the environmental impact scores, covering both PestLCI, USEtox[®] and the respective data input parameters, is not yet available from the scientific consortium. As the most dominant factor in environmental impact scores is often the substance specific characterization factor from USEtox[®], a sensitivity analysis for USEtox[®] is provided in this study.

An additional sensitivity study was also done for understanding how varying input parameters in USEtox[®] influence ecotoxicity impact characterization results. In this sensitivity approach, BCS used the existing USEtox[®] ecotoxicity characterization model, except that data inputs are specified as probability distributions as opposed to point estimates. Input data distributions are sampled independently 10,000 times, and the values were used as input to USEtox[®] to calculate fate, eco-exposure, and ecotoxicity effect factors, and resulting stochastic characterization factors plotted as frequency distributions. To evaluate the relative influence of input parameter variability on calculated characterization factors, we compare Spearman's rank correlation indices for all inputs. This approach has been applied and is further detailed in a previous study on a pharmaceutical tested in USEtox[®] (Wender, Prado, Fantke, Ravikumar, & Seager, 2018). Input data for fate, eco-exposure and ecotoxicity effect modelling that have been varied are presented in Table 9. By default, BCS assumed uniform distributions for all input parameters, with plus-or-minus one order of magnitude variation around the given point estimates, as one possible way of efficiently varying input parameters whenever multiple values per parameters are missing.

Parameter	Description	Units	Point value(s)	Baseline variance	Reference
MW	Molecular weight	g/mol	141.1	141.1	Chemical formula
Kow	Octanol-water partitioning coefficient	I/I	0.16	0.016-1.6	EPISuite, experimental value
Кос	Soil organic carbon-water partitioning coefficient	l/kg	5.01	0.501—50.1	EPISuite, experimental value
Kh	Henry's law constant	Pa m3/mol	8.8×10 ⁻⁵	8.8×10 ⁻⁶ —8.8×10 ⁻⁴	EPISuite, HenryWin
Pvap	Vapour pressure	Ра	4.7×10 ⁻³	4.7x10 ⁻⁴ —0.047	EPISuite, experimental value
Solubility	Solubility in water	mg/l	1×10 ⁶	1×10 ⁵ —1×10 ⁷	EPISuite, experimental value
kdeg, air	Degradation rate constant in air	1/s	2.5×10⁻⁵	2.5×10 ⁻⁶ —2.5×10 ⁻⁴	EPISuite, AopWin
kdeg, water	Degradation rate constant in water	1/s	5.3×10 ⁻⁷	5.3×10 ⁻⁸ —5.3×10 ⁻⁶	EPISuite, BioWin
kdeg, soil	Degradation rate constant in soil	1/s	2×10 ⁻⁶	2×10 ⁻⁷ —2×10 ⁻⁵	PPDB, field DT50 based
kdeg, sediment	Degradation rate constant in sediment	1/s	5.9×10 ⁻⁸	5.9×10 ⁻⁹ —5.9×10 ⁻⁷	EPISuite, BioWin
BAF fish	Bioaccumulatio n factor in fish	l/kg	0.9	0.09—9	EPISuite, BCFBAF upper trophic
HC50	Freshwater aquatic hazard concentration	mg/l	0.94	0.094—9.4	USEtox [®] , precalculated

Table 9: Fate, eco-exposure and ecotoxicity effect relevant input data for USEtox[®] and their modelled variance for the neutral test substance methamidophos (CAS RN: 10265-92-6).

Results of the sensitivity analysis of USEtox[®] input parameter variations are shown in Figure 15 for different emission compartments relevant for pesticide emissions, with related Spearman Rank Correlation results shown for the most influential input parameters per emission scenario given in Figure 16.



Figure 15: Stochastic freshwater aquatic ecotoxicity characterization factors (PAF m³ d/kg emitted) for methamidophos (CAS RN: 10265-92-6) emitted to continental rural air, freshwater, agricultural and natural soil.



Figure 16: Spearman Rank Correlation for model input variables with the largest magnitude of influence on characterization factor variability across four emission scenarios in USEtox[®].

Spearman Rank Correlation identified that USEtox[®] ecotoxicity characterization factor results for methamidophos (CAS RN: 10265-92-6) are mainly influenced by degradation half-lives across compartments, followed by ecotoxicity effect information, and partitioning coefficients (mainly Kaw and Koc for this moderately volatile and rather polar (i.e. not very lipophilic) chemical). Kow would typically become more relevant for more lipophilic chemicals (i.e. log Kow > 3). From this sensitivity analysis, we identify degradation and ecotoxicity information as main aspects that require a careful consideration in refined

scenarios, and where data quality for these aspects should be improved across substances. Moreover, as different input parameters affect both fate and exposure factor, while only the ecotoxicity information affects the effect factor, the ecotoxicity information gains additional importance in terms of influencing variability of characterization factors, which consist of the simple product of fate, exposure and effect factors (i.e. characterization factors are equally sensitive towards these three intermediate factors).

4.3. Qualitative discussion of uncertainty

Dubus et al. (2003) have extensively discussed numerous sources of uncertainty in pesticide emission modeling including **uncertainty in primary data** (from the spatial and temporal variability of environmental variables, from sampling procedures and measurement errors in the field, and from analysis in the laboratory), **uncertainty in the derivation of model input parameters** (when a modeler might decide to (a) leave the parameters at their default values, (b) make an educated guess using expert judgement, (c) extract values from existing databases or (d) derive the values from empirical functions presented in the literature; each procedure may introduce uncertainty into the modelling, depending on the sensitivity of the model), and **other factors** (such as multiplicity of physical, chemical and biological factors affecting the fate of pesticides; the inability of a model to represent reality accurately even when adequate model inputs are being used; subjectivity introduced by the modeler; linguistic imprecision; inappropriate use of concepts implemented in the models; human error through unstable or biased experimental procedures, interpretation, typing error or the simple variation between people; upscaling of models to a scale larger than that for which they were developed) might affect the representativeness of the results.

"Various sensitivity studies have demonstrated that the combined use of the PestLCI and USEtox[®] models lead to a reasonable impact assessment. Nevertheless, users are advised to continue to exercise with great caution when interpreting the results, since, despite their detailed simulation, both methods still exhibit uncertainties" (Roesch & Gaillard, 2017).

