



## ENDURE

European Network for Durable Exploitation of crop protection strategies

Project number: 031499

Network of Excellence  
Sixth Framework Programme

Thematic Priority 5  
FOOD and Quality and Safety

### ***Deliverable DR3.10***

Final report on suitable methods for consideration of pesticides (eco- and human toxicity) in agricultural LCA

**Due date of deliverable:** June 30<sup>th</sup>, 2009

**Actual submission date:** October 15<sup>th</sup>, 2009

**Start date of the project:** January 1<sup>st</sup>, 2007

**Duration:** 48 months

**Organisation name of lead contractor:** AGROS

**Revision:** V2

Project co-funded by the European Commission within the Sixth Framework Programme (2002-2006)	
Dissemination Level	
<b>PU</b> Public	<b>X</b>
<b>PP</b> Restricted to other programme participants (including the Commission Services)	
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## Glossary

AETP <sub>fresh,x,i</sub> :	The fresh water aquatic ecotoxicity potential for a substance x released to compartment I (1,4-DCB equivalents);
AETP <sub>salt,x,i</sub> :	The salt water aquatic ecotoxicity potential for a substance x released to compartment I (1,4-DCB equivalents);
DALY:	Disability Adjusted Life Years = Years of Life Lost (YLL) + Years Lived with Disability (YLD)
DT50:	Hydrolytic stability (in d)
ED10:	Benchmark dose resulting in 10% effect over background (mg/kg/day)
EF:	Equivalence factor for potential ecotoxicity (variable in EDIP method)
ETF:	Ecotoxicity factors Variable in EDIP to describe the damage risk for an environmental compartment. Calculated as the inverse of the compartments PNEC
ETR:	Exposure toxicity ratios
HC50:	The mean hazardous concentration affecting 50% of the species present in the ecosystem
HTF:	Human toxicity factor (variable used in the EDIP method)
HDF:	Human Damage Factor. Variable used to describe damage to human health ion Impact 2002+
HTP <sub>x,i</sub> :	The human toxicity potential for a substance x released to compartment I (1,4-DCB equivalents);
IPEC:	Predicted environmental concentration (long-term)
LC50:	Lethal concentration 50%. Concentration lethal to 50% of test organisms
LOAEL:	Lowest observed adverse effect concentration. The lowest dose observed to result in injurious effects in test organisms
LOEC:	Lowest observed effect concentration. The lowest concentration observed to result in effects in test organisms
NOAEL:	No observed adverse effect level. The highest dose observed to result in no injurious effects in test organisms
NOEC:	No observed effect concentration. The highest concentration observed to result in no effects in test organisms.
PAF:	Potentially affected fraction of species
PDF:	Potentially disappeared fraction of species
APAF:	Potentially Affected Fraction of species per unit of emission
PEC:	Predicted environmental concentration
PNEC:	Predicted no effect concentrations
RCR:	Risk characterisation ratio. Variable used in USES-LCA to describe the damage risk for an environmental compartment. Calculated through dividing the PEC by the PNEC
SETP <sub>fresh,x,i</sub> :	The fresh water sediment ecotoxicity potential for a substance x released to compartment I (1,4-DCB equivalents);
SETP <sub>salt,x,i</sub> :	The sea water sediment ecotoxicity potential for a substance x released to compartment I (1,4-DCB equivalents);
sPEC:	Predicted environmental concentration (short-term)
TETP <sub>x,i</sub> :	The terrestrial ecotoxicity potential for a substance x released to compartment I (1,4-DCB equivalents);
TFI	Treatment frequency index

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## Summary

This report presents the second part of the evaluation of several risk assessment (RA) and life cycle assessment (LCA) methods (EDIP97, EI99, IMPACT2002+, I-PHY, PRZM-USES, SYNOPS, and USES-LCA) to calculate the environmental impacts of pesticide use. The evaluation scheme used in the first part (DR3.4<sup>1</sup>) is mainly based on the work of the ITADA project COMETE (Bockstaller et al., 2006). It is divided into the three dimensions scientific soundness, practical feasibility and stakeholder utility, similarly to the OECD-Report on environmental indicators (OECD, 1999). Eleven criteria for the group scientific soundness, six criteria for the group practical feasibility and three criteria for the group stakeholder utility are presented. Most of the sub-themes for the dimensions practical feasibility and stakeholder utility are divided into three user groups (extension services, authorities and scientists), because it is assumed that their demands are different from each other.

