Report on environmental risk and benefits assessment (TR3.3.)

Christian C. Bockstaller

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ENDURE

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Report on environmental risk and benefits assessment (TR3.3.)

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Dissemination Level	
PU Public	**X**
PP Restricted to other programme participants (including the Commission Services)	
RE Restricted to a group specified by the consortium (including the Commission Services)	
CO Confidential, only for members of the consortium (including the Commission Services)	

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Glossary

a.i.	active ingredient
ATKIS	Authoritative Topographic Cartographic Information System
BÜK1000	Digital soil map for Germany
DT50	Degradation rate in soil
DT50:	Hydrolytic stability (in d)
ETR:	Exposure toxicity ratios
HC50:	The mean hazardous concentration affecting 50% of the species present in the ecosystem
HDF:	Human Damage Factor. Variable used to describe damage to human health ion Impact 2002+
HTPx,i:	The human toxicity potential for a substance x released to compartment I (1,4-DCB equivalents);
KOC	
LC50:	Lethal concentration 50%. Concentration lethal to 50% of test organisms
lPEC:	Predicted environmental concentration (long-term)
NOEC:	No observed effect concentration. The highest concentration observed to result in no effects in test organisms.
PEC:	Predicted environmental concentration
PPP:	Plant Protection Products
sPEC:	Predicted environmental concentration (short-term)
TFI	Treatment frequency index
GPP	good plat protection practice

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Summary

The main objective of this report was focused on comparing model performances for crop protection strategies in wheat and pomefruit using GIS based environmental scenarios for two different regions. The tree available environmental risk models PRZM-USES, SYNOPS and I-PHY were applied, each having their own methodology but also sharing many characteristics and output parameters.

An essential prerequisite for the model comparison was the establishment of a common and harmonised input data base for all three models. A geo-database for environmental data was built for the two case study regions Saxony-Anhalt (wheat) and Lake Constance (pomefruit) including all input parameters relevant to the RA-models on field level. A second database related to the pesticide use in these regions was established for the crops wheat and pomefruit on the basis of former survey conducted at the JKI. For the wheat case study region 156 region specific applications strategies and for the pomefruit 50 region specific applications strategies were analysed. It was further necessary to define a standard database describing the chemical, physical and eco-toxicological properties of the active ingredients.

In total 7488 wheat scenarios and 900 pomefruit scenario were evaluated with the RA-models. The practical application of the three RA-models showed that the model PRZM-USES is not suitable to handle such large numbers of parameter sets and that the parameterisation of I-PHY needed some adoption of the input and output structure of the model.

In a first step the risk potentials assessed with I-PHY and SYNOPS were compared with the treatment frequency index (TFI). The overall comparison of the I-PHY assessments showed only weak correlation for wheat and no correlation for pomefruit. The same is true for the assessments with SYNOPS. No correlation between TFI and risk potential could be found for pomefruit and only weak positive correlations could be found for the wheat scenarios.

The risk assessments of the two models I-PHY and SYNOPS were compared. Considering all scenarios, high correlations between the two models could be found for the wheat and pomefruit scenarios. In all cases the correlation coefficients were around 0.7. Overall, the chronic risk potential showed slightly higher correlation coefficients than the acute risk potential.

Although a good correlation could be found between the model results, there is still a large difference in the classification of the calculated risks between the two models. An analysis of the classified results for the wheat case study region revealed a convergence between the two models of 62 % for the acute risk potential and of 66% for the chronic risk potential. This means that in 34 % (38 %) of all cases, the classification whether a risk was tolerable or not was different between the two models.

1 Introduction

In the last years various indicator models have been developed to assess the risk potential of the usage of plant protection products (PPP) to the environment and human health. Due to the large variety of these risk indicators and their different approaches it is difficult to find a consensus on the methodologies. Some indicators cover a rather large number of compartments, while others are more dedicated to one or a few compartments. Some models consider a wide range of exposure pathways and reference organisms others only a few.

In Europe there are many activities toward a harmonised method of environmental risk assessment. For example, the EU research project HAIR (2007) aimed at developing and integrating scientific expertise on the use, emissions, environmental fate, and the impact of PPP's on agro-ecosystems and human health, in order to develop a harmonised European approach for indicators. Similar goals were achieved by the EU-Project FOOTPRINT (2009). The overall objective of the FOOTPRINT project was to develop a set of unified tools that will allow users to identify the dominant pathways and sources of pesticide contamination in the agricultural landscape and to estimate levels of pesticide concentrations in surface water and groundwater.

There are still well established models in use, which vary in their methodology, in the compartments and exposure pathways they consider and in the form of the results they calculate. Different methods have been developed to compare these agro-ecological assessment models. Some authors use a descriptive (Girardin 2001; Reus et al. 2002; van der Werf and Petit 2002) others a more systematic approach (Gebauer and Bäuerle 2000; Hertwich et al. 1997). Bockstaller et al. (2006 and 2009) developed a new evaluation tool with clearly defined decision rules. Following a similar approach, within sub-activity RA3.4 of the ENDURE-Network three risk assessment models and four LCA toxicity models have been evaluated by means of a multicriteria analysis (see DR3.4).

One objective of the sub-activity RA3.3 is the assessment of the environmental and agronomic risk of current and innovative strategies. Three different risk assessment models, which were developed by the partners of RA3.3, were identified to accomplish this task. These are SYNOPS (Gutsche and Strassemeyer, 2007), I-PHY (Bockstaller et al., 2004 and 2008) and PRZM-USES (Mamy et al. 2007 and 2008). In addition to the risk assessments with these models, the treatment frequency index (TFI) is calculated for the analysed strategies. In section two of this report the applied models are described and characterised.

On the basis of a multicriteria analysis these models have already been evaluated in the deliverable DR3.4. In this report the models will be compared and evaluated on the basis of their modelling results. In order to compare the results it was mandatory to use common databases for the input parameters. Therefore an important task in this sub-activity was to establish a common environmental database including input parameters for climate conditions and field conditions and to link this database to the considered RA-models. Additionally it was essential to agree on a common database for the pesticide properties.

For the comparison of the models, it was planned to apply the risk assessment models to the selected case study regions for wheat and pomefruit. Within the research activity RA 3 main producing areas of winter wheat and pomefruit in Europe were chosen as case-study regions. In section 3 of this report the input data, which are necessary to run the risk assessment models are described for the selected wheat and pomefruit case study regions in detail.

2 Characterisation of the risk assessment models

2.1 General overview of the applied models

2.2 Description of the applied models and indicators

2.2.1 Treatment frequency index

The treatment frequency index (TFI) is a measure of the intensity of Plant protection and is based on the number of applied plant protection products (PPP). For the calculation of the TFI each product is counted separately even if it was applied in a tank mixture.

The TFI is calculated as the number of applied PPP's related to the fraction of the area the product was applied on ($f_{area} = A_{applied}/A_{field}$) and related to the percentage of the used application rate to the maximum allowed application rate ($f_{rate} = AR/AR_{ma}$). For each application of a PPP a sub-index (TFI_x) is calculated as:

$$1 * f_{area} * f_{rate} = TFI_x.$$

The sum of all sub-indices of a pesticide use strategy with n applications is then equal to the TFI of the whole application strategy:

$$TFI = \sum_{x=1}^{n} TFI_x$$

2.2.2 I-PHY

The pesticide risk indicator I-PHY was developed in parallel to other environmental indicators for the assessment method INDIGO (Bockstaller et al., 1997; Bockstaller et al., 2009). The core of the indicator was published by van der Werf and Zimmer (1998) and enhanced, adapted and tested by Bockstaller (2004 and 2008), for arable farming. Since then, I-PHY was adapted to other farming systems like wine growing, fruit production, field vegetable production, palm tree, etc.

For a single application of a pesticide, the calculation of the indicator is based on four modules assessing respectively the risk linked to the amount of active ingredient applied and the risk for groundwater, surface water and air. For some production like wine growing, fruit production, a module addressing the effect on beneficials (natural enemies of pests and pollinators) was added. In a second step, an overall indicator is calculated. Three types of input variables are used:

1. pesticides properties linked to exposure or to eco-toxicological effect,
2. site-specific conditions (e.g. runoff risk)
3. characteristics of the pesticide application (e.g. rate of application).

A fuzzy expert system is used to aggregate all these heterogeneous variables into indicator modules and to subsequently aggregate these modules into a synthetic indicator. Fig. 1 shows an example for ground water risk for which main weight is given to a pesticide property (GUS variable) and less weight to position (crop interception here) and soil sensitivity to leaching. It should be noticed that for surface water, sensitivity of field to runoff and drift plays a major role in comparison with pesticide property (DT50 variable). In all component of I-PHY, toxicity or eco-toxicity variable can increase but not decrease the risk. The use of fuzzy subset enables to avoid effect of knife-edge limit of a given class. Output values for each module as well for the overall indicator are expressed on a qualitative scale used in the INDIGO method: between 0 (maximum risk) and 10 (no risk) with a reference value of 7 (maximum acceptable risk). The first prototype was based on the inverse scale between 0 (no risk) and 1 (maximum risk), which is also used in some recent application (Sadok et al., 2009).

For a programme of pesticides applications, an aggregated indicator is obtained by subtracting to the lowest single indicator value among the pesticides application in the strategy, scores of the other applications. Those depend on the indicator value of each other pesticide in the strategy. By this mean, the aggregated value cannot be better than a single application. Scores are weighted so that most of strategies have a value above 0. Spatial aggregation from field to farm or higher is carried out by calculating a weighted mean by field size.

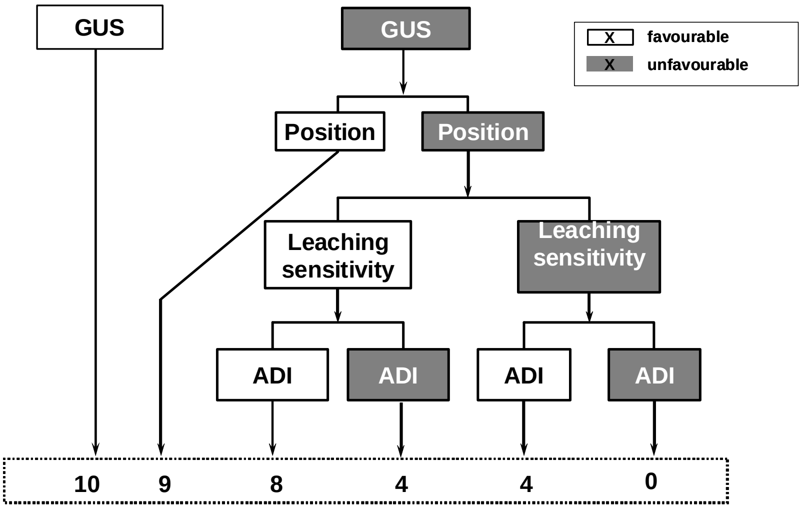


Figure 1: Decision tree of the groundwater component of I-PHY.

In the last five years, the I-PHY indicator was implemented in more than 100 cases in France by advisers mainly working on assessment of risks on field/farms level or working on the development of innovative cropping systems. Some applications were carried out at water catchment level. Adaptation of the indicator to this level is still undergoing.

2.2.3 PRZM-USES

The method of pesticide risk and impact assessment developed by Mamy et al. (2007) combines a pesticide fate model and an exposure and effects model.

The fate of pesticide is assessed by first running the Pesticide Root Zone Model (PRZM 3.21) (Carsel et al., 1998) to estimate the amounts of pesticides in soil, water and air over several years. The performance of PRZM was previously tested by comparing its predictions to experimental data. As a result, PRZM allowed correct predictions of the fate of pesticides (Mamy et al., 2008).

The concentrations of pesticides which were calculated with PRZM are subsequently aggregated with the multi-media fate, exposure and effects model Uniform System for the Evaluation of Substances (USES 2.0) (RIVM, 1998; Huijbregts et al., 2000) to estimate the final impacts of various cropping systems on environment (water, sediment, terrestrial ecosystems) and human health.

The USES model allows calculation of toxicity potentials (TP) of pesticides. These TP are then used to determine the impact scores I of the emission into compartment c (soil, water, ...) of m kg of pesticide p on a particular target t (human, water, ...):

$$I = m \times TP_{c,t,p}$$

where I is expressed in kg eq. 1,4-DCB, TP is the toxicity potential for target t associated with the emission of pesticide p in environmental compartment c, and m is the amounts of pesticide leached or present in soil, water and air calculated with PRZM. Thus, the higher the score, the higher the impact (however, as this method allows only a relative assessment of the impact there are no threshold values for TP and I).

The final impact scores of a technical programme were calculated by summing the impact scores of the various pesticides used in the programme.

2.2.4 SYNOPS

Since published in 1997 (Gutsche and Rossberg, 1997) the model SYNOPS for synoptic assessment of risk potential of chemical plant protection products has been used and further developed within national (Gutsche and Rossberg 1999) and European projects (Gutsche 2004). The model evaluates the risk potential for terrestrial (soil and field margin biotopes) and aquatic (surface water) organisms. It combines use data of pesticides with the environmental conditions linked to the application and the chemical, physical and eco-toxicological properties of the pesticides. Especially the exposure of organisms is calculated by sophisticated sub-models. The recent version of the model was extended to assess the environmental risk potential of plant protection strategies on landscape level using GIS functionalities by linking it to geo-referenced databases for land use, soil conditions and climate data and to a dataset of regionalised surveys of pesticide application. SYNOPS is also used on national level to track the trend of pesticide risks in Germany since 1987 on the basis of sales data (Gutsche and Strassemeyer; 2007). The model is integrated in the national action plan for pesticide risk reduction.

Besides the national and landscape functionality, SYNOPS can be run on field level to assess the environmental risk of pesticide use strategies under different environmental conditions. Within the sub-activity of RA3.4 mainly the field based functionality of the model will be considered.

In general, the risk potentials are calculated as exposure toxicity ratios (*ETR*) for reference organisms in the three compartments soil, surface water and field margin biotopes. These organisms are earthworms for soil, bees for field margin biotopes and Daphnia, algae and fish for surface water.

SYNOPS estimates for each application the loads of an active ingredient (a.i.) into the soil, edge- biotopes and surface water. Based on the estimated loads of a.i.'s a time dependent curve of the predicted environmental concentration (*PEC*) is derived considering temperature dependent degradation according to a first order kinetics.

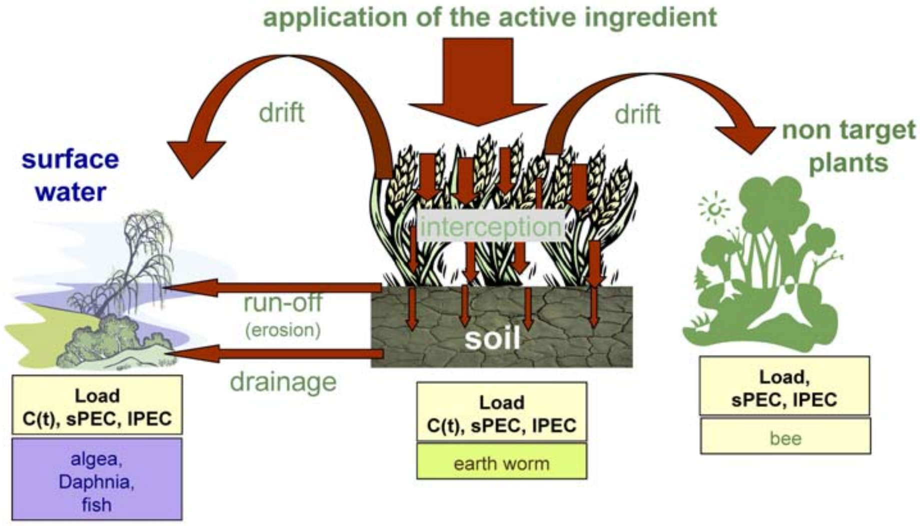


Figure 2: Exposition pathways considered in SYNOPS

Loads and *PEC*'s of an a.i. in the soil are caused directly by pesticide application considering the interception of the crop. The drift into field margin biotopes is estimated by taking into account the distance from the field to the biotope as well as size and structure of the particular biotope. The loads and *PEC*'s in the surface water depend on the minimal distance from the field edge to the edge of the surface water, on the surface water type and dimension, on the slope and on the soil parameters like texture and organic carbon contend. The considered exposure pathways into the surface water are drift, run-off, and drainage. (Fig. 2)

From the time dependent concentration curves the short-term (*sPEC*) and long-term environmental concentration (*lPEC*) are derived. The maximum concentration over a vegetation period (*sPEC*) is used to calculate the acute risk potential. To estimate the chronic risk potential an integral over a time interval, equal to the time period of the NOEC standard test (*tNOEC*) is calculated on daily basis. The maximum of these integrals over the vegetation period (*lPEC*) is then considered for the chronic risk potential.

$$sPEC = \max_{t=1}^{365} CT(t), \qquad lPEC_{sw} = \max_{t=1}^{365} \frac{\int_{t-t_{NOEC}}^{t} CT(t)}{t_{NOEC}}$$

As a measure for the toxicity the lethal concentration (*LC50*) and the no effect concentration (*NOEC*) are considered to estimate the acute and chronic risk potential.

$$ETR_{acute(species)} = \frac{sPEC}{LC50_{species}}, \qquad ETR_{chronic(species)} = \frac{lPEC}{NOEC_{species}}$$

All necessary physico-chemical and eco-toxicological parameters of the applied active ingredients (n=350) are summarised in a database, which is continuously updated at JKI.

2.3 Comparison of the applied models

In order to compare the indicators evaluated in RA3.3 an overview of the different aspects of the indicators is given in Table 1. It summarises the methodologies, the compartments, the assessed effects and the form of the calculated results which are considered by the three. A detailed multicriteria analysis of these models and additional methods used in LCA was conducted within RA3.4.

Looking at Table 1 it becomes clear, that the comparison of the models can only be conducted for risk to surface water and terrestrial organisms, since only these tow compartments are considered by all three models. It was decided to compare the model results on the level of the complete application calendars and not on product or active ingredient level.

Table 1: Overview on the methodology and results of the involved models

		SYNOPS	I-PHY	USES-PRZM
Methodology				
	Scoring system			
	Fuzzy expert system		X	
	Exposure / Toxicity ratios	X		X
Compartments				
	groundwater		X	X
	surface water	**X**	**X**	**X**
	Soil	**X**	**X**	**X**
	Air		X	X
Effects				
	Human health		X	X
	Surface water	**X**	**X**	**X**
	Soil organisms	**X**	**X**	**X**
	bioaccumulation		X	
	Terrestrial organisms	**X**	**X**	**X**
Exposure pathways				
	Run off in SW	X	X	X
	Drainage in SW	X	X	X
	Drift in SW	X	X	

Leaching to GW		X	X
Drift into field margins	X		
Volatilisation to air		X	X
Form of calculated result			
predicted environmental concentration in each compartments	X		X
risk potentials for each compartment	X	X	X
risk potentials for strategies	X	X	X
risk potentials for products	X		X
risk potentials for active ingredients	X	X	X
overall Environmental risk	X	X	X
Human risk potential		X	X

3 Description of the case study regions and available datasets for wheat and pomefruit

For the multicriteria analysis within RA3 the main producing areas of winter wheat and pomefruit in Europe were chosen as case-study regions. During a RA3 workshop in Tänikon, Switzerland in 2007 the following regions were defined for wheat: Saxony-Anhalt (Germany, SA), Denmark (DK), Emilia Romagna (Italy, ER), Wielkopolskie (Poland, WP) and NW of Paris (France, NW-Paris) and for pomefruit: Lake Constance (Germany, LC-D), Lake Constance (Switzerland, LC-CH), Emilia Romagna (Italy ER), Rhone valley (France, RV), Lleida (Spain, LI).

Within the sub-activity RA3.1 an excellent overview of current plant protection strategies was surveyed for different production systems of the case study crops winter wheat and pomefruit (deliverable TR3.1). In all case study regions data on plant protection methods was surveyed (Table 2 and Table 3). This surveyed data tough was raised on an aggregated level, which was not detailed enough for a region specific risk analysis and a model comparison, as it was planned within RA3.3. Furthermore environmental and field data were only available as constructed worst case scenarios and climate data were in most cases available as monthly averages on 50 km^2 grid level. Exceptions were the two German case study regions Saxony-Anhalt for wheat and Lake Constance for pomefruit, where the pesticide use data was raised on field level and the environmental and climate data could be derived on field level using GIS data bases.

Table 2: Data availability for the case-study regions of winter wheat

Region		**crop protection strategies** (active ingredient, date, dose rate)	**field parameters** soil parameters, slope, distance to surface water	**climate data** temperature, precipitation, global radiation
Saxony-Anhalt (Germany)	SA	156 strategies, with used products (a.i.'s), date and application rate	5028 geo referenced	8 climate stations, daily values
Denmark (Denmark)	DK	List of products used products in wheat production with dates and average application rates , derived from sales data	1 worst case (constructed)	Available from MARS-climate database as monthly averages on 50 km^2 grids
Emilia Romagna (Italy)	ER	two strategies (pear, apple)	1 worst case (constructed)	Available from MARS-climate database as monthly averages on 50 km^2 grids
Wielkopolskie (Poland)	WP	one general strategy, dates on monthly basis	1 worst case (constructed)	Available from MARS-climate database as monthly averages on 50 km^2 grids

NW of Paris (France)	NW-Paris	not yet available	not yet available	Available from MARS-climate database as monthly averages on 50 km^2 grids

In order to compare the models I-PHY, SYNOPS and PRZM-USES a variety of pesticide use strategies and a variety of environmental scenarios will be run and analysed with the three RA models. To accomplish this, detailed pesticide use data including the application rate and application date and realistic environmental data including parameters like global radiation are necessary. Since at this stage of the ENDURE-Network detailed enough data to run all there RA-model was only available for two German case study regions it was decided to focus on these two regions.

Table 3: Data availability for the case-study regions of pomefruit

Region	**crop protection strategies** (active ingredient, date, dose rate)	**field parameters** soil parameters, slope, distance to surface water)	**climate data** temperature, precipitation, global radiation
Lake Constance (Germany)	50 apple (IP) 4 pear (IP) 1 apple organic	3836 geo referenced	5 climate stations daily values
Lake Constance (Switzerland)	3 apple (IP) 3 apple organic	1 worst case (constructed)	1 climate station daily values
Emilia Romagna (Italy)	1 pear 1 apple (as date only month)	1 worst case (constructed)	Available from MARS-climate database as monthly averages on 50 km^2 grids
Lleida (Spain)	3 apple (IP) 3 apple organic	not yet available	Available from MARS-climate database as monthly averages on 50 km^2 grids
Rhone Valley (France)	3 apple (IP) 3 apple organic	1 worst case (constructed	Available from MARS-climate database as monthly averages on 50 km^2 grids

In the next sections the available data sets and their sources are summarised. In the two German case study regions the environmental input data was derived on field level via GIS procedures from an extended geographical dataset and the GIS-based risk assessment tool SYNOPS was applied.

To apply the models PRZM-USES and I-PHY and to compare the results of all three models, it was necessary to reduce the geo-referenced and field based environmental dataset to a data subset, which could be handled by all models. This derived subset of input data was used to compare and evaluate the three models without considering the spatial references in the analysis of the results. The goal of this comparison was to point out the differences, advantages and weaknesses of each model and to identify suitable tools for further analysis in RA3.3. In later phases of RA3.3 it is planned to accomplished GIS-based risk analysis for each region.

3.1 GIS-based data sets

The regional risk assessment with the RA-model SYNOPS relies on a GIS database, which includes all necessary environmental parameters on field level to estimate the environmental exposure by drift, run-off and drainage. The database was established by merging information via GIS procedures from an extended geographical dataset (ATKIS, AdV 2001), a digital soil map (BÜK1000, BGR 1995), a digital elevation model (BKG, 2005) and a set of 430 climate stations of the German weather service (DWD).

The input parameters were derived on the basis of a high resolution data set on land use and land cover, the Authoritative Topographic Cartographic Information System (ATKIS). ATKIS is a project of the German Surveying Authorities which is performed uniformly at the Federal level. It provides digital topographic base data suitable for computer-assisted digital processing. ATKIS describes the topographic features of a landscape in vector format and suits the scale range 1:10.000 to 30.000. Using GIS procedures the exact location of all orchards (Lake Constance) and arable fields (Saxony-Anhalt) and their connectivity to surface waters and other landscape object was extracted. The outputs of these procedures are the minimal distance from the edge of the field to the edge of the surface water and the mean width of the field margins.

The slope for each field was calculated by linking the ATKIS dataset to a digital elevation model (DGM-d). For each field the average slope was calculated. According to a digital soil map (BÜK1000) the main soil types for the region were identified and linked to the fields. The relevant input parameters like the organic carbon content, the hydrological soil class or the texture of the soil are linked to the main soil types. Data on precipitation and temperature were available from stations of the German Weather Service. To each field the closest climate station was linked.