Combining fate, exposure and effects yields characterization factors for ecotoxicity. These factors serve as characterization results at the midpoint level in LCA. They can be combined with a damage factor translating ecotoxicity impacts into damages on ecosystem quality, respectively, to arrive at a damage (endpoint) level in LCA. Further details about the general LCA midpoint-damage characterization framework are given in Hauschild and Huijbregts (2015). Thereby, uncertainty has been considered in various steps in USEtox[®], allowing for a comparative assessment of the environmental impacts of chemicals to provide insights on "best in class" products in product comparisons regarding the environmental performance of products in terms of ecotoxicity related to chemical emissions.

Ecotoxicity test results are reported as Effect Concentrations ECx where the effect may be mortality, immobilization, reproduction or other endpoints and 'x' refers to the fraction of the test organisms or replicates showing the effect. EC50 results are determined from statistical evaluation of the concentration-effect values in experiments. The middle of the derived curve is considered to be more robust than the lower ends. Therefore, EC50 are used for determination of the ecotoxicological effect factor to minimize uncertainties in the effect factor.

Results of both models have been evaluated in various other studies, with uncertainty ranges provided that are dominated by effect factors in USEtox[®], and overall ranging from 1 to 3 orders of magnitude for ecotoxicity impacts (see e.g. Dijkman et al. (2012), Rosenbaum et al. (2008))."

In terms of the inventory data on global crop protection product consumption taken from the 'Agrowin' dataset, we argue that Agrowin provides the most extensive and rigorously collected data set currently available that covers agricultural CP consumption data (i.e., consumption data on what has been truly applied on the field). Other existing databases on pesticide use statistics are not consumption data but mostly sales data. For example, the <u>FAOSTAT</u> pesticide use database by the Food and Agriculture Organization (FAO) of the United Nations covers pesticides sales in most countries. In some countries FAO data includes non-agricultural uses such as home and garden use. Furthermore, the FAO pesticide definition varies in some countries. Thus, by using the Agrowin dataset which is based on actual pesticide consumption data (not sales data), we worked to ensure the representativeness of the primary data as much as possible.

BCS acknowledges that a full uncertainty assessment needs to be provided, once available for the scientific consortium. Based on analysis we argue that there are no significant factors that would limit the interpretation of the findings of this study.

4.4. Main limitations and how they are addressed

Regarding limitations of the Agrowin inventory data on agricultural CP consumption data, the frequency and comprehensiveness of the available interview panel data varies, because it depends on the commercial relevance of a market, the accessibility of farmers for panel interviews and other factors. In big and commercially relevant markets, panel data is typically available on a yearly basis. In other markets with a lower commercial relevance, the frequency of panel data collection can be lower and irregular (e.g. only every 2-3 years in the Belgium-potato market). Even if panel data is available in a given crop and country, BCS might decide to not purchase a panel study on a certain market at all. In those cases BCS intends to fill the data from other sources. For such countries and markets where no panel data are available, data gaps are filled by using national statistics (e.g., import and export data). If there are no national statistics, dedicated Bayer market analysis and business intelligence colleagues fill the data gaps based on their expert knowledge of the respective markets (e.g., based on sales information). Even taking those limitations into account, the current AgroWin data set covers about 85-95% of the BCS specific crop protection (coverage varies from year to year) market value and ~90% of all crop protection applied globally. In assessing the BCS hotspots, BCS relies as well on its crop protection sales planning which covers all CP BCS sales (as opposed to application data in AgroWin). BCS therefore does not exclude any CP sales from the analysis of mitigation measures and target delivery and all substances which can be characterized by USEtox® are part of BCS analysis. As of 2020, BCS has decided to buy all available panel data for the entire CP market, which will further improve the completeness, reliability, and comparability of the data set, as most data will be based on panels and not non-panel data sources.

Regarding limitations in the emission modeling via PestLCI, secondary distribution was excluded from the environmental impact assessment, because the level of detail required to model secondary distribution processes are not readily available in the present screening-level assessment, which would introduce large additional uncertainties related to collecting and defining e.g. field-level characteristics at the global scale. To address this issue, BCS and DTU are working on including secondary distribution in the future.

Regarding limitations of the impact assessment via USEtox[®], for this report, only freshwater ecotoxicity impacts have been considered, since it represents the current scope of USEtox[®]. Additionally, freshwater is the best understood biosphere and is the destination of a major share of emissions. More information about freshwater ecotoxicity impacts and how they are assessed with USEtox[®] is provided in section 3.3. To

address this issue, BCS plans to enlarge the scope by integrating the impacts on terrestrial organisms like earthworms and impacts on pollinators, when the models are mature enough.

Overall, both underlying models of the present analysis, namely PestLCI Consensus and USEtox[®], have undergone model evaluations via previous studies. PestLCI results have been compared to results from more sophisticated risk assessment models (Dijkman, Birkved, & Hauschild, 2012), showing overall consistency between the compared models and explaining main differences along considered or omitted processes in each model. USEtox[®], in contrast, was originally built based on a systematic model comparison of models that had been evaluated individually before USEtox[®] was developed. The overall model comparison leading to USEtox[®], SimpleBox, was for instance evaluated for specific chemicals against other models as well as against measurements (Hollander, et al., 2007). Hence, no additional model evaluation was included in the present study.

5. Further developments of this report

Once the second review cycle is completed (review of the present report), the following sections will be developed for the purpose of the final review cycles:

- Review and response by Bayer to comments and feedback of panel members.

In the future, the present report will be complemented by additional sections, not related to the on-going third-party review:

- More detailed sensitivity analyses covering both models (PestLCI and USEtox[®]), and the influence of input and model parameters on the results once this is made available by the academic partners.
- Tiered approach to refined scenarios: a proposal for how to refine the baselines and the performance tracking further, e.g. by adding soil ecotox or by moving from a crop-country level to a regional level to account better for regional agronomic specificities.
- Overview of how BCS intends to deliver against its commitment until 2030.

6. References

Apostol, L. C., Hlihor, R. M., Smaranda, C., Pavel, V. L., Robu, B. M., Caliman, F. A., & Gavrilescu, M. (2009). LIFE CYCLE IMPACT ASSESSMENT OF PESTICIDES: CURRENT ISSUES AND PERSPECTIVES. *Research Gate*.