The methods and results described in the first deliverable are summarised first in this deliverable to give the reader an overview of the work. The main goal of the second part of the evaluation is to expand the assessment for the practical feasibility and stakeholder utility using a set of plant protection strategies. In the second part of the deliverable, the data used for the evaluation are described followed the presentation of the results and the discussion and conclusion.

The assessment performed gives following results:

For the practical feasibility and stakeholder utility the analysis shows that the methods SYNOPS and I-PHY are more favourable in comparison to PRZM-USES and the LCA methods. But because of the different goals of the methods the analysis should be completed by a description of the most appropriated fields of application for each method. Which are:

- For SYNOPS a GIS based evaluation of a large number of plant protection strategies including detailed environmental data.
- For I-PHY in general the same than for SYNOPS but with some small limitations as no GIS modelling is used.
- For PRZM-USES a very detailed fate modelling for a few substances and scenarios
- The LCA toxicity models can't be compared with the risk assessment methods, because of the different targets. Strength of the LCA models is that the results are expressed in units which can be compared to the toxicity of other substances emitted in other steps of the production, other regions and other compartments e.g. hydrocarbons or heavy metals to air during the production of machinery.

The main result of the rank correlation analysis described in section 4.2 is, that the ranking of the strategies according to their risk or toxicity is not comparable over the methods for the aquatic- and terrestrial ecosystem and the human health. Merely between EDIP97 (modified as described in section 2.1.1) and USES-LCA there is a good accordance of the ranking for nearly all case studies and categories.

Regarding the consideration of pesticides in agricultural LCA to our opinion the method USES-LCA is preferable, because on the one hand the method is well known and used and on the other hand the results of the theoretical evaluation are as good or better than for the other LCA methods and the calculation of characterisation factors with the given databases (SYNOPS and Footprint) is possible for more than 300 active ingredients and the categories aquatic and terrestrial eco-toxicity and human toxicity.

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<sup>1</sup> Deliverable DR3.4 Multicriteria evaluation of RA and LCA assessment methods considering pesticide application see [https://workspaces.inra-transfert.fr/QuickPlace/endure/PageLibraryC1257324005BE62D.nsf/h\\_80C07B6C3F3919D0C1257325002FDCCD/973654FEEED09426C12574DB003663CF/?OpenDocument&ResortAscending=12](https://workspaces.inra-transfert.fr/QuickPlace/endure/PageLibraryC1257324005BE62D.nsf/h_80C07B6C3F3919D0C1257325002FDCCD/973654FEEED09426C12574DB003663CF/?OpenDocument&ResortAscending=12)



## Multicriteria evaluation of RA and LCA assessment methods considering pesticide application

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### 1. Introduction

Over the last years, many Life Cycle Assessment (LCA) models have been developed in order to analyse the toxic effect of chemical substances to environment and human health. Experience shows substantial variation between the models, especially when looking at pesticides in agricultural production systems (Nemecek et al., 2005). The main problems are the high number of pesticides applications and the modelling of the fate and effect of the pesticides. Current LCA methods can consider only few active ingredients so far. Furthermore, the fate analysis in the methods is often rather simple in order to be able to assess chemicals with only few known properties. The recent announcement of the newly developed USEtox method (Rosenbaum et al., 2008) should improve the situation in LCA. But so far it is not known whether the improvements in USEtox will be sufficient enough for pesticide applications in agriculture. For these reasons, a closer collaboration between LCA and RA modelling approaches is necessary. Within the ENDURE-Network, one goal of the sub-activity RA3.4 is to compare the risk assessment (RA) toxicity models SYNOPS (Gutsche and Strassemeyer, 2007), IPHY (Bockstaller et al., 2007) and PRZM-USES (Mamy et al., 2007a&b) together with the LCA toxicity models EDIP (Hauschild and Wenzel, 1998), USES-LCA (Guinée et al., 2001), IMPACT2002+ (Jolliet et al., 2003) and EI99 (Goedkoop and Spriensma, 1999) by means of a multicriteria analysis.