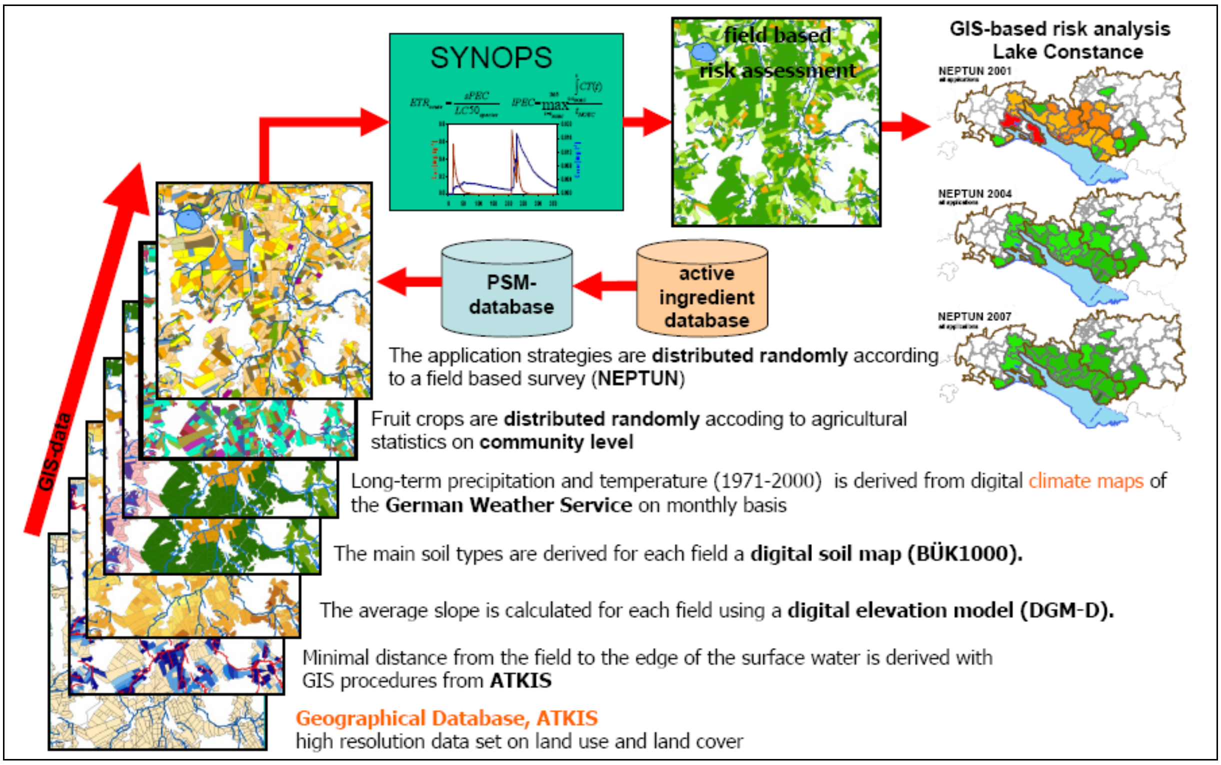


Figure 3: Overview on GIS- related input data and risk analysis with SYNOPS

The information on the cultivated crops is not included in the ATKIS dataset. ATKIS differentiates only between spatial crops like vineyards, orchards and hop and arable crops. Therefore the information on the crop cultivated on field level was achieved by random distribution of the crop types. Within each community the wheat fields were distributed randomly to the derived arable fields according to the agricultural crop statistic on community level.

The pesticide use data is available from field based surveys, which were conducted in the case study regions (NEPTUN, Rossberg 2005). The application strategies of the pesticide use dataset were also distributed randomly to the fields according to the crop related to the field and according to the soil climate region of the field is located in.

This high level of data availability enables us to accomplish a detailed risk analysis on field level for the wheat and orchard case study region.

3.2 Description of wheat case study region: Saxony-Anhalt (Germany)

The state of Saxony-Anhalt was chosen as the ENDURE case study region for wheat in Germany. This corresponds to the three NUTS3 regions DEE1, DEE2 and DEE3 (Figure 4). Agricultural surveys were conducted in this region by the statistical agency of Saxony-Anhalt. The survey on pesticide use (NEPTUN) was conducted by the JKI in the soil climate region (BKR17), which covers about 50% the area of Saxony-Anhalt.

3.2.1 Statistical data and yields

In the region Saxony-Anhalt the last extended statistical survey for crops was conducted in 2005 and is repeated all 5 years. The statistics for the yield are reported every year.

For Saxony-Anhalt the concept of good plant protection practice (GPP) was indicated as the most commonly used production system. In Saxony-Anhalt 90% of the winter wheat is produced according to GPP practices and 3.5% with organic strategies. In this region 3850 farmers (organic 215) produced field crops on an area of 1001860 ha (organic 34318 ha). From these farmers 2950 produced wheat on an area of 349797 ha (35%). The yield for wheat in the years 2005 to 2006 are summarised in Table 4.

Table 4: Yield for wheat in Saxony-Anhalt

Year	farmers N	Area [ha]	Dt	[t/farmer]	[t/ha]
00-05		330416	2372044	804*	7.18
2005	**2950**	**349797**	**2521152**	**854**	**7.22**
2006		337413	2314930	785	6.86

* assuming that the number of farmer did not change in 2006

Wheat Saxony-Anhalt
Statistical surveys: DEE1, DEE2, DEE3
NEPTUN surveys: BKR17
NUTS3-regions: DEE1, DEE2, DEE3

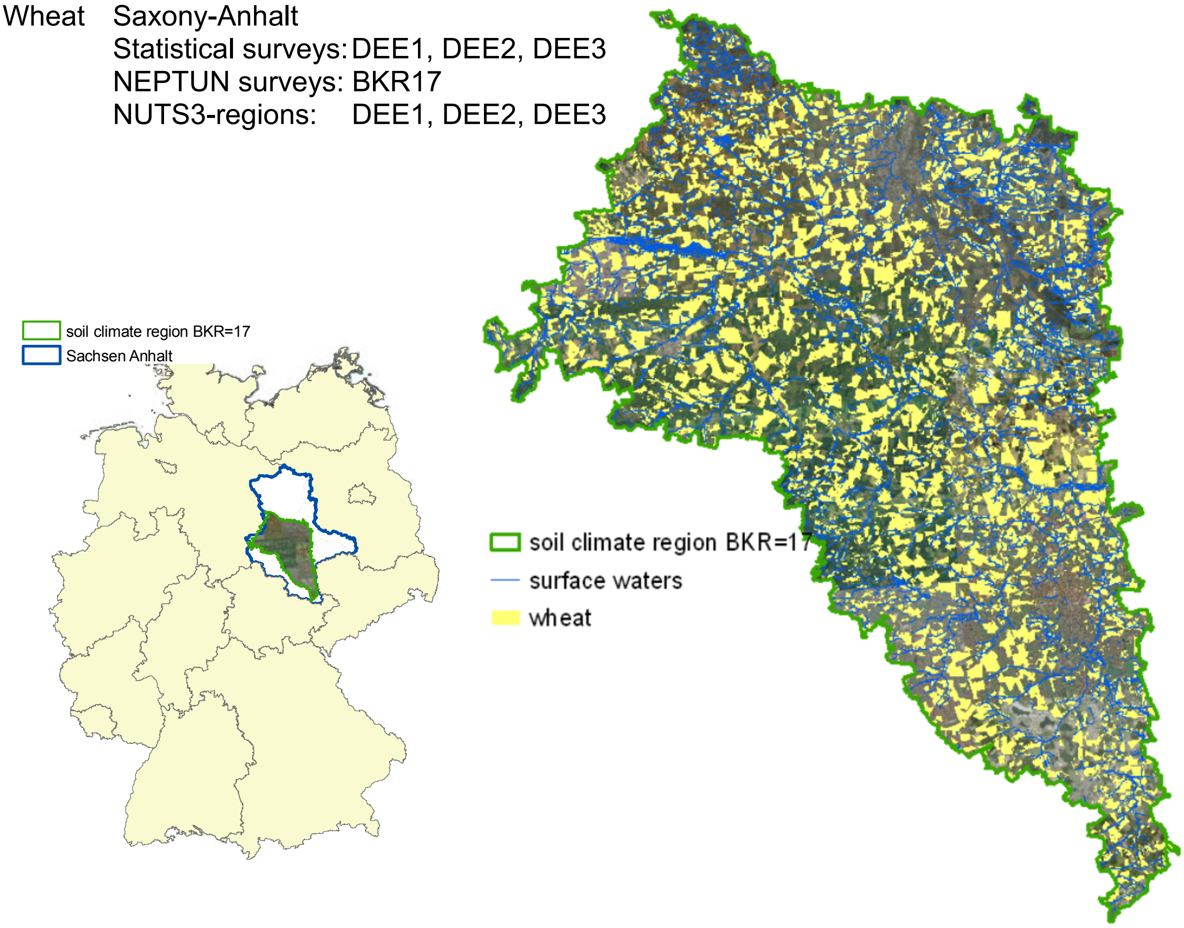


Figure 4: **ENDURE case study region for wheat in Germany. Wheat areas are marked yellow.**

3.2.2 Pesticide use data

The NEPTUN survey for field crops was conducted in the year 2000. A repetition of the survey for the field cops is planned for 2009. In Saxony-Anhalt 29 farmers (1%), which were producing wheat, were surveyed in 2000. They were growing wheat on an area of 9007 ha, which was 3% of the total wheat area. All surveyed farmers were producing according to conventional strategies concept following the concept of good plant protection practice. In total they applied the pesticides according to 112 different application patterns. The frequency treatment indices for all pesticides (herbicides, insecticides and fungicides) range from 0.72 to 8.5. The mean treatment frequency index was 3.77 ±1.61 (Figure 5).

In total 71 different products have been used by the surveyed farmers in Saxony-Anhalt for wheat production. This list of products can be resolved to a list of 55 active ingredients (Table 33). All active ingredients are included in the active ingredient databases, so that the necessary physico-chemical and eco-toxicological parameters are available for the RA models.

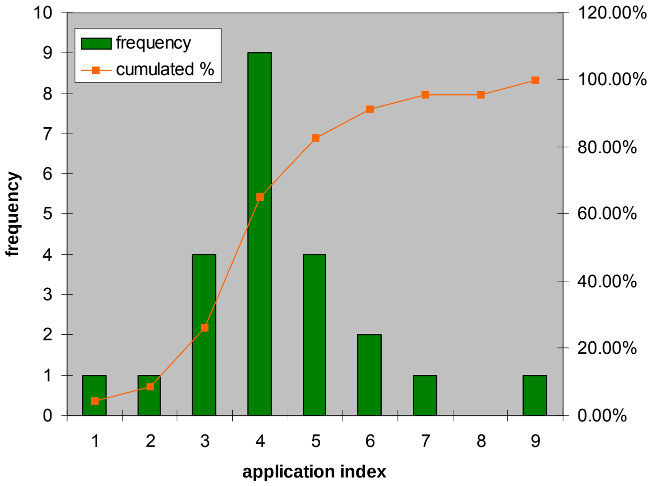


Figure 5: Frequency distribution of the frequency treatment index surveyed in the wheat region Saxony-Anhalt (BKR17)

3.2.3 Environmental and climate data

From the ATKIS database field environmental parameters for all arable fields in the Saxony-Anhalt were derived (n=12000). According to the agricultural statistic on community level wheat fields were distributed randomly to the derived arable fields. In total 5018 wheat fields were selected. The field based input parameters, which are necessary to run the RA-models, as the minimal distance from edge of a field to the edge of the surface water (Figure 6) and the width of surface water (Table 5) were directly derived from ATKIS dataset. Information on the average slope for each field was derived by linking the ATKIS dataset to a digital elevation model (BKG, 2005). In Figure

7 the frequency distribution of all slopes in the case study region is shown. According to a digital soil map (BGR, 1995) the main soil types for the region were identified and linked to the fields (n=6, Table 6). The relevant input parameters like the organic carbon content, the hydrological soil class or the texture of the soil are linked to the main soil types. Data on precipitation and temperature are available from eight stations of the German Weather Service within the considered soil climate region (BKR 17).

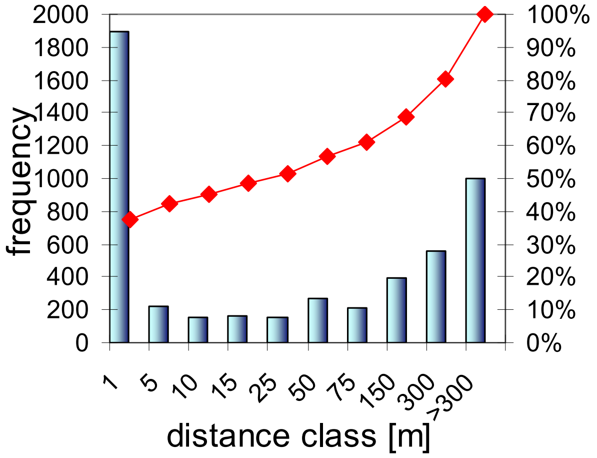


Figure 6: **Frequency distribution of the minimal distance from edge of field to surface water for all fields in the wheat case study region (n=5028)**

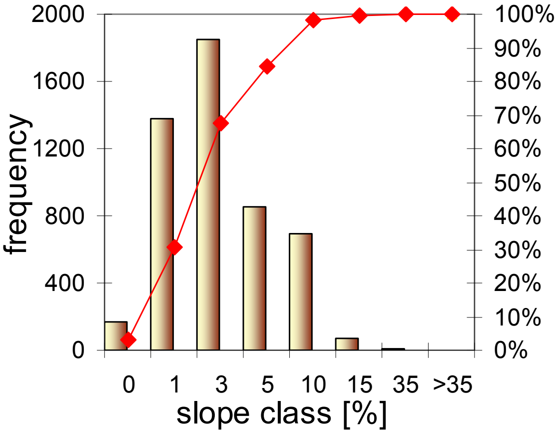


Figure 7: **Frequency distribution of the average slope of all fields within the wheat case study region (n=5028)**

Table 5: **Surface water classes and the probability of occurrence close to a wheat field (p)**

SW type	Definition	width [m]	Depth [m]	n	p
No surface water, mindist > 150 m	-	-	-	1076	0.214
flowing surface water	0.5m - 3m	1	0	2224	0.443
flowing surface water	3m – 6m	3	0.3	128	0.026
flowing surface water	6m- 12m	6	0.5	54	0.011
flowing surface water	15 m	9	0.5	157	0.031
ditch	3	1	0.3	678	0.135
ditch	6	3	0.5	8	0.002
lake	15	9	0.5	683	0.136

Table 6: **Main soil types occurring in wheat fields in the case study region SA. The main soil type are linked to database tables which include the information on the OC-content, hydrological soil type and texture of the soil.**

soil type number	probability of occurrence on a wheat field	Definition
36	0.35	Tschernosem der Mitteldeutschen Trockengebiete aus Löß
37	0.15	Tschernosem / Braunerde aus Löß im Wechsel mit Rendzina aus Mergel und Kalkstein
9	0.10	Gley-tschernosem aus kalkhaltigen, tonig-schluffigen Ablagerungen in Flußtälern der Schwarzerdegebiete
41	0.09	Tschernosem-Braunerde / Griserde / Parabraunerde aus

		sandigen Lößdecken über Sedimenten oder Geschiebelehm
42	0.01	Parabraunerde / Fahlerde / Pseudogley aus Löß oder Lößlehm über verschiedenen Gesteinen
24	0.04	Tschernosem-Parabraunerde / Parabraunerde-Tschernosem aus Löß oder Lößlehm
8	0.04	Auenboden / Gley aus lehmigen bis tonigen Auensedimenten

3.3 Description of pomefruit case study region: Lake Constance (Germany)

The fruit growing region Lake Constance is the leading fruit growing region in Germany. It holds almost half of the orchards in Baden-Württemberg (47%) and 15 % of the German orchards. The region Lake Constance consists of the three counties 'Landkreis Konstanz', 'Bodenseekreis' and 'Landkreis Ravensburg', where the 'Bodenseekreis' contributes with the largest portion of production area (Figure. 6).

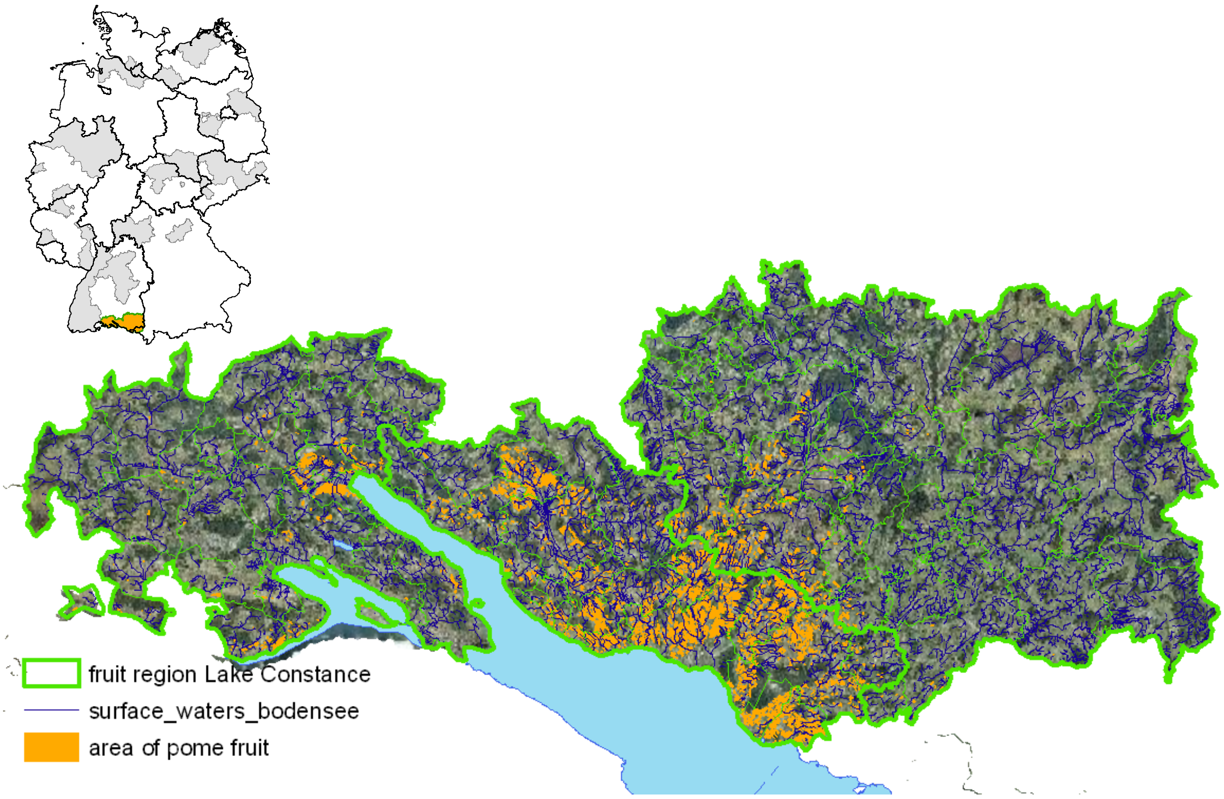


Figure 8: ENDURE sample region for pomefruit in Germany. Pomefruit orchards are marked orange.

The structure of the farms in this region is focused to produce marked fruits with a high percentage of apples (90%). Other agricultural structures only play a secondary role in this region. Due to this specialised structure of the region, the area per farm is with 4.6 ha compared to other regions relatively large and densely planted.

In the region Lake Constance 90% of the fruits are produced with labelled strategies (IP), 6-7% with organic strategies and 3% with conventional strategies.

3.3.1 Statistical data and yields

Extended statistical surveys describing the structure of the farms and fruits and varieties produced by the farmers are repeated all 5 years. The last survey for fruits in the region Lake Constance was conducted in 2007. The surveys show a specialisation and concentration toward fewer farms with larger production areas which reflects the trend of other production branches.

In spring 2007, 1554 producers were surveyed, which means compared to 2002 (1672 producers) a reduction of 7%. The total area used in fruit production slightly increased by 1.1% from 7091 ha in 2002 to 7170 ha in 2007. This means that the area per farm increased in average form 4.2 ha to 4.6 ha. Likewise the percentage of producers with large (>5 ha) production areas significantly increased by 6.5%. The described survey aims at the producers of marked fruits and does not include the extensive ‘Streuobst’ production.

Statistics on the yield of the fruit production are reported every year. Since 2001 they are only evaluated on the regional level of ‘Baden-Württemberg’. Table 8 includes the yield data.

Table 7: statistics on fruits grown in the region Lake Constance

		farmers	**trees**	**Area**	**area per fruit**					
		n	n in 1000	Total	apple	pear	sweet cherry	sour cherry	plums	Others
2002	Konstanz L.	174	2180	739	676	32	14	5	11	1
	Bodenseekreis	1255	14020	5289	4713	212	127	79	153	5
	Ravensburg	243	2346	1063	947	37	40	19	14	5
	Sum	1672	18546	7091	6336	281	181	104	178	11
	Percentage			100	89	4	3	1	3	0
2007	Konstanz L.	171	2397	770	692	41	17	6	15	1
	Bodenseekreis	1157	14882	5383	4758	183	163	67	208	4
	Ravensburg	226	2370	1017	947	37	40	19	14	5
	Sum	1554	19649	7170	6344	254	244	74	244	10
	Percentage			100	88	4	3	1	3	0
	Change 2007/2002	-7.1	5.9	1.1	0.1	-9.5	34.5	-28.6	36.9	-11.9

Table 8: yield for apple in the fruit growing region Lake Constance

Year	**farmers N**	**area [ha]**	**Trees N**	**Yield 1000 [dt]**	**[t/farmer]**	**[t/ha]**	**[kg/tree]**
97-02				2132			
2002	**1672**	**6336**	**176205444**	**2159**	**131.57**	**34.06**	**12.3**
2003				1838*	*112.00**	*29.00**	*10.4**
2004				2145*	*130.71**	*33.84**	*12.2**

* assuming that the number of farmers, the area and the number of trees did not change in 2003 and 2004

3.3.2 Pesticide use data

In Germany repetitive surveys on the pesticide use (NEPTUN) are conducted for fruits, wheat and hop. The NEPTUN survey for fruit crops was conducted in the years 2001, 2004 and 2007 in 9-13 fruit growing regions. All pesticide use data in this report are related to the NEPTUN survey 2004.

In the region Lake Constance 50 farmers (3 %) were surveyed in 2004. They were growing apples on an area of 268 ha (4.3%). All surveyed farmers were producing according to labelled strategies. In total fifty different application patterns are available for labelled pomefruit production. The application indices of these strategies for all pesticides (herbicides, insecticides and fungicides) range from 14.4 to 59. The mean application index for the region Lake Constance was 30.5±8.8. The frequency distribution of the application indices is shown in Figure 9. In total 60 different products have been used by the surveyed farmers. This list of products can be resolved to a list of 55 active ingredients, which is given in appendix (Table 34.)

Table 9: Extent of NEPTUN surveys for apple in the region Lake Constance

	number of strategies		**areas**	farmers		**treatment index**	
	apple	pear	%	%	Mean	min	Max
2001	137	10	9.6	8.3	27,28	9,13	44,90
2004	**50**	**4**	**4.4**	**3.0**	**30,12**	**14,41**	**58,97**
2007	44	40	5.4.	3.3	31.4	4.3	49.1

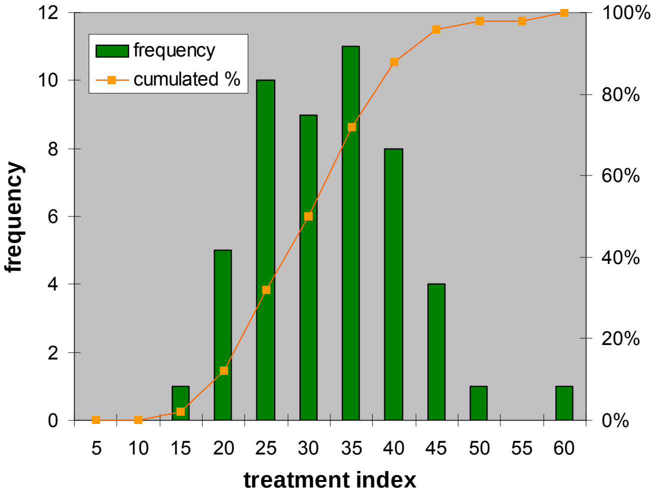


Figure 9: Frequency distribution of the frequency treatment index for pomefruit surveyed in the fruit growing region of Lake Constance

3.3.3 Environmental and climate data

The environmental input parameters were derived as described in section 3.1. The information, if on the fields spatial or arable crops are cultivated is included in the ATKIS dataset. Therefore the position of all orchards is derived from ATKIS. According to the statistical surveys for fruit crops on community level the fruits apple and pear (pomefruit) are distributed randomly to the derived orchards.