Biermann, F., & Kim, R. E. (2020). The boundaries of the planetary boundary framework: a critical appraisal of approaches to define a "safe operating space" for humanity. *Annual Review of Environment and Resources*, *45*, 497-521, doi/10.1146.

Birkved, M., & Hauschild, M. Z. (2006). PestLCI - A model for estimating field emissions of pesticides in agricultural LCA. *Ecological Modelling*, 433-451.

Crenna, E., Sala, S., Polce, C., & Collina, E. (2017). Pollinators in life cycle assessment: towards a framework for impact assessment. *Journal of Cleaner Production*, 525-536.

Dijkman, T. J., Birkved, M., & Hauschild, M. Z. (2012). PestLCI 2.0: A second generation model for estimating emissions of pesticides from arable land in LCA. *The International Journal of Life Cycle Assessment* 17, 973-986.

Dubus, I. G., Brown, C. D., & Beulke, S. (2003). Sources of uncertainty in pesticide fate modelling. *Science of The Total Environment*, S. 53-72.

European Commission; Joint Research Centre; Institute for Environment and Sustainability. (2010). International Reference Life Cycle Data System (ILCD) Handbook - General guide for Life Cycle Assessment - Detailed guidance. First edition. Luxembourg: European Union.

Fantke, P. (2019). Modelling the environmental impacts of pesticides in agriculture. in: Weidema, B.P. (Ed.). Assessing the Environmental Impact of Agriculture. Cambridge, United Kingdom: Burleigh Dodds Science Publishing.

Fantke, P., Aurisano, N., Backhaus, T., Bulle, C., Chapman, P., Cooper, C., . . . Golsteijn, L. (2018a). Toward harmonizing ecotoxicity characterization in life cycle impact assessment. *Environmental Toxicology and Chemistry*.

Fantke, P., Aylward, L., Bare, J., Chiu, W. A., Dodson, R., Dwyer, R., . . . Jolliet, O. (2018b). Advancements in life cycle human exposure and toxicity characterization. *Environmental Health Perspectives 126*.

Fantke, P., Bijster, M., Guignard, C., Hauschild, M., Huijbregts, M., Jolliet, O., . . . van Zelm, R. (2017a). *USEtox®* 2.0 Documentation (Version 1.1). Lyngby, Denmark: USEtox® Team.

Fantke, P., Charles, R., de Alencastro, L. F., Friedrich, R., & Jolliet, O. (2011). Plant uptake of pesticides and human health: Dynamic modeling of residues in wheat and ingestion intake. *Chemosphere 85*, 1639-1647.

Footprint. (2020). The Pesticide Properties Database (PPDB 2.0) of the Footprint Project.

Gentil, C. (2020). Advancing emission and impact modeling for agricultural pesticides under tropical conditions, to improve scientific foundation of the environmental evaluation of tropical agri-food systems. Martinique: University of Montpellier. p. 277.

Gentil, C., Fantke, P., Mottes, C., & Basset-Mens, C. (2019). Challenges and ways forward in pesticide emission and toxicity. *The International Journal of Life Cycle Assessment*, *25*, 1290–1306.

Gentil-Sergent, C., Basset-Mens, C., Gaab, J., Mottes, C., Melero, C., & Fantke, P. (2021). Quantifying pesticide emission fractions for tropical conditions. *Chemosphere*, 275, doi.org/10.1016/j.chemosphere.2021.130014.

Hauschild, M., & Huijbregts, M. (2015). Life Cycle Impact Assessment. Dordrecht: Springer.

Hauschild, M., Huijbregts, M., Macleod, M., Margini, M., van de Meent, D., Rosenbaum, R. K., & McKone, T. E. (2008). Building a Model Based on Scientific Consensus for Life Cycle Impact Assessment of Chemicals: The Search for Harmony and Parsimony. *Environ. Sci. Technol., 42 (19)*, 7032-7037.

Henderson, A. D., Hauschild, M. Z., Meent, D. v., Huijbregts, M. A., Larsen, H. F., Margni, M., . . . Jolliet, O. (2011). USEtox fate and ecotoxicity factors for comparative assessment of toxic emissions in life cycle analysis: sensitivity to key chemical properties. *The International Journal of Life Cycle Assessment*, *16*, Article number: 701.

Hollander, A., Sauter, F., Den Hollander, H., Hujibregts, M., Ragas, A., & Van de Meent, D. (2007). Spatial variance in multimedia mass balance models: Comparison of LOTOS–EUROS and SimpleBox for PCB-153. *Chemosphere*, S. 1318-1326.

ISO. (2006). Environmental management - Life cycle assessment - Principles and framework. Geneva: International Organization for Standardization.

Jenssen, B. M. (2006). Endocrine-disrupting chemicals and climate change: a worst-case combination for Arctic marine mammals and seabirds? *Environmental Health Perspectives* 144, 76-80.

Jolliet, O., Rosenbaum, R., Chapman, P., McKone, T., MD, M., Scheringer, M., . . . Wania, F. (2006). Establishing a framework for life cycle toxicity assessment: Findings of the Lausanne review workshop. *The International Journal of Life Cycle Assessment* 11, 209-212.

Kounina, A., Margni, M., Shaked, S., & Bulle, C. (2014). Spatial analysis of toxic emissions in LCA: A subcontinental nested USEtox model with freshwater archetypes. *Environment International, 69C*, 67-89, DOI:10.1016/j.envint.2014.04.004.

Larsen, H., & Hauschild, M. (2007). GM-troph: A low data demand ecotoxicity effect indicator for use in LCIA. *The International Journal of Life Cycle Assessment 12*, 79-91.

Lexagri. (28. 10 2021). AgroWIn. Von https://www.lexagri.com/service_agrowin.php abgerufen

Linders, J., Mensink, H., Stephenson, G., Wauchope, D., & Racke, K. (2000). Foliar Interception and Retention Values after Pesticide Application. A Proposal for Standardized Values for Environmental Risk Assessment (Technical Report). *Pure and Applied Chemistry, 72 (11)*, 2199-2218 doi.org/10.1351/pac200072112199.

MacLeod, M., Scheringer, M., McKone, T. E., & Hungerbuhler, K. (2010). The State of Multimedia Mass-Balance Modeling in Environmental Science and Decision-Making. *Environ. Sci. Technol.*, 44(22), 8360-8364.