The first part summarised in DR3.4 covers the theoretical part of the multicriteria evaluation. The criteria list is derived from the work of Bockstaller et al (2006) and Gaillard et al. (2005) and was established by the three research institutions represented in RA3.4 (ART, JKI and INRA). The criteria are adapted to the evaluation of indicator methods assessing the impacts of pesticide in an LCA framework. Each author of the method or researcher supporting an indicator first filled in the tables. The method developers not represented in the Network ENDURE were separately consulted. A cross-validation of the evaluation of each indicator has been done in order to avoid evaluation discrepancies.

The second part presented in this deliverable includes the practical test of the methods using a set of 206 surveyed plant protection strategies applied in wheat in Saxony-Anhalt (156) and pomefruit (50 applied at the German side of Lake Constance).

Goals of the analysis presented here are:

- to test if the theoretical assessment of the two dimensions feasibility and stakeholder utility can be confirmed in practise
- to compare the ranking of the strategies according to their toxicity calculated according to several methods to show if conclusions about the risk or toxicity for a given set of strategies are comparable
- and to compare results of the methods with the ranking according to the treatment frequency index to assess if the treatment frequency index can be used as an indicator of the environmental impacts of plant protection

## 2. Summary of DR3.4

The deliverable DR3.10 can be seen as the second part of the deliverable DR3.4. Due to this fact the method evaluation and the results of DR3.4 “Multicriteria evaluation of RA and LCA assessment methods considering pesticide application” are summarised briefly to give the reader a general overview of the work done within the task LCA Methodological work of RA3.4 in the past two years.

### 2.1. Description of the methods compared.

#### 2.1.1. EDIP97

The EDIP97 method was developed under the Danish Environmental Design of Industrial Products programme by a team of the Technical University of Denmark, five industrial companies, the confederation of Danish Industries and the Danish Environmental Protection Agency (Wenzel et al, 1997; Hauschild and Wenzel, 1998).

The EDIP-LCA-method is a problem-oriented midpoint approach with eight impact categories (Global warming potential, ozone depletion, photochemical ozone formation, acidification, nutrient enrichment, eco-toxicity, human toxicity and resource consumption). Only toxicity categories are regarded in this short description.

The eco-toxicity potential is calculated multiplying the magnitude of the emission of a single substance with an equivalence factor. The equivalence factor is expressed in a volume ( $\text{m}^3$ ) of the compartment concerned per g emitted substance which is needed to dilute the substance to a concentration which is low enough to cause no eco-toxic effects. The eco-toxicity potential is calculated for acute eco-toxicity in water (for substances emitted to water), chronic eco-toxicity in water (for substances emitted to air, water and soil) and chronic eco-toxicity in soil (for substances emitted to air, water and soil). The partitioning of a given substance to the different compartments is calculated for emissions to air, soil and water. For substances emitted to air with an atmospheric half live of less than a day, it is assumed that there is no eco-toxicity at all. If the atmospheric half live exceeds one day, the substance will be deposit to soil and water. For the partitioning of emissions to water and soil, the Henry's law constant and the atmospheric half live is used. The eco-toxicity factors (ETF's) are calculated for acute eco-toxicity in water, chronic eco-toxicity in water and chronic eco-toxicity in soil as the inverse of the predicted no effect concentrations (PNEC) in the respective compartment. The PNEC for water are derived using  $\text{LC}_{50}$  and LOEC's for water species. The PNEC in soil is derived using the PNEC water chronic and the coefficient of absorption for the substance in soil.