From the ATKIS database environmental parameters for 3836 pomefruit orchards in the region of Lake Constance could be derived. As for the wheat case study region the minimal distance from the field to the surface water (Figure 10) and width of the surface water (Table 11) were directly derived from ATKIS. The frequency distribution of the calculated average slopes for the orchards are shown in Figure 11. According to the digital soil map BÜK1000 the three main soil types (Table 10) were identified for orchards in the region Lake Constance. Data on precipitation and temperature was available from three stations of the German Weather Service (n=3).

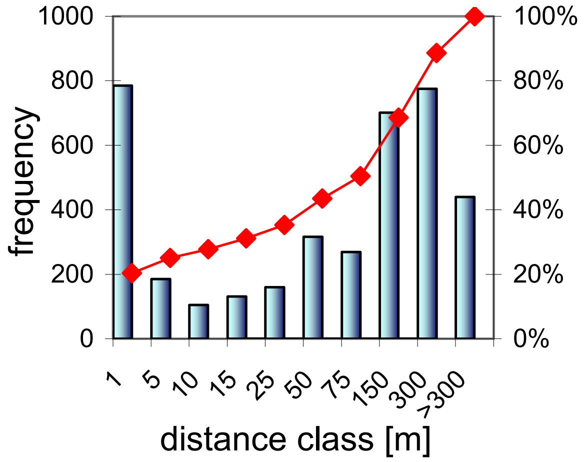


Figure 10: **Frequency distribution of the minimal distance from edge of field to surface water for all pomefruit orchards in the case study region Lake Constance (n=3836)**

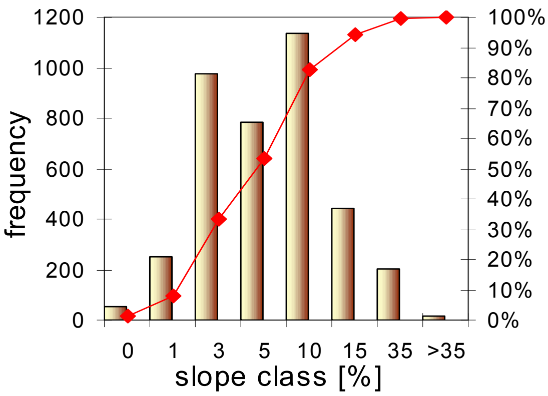


Figure 11: **Frequency distribution of the average slope of all pomefruit orchards in the case study region Lake Constance (n=3836)**

Table 10: Main soil types occurring in pomefruit orchards in the case study region Lake Constance. The main soil types are linked to database tables, which include the information on the OC-content, hydrological soil type and texture of the soil.

soil type number	probability of occurrence on a wheat field	Definition
11	0.11	Auenboden / Gley aus sandigen bis tonigen Flußsedimenten in kleinflächigem Wechsel
14	0.147	Parabraunerde aus schluffig-lehmigen Deckschichten auf eiszeitlichen Schotterplatten
21	0.847	Braunerde / Parabraunerde / Pararendzina aus lehmig-sandigen, kalkhaltigen Moränenablagerungen

Table 11: Surface water classes and the probability of occurrence close to a pomefruit orchard (p)

SW type	Definition	width [m]	depth [m]	n	p
No surface water, mindist > 150 m	-	-	-	1183	0.318
Flowing surface water	0.5m - 3m	1	0	2037	0.547
Flowing surface water	3m - 6m	3	0.3	152	0.041
Flowing surface water	6m- 12m	6	0.5	9	0.002
Flowing surface water	15 m	9	0.5	102	0.027
Ditch	3	1	0.3	115	0.031
Ditch	6	3	0.5	4	0.001
Lake	15	9	0.5	122	0.033

3.4 Input data sets used for the model comparison

Using the environmental datasets described above, it would be possible to assess the maximum range of risk potentials for each region by combining all derived environmental field/orchard data sets with all surveyed pesticide use strategies. For the wheat case study region this would result in 5028 wheat fields * 156 strategies =784368 possible risk evaluations. In the pomefruit region 3836 orchards * 50 strategies=191800 possible risk potentials could be calculated.

This high number of risk calculations could only be handled by the RA-model SYNOPS, which was constructed to analyse large GIS-based datasets. The two other model I-Phy and USES-PRZM, had to be parameterised manually, which was not possible for the complete dataset described above.

It was therefore decided to reduce the number of possible parameter combinations by building representative classes of the parameters slope and minimal distance for each case study region. It was further decided to use only one climate dataset for each region. The station, which was linked to the most fields in each region, was selected.

Since I-PHY and PRZM-USES do not differentiate between Surface water types the worst case situation of a standard ditch with 1m width and 0.3 m depth was chosen as input parameter.

It was also decided to reduce the number of soil types for the wheat case study region to four main soil types. The most common soil types were selected. If two soil types were similar their OC-content and texture only one of the two was selected. In the orchard case study region two main soil types were selected.

Following these assumptions and decisions the complete environmental dataset was reduced to a set of 48 different environmental conditions for the wheat case study region. Applying all 156 different application strategies to each set of environmental parameters would result in 7488 risk evaluations for Saxony Anhalt. In the pomefruit region the data was reduced to a set of 18 environmental conditions, which were combined wit 50 pomefruit strategies. This resulted in 900 different risk evaluations for pomefruit.

The chosen environmental parameter combinations and the probability of its occurrence in each case study region are summarised in Table 12 and in Table 13. In the wheat case study region Saxony-Anhalt they cover about 15% of all possible parameter combinations and in the pomefruit case study region Lake Constance about 30 %. The complete datasets including the tables for climate data soil parameters and pesticide use data were collected in an Access database for each case study region and are published on the ENDURE workspace.

Table 12: Selected environmental scenarios for the wheat case study region Saxony Anhalt and the probability of occurrence (p)

SW type	SW-width [m]	climate station	field margin width [m]	soil type Nr	mindist class [m]	mindist [m]	slope class [%]	slope [%]	P
ditch	1	104	2	9	0-3	1	0-2	1	0.0075
					0-3	1	2-4	3	0.0042
					0-3	1	4-10	5	0.0032
					3-10	3	0-2	1	0.0009
					3-10	3	2-4	3	0.0005
					3-10	3	4-10	5	0.0004
					10- 20	10	0-2	1	0.0016
					10- 20	10	2-4	3	0.0009
					10- 20	10	4-10	5	0.0007
					20-30	20	0-2	1	0.0037
					20-30	20	2-4	3	0.0021
					20-30	20	4-10	5	0.0016
ditch	1	104	2	24	0-3	1	0-2	1	0.0013
					0-3	1	2-4	3	0.0007
					0-3	1	4-10	5	0.0006
					3-10	3	0-2	1	0.0001
					3-10	3	2-4	3	0.0001
					3-10	3	4-10	5	0.0001
					10- 20	10	0-2	1	0.0003
					10- 20	10	2-4	3	0.0002
					10- 20	10	4-10	5	0.0001
					20-30	20	0-2	1	0.0006
					20-30	20	2-4	3	0.0004
					20-30	20	4-10	5	0.0003
ditch	1	104	2	36	0-3	1	0-2	1	0.0266
					0-3	1	2-4	3	0.0150
					0-3	1	4-10	5	0.0115
					3-10	3	0-2	1	0.0031
					3-10	3	2-4	3	0.0017
					3-10	3	4-10	5	0.0013
					10- 20	10	0-2	1	0.0056
					10- 20	10	2-4	3	0.0031
					10- 20	10	4-10	5	0.0024
					20-30	20	0-2	1	0.0134
					20-30	20	2-4	3	0.0075
					20-30	20	4-10	5	0.0058
ditch	1	104	2	41	0-3	1	0-2	1	0.0050
					0-3	1	2-4	3	0.0028
					0-3	1	4-10	5	0.0021
					3-10	3	0-2	1	0.0006
					3-10	3	2-4	3	0.0003
					3-10	3	4-10	5	0.0002
					10- 20	10	0-2	1	0.0010
					10- 20	10	2-4	3	0.0006
					10- 20	10	4-10	5	0.0004
					20-30	20	0-2	1	0.0025
					20-30	20	2-4	3	0.0014
					20-30	20	4-10	5	0.0011
								Sum	0.1470

Table 13: Selected environmental scenarios for the pomefruit case study region Lake Constance and the probability of occurrence (p)

SW type	SW-width	climate station	field margin width	soil type Nr	mindist class	mindist	slope class	slope	P
	[m]		[m]		[m]	[m]	[%]	[%]	
ditch	1	308	4.5	14	0-3	1	0-4	3	0.012
					0-3	1	4-7.5	5	0.008
					0-3	1	7.5-20	10	0.011
					3-10	5	0-4	3	0.004
					3-10	5	4-7.5	5	0.012
					3-10	5	7.5-20	10	0.004
					10- 20	10	0-4	3	0.004
					10- 20	10	4-7.5	5	0.014
					10- 20	10	7.5-20	10	0.003
ditch	1	308	4.5	21	0-3	1	0-4	3	0.069
					0-3	1	4-7.5	5	0.045
					0-3	1	7.5-20	10	0.004
					3-10	5	0-4	3	0.022
					3-10	5	4-7.5	5	0.014
					3-10	5	7.5-20	10	0.021
					10- 20	10	0-4	3	0.020
					10- 20	10	4-7.5	5	0.013
					10- 20	10	7.5-20	10	0.019
								sum	0.299

3.5 Databases for properties of active ingredients

One objective of this analysis was to compare and contrast the indicator methodologies. Consequently a standard database describing the chemical, physical and eco-toxicological properties of the a.i.'s had to be defined to avoid influences of variations in the a.i. parameters. Three different databases were available. The two models I-Phy and SYNOPS have integrated databases on a.i. properties. The model PRZM-USES asks for manual input of the a.i. properties. In addition an online database of the EU-project footprint (FOOTPRINT, 2007) was made available to RA3.3.

The SYNOPS database is holding all necessary a.i. properties for the model calculations in SYNOPS. It includes about 360 active ingredients. The data sources are the monographs relevant to EU review process and to the national legislation process. If both data sources were not available sources like pesticide manual, IVA-Datasheets, Publications per active in the ingredient were used. The database is continuously updated

The FOOTPRINT Pesticide Properties Database (FOOTPRINT PPDB) is a comprehensive relational database of pesticide physicochemical and ecotoxicological data with more than 800 a.i.'s. The database holds data for all EU Annex-1 listed pesticides and selected metabolites. The sources of information for a.i. are the monographs produced as part of the EU review process. These documents have been used in priority for putting together the FOOTPRINT PPDB. Where EU documents were not available, alternative sources were used. FOOTPRINT PPDB is online available and continuously updated.

Similar to FOOTPRINT the I-PHY database is also related to the EU-endpoints.

A rough overview of the differences between these databases was evaluated before a decision was taken, which database will be used in the model comparison. The three a.i. property databases were compared on the basis of selected ecotoxicological parameters and physicochemical parameters. The differences between the databases were evaluated considering two different threshold values. The first threshold value (t1) describes the parameter level, where value differences do not significantly affect the risk potential. If the parameter value is above the threshold t1 (below for DT50), then changes in the parameters are considered to have only little influence on the calculated risk potential.

The second threshold value (t2) describes the range of differences of the parameter values, which are assumed to show little effect on the risk potential. A significant difference between the parameters is considered if i) the value of database 1 and the value of database 2 are lower than threshold 1 (for DT50 larger) and if ii) the difference between value of database 1 and database 2 are larger than threshold 2.

As an example the LC50 values for aquatic organisms of the footprint property database and the SYNOPS database are compared in Figure 12. For the three LC50 values (fish, algae and daphnia) significant differences exist between the SYNOPS and footprint PPDB database in 15-20 % of the values if t2= 10 mg l^{-1} is assumed. This percentage increase if the threshold 2 (t2) is deceased. If t2 is 3 mg l^{-1}, 23-30% of the values differ and if t2 is reduced to 1 mg l^{-1} 29-41% of the values divert in the two databases (Table 14). Similar results are obtained for the non effect concentrations (NoEC).

Table 14: Comparison of the aquatic LC50 concentrations in the footprint and SYNOPS active ingredient database. The analysis was based on three different threshold values(t2), see text.

Thres-hold2	Number of compared values	Significant differences in LC50 Fish		Significant differences in LC50 Algae		Significant differences in LC50 Daphnia	
[mg l^{-1}]		n	%	n	%	n	%
10	354	65	**18**	71	**20**	55	**16**
3	354	92	**26**	108	**30**	80	**23**
1	354	146	**41**	135	**38**	103	**29**

Table 15: Comparison of the aggregated value for aquatic toxicity (Aquatox=min($LC50_{daphnia}$, $LC50_{algae}$, $LC50_{fish}$) in the footprint ,I-PHY and SYNOPS active ingredient database. The analysis was based on three different threshold values(t2), see text.

	SYNOPS-footprint (n=354)		I-PHY-Footprint (n=330)		I-PHY-SYNOPS (n=237)	
Threshold2	Significant differences in Aquatox		Significant differences in Aquatox		Significant differences in Aquatox	
[mg l^{-1}]	N	%	n	%	n	%
t10	41	**12**	22	**7**	14	**9**
t3	62	**18**	40	**12**	18	**11**
t1	88	**25**	55	**17**	30	**21**

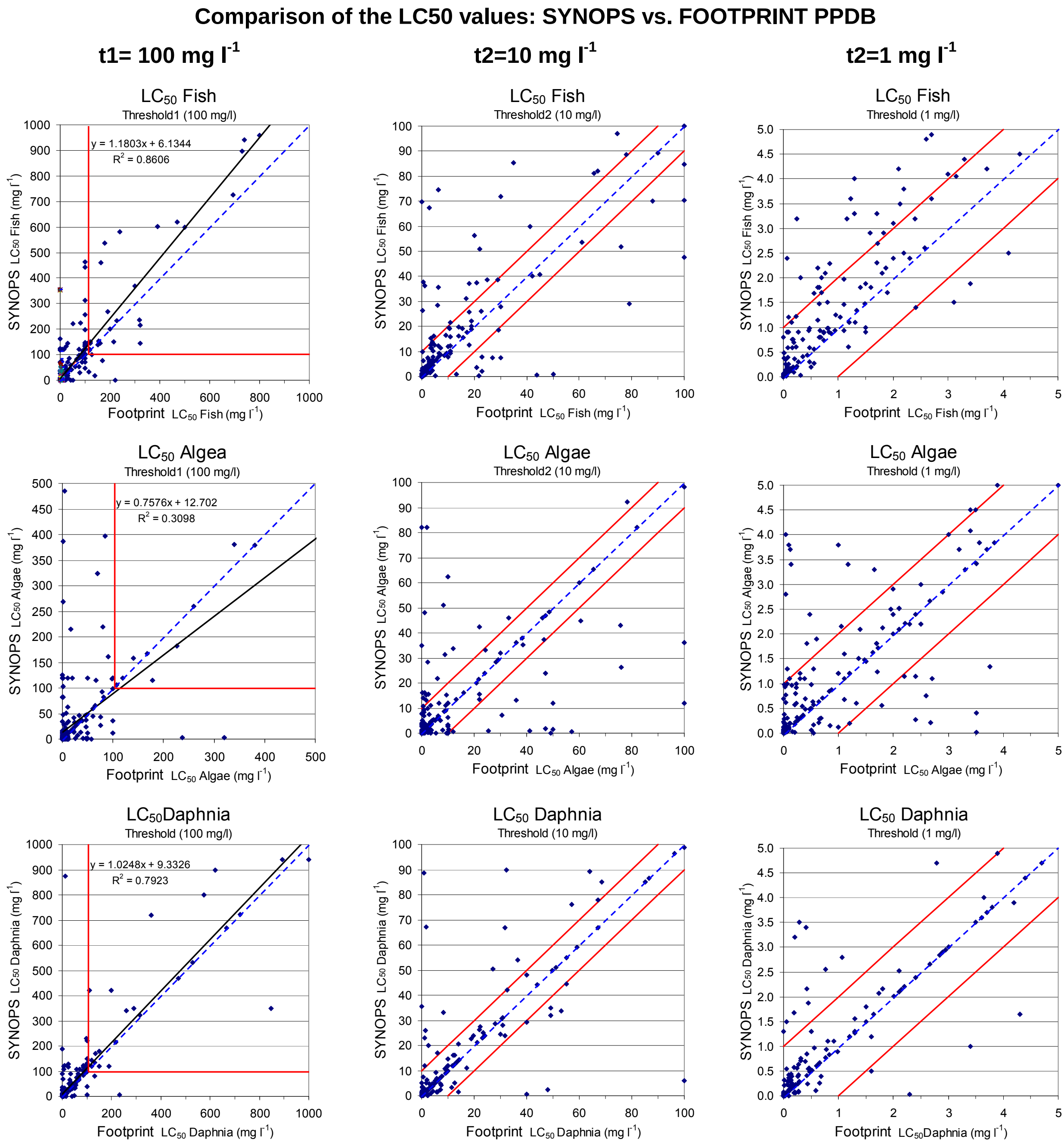


Figure 12: **Comparison of the LC50 values for fish (a), algae (b) and daphnia (c). Left column: correlation between the LC50 values of the SYNOPS and footprint database and the treshhold1 (red line); middle column: subset of all data points (<100 mg l^{-1}) including the threshold2 with t2=10 mg l^{-1} (red lines); right column: subset of all data points (<5 mg l^{-1}) including the threshold2 with t2=1 mg l^{-1} (red lines)**

The I-PHY database was available only with aggregated values for the aquatic toxicity were the minimum value of the available toxicity data was calculated as AquaTox=min(LC50,NOEC). Therefore the comparison of all three databases was conducted on the basis of the aggregated values for aquatic toxicity (Figure 13, Table

15). When using these values the percentages of significant differences are reduced, compared to the organism specific values.

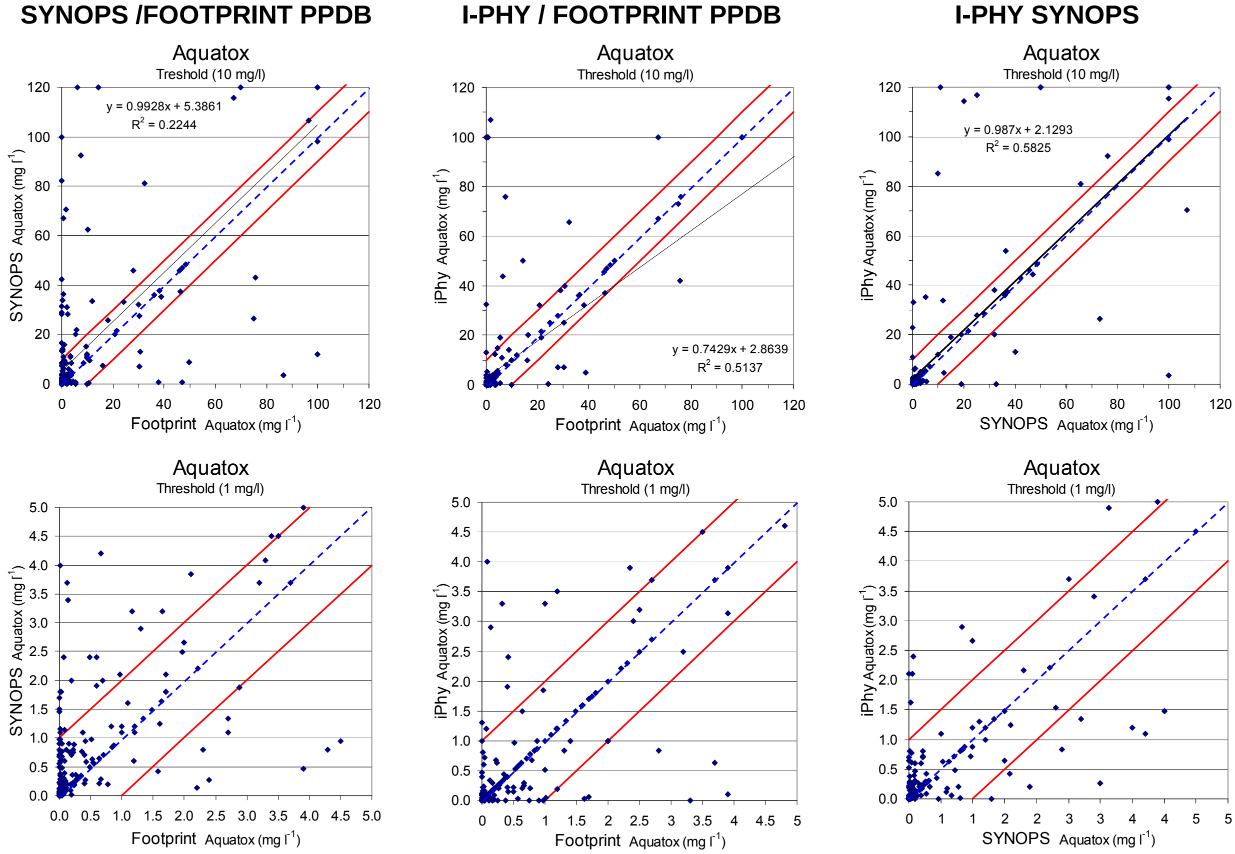


Figure 13: **Comparison of Aquatox values. Left column: SYNOPS/footprint PPDB, middle column: I-PHY / footprint PPDB, right column: I-PHY SYNOPS**

The three databases were also analysed for differences in the soil degradation rate (DT50) and partitioning constant (Koc). The results of this analysis are summarised Figure 14. The difference of a pair-wise comparison of the Koc values range from 13-17% if the threshold value is assumed to be t2=150 mg g^{-1} and from 21-34% if the threshold value is t2=50 mg g^{-1}. (Table 16)

The differences in the degradation rate in soil were clearly larger. They ranged from 35-45% if threshold2 was assumed to be 10 days and from 43-51% if threshold2 was assumed to be 2 days (Table 17).

Table 16: Comparison of KOC values in the footprint, I-PHY and SYNOPS active ingredient database. The analysis was based on three different threshold values (t2), see text.

parameter	t1	t2	SYNOPS-footprint (n=182)		I-PHY-Footprint (n=321)		I-PHY-SYNOPS (n=143)	
	[mg g^{-1}]	[mg g^{-1}]	n	% different	n	% different	n	% different
Koc	<1000	150	23	**13**	67	**21**	24	**17**
Koc	<1000	100	27	**15**	86	**27**	45	**31**

parameter	t1	t2	SYNOPS-footprint (n=182)		I-PHY-Footprint (n=321)		I-PHY-SYNOPS (n=143)	
	[mg g^{-1}]	[mg g^{-1}]	**n**	**% different**	**n**	**% different**	**n**	**% different**
Koc	<1000	50	39	**21**	110	**34**	42	**29**

Table 17: Comparison of DT50 values in the footprint, I-PHY and SYNOPS active ingredient database. The analysis was based on three different threshold values (t2), see text.

parameter	t1	t2	SYNOPS-footprint (n=348)		I-PHY-Footprint (n=329)		I-PHY-SYNOPS (n=237)	
	[days]	[days]	**n**	**% different**	**n**	**% different**	**n**	**% different**
DT50	>30	10	156	**45**	115	**35**	102	**43**
DT50	>30	5	165	**47**	129	**40**	110	**46**
DT50	>30	2	170	**49**	141	**43**	121	**51**

Overall it can be concluded, that all three databases had a certain percentage of diverting values, and that all of these percentages were more or less in the same range for the pair-wise comparison of the databases. On the basis of this result and considering technical feasibility it was decided to use the SYNOPS database as input database for the risk assessment and the comparison of the three models.

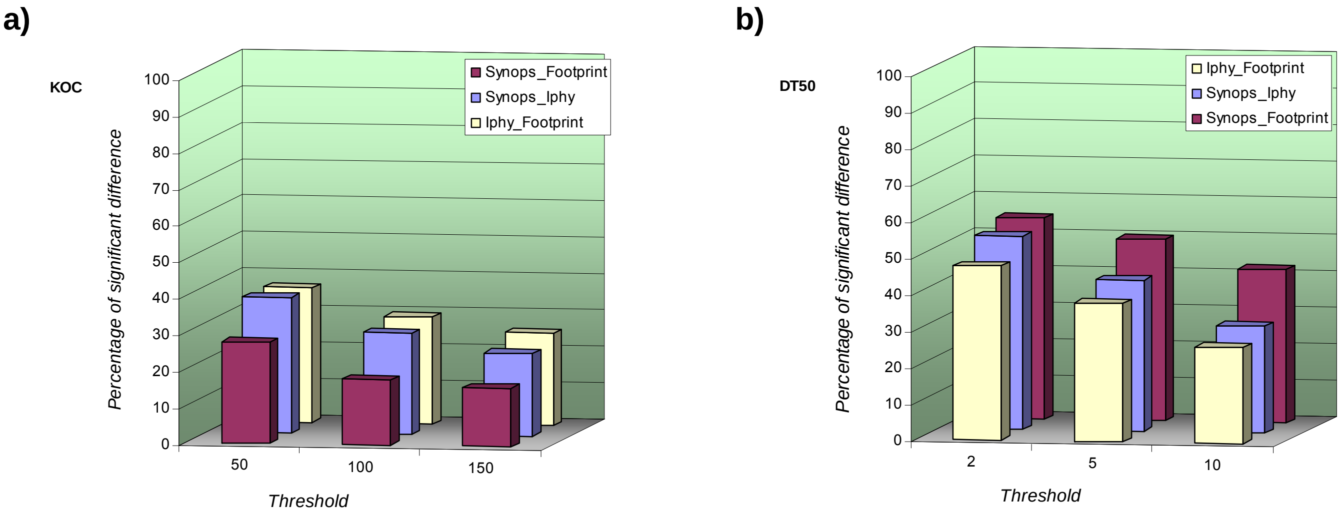


Figure 14: Comparison of Koc and DT50 values in the footprint, I-PHY and SYNOPS active ingredient database. The analysis was based on three different threshold values (t2).