Mansouri, K., Williams, A. J., Grulke, C. M., & Judson, R. S. (2018). OPERA models for predicting physicochemical properties and environmental fate endpoints. *Journal of Cheminformatics*.

Mariana Furio Franco Bernardes, M. P. (2015). Impact of Pesticides on Environmental and Human Health. *Toxicology Studies - Cells, Drugs and Environment*.

McDougall, P. (2018). *Evolution of the crop protection industry since 1960.* Midlothian: Vineyard Business Centre,.

McDougall, Phillips. (2018). *Evolution of the crop protection industry since 1960* (EH37 5XP, p.10 Ausg.). Pathhead, Midlothian, Scotland: Vineyard Business Centre.

Meier, U. (2018). Growth stages of mono- and dicotyledonous plants : BBCH Monograph. DOI: 10.5073/20180906-075119.

Noyes, P. D., McElwee, M. K., Miller, H. D., Clark, B. W., Tiem, L. A., Walcott, K. C., . . . Levin, E. D. (2009). The toxicology of climate change: environmental contaminants in a warming world. *Environment International 35*, doi:10.1016/j.envint.2009.02.006.

Posthuma, L., van Gils, J., van de Meent, D., & de Zwart, D. (2019). Species sensitivity distributions for use in environmental protection, assessment, and management of aquatic ecosystems for 12 386 chemicals. *Environmental Toxicology and Chemistry*, 905-917.

Postshuma, L., Suter II, G., & Traas, T. (2002). *Species Sensitivity Distributions in Ecotoxicology*. Boca Raton: CDC Press.

Rockström, J. W. (2009). Planetary Boundaries: Exploring the Safe Operating Space for Humanity. *Ecology* and society.

Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F. S., Lambin, E., . . . Costanza, R. (2009). Planetary Boundaries: Exploring the Safe Operating Space for Humanity. *Ecology and Society 14 (2)*.

Roesch, A., & Gaillard, G. (2017). Comprehensive Farm Sustainability Assessment. *Agroscope Science | No* 47.

Rosenbaum, R., Assumocío, A., & Wallman, M. (2015). The Glasgow consensus on the delineation between pesticide emission inventory and impact assessment for LCA. *The International Journal of Life Cycle Assessment, 20,* 765-776.

Rosenbaum, R., Bachmann, T., Gold, L., & Huijbregts, M. (2008). The UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in Life Cycle Impact Assessment. *The International Journal of Life Cycle Assessment*, *13*(7), 532-546.

Rosenbaum, R., Margni, M., & Jolliet, O. (2007). A flexible matrix algebra framework for the multimedia multipathway modeling of emission to impacts. *Environment International*, *33*(5), 624-634.

Saouter, E., Biganzoli, F. C., Versteeg, D., Crenna, E., Zampori, L., Sala, S., & Pant, R. (2020). Environmental Footprint: Update of Life Cycle Impact Assessment Methods – Ecotoxicity freshwater, human toxicity cancer, and non-cancer. *Publications Office of the European Union, Luxembourg*, doi:10.2760/300987.

Spatial variance in multimedia mass balance models: Comparison of LOTOS–EUROS and SimpleBox for PCB-153. (2007). *Chemosphere*, S. 1318-1326.

Stockholm Resilience Center (SRC). (2015). *The nine planetary resilience*. Abgerufen am 26. 02 2021 von https://www.stockholmresilience.org/research/planetary-boundaries/planetary-boundaries/about-the-research/the-nine-planetary-boundaries.html

UNEP. (2021). Environmental and health impacts of pesticides and fertializers and ways of minimizing them.

UNEP, United Nations Environmental Programme. (2021). *Environmental and Health Impacts of Pesticides and Fertilizers and Ways of Minimizing Them: Summary for Policymakers.* Von https://wedocs.unep.org/xmlui/bitstream/handle/20.500.11822/34463/JSUNEPPF.pdf?sequence=13 abgerufen

Wender, B., Prado, V., Fantke, P., Ravikumar, D., & Seager, T. (2018). Sensitivity-based research prioritization through stochastic characterization modeling. *The International Journal of Life Cycle Assessment*, S. 324-332.

Westh, T. B., Hauschild, M. Z., Birkved, M., Jørgensen, M. S., Rosenbaum, R. K., & Fantke, P. (2015). The USEtox story: a survey of model developer visions and user requirements. *International Journal of Life Cycle Assessment*, 299-310.

Williams, A. J., Grulke, C. M., McEachran, A. D., Mansouri, K., Baker, N. C., Patlewicz, G., . . . Richard, A. M. (2017). The CompTox Chemistry Dashboard: A community data resource for environmental chemistry. *Journal of Cheminformatics*, 9-61.

Appendix I – External Sources in Agrowin 2019 (all other cropcountry combinations are based on non-panel data)

Market	Country	Source	Crop Main Group	Data purchased by Bayer
СР	ARGENTINA	KLEFFMANN	CORN/MAIZE	Х
СР	ARGENTINA	KLEFFMANN	SOYBEANS	х
СР	ARGENTINA	KLEFFMANN	CEREALS	х
СР	BELGIUM	KYNETEC	CEREALS	х
СР	BELGIUM	KYNETEC	CORN/MAIZE	Х
СР	BELGIUM	KYNETEC	POTATOES	х
СР	BELGIUM	KYNETEC	FRUITS	х
СР	BELGIUM	KYNETEC	LEEKS	х
СР	BRAZIL	SPARK	CORN/MAIZE	х
СР	BRAZIL	SPARK	COTTON	х
СР	BRAZIL	SPARK	COFFEE	Х
СР	BRAZIL	SPARK	SOYBEANS	Х
СР	BRAZIL	KLEFFMANN	COTTON	х
СР	BRAZIL	KLEFFMANN	CORN/MAIZE	х
СР	BRAZIL	KLEFFMANN	SOYBEANS	х
СР	BULGARIA	KLEFFMANN	CEREALS	х