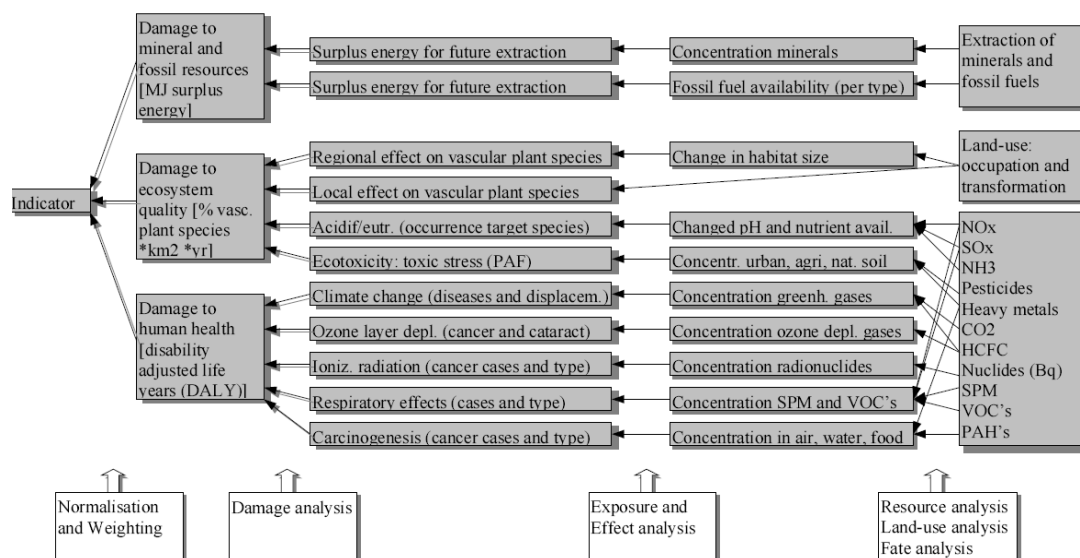
For the human toxicity potential the dispersion of the substance to the compartments is calculated in the same way as for eco-toxicity, but the procedure to estimate the equivalence factors differs. The human toxicity potential is also expressed in a volume ( $\text{m}^3$ ) of the compartment per g emitted substance which is needed to dilute the substance to a concentration which is low enough to cause no toxic effects on humans. The fraction (f) which reaches the different environmental compartments, the transfer factor (T) for the substance via the actual exposure route, the intake factor for the single exposure routes (I) and the human toxicity factors (HTF), which is the inverse from the human reference concentration or the human reference dose, are used to calculate the equivalence factor. For the exposure via soil and surface water also the biodegradability factor is regarded.

As a result of the simple fate model of EDIP97 there is no transfer of substances from the compartment soil to the water compartment for any of the active ingredients. For that reason the

method was adapted for the present evaluation. The partitioning of the active ingredient is modelled with SYNOPS and then the toxicity is assessed following the EDIP97 methodology.

### 2.1.2. EI99

The EcoIndicator 99 (EI99) method developed in the Netherlands (Goedkoop and Spriensma, 2001) is an LCIA method with endpoint approach and a subsequent aggregation of the three endpoints (damage to mineral and fossil resources, - to ecosystem quality and - to human health) to a single value (Indicator). For a general overview of the method see Figure 1.



**Fig. 1 :** General representation of the EI99 method (source: Goedkoop and Spriensma, 2001).

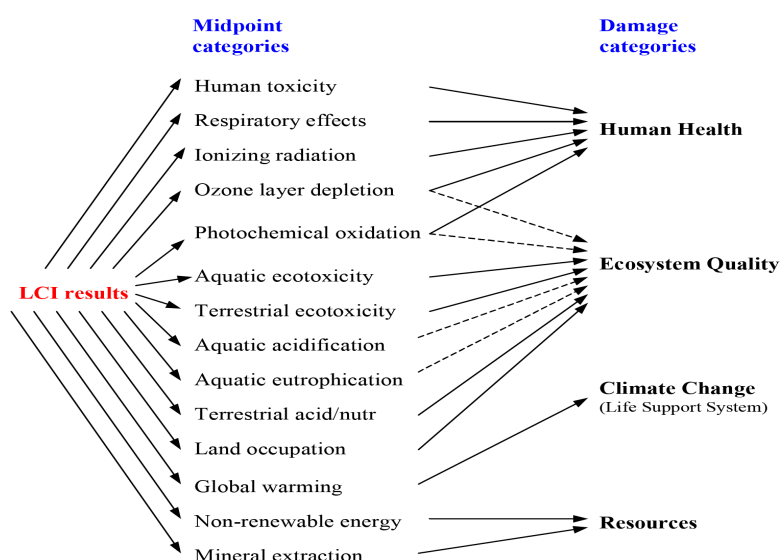
The white boxes represent processes and the grey ones intermediate results. Eleven mid point categories are calculated and summarised by a damage analysis into the three endpoint categories. The toxicity of systems is regarded as a damage to ecosystems (expressed in the percentage of species that has disappeared in a certain area) and damage to human health (DALY Disability Adjusted Life Years). The damage to human health is related to the midpoint categories climate change, ozone layer depletion, ionising radiation, carcinogenesis and respiratory effects.