4 Result of the RA-models calculated for the wheat and pomefruit case study regions

The three available RA-models SYNOPS, I-PHY and PRZM-USES were run with the datasets described in section 3.4. When applying and parameterising the models it became evident that not all models could be applied to the complete input dataset. Due to the time consuming manual parameterisation of PRZM only 16 scenarios for wheat and none for pomefruit could be evaluated with the method PRZM-USES. From the 900 scenarios for pomefruit only 66 could be evaluated using I-PHY. The following sections summarise the results of each model separately for the two case study regions. In section 5 the results of the models will be compared.

4.1 Wheat case study region: Saxony Anhalt

4.1.1 Results of I-PHY

The risk values calculated with I-PHY are expressed as scores in the range from 0 to 1, where 0 is low risk and 1 is high risk. A risk score of 0.3 is considered as the maximal still tolerable risk potential. Scores above 0.7 are considered as high risk. The basic statistics of the I-PHY results over all 7488 scenarios and the corresponding frequency distribution of the calculated risk scores are summarised in Table 18 and Figure 15.

Overall I-PHY estimates relative high risk scores for the wheat case study region in Saxony Anhalt. The lowest risk scores are estimated for groundwater with a median of 0.24 and a 90th percentile of 0.37. In total 24 % of the scenarios are above the maximum tolerable groundwater risk of 0.3. For the risk in air much higher values were estimated. A median of 0.43 and a 90th percentile of 0.58 was calculated. More than 93 % of the values lie above the tolerable risk of 0.3. The aquatic risk potentials (surface waters) reach the highest values with a median of 0.53 and a 90th percentile of 0.91. Compared to the other two risk potentials the aquatic risk scores are spread over a wider range and 82 % of the scenarios have a larger value than the maximal tolerable risk level of 0.3.

Table 18: Risk scores for wheat case study region Saxony Anhalt calculated with I-PHY. Statistical evaluation for the global environmental risk, and the risk scores of the three compartments groundwater, surface water and air.

	N	mean	std	median	**p90**	max	min	**% above max. tolerable risk**
global environmental risk	7488	0.63	0.13	0.61	**0.79**	1.00	0.28	
risk in air	7488	0.44	0.11	0.43	**0.58**	0.76	0.09	93
groundwater risk	7488	0.25	0.09	0.24	**0.37**	0.48	0.06	24
aquatic risk	7488	0.53	0.26	0.53	**0.90**	1.00	0.03	82

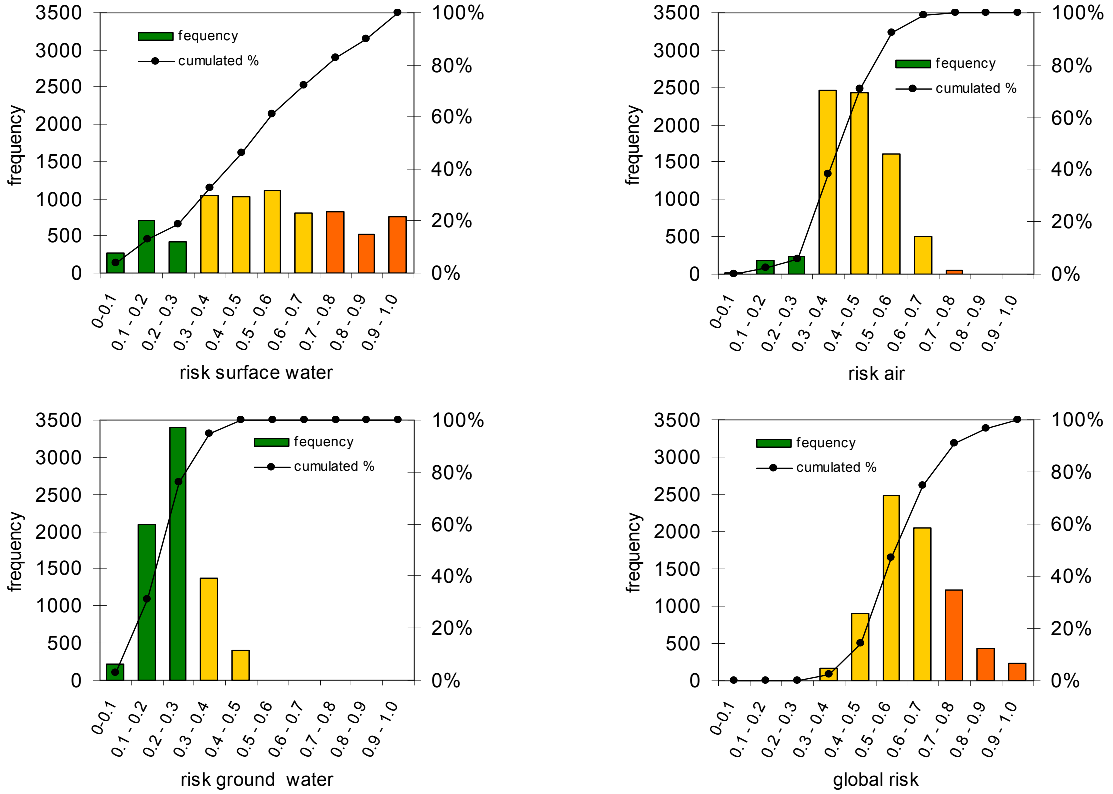


Figure 15: Risk scores for wheat case study region Saxony Anhalt calculated with I-PHY. Frequency distributions for the global environmental risk, and the risk scores of the three compartments groundwater, surface water and air. 🟩low risk, 🟨 intermediate risk, 🟧 high risk

In Table 19 the calculated risk scores are evaluated for three environmental parameters (slope, mindist and soil type) separately. The statistical analysis was conducted for all possible values of each environmental parameter. For example, the means and percentiles were calculated for the parameter mindist at 1m, 3m, 10m and 20m distance.

The environmental parameter ‘minimal distance’ has a strong impact on the median and 90th percentile of the aquatic risk, whereas the impact of the slope and soil type is much smaller. If the minimal distance increases from 1 m to 20 m the median of the aquatic risk score decreases by 0.66 and the 90th percentile by 0.486. A trend in the opposite direction can be observed for the slope but the effects are much smaller. An increase of the slope from 1 to 5 % causes an increase of the median of the aquatic risk score by 0.13 and of the 90th percentile only by 0.02. The different four soil types cause a variation of the median by 0.1 and of the 90th percentile by 0.04.

The risk of groundwater is only influenced by the slope of the fields. The influence of all three environmental parameter on the risk in air can be neglected.

It can be summarised, that the risk assessment with I-PHY calculates overall environmental risk scores for the used wheat strategies in the case study region Saxony Anhalt, which can not be considered acceptable. The same can be clearly concluded for the risk scores in surface water and in air. The groundwater risk potential shows the lowest values with 24% above the tolerable risk level, but this still would not be an acceptable value for the wheat case study region.

Table 19: Statistical evaluation of the risk scores grouped for each environmental parameter separately. Risk scores for wheat case study region Saxony Anhalt were calculated with I-PHY

Risk score	Mindist [m]	Slope [%]	soil-type number	number of scenarios	risk scores				max differences in median	max differences in p90
					mean	std	median	p90		
risk in air	**1**			1872	0.47	0.11	0.45	0.63	**0.058**	**0.089**
	3			1872	0.45	0.11	0.43	0.60		
	10			1872	0.44	0.10	0.42	0.58		
	20			1872	0.42	0.10	0.40	0.54		
groundwater risk	**1**			1872	0.25	0.09	0.24	0.37	**0.000**	**0.000**
	3			1872	0.25	0.09	0.24	0.37		
	10			1872	0.25	0.09	0.24	0.37		
	20			1872	0.25	0.09	0.24	0.37		
aquatic risk	**1**			1872	0.84	0.13	0.86	1.00	**0.666**	**0.486**
	3			1872	0.59	0.13	0.58	0.77		
	10			1872	0.45	0.13	0.41	0.63		
	20			1872	0.25	0.16	0.19	0.51		
risk in air		**1**		2496	0.44	0.11	0.43	0.58	**0.007**	**0.004**
		3		2496	0.44	0.11	0.43	0.58		
		5		2496	0.45	0.11	0.43	0.59		
groundwater risk		**1**		2496	0.25	0.09	0.24	0.37	**0.000**	**0.000**
		3		2496	0.25	0.09	0.24	0.37		
		5		2496	0.25	0.09	0.24	0.37		
aquatic risk		**1**		2496	0.48	0.28	0.45	0.89	**0.133**	**0.019**
		3		2496	0.53	0.25	0.51	0.90		
		5		2496	0.59	0.23	0.58	0.91		
risk in air			**9**	1872	0.44	0.11	0.43	0.58	**0.006**	**0.004**
			24	1872	0.44	0.11	0.43	0.58		
			36	1872	0.45	0.11	0.43	0.59		
			41	1872	0.44	0.11	0.43	0.58		
groundwater risk			**9**	1872	0.21	0.06	0.22	0.29	**0.137**	**0.133**
			24	1872	0.32	0.10	0.36	0.43		
			36	1872	0.21	0.06	0.22	0.29		
			41	1872	0.25	0.08	0.26	0.34		
aquatic risk			**9**	1872	0.53	0.25	0.52	0.89	**0.101**	**0.041**
			24	1872	0.49	0.27	0.47	0.88		
			36	1872	0.58	0.24	0.57	0.92		
			41	1872	0.53	0.25	0.52	0.89		

4.1.2 Results of SYNOPS

The risk potentials calculated with SYNOPS are given as Exposure – Toxicity – Ratios (ETR). The aquatic risk is evaluated as the maximum risk potential of the three reference organisms Daphnia, fish and algae and the terrestrial risk as the maximum of the risk potentials for bees and earthworms.

Compared to the results calculated with I-PHY the model SYNOPS only considers terrestrial and aquatic risk potentials. On the other hand SYNOPS differentiates between acute and chronic risk potential (see 2.2.3). For the acute risk potential the maximal tolerable ETR value is $ETR_{acute}=0.1$. In this case the predicted environmental concentration is one 1/10 of the LC50 concentration. For the chronic risk the maximal tolerable ETR value is $ETR_{chronic}=1$, where the PEC is equal to the NOEC.

Furthermore it is possible to consider the labelled buffer zone requirements for each product, when estimating risk potentials with SYNOPS. Since this strongly affects the outcome of the model, the two scenarios: all farmers **A) don't meet / B) meet** the buffer zone requirements are evaluated in this section. Since I-PHY does not consider buffer zone requirements only the scenario A) is evaluated in the model comparison.

The statistical evaluation for the risk scores of the reference organisms is aggregated in Table 20. In scenario B) were all buffer zone requirements were met, none oft the calculated acute terrestrial risk potentials and only 1.3 % of the chronic terrestrial risk potentials were above the maximal tolerable ETR. The corresponding 90th percentiles were 0.76 for the chronic terrestrial risk potential and 0.006 for the acute terrestrial risk potential. Almost identical results were calculated for the terrestrial risk potentials in scenario A). The frequency distributions of the terrestrial risk potentials are shown in Figure 16.

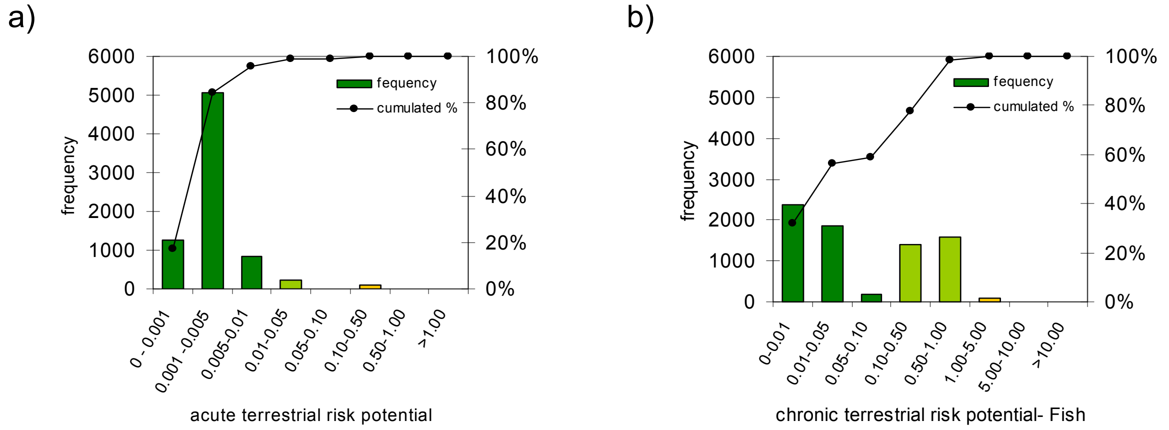


Figure 16: Frequency distributions of the acute (A) and chronic (B) terrestrial risk potentials for the wheat case study region Saxony Anhalt calculated with SYNOPS. 🟩low risk, 🟩 acceptable risk, 🟨 intermediate risk, 🟧 high risk

The aquatic risk potentials were significantly higher than the terrestrial risk potentials. If the buffer zone requirements were met, 6 % of all calculated acute aquatic risk potentials were above the maximal tolerable risk level (ETR>0.1). But both the median and the 90th percentile were below this level with values of 0.030 for the median and 0.091 for the 90th percentile. In scenario A these values were significantly higher: 46 % oft the acute aquatic risk potential were above the maximal tolerable risk level. In Figure 17 the frequency distributions of the calculated acute risk potentials for surface water are shown for both scenarios.

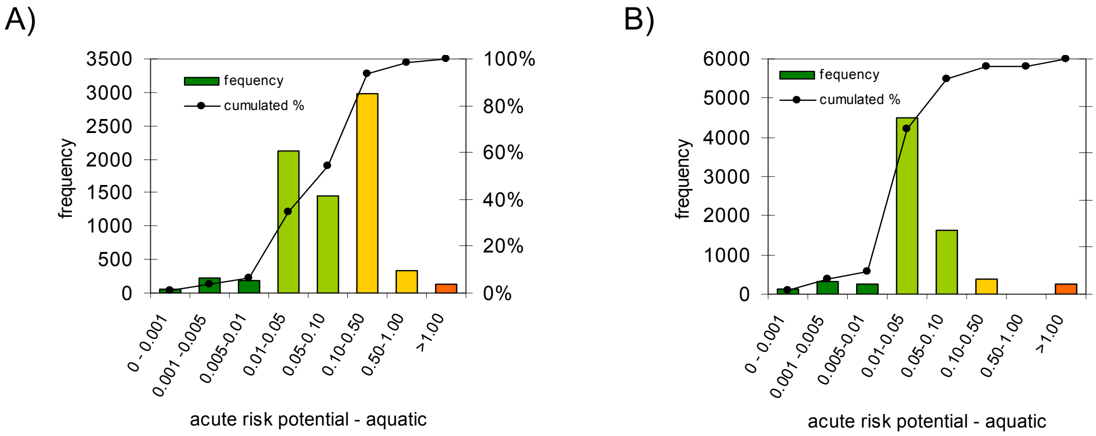


Figure 17: Frequency distributions of the acute aquatic risk potentials for the wheat case study region Saxony Anhalt calculated with SYNOPS. (A) buffer zone requirements were not met, (B) buffer zone requirements were met. 🟩low risk, 🟩 acceptable risk, 🟨 intermediate risk, 🟧 high risk.

Table 20: Statistical evaluation of the risk potentials for the wheat case study region Saxony Anhalt calculated with SYNOPS.

						ETR (n=7488)			% above maximal tolerable ETR
scenario	**risk potential**		**mean**	**Std**	**median**	**90th percentile**	**maximum**	**minimum**	
scenario A buffer zone requirements are **not met**	acute	daphnia	0.02	0.08	0.00	0.02	1.43	0.00	4.8
		fish	0.01	0.02	0.00	0.02	0.23	0.00	1.4
		algae	0.18	0.36	0.09	0.35	4.07	0.00	45.4
		aquatic	**0.18**	**0.36**	**0.09**	**0.36**	**4.07**	**0.00**	**46.0**
		earthworm	0.00	0.00	0.00	0.00	0.03	0.00	0.0
		bee	0.00	0.02	0.00	0.00	0.20	0.00	0.0
		terrestrial	**0.01**	**0.02**	**0.00**	**0.01**	**0.20**	**0.00**	**0.0**
	chronic	daphnia	0.36	1.79	0.01	0.65	37.43	0.00	8.9
		fish	0.24	1.08	0.03	0.37	21.03	0.00	5.6
		algae	1.87	2.36	1.05	4.65	18.77	0.00	51.4
		aquatic	**1.98**	**2.82**	**1.08**	**4.73**	**37.43**	**0.00**	**52.0**
		earthworm	0.24	0.32	0.03	0.80	1.05	0.00	1.3
		Bee	0.00	0.01	0.00	0.00	0.11	0.00	0.0
		terrestrial	**0.24**	**0.32**	**0.03**	**0.80**	**1.05**	**0.00**	**1.3**
scenario B buffer zone requirements **met**	acute	Daphnia	0.00	0.01	0.00	0.01	0.11	0.00	0.8
		Fish	0.00	0.00	0.00	0.00	0.02	0.00	0.7
		Algae	0.10	0.35	0.03	0.09	2.65	0.00	6.6
		aquatic	**0.10**	**0.35**	**0.03**	**0.09**	**2.65**	**0.00**	**6.6**
		earthworm	0.00	0.00	0.00	0.01	0.03	0.00	0.0
		Bee	0.00	0.02	0.00	0.00	0.20	0.00	0.0
		terrestrial	**0.01**	**0.02**	**0.00**	**0.01**	**0.20**	**0.00**	**0.0**
	chronic	Daphnia	0.10	0.28	0.00	0.33	2.84	0.00	0.6
		Fish	0.04	0.14	0.01	0.05	1.60	0.00	0.0
		Algae	0.62	0.73	0.39	1.24	5.01	0.00	7.8
		aquatic	**0.65**	**0.74**	**0.41**	**1.26**	**5.01**	**0.00**	**8.5**
		earthworm	0.23	0.31	0.03	0.77	1.01	0.00	1.3

scenario	**risk potential**	**ETR (n=7488)**						**% above maximal tolerable ETR**
		mean	**Std**	**median**	**90th percentile**	**maximum**	**minimum**	
	bee	0.00	0.01	0.00	0.00	0.11	0.00	0.0
	terrestrial	**0.23**	**0.31**	**0.03**	**0.77**	**1.01**	**0.00**	**1.3**

Similar results as for the acute aquatic risk potential were calculated for the chronic risk in surface water. If the buffer zone requirements were met (scenario B), 8.5 % of the chronic risk potentials were above the maximal tolerable risk level (ETR>1). The median was 0.421 and 90th percentile 0.956. Again with scenario A) these values were significantly higher. 52 % oft the chronic aquatic risk potential were above the maximal tolerable risk level. In Figure 18 the frequency distributions of the calculated chronic risk potentials for surface water are shown for both scenarios.

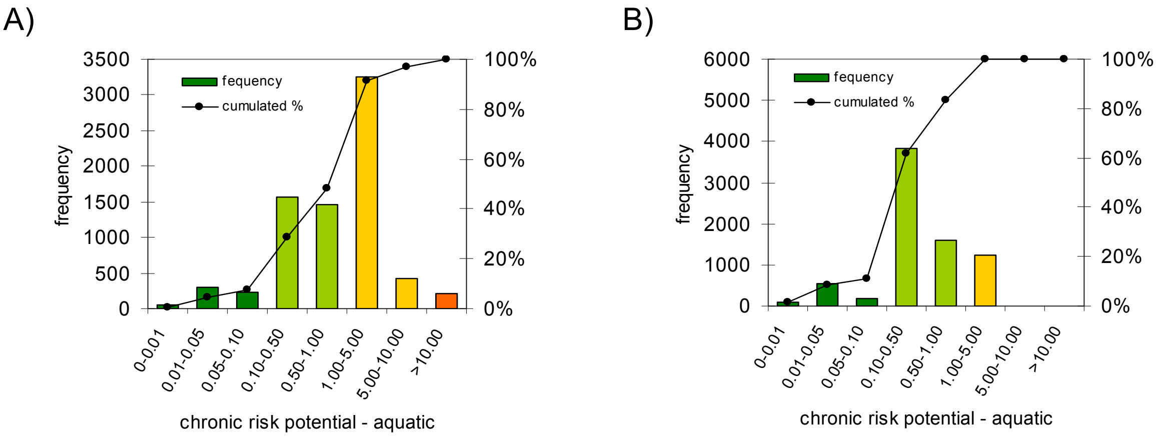


Figure 18: Frequency distributions of the chronic aquatic risk potentials for the wheat case study region Saxony Anhalt calculated with SYNOPS. (A) buffer zone requirements were not met, (B) buffer zone requirements were met. 🟩low risk, 🟩 acceptable risk, 🟨 intermediate risk, 🟧 high risk

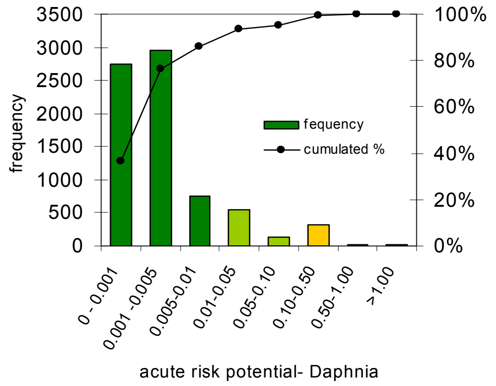
The chronic and acute aquatic risk potentials of the analysed strategies for wheat are clearly driven by the risk potential for algae. Figure 19 shows the frequency distributions of the acute risk potentials for all three aquatic reference organisms. Following the assumption, that the buffer zone requirements are met (scenario A), the chronic and acute risk potentials for daphnia and fish exceed only in 1% the maximal tolerable ETR. On the other hand the risk potentials of algae exceed this level in more than 6.5%. For scenario A) the conclusion can be driven. The chronic and acute risk potentials for daphnia and fish exceed the maximal tolerable ETR by less than 9% but the risk potentials for algae exceed this level by more than 45%.

It can be summarised, that the risk assessment with SYNOPS evaluates acceptable aquatic and terrestrial risk potentials for the wheat case study region Saxony Anhalt, if it is assumed that the farmers follow the concept of good plant protection practice and meet the labelled buffer zone requirements (scenario **B**). In no case the 90th percentile of the calculated chronic or acute risk potentials was larger than the maximal tolerable risk potential. The worst values were calculated for the chronic aquatic risk, where 8.5% of the calculated ETR where above the maximal tolerable risk potential.

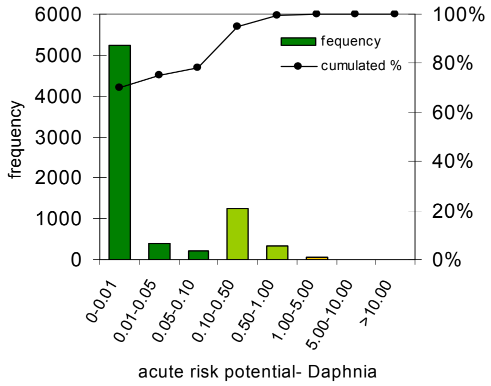
The situation looks different, if it is assumed that the all farmers don't meet the labelled buffer zone requirements (scenario **A**). In this case the chronic and acute aquatic risk potentials reach unacceptable values with more than 44% above the maximal tolerable risk potential. The terrestrial risk is not influenced in scenario **A** since the applied products don't require buffer zones to field margins.

Since the risk assessment model I-PHY is not considering buffer zone requirements the results calculated with I-PHY are comparable with scenario **A**. The aquatic risk scores of calculated with I-PHY lie in 81.8 % above the tolerable risk level. Compared to the aquatic risk potentials assessed with SYNOPS, where more than 44% are lager than the tolerable ETR, the results of I-PHY seem to be more conservative. A detailed comparison of the results will be conducted in section 4.3.