СР	BULGARIA	KLEFFMANN	CORN/MAIZE	Х
СР	BULGARIA	KLEFFMANN	OILSEED-RAPE/CANOLA	х
СР	CANADA	AGDATA		х
СР	CHINA	KLEFFMANN	CORN/MAIZE	х
СР	CHINA	KLEFFMANN	RICE	х
СР	CHINA	ARN/SHANGHAI	All available crops	х
СР	CZECH REP.	KLEFFMANN	CEREALS	х
СР	CZECH REP.	KLEFFMANN	CORN/MAIZE	х
СР	CZECH REP.	KLEFFMANN	OILSEED-RAPE/CANOLA	х
СР	CZECH REP.	KLEFFMANN	POTATOES	х
СР	CZECH REP.	KLEFFMANN	BEETS	х
СР	CZECH REP.	KLEFFMANN	GRAPES	Х
СР	DENMARK	KLEFFMANN	CEREALS	х
СР	FINLAND	KLEFFMANN	CEREALS	х
СР	FRANCE	ADQUATION-FRANCE	BEETS	Х
СР	FRANCE	ADQUATION-FRANCE	CEREALS	Х
СР	FRANCE	ADQUATION-FRANCE	CORN/MAIZE	х
СР	FRANCE	ADQUATION-FRANCE	OILSEED-RAPE/CANOLA	х
СР	FRANCE	ADQUATION-FRANCE	FORAGE CROPS	х
СР	FRANCE	ADQUATION-FRANCE	SORGHUM & MILLET	х
СР	FRANCE	ADQUATION-FRANCE	SUNFLOWER	х
СР	FRANCE	ADQUATION-FRANCE	SOYBEANS	х
СР	FRANCE	ADQUATION-FRANCE	POTATOES	Х
СР	FRANCE	ADQUATION-FRANCE	TOP FRUITS	Х
СР	GERMANY	KLEFFMANN	BEETS	х

СР	GERMANY	KLEFFMANN	CEREALS	Х
СР	GERMANY	KLEFFMANN	CORN/MAIZE	Х
СР	GERMANY	KLEFFMANN	OILSEED-RAPE/CANOLA	Х
СР	GERMANY	KLEFFMANN	FORAGE CROPS	Х
СР	GERMANY	KLEFFMANN	OILSEEDS: OTHER	Х
СР	GERMANY	KLEFFMANN	POTATOES	Х
СР	GERMANY	KLEFFMANN	FRUITS	х
СР	GERMANY	KLEFFMANN	ASPARAGUS	Х
СР	GERMANY	KLEFFMANN	GRAPES	х
СР	GERMANY	KLEFFMANN	STRAWBERRY	Х
СР	HUNGARY	KLEFFMANN	BEETS	Х
СР	HUNGARY	KLEFFMANN	CEREALS	Х
СР	HUNGARY	KLEFFMANN	CORN/MAIZE	Х
СР	HUNGARY	KLEFFMANN	OILSEED-RAPE/CANOLA	Х
СР	HUNGARY	KLEFFMANN	SUNFLOWER	Х
СР	HUNGARY	KLEFFMANN	VEGETABLES & FLOWERS	Х
СР	HUNGARY	KLEFFMANN	FRUITS	Х
СР	HUNGARY	KLEFFMANN	GRAPES	Х
СР	INDONESIA	KLEFFMANN	CORN/MAIZE	Х
СР	KAZAKHSTAN	KLEFFMANN	CEREALS	Х
СР	KAZAKHSTAN	KLEFFMANN	COTTON	Х
СР	KAZAKHSTAN	KLEFFMANN	FLAX/LINSEED	Х
СР	KAZAKHSTAN	KLEFFMANN	SUNFLOWER	х
СР	KAZAKHSTAN	KLEFFMANN	RICE	х
СР	KAZAKHSTAN	KLEFFMANN	VEGETABLES & FLOWERS	х

СР	KAZAKHSTAN	KLEFFMANN	FRUITS	Х
СР	KAZAKHSTAN	KLEFFMANN	LENTIL	х
СР	KAZAKHSTAN	KLEFFMANN	POTATOES	х
СР	LATVIA	KLEFFMANN	CEREALS	х
СР	LATVIA	KLEFFMANN	OILSEED-RAPE/CANOLA	х
СР	LITHUANIA	KLEFFMANN	CEREALS	х
СР	LITHUANIA	KLEFFMANN	OILSEED-RAPE/CANOLA	х
СР	MEXICO	KLEFFMANN	CORN/MAIZE	х
СР	MEXICO	KLEFFMANN	POTATOES	х
СР	MEXICO	KLEFFMANN	TOMATOES	х
СР	NETHERLANDS	BRANCHES&TRENDS	ARABLE CROPS	х
СР	NETHERLANDS	BRANCHES&TRENDS	FLOWER BULBS	х
СР	NETHERLANDS	BRANCHES&TRENDS	CAULIFLOWER	х
СР	NETHERLANDS	BRANCHES&TRENDS	BROCCOLI	х
СР	NETHERLANDS	BRANCHES&TRENDS	FRUITS	х
СР	PARAGUAY	KLEFFMANN	CEREALS	х
СР	PHILIPPINES	KLEFFMANN	CORN/MAIZE	х
СР	PHILIPPINES	KLEFFMANN	RICE	х
СР	POLAND	KLEFFMANN	BEETS	х
СР	POLAND	KLEFFMANN	CEREALS	х
СР	POLAND	KLEFFMANN	CORN/MAIZE	х
СР	POLAND	KLEFFMANN	OILSEED-RAPE/CANOLA	х
СР	POLAND	KLEFFMANN	POTATOES	х
СР	POLAND	KLEFFMANN	FRUITS	х
СР	POLAND	KLEFFMANN	BERRIES	х