For eco-toxicity, a method developed by RIVM for the Dutch Environmental Outlook (Meent and Klepper, 1997) is used. This method determines the Potentially Affected Fraction (PAF) of species in relation to the concentration of toxic substances. The PAFs are determined on the basis of toxicity data for terrestrial and aquatic organisms like micro-organisms, plants, worms, algae, amphibians, molluscs, crustaceans and fishes. The PAF expresses the percentage of species that is exposed to a concentration above the NOEC. The higher the concentration is, the larger the number of species is affected (Goedkoop and Spriensma, 2001).

Human toxicity is expressed in DALY (Disability Adjusted Life Years). The core of the DALY system is a disability weighting scale. This scale has been developed in a number of panel sessions and lists many different disabilities on a scale between 0 and 1, where 0 means being healthy and 1 means death (Goedkoop and Spriensma, 2001).

### 2.1.3. IMPACT2002+

The IMPACT 2002+ method described by Jolliet et al. (2003) is a combination of midpoint and damage approaches. Four damage categories (Human Health, Ecosystem Quality, Climate Change and Resources) are assessed using 14 midpoint categories (human toxicity, respiratory effects, ionizing radiation, ozone layer depletion, photochemical oxidation, aquatic eco-toxicity, terrestrial eco-toxicity, terrestrial acidification/nutritation, aquatic acidification, aquatic eutrophication, land occupation, global warming, non-renewable energy, mineral extraction). See Fig. 2 and Tab. 1 for an overview and a description of reference substances and damage units.



**Fig. 2: Overall scheme of the IMPACT 2002+ framework, linking LCI results via the midpoint categories to damage categories (source: Jolliet et al, 2003)**

**Tab. 1: Impact - and damage categories, reference substances, and damage units used in IMPACT 2002+ (adapted from Jolliet et al, 2003).**

Midpoint category	Midpoint reference substance	Damage Category	Damage unit
Human toxicity	kg <sub>eq</sub> chlorethylene into air	Human health	DALY
Respiratory	kg <sub>eq</sub> PM2.5 into air		
Ionizing radiations	Bq <sub>eq</sub> carbon-14 into air		
Ozone layer depletion	kg <sub>eq</sub> CFC-11 into air		
Photochemical oxidation	kg <sub>eq</sub> ethylene into air	Ecosystem quality	-
Aquatic eco-toxicity	kg <sub>eq</sub> triethylene glycol into water	Ecosystem quality	PDF · m <sup>2</sup> · year
Terrestrial eco-toxicity	kg <sub>eq</sub> triethylene glycol into water		
Terrestrial acidification	kg <sub>eq</sub> SO <sub>2</sub> into air		
Aquatic acidification	kg <sub>eq</sub> SO <sub>2</sub> into air		
Aquatic eutrophication	kg <sub>eq</sub> PO <sub>4</sub> <sup>3-</sup> into water	Climate change	(kg <sub>eq</sub> CO <sub>2</sub> into air)
Land occupation	m <sup>2</sup> <sub>eq</sub> organic arable land-year		
Global warming	kg <sub>eq</sub> CO <sub>2</sub> into air		
Non-renewable energy	MJ Total primary non-renewable or kg <sub>eq</sub> crude oil		
Mineral extraction	MJ Additional energy of kg <sub>eq</sub> iron (in ore)	Resources	MJ

Only human, aquatic and terrestrial toxicity are regarded in the following description.