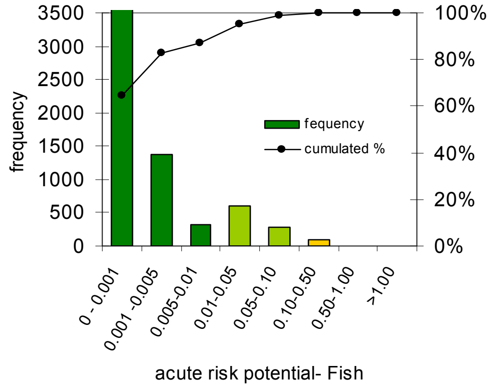
A1)



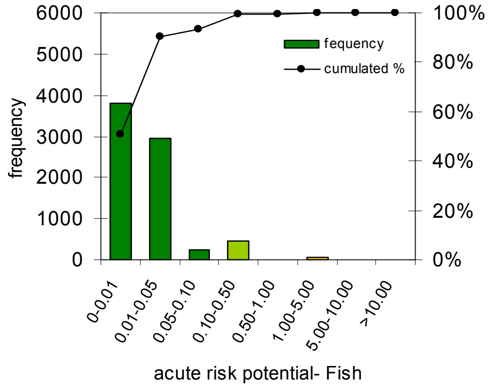
B1)



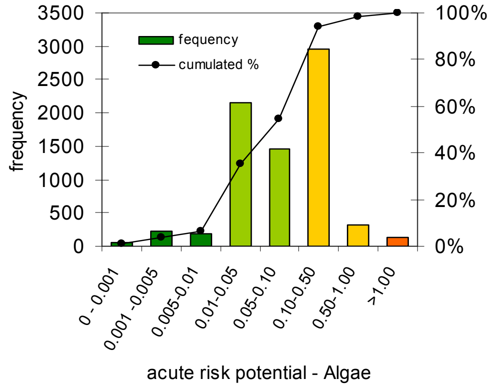
A2)



B2)



A3)



B3)

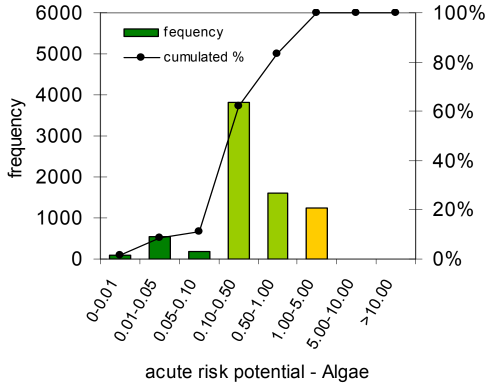


Figure 19: Frequency distributions of the acute aquatic risk potentials for the wheat case study region Saxony Anhalt calculated with SYNOPS. (A) buffer zone requirements were not met, (B) buffer zone requirements were met. 🟩low risk, 🟩 acceptable risk, 🟨 intermediate risk, 🟧 high risk

If the calculated aquatic risk potentials are evaluated for three environmental parameters (slope, mindist and soil type) separately. The statistical analysis was conducted for all possible values of each environmental parameter. For this evaluation only scenario A was considered, since the results will be compared with the results from I-PHY.

Like I-PHY the aquatic indicator of SYNOPS reacts most sensitive to the parameter mindist, whereas the impacts of the slope and soil type are clearly smaller. If the minimal distance increases from 1 to 20 m the median of the acute aquatic risk decreases by 0.26 and the 90th percentile by 0.56. Much larger reductions are observed for the chronic aquatic risk, where the median decreases by 3.17 and the 90th percentile by 9.51.

A opposite trend can be observed for the slope. This is also comparable to the results achieved with I-PHY. If the slope increases from 1 to 5 %, the median of the acute aquatic risk increases by 0.026 and the 90th percentile by 0.040. The median of the chronic risk is decreased by 0.365 and the 90th percentile by 0.315.

The four different soil types cause a variation of the median by 0.032 and of the 90th percentile by 0.047 for the acute risk and by 0.499 and of the 90th percentile by 0.365 for the chronic risk.

Table 21: Statistical evaluation of the risk scores grouped for each environmental parameter separately. Risk scores for wheat case study region Saxony Anhalt were calculated with SYNOPS. Buffer zone requirements were not considered (scenario A).

Risk sore	Mindist [m]	Slope [%]	soil-type number	number of scenarios	risk potential ETR				max differences in median	max differences in p90
					mean	std	median	p90		
acute aquatic risk	**1**			1872	0.41	0.60	0.29	0.65	**0.264**	**0.557**
	3			1872	0.19	0.26	0.13	0.29		
	10			1872	0.08	0.10	0.05	0.12		
	20			1872	0.05	0.06	0.03	0.09		
chronic aquatic risk	**1**			1872	4.46	4.25	3.56	10.74	**3.172**	**9.509**
	3			1872	2.03	1.86	1.57	4.63		
	10			1872	0.85	0.76	0.64	1.78		
	20			1872	0.56	0.53	0.39	1.23		
acute aquatic risk		**1**		2496	0.17	0.36	0.08	0.33	**0.026**	**0.040**
		3		2496	0.18	0.36	0.09	0.36		
		5		2496	0.19	0.37	0.10	0.37		
chronic aquatic risk		**1**		2496	1.84	2.78	0.90	4.62	**0.365**	**0.315**
		3		2496	1.97	2.81	1.06	4.72		
		5		2496	2.12	2.85	1.27	4.94		
acute aquatic risk			**9**	1872	0.17	0.36	0.07	0.33	**0.032**	**0.047**
			24	1872	0.20	0.37	0.11	0.38		
			36	1872	0.17	0.36	0.08	0.34		
			41	1872	0.18	0.37	0.09	0.35		
chronic			**9**	1872	1.84	2.78	0.87	4.62	**0.499**	**0.365**

Risk sore	Mindist [m]	Slope [%]	soil-type number	number of scenarios	risk potential ETR mean	std	median	p90	max differences in median	max differences in p90
aquatic risk			**24**	1872	2.21	2.88	1.37	4.98		
			36	1872	1.89	2.79	0.94	4.63		
			41	1872	1.96	2.81	1.04	4.75		

4.1.3 Results of PRZM

Among the JKI database, four pesticide use strategies were selected for PRZM-USES. Two strategies with maximum amount and number of applied pesticide and two strategies with the minimum amount and number of applied pesticides were selected (Table 22). In total 16 scenarios (combinations of strategies and field conditions) were analysed. This resulted in 176 simulations with PRZM and USES. The climate of year 2000 was used for the model calculations (JKI database).

Among the defined environmental scenarios (section 3.4) two soil types (Nr. 9 and 36) and two slopes (1% and 5%) could be parameterised. PRZM and USES do not consider the exposition pathway drift. Therefore the parameter distance to surface water was not taken into account.

Table 22: Selected strategies analysed with PRZM-USES

Name	JKI strategy ID		Definition	TFI
Qmax	1701339105	maximum amount of substances	> 6000 kg/ha	6.95
Qmin	1701353321	minimum amount of substances	800 kg/ha	2.76
ASmax	1701342130	maximum number of substances	16	6.50
ASmin	1701349266	minimum number of substances	6	3.66

Table 23: Soil characteristics of soils 9 and 36 (Data from JKI database, except when indicated)

Depth (cm)	OC content (%)	Clay (%)	Silt (%)	Sand (%)	Bulk density	Field capacity (%)	Wilting point [1] (%)
Soil 9							
0-15	3.0	14.33	64.73	20.94	1.35	40.00	18.01
15-70	2.0	14.33	64.73	20.94	1.35	37.00	15.69
70-100	0.1	14.33	64.73	20.94	1.35	37.00	11.67
100-130	0.1	14.33	64.73	20.94	1.35	37.00	11.67
Soil 36							
0-30	1.8	14.33	64.73	20.94	1.35	40.00	15.82
30-60	1.1	14.33	64.73	20.94	1.35	39.00	13.99
60-100	1.0	23.53	49.66	20.81	1.55	36.00	16.82
100-140	0.1	14.33	64.73	20.94	1.35	36.00	11.67

[1] From Rawls et al. (1982)

The complete input data of PRZM and USES are summarized in the appendix (Table 35 and Table 36). Toxicity potentials (TP) were available for bentazone, carbendazim, deltamethrine, dichlorprop P, isoproturon and MCPA in Huijbregts et al. (2000), but they were calculated with USES for the other 20 pesticides (Annex 2). For six pesticides (chlormequat, fenvalerat, fluquinconazole, metconazole, tribenuron and trinexapac), no aquatic PNEC (Predicted No Effect Concentration) were available in the database nor in literature, therefore the TP and the impact scores were only calculated for Human.

Figure 20 shows the impact scores of the different strategies on Human, terrestrial ecosystems, fresh and seawater and fresh and sea sediment. The higher the score is, the highest the impact is. Results are presented only for a soil slope of 5% as the results for a slope of 1% were similar (losses of pesticides with erosion, runoff and lateral outflow were negligible in both cases).

Differences among the two soils were observed. Soil 36 seems to lead to highest impacts, except for ASmax and Qmax scenarios. This can be due to lower organic carbon content therefore, lower sorption of pesticides.

In general, the highest impacts were observed with the scenarios of Qmax, except for sediment where the highest impact was observed for the ASmax scenario. This is due to high impact of carbendazim on sediment. The highest impact scores were found for human, the lowest for seawater and sea sediment.

The method allows discrimination of soil context and of different crop protection strategies. Highest impacts were found for strategies using the highest amounts of pesticides, lowest impacts for the lowest amounts.

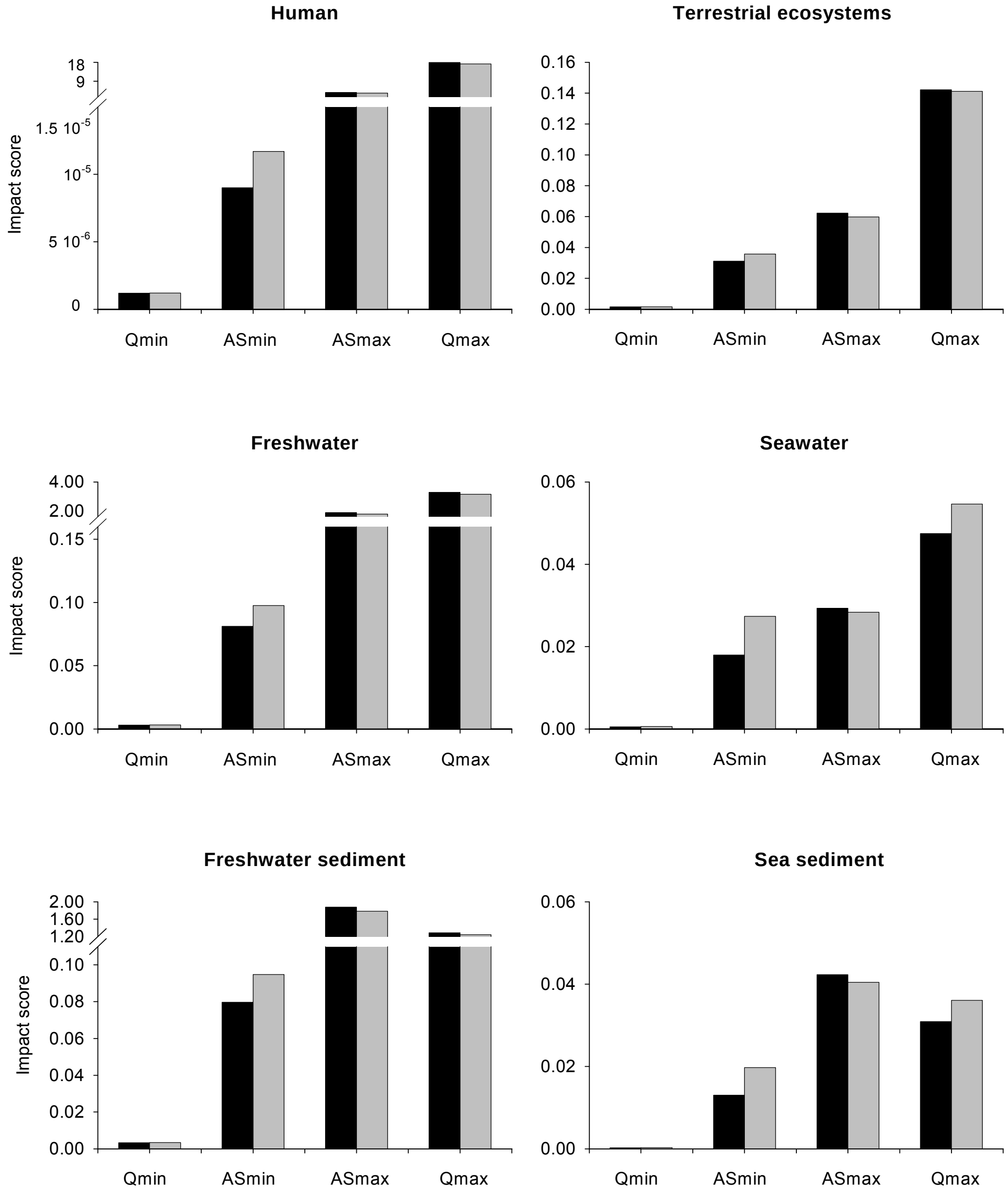


Figure 20: Impact scores of crop protection strategies with minimum amounts of pesticides (Qmin), minimum number of active substances (ASmin), maximum amounts of pesticides

(Qmax), maximum number of active substances (ASmax) on Human, terrestrial ecosystems, fresh and seawater, fresh and sea sediment, in soils 9 (■) and 36 (□).

4.2 Pomefruit case study region: Lake Constance

Due to technical reasons only 66 of the 900 defined scenarios for the pomefruit region could be evaluated with I-Phy and none were evaluated with PRZM-USES. The following sections summarise the results for the region Lake Constance.

4.2.1 Results of I-PHY

For the pomefruit region Lake Constance only results for the aquatic risk potential were available from risk assessments with I-PHY. For the analysis with I-PHY the number of strategies was reduced to eleven pomefruit strategies, three with high frequency index, four with medium frequency index and 3 with low frequency index. These were analysed with 6 different environmental scenarios considering only one soil type (Iba=21), two slopes (1% and 5%) and three distance classes (1m, 5m, 10m).

The frequency distribution of the calculated aquatic risk scores is shown in Figure 21. For the pomefruit region the evaluated risk scores were significantly higher, than for the wheat region Saxony Anhalt. 100% of the calculated risk scores were lager than the maximal tolerable sore of 0.3. The median was in the high risk range with 0.710 and the 90th percentile reached a value of 0.95 (Table 24).

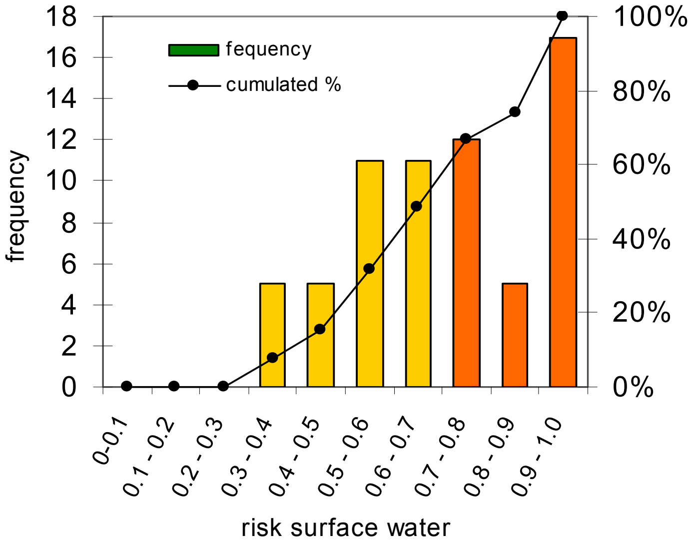


Figure 21: Aquatic risk scores for pomefruit case study region Lake Constance calculated with I-PHY.
🟩low risk, 🟨 intermediate risk, 🟧 high risk

A decrease of the 90th percentile from 0.99 to 0.68 could be observed, when the distance form the field to the surface water was increased form 1 to 10 m. The range of variation was slightly larger for the median from 0.94 to 0.52. An increase of slope resulted in a slight increase of the aquatic risk scores for the median by 0.35. The 90th percentile was not affected.

Table 24: Statistical evaluation of the aquatic risk scores for the pomefruit case study region Lake Constance calculated with I-PHY

Risk sore	Mindist [m]	Slope [%]	soil-type number	number of scenarios	risk scores (n=66) Mean	std	median	p90	max differences in median	max differences in p90
aquatic risk			21	66	0.71	0.19	0.71	0.95		
aquatic risk	1		21	22	0.93	0.05	0.94	0.99	0.416	0.308
	5		21	22	0.69	0.09	0.70	0.78		
	10		21	22	0.52	0.12	0.52	0.68		
aquatic risk		3	21	33	0.69	0.218	0.70	0.95	0.035	0.000
		5	21	33	0.73	0.18	0.73	0.95		

4.2.2 *Results of SYNOPS*

For the pomefruit region of Lake Constance all 900 suggested scenarios could be evaluated with SYNOPS. Again, like for wheat, the labelled buffer zone requirements for each product were not considered in scenarios **A)** assuming **all farmers don't meet the buffer zone requirements** and were considered in scenario **B)** assuming that **all farmers meet the buffer zone requirements**. Since I-PHY does not consider buffer zone requirements only scenario A) can be compared with the results of I-PHY.

Compared to the risk potentials in wheat, SYNOPS calculates higher risk potentials for the pomefruit region Lake Constance. For scenario A) 100 % of the calculated acute aquatic risk potentials and 80.7 % of the chronic aquatic risk are above the tolerable risk and level. As expected, the risk potentials are significantly reduced for scenario B. Here the percentages of risk potentials above the tolerable risk level are reduced to 31.9 % for the acute risk and to 4.9% for the chronic risk. The two frequency distributions of the acute aquatic risk for scenario A and B are shown in Figure 22. The frequency distributions of chronic risk are demonstrated in Figure 23.

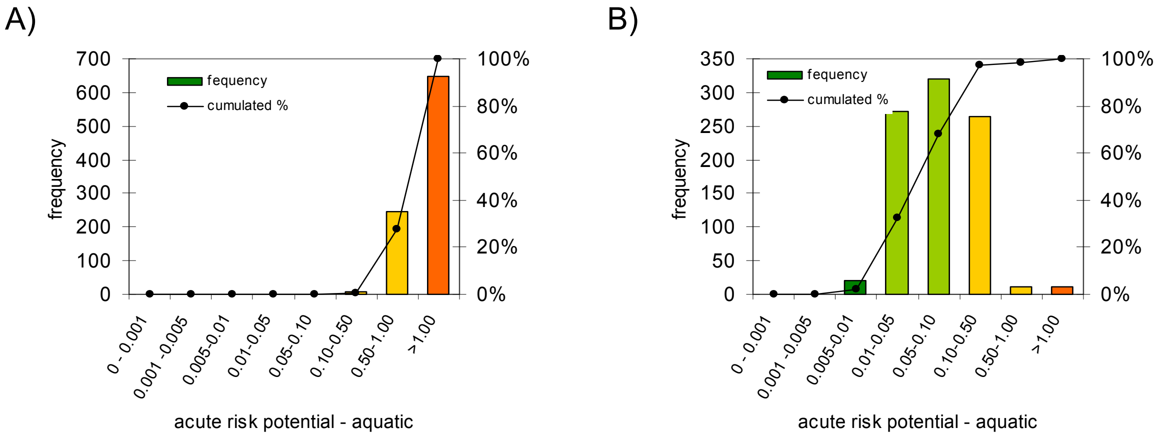


Figure 22: Frequency distributions of the acute aquatic risk potentials for the pomefruit case study region Lake Constance calculated with SYNOPS. (A) buffer zone requirements were not met, (B) buffer zone requirements were met. 🟩low risk, 🟩 acceptable risk, 🟨 intermediate risk, 🟧 high risk

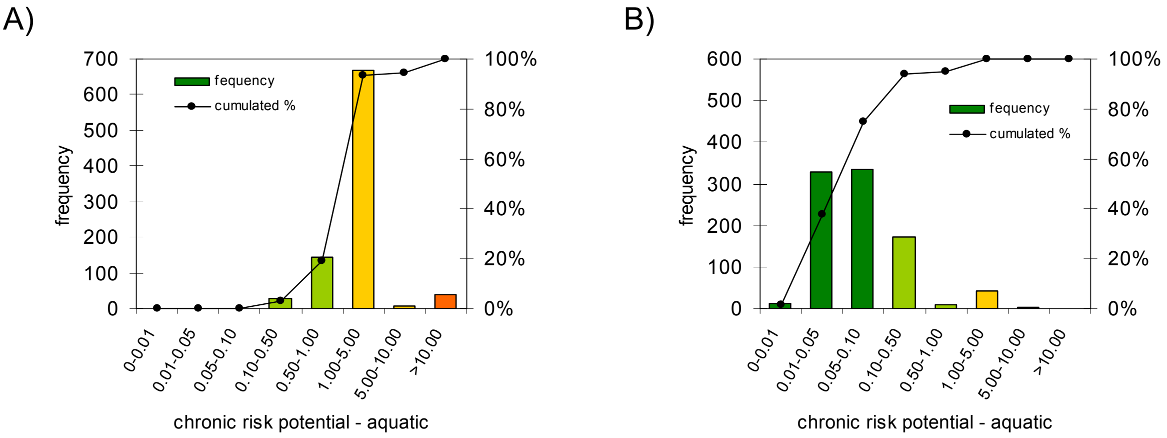


Figure 23: Frequency distributions of the chronic aquatic risk potentials for the pomefruit case study region Lake Constance calculated with SYNOPS. (A) buffer zone requirements were not met, (B) buffer zone requirements were met. 🟩low risk, 🟩 acceptable risk, 🟨 intermediate risk, 🟧 high risk

Similar high values are achieved for the terrestrial risks with 70 % of the acute risk potential and 80.7 % of the chronic risk potentials above the tolerable risk potential. The terrestrial indicator is clearly driven by the risk for bees (see Figure 24). One reason for the high risk potentials is the in crop exposition of the bees. Some active ingredients, which are dangerous for bees, have spraying restrictions, like spraying only during night or not during the pomefruit blossom. These restrictions could not be considered with the current version of SYNOPS, which explains the high scores for bees and therefore for the terrestrial risk.

The statistical analysis of the aquatic and terrestrial risk potentials and of the risk potentials for the different reference organisms are summarised Table 25.

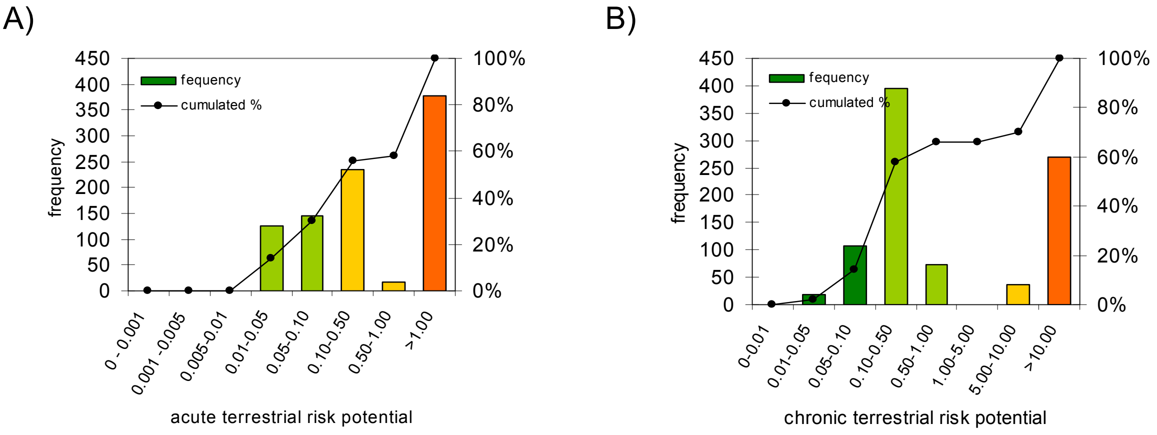


Figure 24: Frequency distributions of the acute (A) and chronic (B) terrestrial risk potentials for the pomefruit case study region Lake Constance calculated with SYNOPS. 🟩low risk, 🟩 acceptable risk, 🟨 intermediate risk, 🟧 high risk

Table 25: Statistical evaluation of the risk potentials for the pomefruit case study region Lake Constance calculated with SYNOPS.

scenario	risk potential		ETR (n=900)						% above maximal tolerable ETR
			mean	std	median	90th percetile	maximum	minimum	
scenario A buffer zone requirements are **not met**	acute	daphnia	1.82	2.79	1.16	2.90	28.93	0.37	100
		fish	1.57	1.99	1.02	1.91	16.65	0.33	100
		algae	1.26	0.77	1.06	2.44	5.43	0.05	97.3
		aquatic	**2.09**	**3.00**	**1.26**	**2.90**	**28.93**	**0.43**	**100**
		earthworm	0.01	0.00	0.01	0.01	0.02	0.00	0
		bee	9.03	13.14	0.35	26.98	44.70	0.02	70
		terrestrial	**9.03**	**13.14**	**0.35**	**26.98**	**44.70**	**0.02**	**70.0**
	chronic	daphnia	3.25	11.63	0.64	1.72	132.67	0.17	25.9
		fish	6.06	19.05	1.60	3.32	140.39	0.31	79.4
		algae	1.50	4.53	0.44	0.93	36.90	0.04	8.56
		aquatic	**6.30**	**19.77**	**1.65**	**3.39**	**140.39**	**0.44**	**80.67**
		earthworm	0.30	0.29	0.13	0.81	0.92	0.02	0
		bee	8.81	12.98	0.33	26.54	44.02	0.02	66
		terrestrial	**8.86**	**12.94**	**0.39**	**26.54**	**44.02**	**0.04**	**66.0**
scenario B buffer zone requirements **met**	acute	Daphnia	0.08	0.39	0.02	0.09	5.15	0.01	9.67
		Fish	0.06	0.20	0.02	0.10	2.71	0.01	8.56
		Algae	0.09	0.09	0.07	0.24	0.59	0.00	25.89
		aquatic	**0.14**	**0.39**	**0.07**	**0.24**	**5.15**	**0.01**	**31.89**
		earthworm	0.01	0.00	0.01	0.01	0.02	0.00	-
		Bee	9.03	13.14	0.35	26.98	44.70	0.02	-
		terrestrial	9.03	13.14	0.35	26.98	44.70	0.02	**-**
	chronic	Daphnia	0.12	0.49	0.02	0.08	9.02	0.00	3.0
		Fish	0.15	0.63	0.04	0.12	13.77	0.01	3.89
		Algae	0.14	0.49	0.05	0.15	5.21	0.00	3.33
		aquatic	**0.22**	**0.75**	**0.06**	**0.18**	**13.77**	**0.01**	**4.89**
		earthworm	0.30	0.29	0.13	0.81	0.92	0.02	-
		Bee	8.81	12.98	0.33	26.54	44.02	0.02	-
		terrestrial	8.86	12.94	0.39	26.54	44.02	0.04	**-**

Looking at three different aquatic reference organisms, SYNOPS calculates the highest acute risk potentials for algae (Figure 25). Following the assumption, that the buffer zone requirements are met (scenario B), acute risk potentials for daphnia and fish exceed in 9.6% or 8.6% the maximal tolerable ETR=0.1 but for algae this level is exceed by more than 25.9%. In scenario A for all three reference organisms 100% exceed the tolerable ETR for acute risk.