СР	POLAND	KLEFFMANN	VEGETABLES & FLOWERS	Х
СР	ROMANIA	KLEFFMANN	CEREALS	Х
СР	ROMANIA	KLEFFMANN	CORN/MAIZE	Х
СР	ROMANIA	KLEFFMANN	OILSEED-RAPE/CANOLA	Х
СР	ROMANIA	KLEFFMANN	SUNFLOWER	Х
СР	ROMANIA	KLEFFMANN	POTATOES	Х
СР	ROMANIA	KLEFFMANN	SOYBEANS	Х
СР	ROMANIA	KLEFFMANN	FRUITS	х
СР	ROMANIA	KLEFFMANN	VEGETABLES & FLOWERS	Х
СР	ROMANIA	KLEFFMANN	GRAPES	Х
СР	RUSSIAN FED.	KLEFFMANN	CEREALS	Х
СР	RUSSIAN FED.	KLEFFMANN	CORN/MAIZE	х
СР	RUSSIAN FED.	KLEFFMANN	OILSEED-RAPE/CANOLA	Х
СР	RUSSIAN FED.	KLEFFMANN	SORGHUM & MILLET	Х
СР	RUSSIAN FED.	KLEFFMANN	SUNFLOWER	Х
СР	RUSSIAN FED.	KLEFFMANN	SOYBEANS	Х
СР	RUSSIAN FED.	KLEFFMANN	FRUITS	Х
СР	RUSSIAN FED.	KLEFFMANN	POTATOES	Х
СР	RUSSIAN FED.	KLEFFMANN	BEETS	Х
СР	RUSSIAN FED.	KLEFFMANN	VEGETABLES & FLOWERS	Х
СР	RUSSIAN FED.	KLEFFMANN	GRAPES	Х
СР	SLOVAKIA	KLEFFMANN	CEREALS	Х
СР	SLOVAKIA	KLEFFMANN	CORN/MAIZE	х
СР	SLOVAKIA	KLEFFMANN	SUNFLOWER	х
СР	SLOVAKIA	KLEFFMANN	OILSEED-RAPE/CANOLA	х

СР	SLOVAKIA	KLEFFMANN	POTATOES	Х
СР	SLOVAKIA	KLEFFMANN	BEETS	Х
СР	SLOVAKIA	KLEFFMANN	GRAPES	Х
СР	SWEDEN	KLEFFMANN	CEREALS	х
СР	THAILAND	KLEFFMANN	CORN/MAIZE	х
СР	TURKEY	KLEFFMANN	CEREALS	х
СР	U.KINGDOM(UK)	KYNETEC-SEED- DRESSING	BEETS	х
СР	U.KINGDOM(UK)	KYNETEC-SEED- DRESSING	CEREALS	х
СР	U.KINGDOM(UK)	KYNETEC-SEED- DRESSING	CORN/MAIZE	Х
СР	U.KINGDOM(UK)	KYNETEC-SEED- DRESSING	OILSEED-RAPE/CANOLA	х
СР	U.KINGDOM(UK)	KYNETEC-SEED- DRESSING	FLAX/LINSEED	Х
СР	U.KINGDOM(UK)	KYNETEC-SEED- DRESSING	FORAGE CROPS	Х
СР	U.KINGDOM(UK)	KYNETEC-SEED- DRESSING	OILSEEDS: OTHER	Х
СР	U.KINGDOM(UK)	KYNETEC-SEED- DRESSING	POTATOES	х
СР	U.KINGDOM(UK)	KYNETEC	BEETS	х
СР	U.KINGDOM(UK)	KYNETEC	CEREALS	х
СР	U.KINGDOM(UK)	KYNETEC	CORN/MAIZE	х
СР	U.KINGDOM(UK)	KYNETEC	OILSEED-RAPE/CANOLA	х
СР	U.KINGDOM(UK)	KYNETEC	FALLOW-LAND/SET-ASID	х
СР	U.KINGDOM(UK)	KYNETEC	FLAX/LINSEED	х
СР	U.KINGDOM(UK)	KYNETEC	FORAGE CROPS	х

СР	U.KINGDOM(UK)	KYNETEC	OILSEEDS: OTHER	Х
СР	U.KINGDOM(UK)	KYNETEC	POTATOES	х
СР	UKRAINE	KLEFFMANN	BEETS	Х
СР	UKRAINE	KLEFFMANN	CEREALS	Х
СР	UKRAINE	KLEFFMANN	CORN/MAIZE	х
СР	UKRAINE	KLEFFMANN	OILSEED-RAPE/CANOLA	Х
СР	UKRAINE	KLEFFMANN	SORGHUM & MILLET	х
СР	UKRAINE	KLEFFMANN	SUNFLOWER	х
СР	UKRAINE	KLEFFMANN	FRUITS	Х
СР	UKRAINE	KLEFFMANN	GRAPES	х
СР	UKRAINE	KLEFFMANN	VEGETABLES & FLOWERS	х
СР	UKRAINE	KLEFFMANN	POTATOES	Х
СР	UKRAINE	KLEFFMANN	SOYBEANS	Х
СР	URUGUAY	KLEFFMANN	SOYBEANS	Х
СР	USA	KYNETEC	CORN/MAIZE	х
СР	USA	KYNETEC	SOYBEANS	х
СР	USA	KYNETEC	COTTON	х
СР	USA	KYNETEC	SPECIALTY CROPS	х
СР	USA	KYNETEC	OTHER ROW CROPS	Х
СР	VIETNAM	KLEFFMANN	CORN/MAIZE	Х
СР	VIETNAM	KLEFFMANN	RICE	х

8. Appendix II: Checklist Quality Standards for Panel Providers

Checklist Panel Quality Standards for Panel Providers

-1-

/ /			Documentation		Cor	trol
	Recom- mended	Must	Internal	To client	Carried out?	Result OK?
. Information about agricultural universe						
1.1. Country:		X		Х		
1.2. Definition of the covered region, sub-regions relevant to the evaluation		X		X		
1.3. Statistics about:						
Cultivated areas by crops		X		Х		
 Farm structures according to country specific farm sizes for crops, according to the regions (smallest unit: farm size specific to the crop for a crop in a region) 		X		x		
1.4. Special features (e.g. peculiar significance of small or large farms)		X		X		
1.5. Data source: publisher and date / period for all statistics used in 1.3 / for the extrapolation		X		Х		