The assessed chronic aquatic risk potentials are for all three reference organisms lower than the acute risks. Only 3 to 4% exceed the maximum tolerable risk level and no significant difference between the organisms could be found.

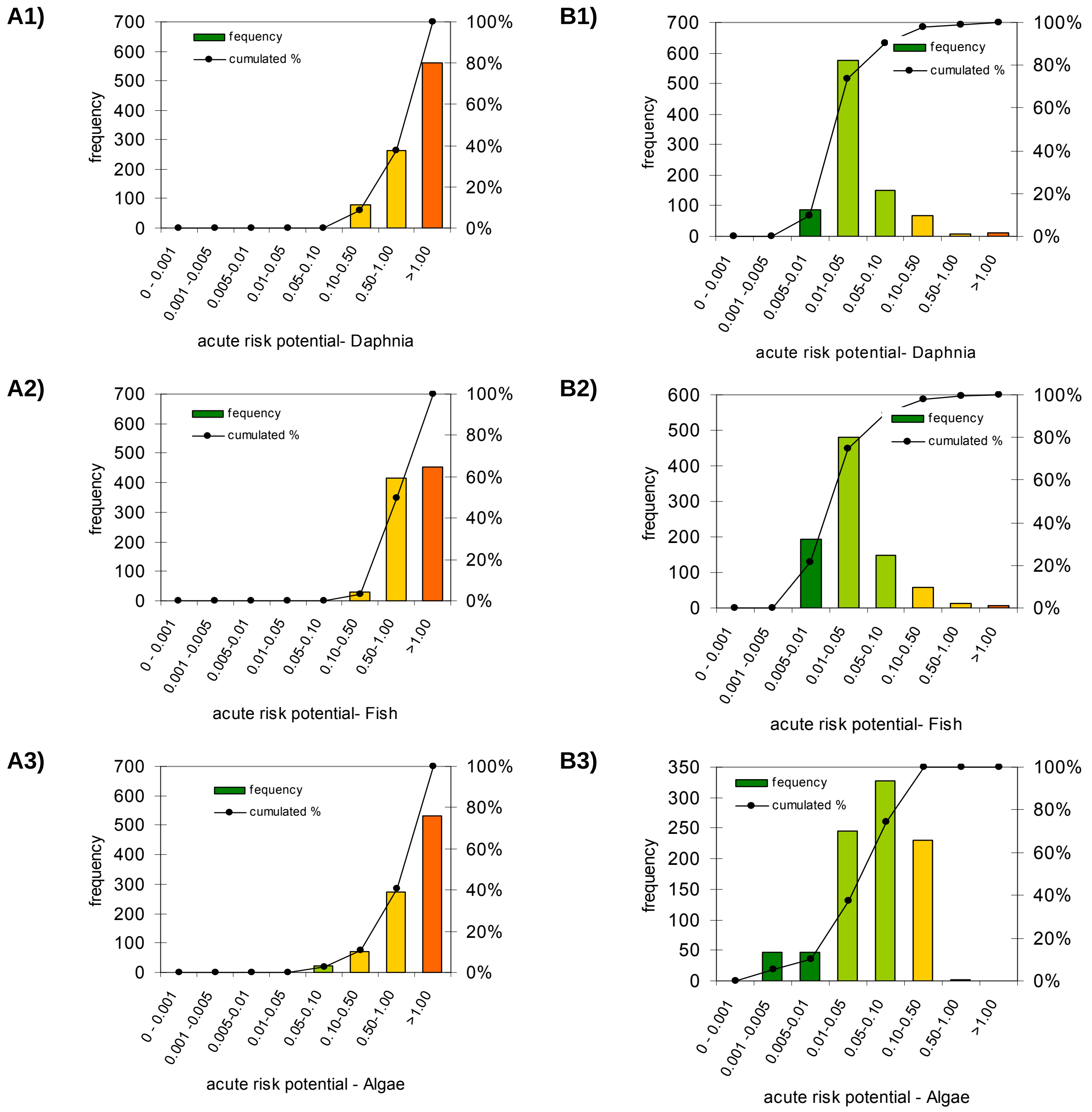


Figure 25: Frequency distributions of the acute aquatic risk potentials for the pomefruit case study region Lake Constance calculated with SYNOPS. (A) buffer zone requirements were not met, (B) buffer zone requirements were met. 🟩low risk, 🟩 acceptable risk, 🟨 intermediate risk, 🟧 high risk

Considering the separate evaluation of the environmental parameters, comparable relations are found as for the wheat case study region (Table 26). The three environmental parameters had no influence on the terrestrial risk potentials, since the exposition pathway is drift into the field margins at a fixed distance of 0.5m. The aquatic indicator reacts most sensitive to the parameter mindist, whereas the impacts of the slope and soil type are clearly smaller. If the minimal distance increases from 1 to 10 m the median of the acute aquatic risk decreases by 1 and the 90th percentile by 5. Much larger reductions are observed for the chronic aquatic risk, where the median decreases by 1.6 and the 90th percentile by 76.

The effects of the slope were lager than in the wheat case study region, since the range of the slopes was larger in the pomefruit region. The two different soil types also cause a larger variation of the aquatic risk potential than in the variation of the four soil types in the wheat region.

Table 26: Statistical evaluation of the risk scores grouped for each environmental parameter separately. Risk scores for pomefruit case study region Lake Constance were calculated with SYNOPS. Buffer zone requirements were not considered (scenario A).

Risk sore	Mindist [m]	Slope [%]	Soil-type number	number of scenarios	risk potential ETR				max differences in median	max differences in p90
					mean	std	median	p90		
acute aquatic risk	**1**			300	3.36	4.03	1.78	6.64	1.03	5.38
	5			300	1.81	2.42	1.22	2.06		
	10			300	1.11	1.49	0.75	1.26		
chronic aquatic risk	**1**			300	15.96	32.14	2.76	77.06	1.60	75.47
	3			300	1.81	0.75	1.90	2.55		
	10			300	1.12	0.47	1.17	1.59		
acute aquatic risk		**3**		300	1.82	2.63	1.26	2.90	0.00	3.75
		5		300	1.82	2.63	1.26	2.90		
		10		300	2.64	3.57	1.26	6.64		
chronic aquatic risk		**3**		300	1.81	0.96	1.62	3.00	0.22	74.06
		5		300	1.81	0.97	1.62	3.00		
		10		300	15.26	32.43	1.83	77.06		
acute aquatic risk			**14**	450	1.82	2.63	1.26	2.90	0.00	2.06
			21	450	2.36	3.31	1.26	4.95		
chronic aquatic risk			**14**	450	1.82	0.98	1.62	3.01	0.16	44.49
			21	450	10.77	27.22	1.78	47.50		

5 Comparison of the assessment results

In this section the results of the models I-PHY and SYNOPS will be compared: Due to the small number of analysed scenarios PRZM-USES was not included in the model comparison. Only four pesticide use strategies were analysed with four different environmental scenarios for wheat and none were analysed for pomefruit.

The intensity of plant protection, which is expressed with the treatment frequency index, is often related to the risk potential of the applied strategies. With the accomplished assessment of 156 wheat strategies and 50 pomefruit strategies it is possible to set the TFI in relation to the risk potentials calculated SYNOPS and I-PHY. In the first two sections the result of the two models will be compared to the calculated frequency treatment indices (TFI) of the analysed pesticide use strategies. In the last section the results of the two models will be compared to each other.

5.1 Comparison of the TFI with the risk scores calculated with I-PHY

For the wheat case study region Saxony Anhalt 156 strategies were analysed considering 48 different environmental scenarios, resulting in 7488 risk assessments with I-PHY. The TFI of these strategies ranged form 14.4 to 59.3. The large variation of the results is demonstrated in Figure 26, where the complete set of results (aquatic risk score) is set into relation to the frequency treatment index (TFI).

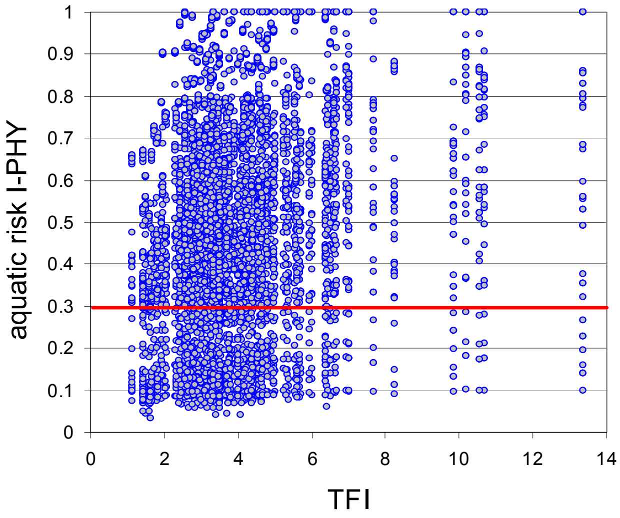


Figure 26: Aquatic risk scores for wheat strategies calculated with IPH vs. TFI (n=7488). The red line marks the maximum tolerable risk.

The correlation matrix according to a Spearman rank analysis is listed in Table 27. In most cases only very weak (0.2<r>0.5) positive correlation were evaluated between the risk scores calculated with I-PHY and the TFI. If the scores were grouped by the environmental parameters only the global risk and the aquatic risk showed a weak positive correlation (0.5<r>0.7) when the mindist was 1 m and 5m. In all other parameter combinations only very weak correlations were evaluated.

Table 27: Correlation matrix for I-PHY risk scores vs. TFI according to a Spearman rank analysis. Risk potentials were evaluated for wheat case study region.

	grouped by				**Correlation coefficient (r)**			
	Mindist [m]	**Slope [%]**	**soil-type number**	**number of scenarios**	**Global risk**	**Groundw. risk**	**Risk in air**	**Aquatic risk**
Correlated with TFI	all			7488	0.40	0.35	0.38	0.24
	1			1872	**0.69**	0.35	0.45	**0.60**
	5			1872	**0.67**	0.35	0.41	**0.56**
	10			1872	0.47	0.35	0.39	0.42
	20			1872	0.46	0.35	0.33	0.29
		1		2496	0.34	0.35	0.37	0.16
		3		2496	0.40	0.35	0.38	0.24
		10		2496	0.48	0.35	0.40	0.33
			9	1872	0.39	0.41	0.38	0.24
			24	1872	0.44	0.41	0.39	0.30
			36	1872	0.44	0.41	0.39	0.30
			41	1872	0.40	0.38	0.38	0.24

Mean values were calculated for each strategy to avoid the large variation, which is determined by the varying environmental conditions. The mean risk scores for each strategy expresses the average of all considered environmental conditions (n=48) for the wheat case study region.

In Figure 27 the average values of the calculated risk scores for surface water (a), groundwater (b), air (c) and the global risk (d) are related to the TFI and regression analysis were conducted. A fairly good regression according to a power function ($y=a*x^b$, $r^2=0.57$) could be found for the means oft the global risk (Figure 27d). Also the average aquatic risk showed a positive regression according to a power function, but the regression coefficient was much lower ($r^2=0.39$). Very weak regression coefficients were for the means of groundwater risk and the risk in air ($r^2<0.16$).

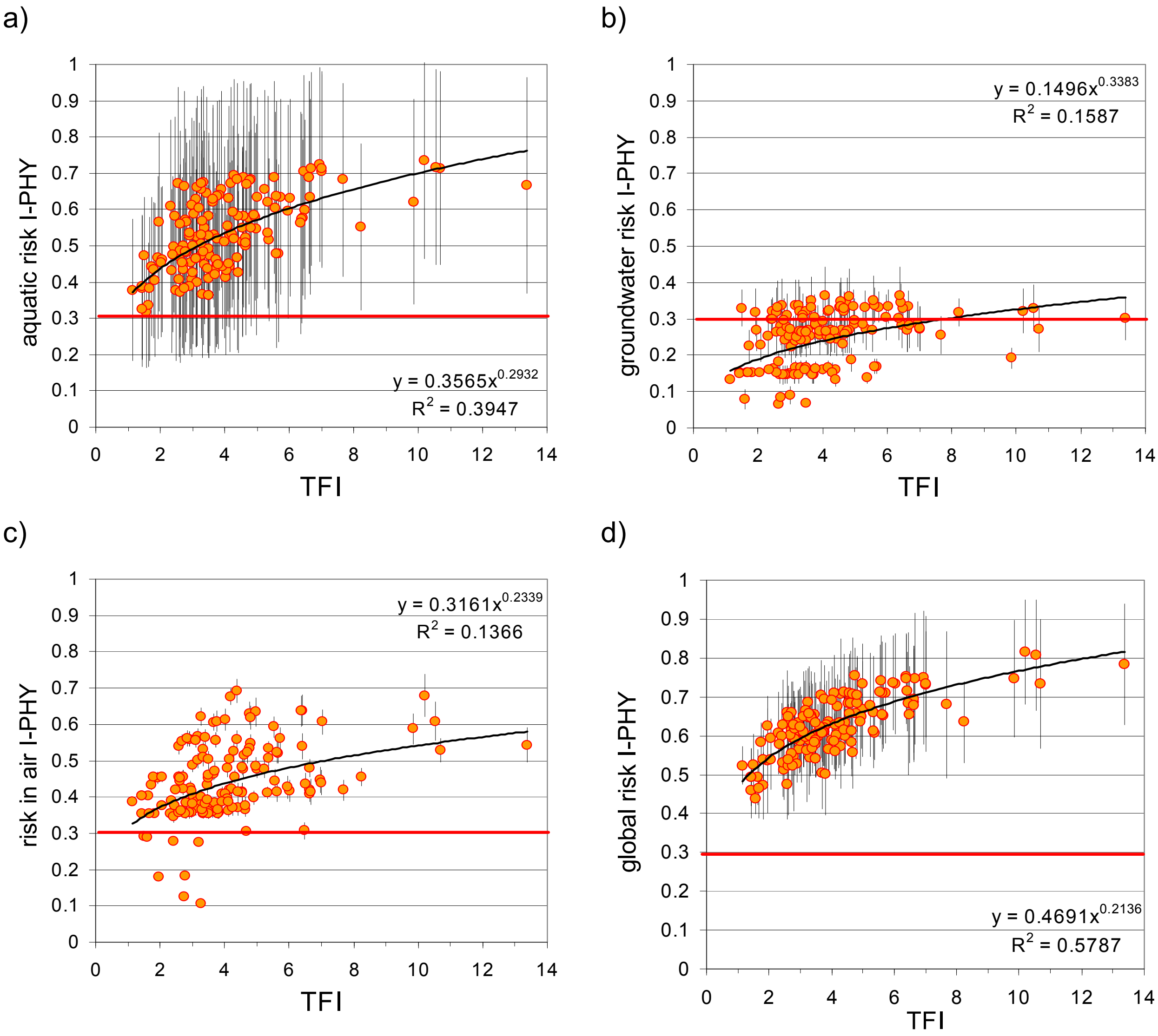


Figure 27: **Mean risk scores for wheat strategies calculated with I-PHY in relation to the TFI (n=156). surface water (a), groundwater (b), air (c) and the global risk (d) - the red line marks the maximum tolerable risk.**

For the pomefruit region only 11 strategies were analysed with I-PHY. These strategies had a range of the frequency treatment index from 14.4 to 49.1. With a Spearman correlation coefficient of r=0.023 no correlation could be shown between the aquatic risk score and the TFI (Figure 28).

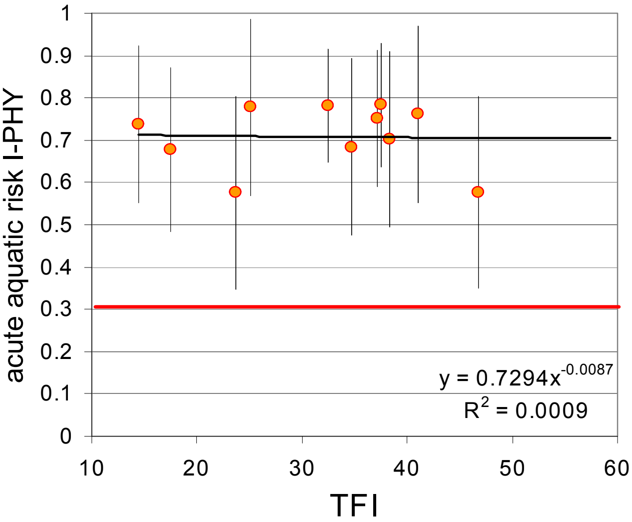


Figure 28: Mean aquatic risk scores for pomefruit strategies calculated with I-PHY in relation to the TFI (n=11). The red line marks the maximum tolerable risk.

5.2 Comparison of the TFI with the risk scores calculated with SYNOPS

The result for the wheat case study region calculated with SYNOPS show a similar picture as the I-PHY results. Only very weak correlations can be found, if all 7488 strategy - environmental scenario combinations are related to the TFI. The SYNOPS results are represented on a logarithmic scale, since the calculated risk potentials range 0.0001 to 10 (Figure 29).

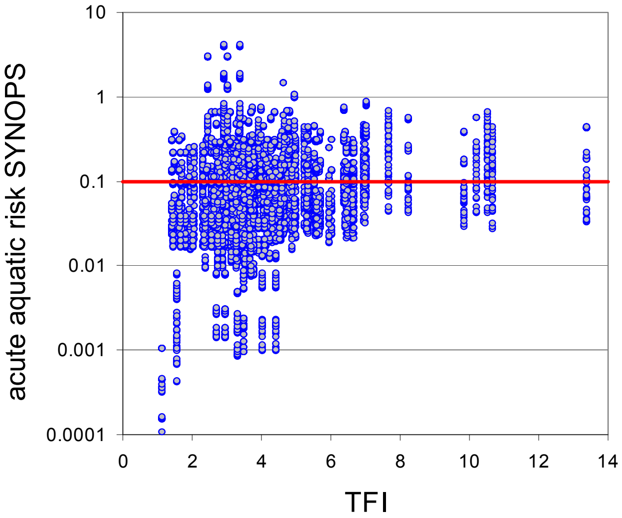


Figure 29: Aquatic risk scores calculated with SYNOPS vs. TFI (n=7488). The red line marks the maximum tolerable risk.

A rank analysis according to Spearman was conducted for all combinations of environmental conditions and pesticide use strategies. The correlation matrix is shown in Table 28. All analysed risk potentials showed very weak ($0.2<r>0.5$) positive correlations, when the results were grouped by the three environmental parameters slope, mindist and soil type. The correlations of the terrestrial risk potentials were slightly stronger. As described in section 4.2.2, the scores were not influenced by the environmental parameters.

Table 28: Correlation matrix for SYNOPS risk potentials vs. TFI according to a Spearman rank analysis. Risk potentials were evaluated for wheat case study region.

	grouped by			number of scenarios	Correlation coefficient (r)			
	Mindist [m]	**Slope [%]**	**soil-type number**		**acute aquatic risk**	**chronic aquatic risk**	**acute terrestrial risk**	**chronic terrestrial risk**
Correlated with TFI	all			7488	0.17	0.20	0.50	0.47
	1			1872	0.31	0.27	0.49	0.47
	5			1872	0.31	0.28		
	10			1872	0.31	0.28		
	20			1872	0.30	0.29		
		1		2496	0.16	0.18	0.49	0.47
		3		2496	0.18	0.20		
		10		2496	0.19	0.22		
			9	1872	0.16	0.18	0.49	0.47
			24	1872	0.21	0.23		
			36	1872	0.16	0.19		
			41	1872	0.17	0.20		

Again average values were calculated for each strategy (n=48) to avoid the large variation and regression analysis on the mean terrestrial and aquatic risk potentials were conducted. No regression could be found between the acute aquatic risk potential and the TFI or between the chronic aquatic risk potential and the TFI (Figure 30). This is true for scenario A (buffer zone requirements are not met) and scenario B (buffer zone requirements are met). The maximum regression coefficient was $r^2= 0.10$.

The average values of the calculated terrestrial risk potential showed for both scenarios (A and B) a weak regression according to a power function with regression coefficients of $r^2>0.22$ (Figure 31).

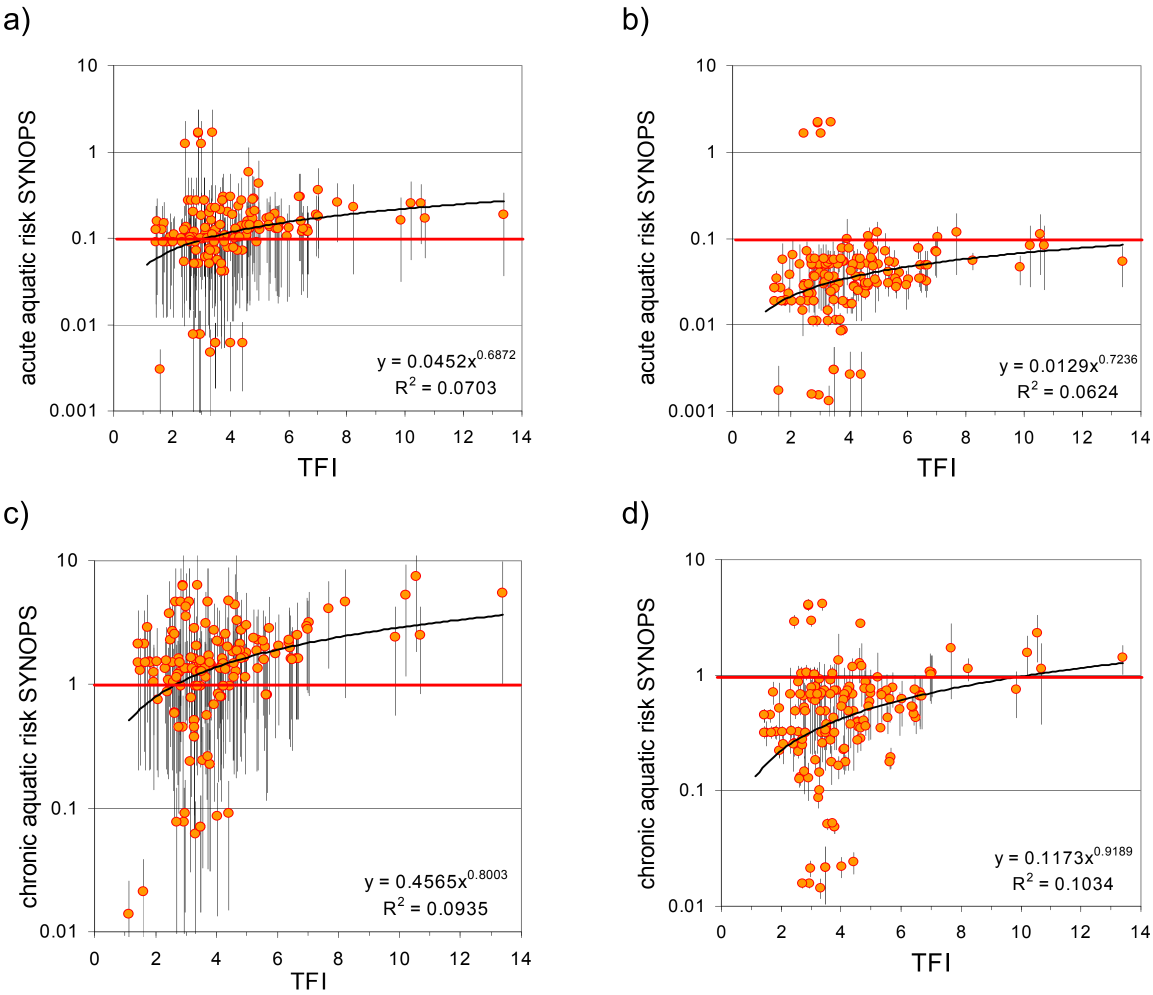


Figure 30: Mean aquatic risk potentials for wheat strategies calculated with SYNOPS in relation to the TFI (n=156). (a) acute, scenario A (b) acute, scenario B (c) chronic, scenario A (d) chronic, scenario B- the red line marks the maximum tolerable risk.