- 2 -

Recom- mendedMustInternal clientTo clientCarried out?2.1. Targeted sample according to farm sizes per crop and region••					Docume	ntation	Con	ntrol	
Description of sampling 2.1. Targeted sample according to farm sizes per crop and region Representative for the total cultivated area of the respective crop Coverage: at least 90% of the respective cultivated crop area Coverage: at least 50% of the farmers of the respective crop X X Coverage: at least 50% of the farmers of the respective crop X X Consideration of "cut offs" = farm size classes, grown/cultivated crop area Safety level = 95% at an error probability of 5% X Safety level = 95% at an error probability of 5% X Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%: for each crop per country X X Tor each farm size class per crop / country X X X Tor each farm size class per crop / country X X X Tor each farm size class per crop / country X X			Recom- mended	Must	Internal	To client	Carried out?	Result OK?	
2.1. Targeted sample according to farm sizes per crop and region Representative for the total cultivated area of the respective crop X Coverage: at least 90% of the respective cultivated crop area X X Coverage: at least 50% of the farmers of the respective crop X X Coverage: at least 50% of the farmers of the respective crop X X	Descriptio	on of sampling							
• Representative for the total cultivated area of the respective crop X X • Coverage: at least 90% of the respective cultivated crop area X X • Coverage: at least 50% of the farmers of the respective crop X X • At least 30 interviews per cell X X • Consideration of "cut offs" = farm size classes, grown/cultivated crop areas X X • Consideration of "cut offs" = farm size classes, grown/cultivated crop areas X X • Safety level = 95% at an error probability of 5% X X X • Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%: X X X • for each crop per country X X X X • for each crop per country X X X X • for each farm size class per crop / country X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X	2.1. Targete	ed sample according to farm sizes per crop and region							
• Coverage: at least 90% of the respective cultivated crop area X X • Coverage: at least 50% of the farmers of the respective crop X X • At least 30 interviews per cell X X • Consideration of "cut offs" = farm size classes, grown/cultivated crop areas X X • Safety level = 95% at an error probability of 5% X X • Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%: X X • for each crop per country X X X • for each crop per country X X X • for each farm size class per crop / country X X X • for each farm size class per crop / country X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region </td <td>•</td> <td>Representative for the total cultivated area of the respective crop</td> <td></td> <td>X</td> <td></td> <td>Х</td> <td></td> <td></td>	•	Representative for the total cultivated area of the respective crop		X		Х			
Coverage: at least 50% of the farmers of the respective crop X X X At least 30 interviews per cell X X Consideration of "cut offs" = farm size classes, grown/cultivated crop areas Safety level = 95% at an error probability of 5% X X Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%: for each crop per country for each crop per region X X X A for each farm size class per crop / country X X X Consideration data (confidence intervals) for market share levels of 5/10/20%: for each crop per country X X X Consideration Safety level = 95% at an error probability of 5% X X Consideration data (confidence intervals) for market share levels of S10/20%: for each crop per country X X X Consideration Safety level = 0, so the stratification method (distribution of the interviews X X X	•	Coverage: at least 90% of the respective cultivated crop area		X		Х			
• At least 30 interviews per cell X X X • Consideration of "cut offs" = farm size classes, grown/cultivated crop areas X X X • Safety level = 95% at an error probability of 5% X X X X • Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%: X X X • for each crop per country X X X • for each crop per region X X X • for each farm size class per crop / country X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • Statistication method (distribution of the interviews X X X	•	Coverage: at least 50% of the farmers of the respective crop		X		Х			
Consideration of "cut offs" = farm size classes, grown/cultivated crop areas Safety level = 95% at an error probability of 5% X X Safety level = 95% at an error probability of 5% X X Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%: for each crop per country X X X for each crop per region X X X for each farm size class per crop / country X X for each farm size class per crop / region X X X Safety level Safety Safety level Safety level Safety Safety	•	At least 30 interviews per cell		X		Х			
Safety level = 95% at an error probability of 5% X X X Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%: for each crop per country X X X for each crop per region X X X for each farm size class per crop / country X X for each farm size class per crop / region X X 2.2. Actual sample (criteria the same as for targeted sample) X X 2.3. Description of the stratification method (distribution of the interviews X X	•	Consideration of "cut offs" = farm size classes, grown/cultivated crop areas		X		Х			
Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%: for each crop per country for each crop per region X X X	•	Safety level = 95% at an error probability of 5%		X		Х			
• for each crop per country X X X • for each crop per region X X X • for each farm size class per crop / country X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X • for each farm size class per crop / region X X X <td>•</td> <td>Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%:</td> <td></td> <td>X</td> <td></td> <td>Х</td> <td></td> <td></td>	•	Information regarding deviations for percentages / extrapolation data (confidence intervals) for market share levels of 5/10/20%:		X		Х			
for each crop per region X X X		 for each crop per country 		X		Х			
for each farm size class per crop / country X X X		 for each crop per region 		X		Х			
for each farm size class per crop / region X X X 2.2. Actual sample (criteria the same as for targeted sample) X X 2.3. Description of the stratification method (distribution of the interviews X X		 for each farm size class per crop / country 		X		X			
2.2. Actual sample (criteria the same as for targeted sample) X X 2.3. Description of the stratification method (distribution of the interviews X X		 for each farm size class per crop / region 		X		X			
2.3. Description of the stratification method (distribution of the interviews X X	2.2. Actual	sample (criteria the same as for targeted sample)		X		Х			
with regard to cultivated areas, crops and regions)	2.3. Descrip with re	otion of the stratification method (distribution of the interviews gard to cultivated areas, crops and regions)		X	X				
	WITTE	garu to cultivated areas, crops and regions)							

		IS		Cantral																																																							
		-	Decem	Decem	Decem	Decem	_	_	Decem	Decem	Decem	Decem						_	-	_	-	-	-	Decem	Decem	Decem	Decem	-					_								_	Recom-	Recom-					-		-			Decem		Docume	cumentation	mentation Co	Con	trol
		Recom- mended	Must	Internal	client	Carried out?	Result OK?																																																				
2.4. Su	rvey periods																																																										
a)	Conducted waves in the same crop (time/date)		X	X																																																							
b)	Number of interviews in the individual waves (for panel approach = number		X	X																																																							
	of the constant panel farms / mortality rate)																																																										
2.5.Ch	anges to sampling compared to the previous years																																																										
•	Panel: panel mortality in percent		X	X																																																							
•	Changes to the number of interviews in the individual cells		X	X																																																							

Checklist Panel Qua	lity Standards					
	-		Docume	Documentation		trol
	Recom- mended	Must	Internal	To client	Carried out?	Result OK?
3. Description of the recruiting method						
3.1. Survey methods				X		
Panel approach						
Ad-hoc survey						
3.2. Methods of data collection				X		
Farm by farm						
Crop by crop						
Field by field						
3.3. Interview technique				X		
 Face to face = % of the interviews 						
 CATI = % of the interviews 						
 Online = % of the interviews 						
 Self-completion = % of the interviews 						
3.4. Selection method				X		
Random						
Quotas						
Cluster sampling						
Others						