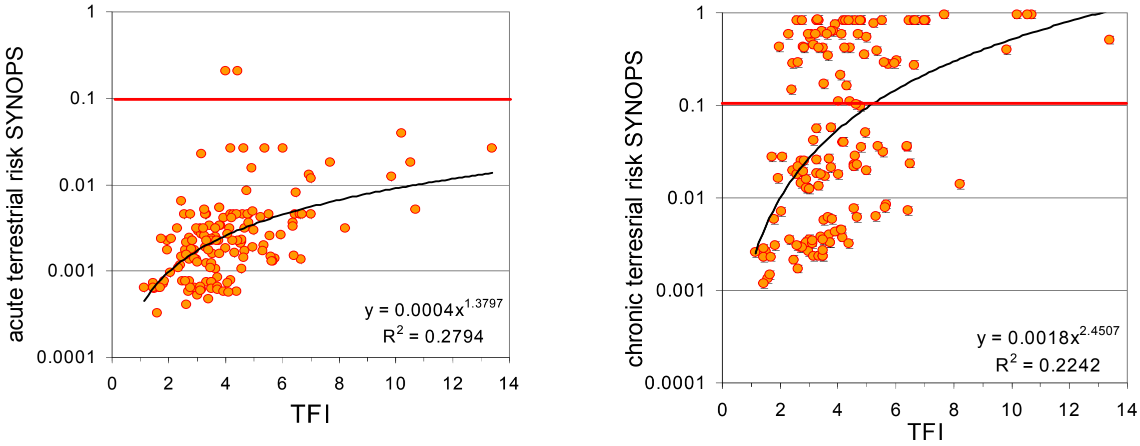


Figure 31: Mean terrestrial risk potentials for wheat strategies calculated with SYNOPS in relation to the TFI (n=156). The red line marks the maximum tolerable risk.

For the pomefruit strategies no or only very weak significant correlation could be found between the aquatic or terrestrial risk potentials calculated with SYNOPS and the TFI. This is also the case if the results are grouped by the environmental parameters. (Table not shown) And it is applicable for scenario A (buffer zone requirements are not met) and scenario B (buffer zone requirements are met).

Figure demonstrates that no or very weak regressions could be found between the average values of the aquatic risk potentials and the TFI. The maximum regression coefficient was r^2= 01469.

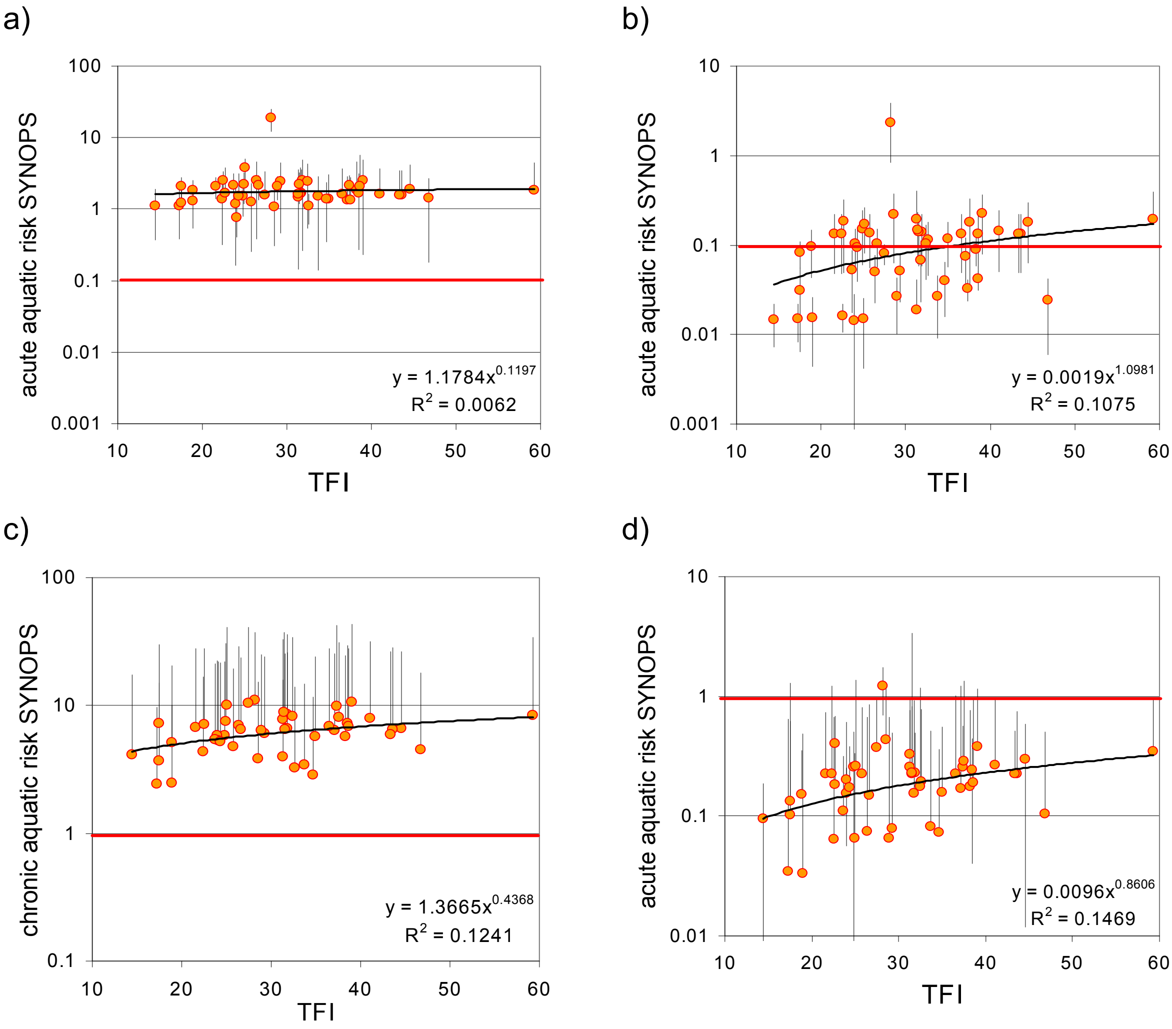


Figure 32: **Mean aquatic risk potentials for pomefruit strategies calculated with SYNOPS in relation to the TFI (n=50). (a) acute, scenario A (b) acute, scenario B (c) chronic, scenario A (d) chronic, scenario B- the red line marks the maximum tolerable risk.**

5.3 Comparison of the results of SYNOPS and I-PHY

Looking at the evaluations above it becomes evident, that the models SYNOPS and I-PHY can only be compared on the level of the aquatic risk, since SYNOPS did not calculate risk potentials for groundwater and air and I-PHY did not consider terrestrial risk. As mentioned above only the SYNOPS results of Scenario A could be compared to the results of I-PHY, since I-PHY could not consider the product labelled buffer zones. Therefore the aquatic risk calculated with I-PHY will be compared with both the acute and the chronic aquatic risk calculated with SYNOPS.

In Figure 33 the results for the wheat case study region calculated with SYNOPS are plotted against the result calculated with I-PHY. The corresponding correlation matrix according to a Spearman rank analysis is summarised in Table 29.

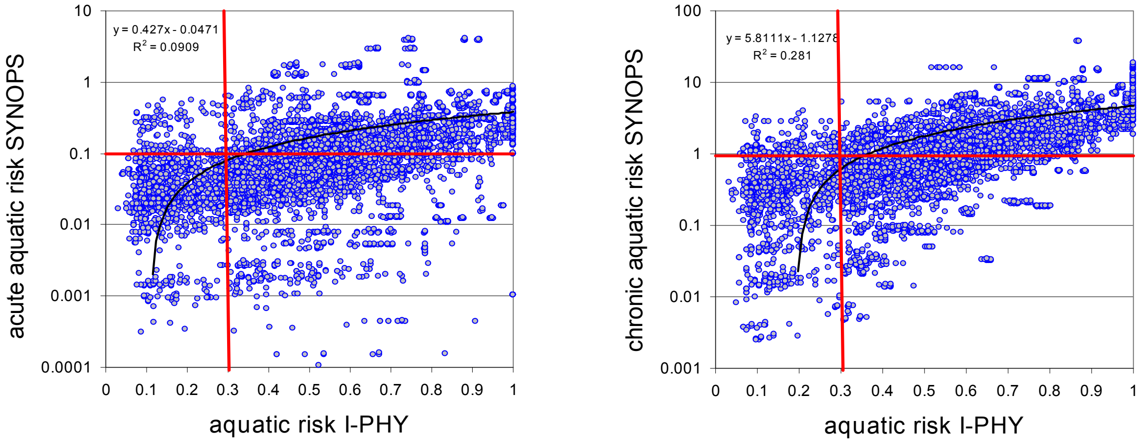


Figure 33: Acute and chronic aquatic risk calculated with SYNOPS in relation to the aquatic risk scores calculated with I-PHY. Risk assessments were conducted for wheat case study region

Considering all scenarios, high correlations between the two models could be found with correlation coefficients lager than 0.7. Overall, the chronic risk potential showed slightly higher correlation coefficients than the acute risk potential.

Besides the comparison of all scenarios in Table 29 the results were also grouped by the environmental parameters slope, soil type and mindist. It becomes evident, that the lowest correlation coefficients (0.33>r>0.52) are achieved, when they are grouped by the minimal distance. In this case, that the two variable parameters soil type and slope have less impact on the correlation than the parameter mindist. Therefore higher correlation coefficients are found if the results are grouped by the soil type (0.66>r>0.74) and slope (0.70>r>0.76). This is consistent with the findings in section 4, that a variation of the slope or soil type has less impact on the risk scores than a variation in the minimal distance.

Although a fairly good correlation between the model results could be found, there is still a large difference in the classification of the calculated risks between the two models. With I-PHY it is assessed, that 84% of the risk sores are above the maximum tolerable risk level. These are all points to the right of the vertical red line in Figure 33. SYNOPS assesses that 46% of the acute and 52 % of the chronic aquatic risk potential are above the max tolerable risk level. These are all points above the horizontal red line in Figure 33.

Table 29: Correlation matrix according to a Spearman rank analysis. Analysed were the aquatic risk potentials calculated with SYNOPS vs. aquatic risk scores calculated with I-PHY. Risk assessments were conducted for wheat case study region.

	grouped by			**number of scenarios**	**Correlation coefficient (r)**	
	Mindist [m]	**Slope [%]**	**soil-type number**		**acute aquatic risk SYNOPS**	**chronic aquatic risk SYNOPS**
Correlated with Aquatic risk scores I-PHY	All			7488	0.71	0.72
	1			1872	0.35	0.43
	5			1872	0.46	0.52
	10			1872	0.35	0.38
	20			1872	0.33	0.33
		1		2496	0.74	0.73
		3		2496	0.71	0.72
		10		2496	0.66	0.68
			9	1872	0.74	0.75
			24	1872	0.74	0.73
			36	1872	0.70	0.73
			41	1872	0.75	0.76

The assessed scenarios can be grouped in five categories according to Table 30. The assessment of the two models converge, if both models calculate a risk potential above the tolerable risk level (category A) or if both calculated risk potentials are below the tolerable risk level (category B). The assessment of the two models diverge, if SYNOPS calculates risk potentials above the maximum tolerable risk level and I-PHY calculates risk potentials below the maximum tolerable risk (category D). The same applies, if SYNOPS calculates risk potentials below the maximum tolerable risk level and I-PHY calculates risk potentials above the maximum tolerable risk (category E). Finally the models are considered to converge if both calculated risk potentials are around the maximum tolerable risk (category C). If both calculated risk values are within a range of ± 0.01 of the tolerable risk level the two models considered to converge.

Table 30 shows, that 62.2 % of the assessed risks convert and 37.8% divert if the I-PHY risk scores are compared with the acute risk potentials of SYNOPS. A slightly higher convergence of 65.8% is achieved if the I-PHY scores are compared with the chronic risk potentials.

It is also evident, that a high percentage (>31.6%) of the assessed scenarios is risky when analysed with I-PHY but not risky when analysed wit SYNOPS (category E). Only low percentage (<2.6%) are reached were SYNPOS assesses the scenarios as risky but I-PHY on the other hand as not risky (category D).

Table 30: Percentages of convergence and divergence of the RA-models I-PHY and SYNOPS

Cat.	Assessment with			acute risk potential		chronic risk potential	
	SYNOPS max. tolerable risk ETR=0.1	**I-PHY max. tolerable risk score=0.3**					
A	**> max tolerable ETR**	**> max tolerable score**	Convergence	44.5 %	62.2 %	49.4 %	65.8 %
B	< max tolerable ETR	< max tolerable score	Convergence	17.2 %		16.1 %	
C	$0,09 \le ETR_{acute} \le 0.11$ $0,9 \le ETR_{chronic} \le 1.1$	$0.29 \le score \le 0.31$	Convergence	0.5 %		0.3 %	
D	**> max tolerable ETR**	< max tolerable score	Divergence	1.5 %	37.8 %	2.6 %	34.2 %
E	< max tolerable ETR	**> max tolerable score**	Divergence	36.4 %		31.6 %	

Since for the pomefruit case study region much less scenarios have been assessed with I-PHY, the achieved results of the model comparison are less meaningful than for the wheat case study region. In Figure 34 the results for the pomefruit case study region calculated with SYNOPS are plotted against the result calculated with I-PHY. A weak linear regression (r2=0.25) of the two model results could be found for the acute risk potential and a medium linear regression (r2=0.47) for the chronic risk potential. The corresponding correlation matrix according to a Spearman rank analysis is summarised in Table 31.

Similar comparison results as for the wheat case study are achieved for the pomefruit case study. Good correlations (r>0.69) are found between the two models, if all 66 scenarios are considered. Again, the chronic risk potential shows slightly higher correlation coefficients than the acute risk potential.

When the model results are grouped by the parameter mindist, no correlations to medium could be found between the risk potentials calculated with SYNOPS and the aquatic risk score calculated with I-Phy (-0.11<r<0.54). Higher correlation coefficients are found if the results are grouped by the slope (0.62>r>0.73).

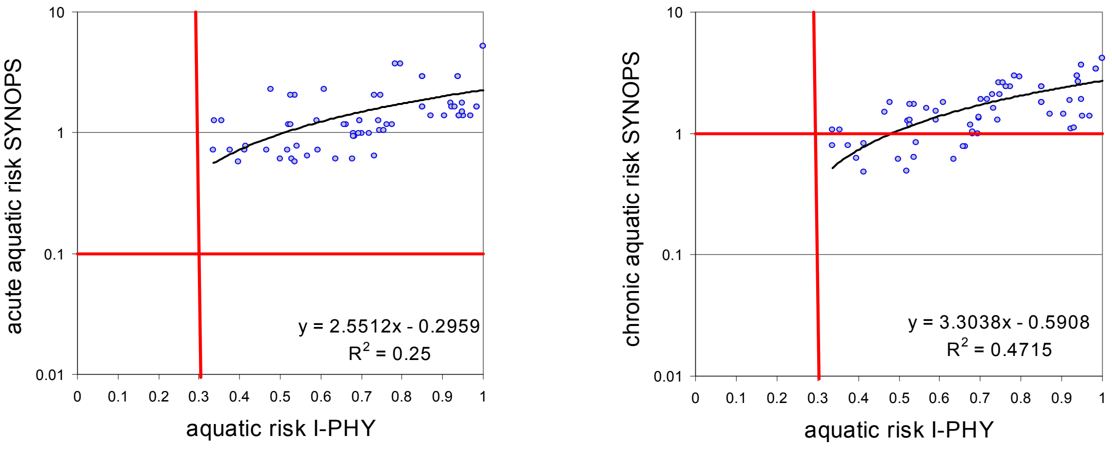


Figure 34: Acute and chronic aquatic risk calculated with SYNOPS in relation to the aquatic risk scores calculated with I-PHY. Risk assessments were conducted for pomefruit case study region

Table 31: Correlation matrix according to a Spearman rank analysis. Analysed are the aquatic risk potentials calculated with SYNOPS vs. aquatic risk scores calculated with I-PHY. Risk assessments were conducted for pomefruit case study region.

	grouped by			number of scenarios	Correlation coefficient (r)	
	Mindist [m]	**Slope [%]**	**soil-type number**		**acute aquatic risk SYNOPS**	**chronic aquatic risk SYNOPS**
Correlated with **Aquatic risk scores** **I-PHY**	all			66	0.69	0.70
	1		**21**	22	0.05	0.54
	5		**21**	22	0.21	0.40
	10		**21**	22	-0.11	0.44
		1	**21**	33	0.66	0.73
		5	**21**	33	0.62	0.72

The convergence of the two models for pomefruit case study region is very high. The assessment of the acute risk with SYNOPS converges to 100% with the calculated risk sores of I-PHY. In all case the calculate risks are above the tolerable risk level (category A). A convergence of 78.8% can be found for the chronic risk and 21 % of the results are diverging with risk scores calculated with I-PHY above the maximum tolerable risk and the chronic risk potential assessed with SYNOPS below the max tolerable risk level (category D).

Table 32; Percentages of convergence and divergence of the RA-models I-PHY and SYNOPS

	Assessment with						
Cat.	**SYNOPS max. tolerable risk ETR=0.1**	**I-PHY max. tolerable risk score=0.3**		**acute risk potential**		**chronic risk potential**	
A	**> max tolerable ETR**	**> max tolerable score**	Convergence	100 %	100 %	78.9 %	78.8%
B	< max tolerable ETR	< max tolerable score	Convergence	0 %		0 %	
C	$0,09 \leq ETR_{acute} \leq 0.11$ $0,9 \leq ETR_{chronic} \leq 1.1$	$0.29 \leq score \leq 0.31$	Convergence	0 %		0 %	
D	**> max tolerable ETR**	< max tolerable score	Divergence	0 %	0 %	0 %	21.1%
E	< max tolerable ETR	**> max tolerable score**	Divergence	0 %		21.1 %	

6 Discussion and Conclusion

In this study a geo-database for environmental data was established for the two case study regions Saxony-Anhalt (wheat) and Lake Constance (pomefruit) including all input parameters relevant to the RA-models on field level. The structure of this geo-database will be the basis for regional risk assessments on landscape level for further tasks within RA3.3:

A second database related to the pesticide use in these regions was established for the crops wheat and pomefruit on the basis of former survey conducted at the JKI. For the wheat case study region 156 region specific applications strategies and for the pomefruit 50 region specific applications strategies were made available to the RA-models.

The high number datasets in the geo-database was reduced in order to facilitate the parameterisation of the models I-PHY and PRZM-USES. This was done by building representative parameters combination of soil-type, slope and minimal distance and climate scenario for each case study region and combining them with all available pesticide use strategies. This resulted in 7488 sets of environmental data / pesticide use data combinations for wheat and 900 for pomefruit. Both databases were made available on the workspace of ENDURE.

The practical application of the three RA-models showed that the model PRZM-USES is not suitable to handle such large numbers of parameter sets and that the parameterisation of I-PHY needed some adoption of the input and output structure of the model. Therefore one conclusion of this exercise is that for further GIS-based risk assessments within the sub-activity in RA3.3 only SYNOPS or I-PHY with modified input and output structure can be used.

To compare and contrast the RA-Models it was necessary to define a standard database describing the chemical, physical and eco-toxicological properties of the a.i.’s. In the models I-PHY and SYNOPS, databases on a.i. properties were integrated. In addition an online database of the EU-project FOOTPRINT (FOOTPRINT, 2007) was made available to RA3.3. The comparison of these three active ingredient databases in section 3.6 revealed a certain percentage of diverting values, even tough all three databases are related to some extend on the EU monographs. Depending on the databases and the assumed threshold values the comparison revealed that for the parameter AquaTox 10%-25% of the values are diverging. Even higher percentage of diverging values were found for the parameters Koc with a range of 12 -34 % and DT50 with a range of 35 -51%. On the basis of this result and considering technical feasibility it was decided to use the SYNOPS database as input database for the risk assessment and the model comparison.

Concerning the assessment results of the wheat case study region Saxony Anhalt the following can be concluded. I-PHY assesses overall environmental risk scores for the used wheat strategies, which can not be considered acceptable. The same can be clearly concluded for the risk scores in surface water and in air. The groundwater risk potential shows the lowest values with 24% above the tolerable risk level, which still is not an acceptable value for the wheat case study region.

With SYNOPS acceptable aquatic and terrestrial risk potentials are assessed for the wheat case study region Saxony Anhalt, if it is assumed that the farmers follow the concept of good plant protection practice and meet the labelled buffer zone requirements. In no case the 90th percentile of the calculated chronic or acute risk potentials was larger than the maximal tolerable risk potential. The worst values were calculated for the chronic aquatic risk, where 8.5% of the calculated ETR where above the maximal tolerable risk potential. The situation looks different, if it is assumed that the all farmers don't meet the labelled buffer zone requirements. In this case the chronic and acute aquatic risk potentials reach unacceptable values with more than 44% above the maximal tolerable risk potential.

Since the risk assessment model I-PHY is not considering buffer zone requirements the results calculated with I-PHY are only comparable with scenario A. The aquatic risk scores calculated with I-PHY lie in 81.8 % above the tolerable risk level. Compared to the aquatic risk potentials assessed with SYNOPS, where more than 44% are lager than the tolerable ETR, the results of I-PHY seem to be more conservative.

Compared to the wheat scenarios the assessed risk potentials for the pomefruit region Lake Constance were significantly higher. 100 % of the aquatic risk scores assessed with I-PHY were above the maximum risk level. Similar high risk potentials were calculated with SYNOPS, if it is assumed that all farmers do not meet the buffer zone requirements. In this case 100 % of the calculated acute aquatic risk potentials and 80.7 % of the chronic aquatic risk are above the tolerable risk and level. As expected, the risk potentials are significantly reduced, if it is assumed that all farmers meet the labelled buffer zone requirements. In this case the percentages of risk potentials above the tolerable risk level are reduced to 31.9 % for the acute risk and to 4.9% for the chronic risk.

An important conclusion of these results is that RA-models should account for risk mitigation regulations like buffer zone requirements; otherwise the assessed risks overestimate the actual risk within the considered region. Assuming, that 100 % of the applied strategies within a region are unacceptable concerning the environmental risk, is not a result which can be communicated and which reflects the actual risk situation. The information about the risk mitigation requirements is varying within the EU-member states and could be linked as a database table to the applied plant protection products.

In a first step the risk potentials assessed with I-PHY and SYNOPS were compared with the treatment frequency index (TFI). The overall comparison of the I-PHY assessments showed only weak correlation for wheat and no correlation for orchards. The same is true for the assessments with SYNOPS. No correlation between TFI and risk potential could be found for pomefruit and only weak positive correlations could be found for the wheat scenarios. An exception was the correlation for the wheat scenarios between the terrestrial risk potential and the TFI. Here weak to medium correlations could be found

In addition regression analyses were conducted based on the average risk values for each strategy to avoid the large variation of the risk values, which is determined by the varying environmental conditions. No relevant regression could be analysed between the average SYNOPS risk potentials and TFI for wheat and pomefruit. The same is applicable for average values of I-PHY and the TFI. The only exception are the global risk scores calculated with I-PHY for the 156 wheat strategies. Here a medium regression according to a power function ($y=a*x^b$, $r^2=0.57$) could be found. I seem that the weak regression of the risk scores for air, groundwater and surface water merge to a medium regression for the global risk

Nevertheless all these results lead to the conclusion that the TFI is not a suitable index to predict the environmental risk related to plant protection products.

Finally the risk assessments of the two modes I-PHY and SYNOPS were compared. One has to bear in mind that a comparison of the models was only possible under the assumption, that no buffer zone requirements were met. This explains the high risk sores.