- 5 -

				Documer	ntation	Con	trol
	Recom- mended	Must	Internal	To client	Carried out?	Result OK?	
4. Questionnaire							
4.1. Contents / structure of questionnaire							
4.1.1. Screening questions to control target group		X		Х			
4.1.2. Logic checks in the questionnaire	X		Х				
4.1.3 Main part plant protection measures:							
Recording the cultivated area per crop		X		X			
Recording the number of crops per field and year (rotations)		X		X			
 Definition of the treated area (information should refer to the 		X		X			
effectively treated area, including band/row and partial							
treatment/patches, and even if a part of land is used several times per							
year for one crop).							
 Recording of the non-treated area in the crop (to estimate potentials) 		X		X			
 Recording of products, mixtures, spraying sequences, reasons for 		X		X			
use							
Net area		X		X			
 Super-developed area (= area treated with product) 		X		X			
 Tractor-treated area (= treated basic area, number of tractor crossings) 		X		X			
 Dose rate in I/ha or I/100I water or litres per water (concentration) 		X		X			
 Dose rate in the cultivation of grapes, fruit, hops, etc. : 		X		X			
- Dose rate per ha.		X		X			
 Dose rate per 100l of spray mixture + applied volume of water or volume of water and concentration of the spray mixture 		X		X			
Dose rate for seed dressings:		X		X			
 Seed sowing rate, sowing amount per ha. For corn / rapeseed, also quantity of seed units per ha. 		X		Х			

			Docume	ntation	Con	trol
	Recom- mended	Must	Internal	To client	Carried out?	Result OK?
 Dose rate of seed dressing per 100kg seeds 		X		X		
 Assignment of twin packs / combi packs or products with additives/ adjuvants and their use (together/separately) 		X		X		
 Aims of control (most important pests/weeds/grass weeds/ diseases) per product used 		X		Х		
4.2. Show cards						
4.2.1. Development stages (with BBCH code and standard name as a graphic)		X		X		
4.2.2. Lists of pasts/waads/grass waads/diseases (the 15 most important of pac	h)					
Colloquial nomenclature	<u> </u>	X		X		
Latin nomenclature		X		X		
4.2.3. Product lists par crop						
If the market bas generic products		X		X		
If the market has no generic products		X		X		
				~		
4.3. Price records				·		
 Wherever possible, based on submitted invoices (ratio of prices from invoices:%) 	X			X		
Record as price per kg/l		X		X		
Including or excluding VAT		X		X		
Discounts and discount amount		X		X		
4.4. Providing of questionnaire including show cards in English and the national language		X		X		
		V		Y		

			Docume	ntation	tion Con	
	Recom- mended	Must	Internal	To client	Carried out?	Resu OK
5. Interviewers						
5.1. Number and distribution of the interviewers over the regions		X	Х			
5.2. Information on the qualifications of the interviewer (e.g. education, background, experience, mastery of regional dialects)		X	Х			
5.3. The training methods used						
Training documentation		X	Х			
Supervision		X	Х			

- 8 -
| | | | Docume | ntation | Con | trol |
|--|------------------|-------------|----------|--------------|--------------|---------------|
| | Recom-
mended | Must | Internal | To
client | Carried out? | Result
OK? |
| Weighting and extrapolation processes | | | | | | |
| 1. Method, general | | X | | X | | |
| Weighting by farms | | | | | | |
| Weighting by areas | | | | | | |
| 2. Weighting process | | X | | X | | |
| Stage (single-stage, multi-stage) | | | | | | |
| Definition of the weighting cells (crops/regions/farm size classes) | | | | | | |
| 3. Weighting factors | | | | | | |
| Number of interviews per weighting cell (minimum = 30) | | X | | X | | |
| Size of the weighting factors (specification = no more than 100) | | X | | X | | |
| 3. Evaluation of the confidence intervals (at an error probability of 5%,
For market share levels of 5/10/20%: | 95% safety lev | el) | | | | |
| for each crop and country | | X | | X | | |
| for each crop and region | | X | | X | | |
| for each crop and farm size class | | X | | X | | |
| for each region/crop/farm size (so far as it is relevant) | | X | | Х | | |
| for each crop and region for each crop and farm size class for each region/crop/farm size (so far as it is relevant) | | X
X
X | | X
X
X | | |

			Docume	ntation	Con	ntrol	
	Recom-	Must	Internal	To	Carried	Result	
Evaluation / Reporting	menueu			chent	out		
. Quality controls before the evaluation							
7.1.1. Method and ratio of controlled interviews (at least 10%, yet not only about problem farms) and controlled interviewers		X	Х				
7.1.2. Information regarding the identification method for illogical data (two- stage data check: first of all plausibility, then logical consistency)		X	X				
7.1.3. Recording of the controls		X	X				
7.1.4. Recording of the initiatives to participate due to possible influence on the data quality		X	Х				
7.1.5. Problem report (design of the questionnaire, illogical entries, rejects, callbacks due to problems in interview,)		X	X				

· · · · · · · · · · · · · · · · · · ·	Recom-	Must	Docume Internal	ntation To	Con Carried	trol Result
	mended			client	out?	OK?
7.2. Basic results						
7.2.1. per country, defined region, crop and pesticide segments:		X		X		
• areas						
market shares						
dose rates						
tons						
turnovers						
for total market, product and ingredient						
7.2.2. per country, crop and pesticide segment:		X		X		
tank mixtures						
spraying sequences						
7.3. Specifics						
7.3.1. Identification of twin packs applied together or separately		X		X		
7.3.2. Identification of the aims of control in Latin nomenclature		X		X		
7.3.3. Identification of the application times according to the BBCH code		X		X		
7.3.4. Orientation towards the data format by Kleffmann		X	<u> </u>			

- 11 -

					Docume	ntation	Cor	ntrol
			Recom- mended	Must	Internal	To client	Carried out?	Result OK?
7.4.	Data	transfer and submission						
	٠	Data delivery within 4-6 weeks after the last interview is done		Х		X		
	•	Forwarding of the data simultaneously to local clients and Agrobase		Х		X		
		, <u> </u>						