Considering all scenarios, high correlations between the two models could be found for the wheat and pomefruit scenarios. In all cases the correlation coefficients were around 0.7. Overall, the chronic risk potential showed slightly higher correlation coefficients than the acute risk potential.

Although a good correlation could be found between the model results, there is still a large difference in the classification of the calculated risks between the two models. An analysis of the classified results for the wheat case study region revealed a convergence between the two models of 62 % for the acute risk potential and of 66% for the chronic risk potential. This means that in 34 % (38 %) of all cases, the classification whether a risk was tolerable or not was different between the two models.

An adjustment of the tolerable risk levels would improve these percentages. Maximum tolerable risk level of SYNOPS relates to a measured toxicity value, the no effect concentration (NOEC). The maximum tolerable risk potential considered in I-PHY has been defined. Possibly a comparison analysis as accomplished in this study could be used to calibrate the maximum tolerable risk level in I-PHY by optimizing the convergence of the two models. An increase of the maximum tolerable risk level defined in I-PHY form 0.3 to 0.4 would cause an increase of the convergence to 73% for the acute risk and to 75 % for the chronic risk.

7 References

AdV. (2002): ATKIS Amtliches Topographisch - Kartographisches Informationssystem, Objektartenkatalog Basis-DLM, Arbeitsgemeinschaft der Vermessungsverwaltungen, http://www.atkis.de

Agritox, 2008. www.dive.afssa.fr/agritox

BGR (1995): Bodenübersichtskarte der Bundesrepublik Deutschland 1:1.000.000 (BÜK 1000), http://www.bgr.bund.de/cln_092/nn_325378/DE/Themen/Boden/Produkte/Karten/

BKG (2005): DGM-Deutschland / Digitales Geländemodell Bundesrepublik Deutschland 25 x 25, http://www.bkg.bund.de/

Bockstaller C.,Guichard L.,Keichinger O.,Girardin P.,Galan M. B., Gaillard G., 2009. Comparison of methods to assess the sustainability of agricultural systems. A review. Agronomy for Sustainable Development, 29, 223-235.

Bockstaller C.,Wohlfahrt J.,Huber A.,Hennebert P.,Zahm F.,Vernier F.,Keichinger O., Girardin P., 2008. Les indicateurs de risque de transfert de produits phytosanitaires et leur validation: exemple de l'indicateur I-PHY. Ingénieries, n°86, 103-114.

Bockstaller, C. (2004): Elaboration et utilisation des indicateurs. Exemple de I-PHY, in: Barriuso, E. (Ed.), Estimation des risques environnementaux des pesticides, INRA Editions, Paris, pp. 75-86.

Bockstaller, C., Gaillard, G., Baumgartner, D., Freiermuth Knuchel, R., Reinsch, M., Brauner, R., Unterseher, E., (2006): Méthodes d'évaluation agro-environnementale des exploitations agricoles : Comparaison des méthodes INDIGO, KUL/USL, REPRO et SALCA, Colmar, ITADA, p. 112. (http///www.itada.org). German version available

Bockstaller, C., Girardin, P., Van der Werf, H.G.M. (1997): Use of agro-ecological indicators for the evaluation of farming systems, European Journal of Agronomy 7, 261-270.

Carsel, R.F., Imhoff, J.C., Hummel, P.R., Cheplick, J.M., Donigian, A.S. Jr. (1998): PRZM-3, a model for predicting pesticide and nitrogen fate in the crop root and unsaturated soil zones: Users manual for release 3.0. Natl. Exposure Res. Lab., Office of Res. and Dev., USEPA, Athens, GA

FOCUS, 2000. FOCUS groundwater scenarios in the EU review of active substances, Report of the FOCUS Groundwater Scenarios Workgroup, EC document references Sanco/321/2000 rev.2, 202 pp.

FOOTPRINT (2007). The FOOTPRINT Pesticide Properties Database. Collated by the University of Hertfordshire as part of the EU-Funded FOOTPRINT project (FP6-SSP-022704). Http://www.eu-footprint.org/ppdb.html. Database version of 05/04/2008 subsection created specifically for the ENDURE network research project under licence. See also http://sitem.herts.ac.uk/aeru/footprint.

FOOTPRINT (2009): FOOTPRINT : creating tools for pesticide risk assessment and management in Europe, http://www.eu-footprint.org/index.html

Gebauer, J., Bäuerle, A.S. (2000): Betriebliche Umweltinformationstechnik für die Landwirtschaft. Berichte über Landwirtschaft, 78, 354-392.

GIRARDIN, P. (2001): Französische Verfahren zur Bewertung von Umweltwirkungen landwirtschaftlicher Betriebe. Beitrag anlässlich des ITADA Forum in Sissach, Schweiz, am 26. Juni 2001.

Gutsche, V. und Rossberg, D. (1997): SYNOPS 1.1: A model to assess and to compare the environmental risk potential of active ingredients in plant products. Agriculture, Ecosystems & Environment 64, 1997, 181-188.

Gutsche, V. und Rossberg, D. (1999): A proposal for estimating the quantity of pesticide active ingredients applied by crop based on national sales data. Report of the OECD Project in Pesticide Aquatic Risk Indicators – Report of Phase 1, Annex 1, OECD, Paris, 1999, 44-49.

Gutsche, V.(2004):, Pflanzenschutzindikatoren in Deutschland, Tagungsbericht Nachhaltigkeit- und Agrarumweltindikatoren, Bonn, 25.-26. März 2004, Bundesministerium f. Ernährung u. Landwirtschaft, S. 83-99.

Gutsche, V., Roßberg, D. (2000): Bewertung von Pflanzenschutz – Strategien mittels Risikoindikatoren. Mitt. Biol. Bundesanst. Land-Forstwirtsch. 371 (2000), 68-83.

Gutsche, V., Strassemeyer, J. (2007) SYNOPS - ein Modell zur Bewertung des Umwelt-Risikopotentials von chemischen Pflanzenschutzmitteln, Institut für Folgenabschätzung im Pflanzenschutz, Biologische Bundesanstalt für Land- und Forstwirtschaft.

HAIR (2007) Final report, http://www.rivm.nl/rvs/risbeoor/Modellen/Results_of_HAIR_project.jsp

Hertwich, E.G., Pease, W.S., Koshland, C.P. (1997): Evaluating the Environmental Impact of Products and Production Processes – A Comparison of Six Methods. Science of the Total Environment, 196, 13-29.

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

Mamy, L., Gabrielle, B. and Barriuso, E. (2007): Compared environmental balances of broad-spectrum and selective herbicides. In Proceedings XIII Symposium in Pesticide Chemistry, 3-6 Sept. 2007, Piacenza, Italy, pp 332-339..

Mamy, L., Gabrielle, B. and Barriuso, E. (2008): Measurement and modelling of glyphosate fate compared with that of herbicides replaced as a result of the introduction of glyphosate-resistant oilseed rape. Pest Management Science, 64, 262-275.

OECD, (1999): Environmental Indicators for Agriculture, vol.1: Concepts and Framework. Publications Service, OECD, Paris

Reus, J., Leendertse, P., Bockstaller, C., Fomsgaard, I., Gutsche, V., Lewis, K., Nilson, C., Pussemeier, L., Trevisan, M., van der Werf, H., Alfarroba, F., Blümel, S., Isart, J., McGrath, D., Seppälä, T..(1999): Comparing Environmental Risk Indicators for Pesticides. Results of the European CAPER Project. Centre for Agriculture and Environment Utrecht, CLM 426, 1999, ISBN 90-5634-106-5), 184 pp

Reus, J., Leendertse, P., Bockstaller, C., Fomsgaard, I., Gutsche, V., Lewis, K., Nilson, C., Pussemeier, L., Trevisan, M., van der Werf, H., Alfarroba, F., Blümel, S., Isart, J., McGrath, D., Seppälä, T. (2002): Comparison and evaluation of eigth pesticide environmental risk indicators development in Europe and recommendations for future use. Agriculture Ecosystems & Environment 90, 177 - 187.

RIVM, VROM, VWS (1998): Uniform System for the Evaluation of Substances 2.0 (USES 2.0). National Institute of Puplic Health and the Environment (RIVM), Ministry of Housing, Spatial Planning and the Environment (VROM), Ministry of Health, Welfare and Sport (VWS), The Netherlands. RIVM report no. 679102044.

Roßberg, D., H. Eckert, and U. Gernand, (2005): Farm assessment regarding the environmental sustainability. Part: quantitative assessment of the intensity of applications of plant protection products. Nachrichtenblatt des Deutschen Pflanzenschutzdienstes, 57(6), p. 121-125

Sadok W.,Angevin F.,Bergez J.-E.,Bockstaller C.,Colomb B.,Guichard L.,Reau R.,Messean A., Doré T., 2009. MASC: a qualitative multi-attribute decision model for ex ante assessment of the sustainability of cropping systems. Agronomy for Sustainable Development, 29, 447-461.

van der Werf, H.M.G., Petit, J. (2002): Evaluation of the environmental impact of agriculture at the farm level: a comparison and analysis of 12 indicator-based methods. Agriculture, Ecosystems & Environment, Volume 93, Issues 1-3, Pages 131-145.

van der Werf, H.M.G., Zimmer C. (1998): An indicator of pesticide environmental impact based on a fuzzy expert system, Chemosphere 36, 2225-2249.

Wenzel, H., Hauschild, M., Alting, L. (1997): Environmental Assessment of Products. Vol. 1: Methodology, tools and case studies in product development. Boston, Kluwer.

8 Appendix

Table 33: List of all active ingredients surveyed for wheat production in soil climate region BkR17 (Saxony-Anhalt). In total 156 application strategies were surveyed in this region.

HIF	Active ingredient	CAS_Nr	applications n	mean dosis [g ha-1]
Fungicides	Tebuconazol	107534-96-3	119	92.3
	Epoxiconazol	133855-98-8	103	75.3
	Fenpropimorph	67564-91-4	94	149.1
	Azoxystrobin	131860-33-8	91	114.6
	Kresoxim-methyl	143390-89-0	84	72.1
	Propiconazol	60207-90-1	76	65.1
	Fenpropidin	67306-00-7	71	175.5
	Spiroxamine	118134-30-8	40	217.8
	Metconazol	125116-23-6	27	32.7
	Quinoxyfen	124495-18-7	22	80.7
	Fluquinconazol	136426-54-5	16	133.0
	Prochloraz	67747-09-5	15	252.1
	Carbendazim	10605-21-7	10	72.8
	Cyprodinil	121552-61-2	4	384.4
	Difenoconazol	119446-68-3	3	87.5
	Dithianon	3347-22-6	2	165.0
	Cyproconazol	94361-06-5	2	24.0
	Tridemorph	81412-43-3	2	562.5
Herbicides	Isoproturon	34123-59-6	71	797.5
	Tribenuron	101200-48-0	60	13.3
	Diflufenican	83164-33-4	49	68.9
	Mecoprop-P	16484-77-8	48	752.5
	Fluroxypyr	69377-81-7	31	82.5
	Flurtamone	96525-23-4	26	195.7
	Florasulam	145701-23-1	24	4.8
	MCPA	94-74-6	24	620.8
	Thifensulfuron	79277-27-3	16	13.5
	Amidosulfuron	120923-37-7	15	12.8
	Carfentrazone	128639-02-1	14	14.0
	Cinidon-ethyl	142891-20-1	12	30.5
	Flupyrsulfuron	144740-54-5	11	7.3
	Dichlorprop-P	15165-67-0	10	434.5
	Bentazon	25057-89-0	10	621.0
	Iodosulfuron	144550-36-7	6	8.0
	Bifenox	42576-02-3	5	450.0
	Fenoxaprop-P	71283-80-2	4	60.4
	Ioxynil	1689-83-4	4	182.5
	Metsulfuron	74223-64-6	3	3.3
	Flufenacet	142459-58-3	3	186.7
	Clodinafop	105512-06-9	3	29.7
	Glyphosat	1071-83-6	3	720.0
	2,4-D	94-75-7	2	550.0

HIF	Active ingredient	CAS_Nr	applications n	mean dosis [g ha-1]
	Metribuzin	21087-64-9	2	70.0
	Pendimethalin	40487-42-1	1	600.0
Insecticides	Fenvalerat	51630-58-1	10	21.0
	Deltamethrin	52918-63-5	9	7.4
	alpha-Cypermethrin	67375-30-8	9	10.0
	Parathion	56-38-2	4	101.5
	Lambda-Cyhalothrin	91465-08-6	4	8.8
	Dimethoat	60-51-5	2	200.0
	beta-Cyfluthrin	68359-37-5	2	5.2
	Esfenvalerat	66230-04-4	1	7.5
growth regulators	Chlormequat	999-81-5	256	474.3
	Trinexapac	95266-40-3	36	65.4
	Ethephon	16672-87-0	16	158.5

Table 34: List of all active ingredients surveyed for apple production in soil climate region Lake Constance. In total 50 application strategies were surveyed in this region.

HIF	active ingredient	CAS_Nr	applications n	mean dosis [g ha-1]
Fungicides	Captan	133-06-2	256	1011.6
	Schwefel	7704-34-9	198	2202.4
	Penconazol	66246-88-6	155	23.9
	Tolylfluanid	731-27-1	154	726.0
	Pyrimethanil	53112-28-0	150	203.9
	Fluquinconazol	136426-54-5	140	49.6
	Dithianon	3347-22-6	108	355.4
	Mancozeb	8018-01-7	104	1446.2
	Myclobutanil	88671-89-0	55	47.5
	Cyprodinil	121552-61-2	54	143.3
	Kresoxim-methyl	143390-89-0	44	62.7
	Trifloxystrobin	141517-21-7	41	48.7
	Kupferoxychlorid	1332-40-7	32	2126.3
	Flusilazol	85509-19-9	28	22.6
	Thiophanat-methyl	23564-05-8	15	332.0
	Metiram	9006-42-2	10	1253.0
	Bitertanol	55179-31-2	2	81.3
	Fenarimol	60168-88-9	1	21.6
	Kupferhydroxid	20427-59-2	1	2073.0
	Triadimenol	55219-65-3	1	26.0
Herbicides	Diuron	330-54-1	58	2304.1
	Glyphosat	1071-83-6	58	1281.3
	Amitrol	61-82-5	56	2328.6
	MCPA	94-74-6	26	883.8
	Glufosinat	77182-82-2	16	794.9

HIF	active ingredient	CAS_Nr	applications n	mean dosis [g ha-1]
	Mecoprop-P	16484-77-8	2	24.0
	Fluazifop-P	79241-46-6	1	107.0
Insecticides	Codling Moth-Granulosevirus	Nn	176	0.1
	Methoxyfenozide	161050-58-4	58	88.8
	Pirimicarb	23103-98-2	44	219.9
	Thiacloprid	111988-49-9	35	92.6
	Fenoxycarb	79127-80-3	33	99.2
	Tebufenozid	112410-23-8	33	122.9
	Codling Moth-Granulosevirus /Granuprom	Nn	30	24.3
	Imidacloprid	138261-41-3	18	65.7
	Mineraloil	Nn	16	10782.8
	Indoxacarb	173584-44-6	14	49.1
	Schalenwickler-Granulosevirus /Carpex 2	Nn	13	1.0
	Fenpyroximat	134098-61-6	18	70.5
	Oxydemeton-methyl	301-12-2	14	204.7
	Tebufenpyrad	119168-77-3	2	37.5
	Abamectin	71751-41-2	1	13.5
growth regulators	Prohexadion	127277-53-6	19	104.9
	Ethephon	16672-87-0	7	75.0
	Streptomycin	nn	6	106.5

Table 35: PRZM input data: sorption coefficient Kd and degradation rates k

Pesticide	Soil 9												Soil 36							
	Kd (L/kg)						k (day^{-1})						Kd (L/kg)				k (day^{-1})			
Soil depth (cm)	0-15	15-30	30-60	60-70	70-100	100-130	0-15	15-30	30-60	60-70	70-100	100-130	0-30	30-60	60-100	100-140	0-30	30-60	60-100	100-140
Azoxystrobin	12.720	8.480	8.480	8.480	0.424	0.424	0.002	0.002	0.001	0.001	0.001	0.000	7.632	4.664	4.240	0.424	0.002	0.001	0.001	0.000
Bentazone	0.224	0.149	0.149	0.149	0.007	0.007	0.027	0.027	0.013	0.008	0.008	0.000	0.134	0.082	0.074	0.007	0.027	0.013	0.008	0.000
Carbendazime	1.996	1.331	1.331	1.331	0.066	0.066	0.017	0.017	0.008	0.005	0.005	0.000	1.198	0.732	0.665	0.066	0.07	0.008	0.005	0.000
Chlormequat	0.030	0.020	0.020	0.020	0.010	0.010	0.173	0.173	0.086	0.052	0.052	0.000	0.018	0.011	0.010	0.001	0.173	0.086	0.052	0.000
Clodinafop	43.170	28.780	28.780	28.780	1.439	1.439	0.770	0.770	0.385	0.231	0.231	0.000	25.902	15.829	14.390	1.439	0.770	0.385	0.231	0.000
Deltamethrine	53.594	35.729	35.729	35.729	1.786	1.786	0.015	0.015	0.007	0.007	0.004	0.000	32.156	19.651	17.864	17.864	0.015	0.007	0.004	0.000
Dichlorprop P	2.040	1.360	1.360	1.360	0.068	0.068	0.054	0.054	0.027	0.016	0.016	0.000	1.224	0.748	0.680	0.068	0.053	0.027	0.016	0.000
Diflufenican	59.670	39.780	39.780	39.780	1.989	1.989	0.005	0.005	0.002	0.002	0.001	0.000	35.802	21.879	19.890	1.989	0.005	0.002	0.001	0.000
Epoxiconazol	26.490	17.660	17.660	17.660	0.883	0.883	0.002	0.002	0.001	0.001	0.001	0.000	15.894	9.713	8.830	0.883	0.002	0.001	0.001	0.000
Fenpropidin	113.94	75.960	75.960	75.960	3.798	3.798	0.010	0.010	0.005	0.003	0.003	0.000	68.364	41.778	37.980	3.798	0.010	0.005	0.003	0.000
Fenpropimorph	29.875	19.917	19.917	19.917	0.995	0.995	0.018	0.018	0.009	0.005	0.005	0.000	17.925	10.954	9.958	0.995	0.018	0.009	0.005	0.000
Fenvalerat	384.1	256.1	256.1	256.1	12.805	12.805	0.016	0.016	0.008	0.005	0.005	0.000	230.5	140.8	128.0	12.805	0.016	0.008	0.005	0.000
Florasulam	0.660	0.440	0.440	0.440	0.022	0.022	0.385	0.385	0.192	0.115	0.115	0.000	0.396	0.242	0.220	0.022	0.385	0.192	0.115	0.000
Fluquinconazol	25.710	17.140	17.140	17.140	0.857	0.857	0.002	0.002	0.001	0.001	0.001	0.000	15.426	9.427	8.570	0.857	0.002	0.001	0.001	0.000
Flurtamone	9.885	6.590	6.590	6.590	0.329	0.329	0.008	0.008	0.004	0.002	0.002	0.000	5.931	3.624	3.295	0.329	0.008	0.004	0.002	0.000
Ioxynil	16.474	10.983	10.983	10.983	0.549	0.549	0.099	0.099	0.049	0.049	0.029	0.000	9.884	6.041	5.491	0.549	0.099	0.049	0.029	0.000
Isoproturon	5.404	3.603	3.603	3.603	0.180	0.180	0.038	0.038	0.019	0.011	0.011	0.000	3.242	1.981	1.801	0.180	0.038	0.019	0.011	0.000
Kresoxim-methyl	9.240	6.160	6.160	6.160	0.308	0.308	0.138	0.138	0.069	0.041	0.041	0.000	5.544	3.388	3.080	0.308	0.138	0.069	0.041	0.000
MCPA	0.153	0.102	0.102	0.102	0.005	0.005	0.051	0.051	0.025	0.015	0.015	0.000	0.092	0.056	0.051	0.005	0.050	0.025	0.015	0.000
Metconazol	30.030	20.020	20.020	20.020	1.001	1.001	0.002	0.002	0.001	0.001	0.001	0.000	18.018	11.011	10.010	1.001	0.002	0.001	0.001	0.000
Prochloraz	30.030	20.020	20.020	20.020	1.001	1.001	0.007	0.007	0.003	0.002	0.002	0.000	18.018	11.011	10.010	1.001	0.007	0.003	0.002	0.000
Propiconazol	20.678	13.785	13.785	13.785	0.689	0.689	0.007	0.007	0.004	0.002	0.002	0.000	12.407	7.582	6.892	0.689	0.007	0.003	0.002	0.000
Quinoxyfen	57.190	38.126	38.126	38.126	1.906	1.906	0.002	0.002	0.001	0.001	0.001	0.000	34.314	20.969	19.063	1.906	0.002	0.001	0.001	0.000
Tebuconazol	27.192	18.128	18.128	18.128	0.906	0.906	0.006	0.006	0.003	0.002	0.002	0.000	16.315	9.970	9.064	0.906	0.006	0.003	0.002	0.000
Tribenuron	0.930	0.620	0.620	0.620	0.031	0.031	0.173	0.173	0.086	0.052	0.052	0.000	0.558	0.341	0.310	0.031	0.173	0.086	0.052	0.000
Trinexapac	8.400	5.600	5.600	5.600	0.280	0.280	0.138	0.138	0.069	0.041	0.041	0.000	5.040	3.080	2.800	0.280	0.138	0.069	0.041	0.000

Table 36: Summary of USES input data (Data from JKI database except when indicated)

Pesticide	ADI (mg/kg/d)	PNECaq (µg/L)	PNECterr	Mw (g/mol)	log Kow	Melting point (°C)	Pvap 25°C (Pa)	Sw 25°C (mg/L)	Koc (L/kg)	DT50sw (days)	DT50soil (days)	DT50sed (days)	pKa
Azoxystrobin	0.1	1.5 10-3 *	EP ***	403.4	2.5	116 ****	1.1 10-10	6.7	424	47.7	279	57.5	
Chlormequat	0.05 *	-	EP	158.1	-2.3	245 ****	1.01 10-4	1200000	1.02	13.8	4	22.7	
Clodinafop	0.003	2.1 10-3 *	EP	311.7	3.9	48.2 ****	1.6 10-4	4	1439	66.1	0.9	109.5	
Diflufenican	0.2	2.5 10-5 *	EP	394.3	4.9	160 **	3.1 10-5	0.05	1989	39.4	141.6	151.9	
Epoxiconazol	0.008	1.0 10-3 *	EP	329.76	3.33	136.7 **	0.02	7.05	883	33	402.7	181.8	
Fenpropidin	0.02	1.2 10-4 *	EP	273.5	2.59	-	0.021	530	3798	6.3	69.3	21.2	10.5 *
Fenpropimorph	0.003 **	1.6 10-5 *	EP	303.5	4.06	-	2.3 10-3	4.3	995	31.7	37.4	43.3	6.98 *
Fenvalerat	0.02 **	-	EP	419.9	6.42	-	1.92 10-5	0.001	12805	7.6	42.4	23.1	
Florasulam	0.05	1.18 10-4 *	EP	359.3	-1.22	212 **	1 10-5	6360	22	86.3	1.8	88.1	4.54 *
Fluquinconazol	0.005 **	-	EP	376.2	3.24	192.4 **	6.4 10-9	1.15	857	33.5	377.8	257.6	
Flurtamone	0.03	9.9 10-4 *	EP	333.3	3.24	148.5 ****	1 10-5	11.5	329	31.4	87.3	333.8	
Ioxynil	0.005 **	1.1 10-3 *	EP	370.9	3.51	207.8 **	2.04 10-6	15	549	13.2	7	37.6	
Kresoxim-methyl	0.4	1.5 10-2 *	EP	313.3	3.4	101.6 ****	2.3 10-6	2	308	131.8	5	64.6	
Metconazol	0.048	-	EP	319.8	3.85	104.2 **	1.3 10-5	30.4	1001	17	350.5	279	1.5 *
Prochloraz	0.01 **	4 10-3 *	EP	376.7	4.12	48.3 **	4.5 10-6	26.5	1062	15.4	99.2	1615.4	
Propiconazol	0.04 *	5.1 10-3 *	EP	342.2	3.72	-	5.6 10-5	110	689	140.1	95.8	46.9	1.09 *
Quinoxyfen	0.2	8 10-4 *	EP	308.14	4.66	103 **	2 10-5	0.047	1906	22	322.7	222.7	3.56 *
Tebuconazol	0.03	1.2 10-3 *	EP	307.8	3.7	105 **	9.69 10-7	32	906	21.9	117.8	46.7	
Tribenuron	0.01	-	EP	381.4	0.78	141 ****	5.3 10-8	2040	31	70.1	4	67.4	4.7 *
Trinexapac	0.3	-	EP	224.2	-0.29	36 ****	2.16 10-3	200000	280	3.2	5	2.1	4.57 *

* Data from Agritox
** Data from Footprint
*** RIVM et al. (1998)
**** Other sources of information
\- No data