### Human Toxicity

The human toxicity is described as Human Damage Factor (HDF) in DALY (Disability Adjusted Life Years) and is calculated as follows:

$$\text{HDF}_i = iF_i \cdot \text{EF}_i = iF_i \cdot \beta_i \cdot D_i$$

where  $iF_i$  is the fraction of mass of a chemical which is finally taken in by human population,  $\text{EF}_i$  is the effect factor which is the product the dose-response factor  $\beta_i$  and the DALY per incidence  $D_i$ .

### Aquatic and terrestrial eco-toxicity

The aquatic - and terrestrial eco-toxicity are calculated similar to the human toxicity with the exception that the calculations are based rather on species than on individuals. Therefore, the level of concentration is used to estimate the effect from fate. In IMPACT2002+ for aquatic freshwater ecosystems the Potentially Damaged Fraction of species per unit of emission (APDF) is estimated from the Potentially Affected Fraction of species used in IMPACT2002:

$$\text{APAF}_i = F_i^{\text{mw}} \cdot \theta_i^{\text{w}} \cdot \beta_i, \text{ in PAF} \cdot \text{m}^3 \cdot \text{year} \cdot \text{kg}^{-1}$$

$$\text{APDF}_i = \text{APAF}_i \cdot 0.5^{-1} \cdot 17.8 \text{m}^{-1}, \text{ in PDF} \cdot \text{m}^2 \cdot \text{year} \cdot \text{kg}^{-1}$$

with the fate factor  $F_i^{\text{mw}}$  describing the fraction of substance which is transferred to the freshwater ecosystems,  $\theta_i^{\text{w}}$  describing the residence time of the substance in water and  $\beta_i$  describing the dose-response factor (estimated using the  $\text{HC50}_{\text{w}}$ ). The terrestrial eco-toxicity is calculated similar to the described procedure extrapolating the  $\text{HC50}_{\text{Soil}}$  from  $\text{HC50}_{\text{Water}}$ .

## 2.1.4. I-PHY

### Short description of 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., 2007). The core of the indicator was published by van der Werf and Zimmer (1998) and enhanced, adapted and tested by Bockstaller et al. (2008) for arable farming. Since then, I-PHY was adapted to other farming systems like wine growing, fruit production, field vegetable production or palm tree.

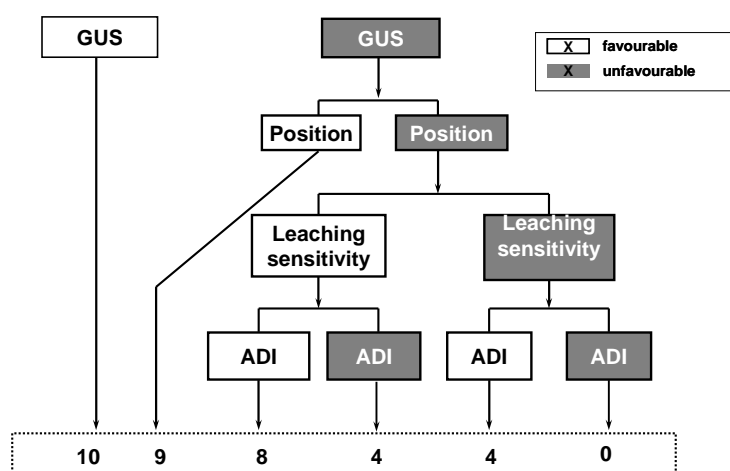
For a single application of a pesticide, the calculation of the indicator is based on four modules assessing respectively the risk linked to the amount of active ingredient applied and the risks for groundwater, surface water and air. In a second step, an overall indicator is calculated. Three types of input variables are used:

1. Pesticides properties linked to exposure or to ecotoxicological 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. 3 shows an example for ground water risk for which the main weight is given to a pesticide property (GUS variable) where as less weight is attributed to position (crop interception here) and soil sensitivity to leaching. It should be noticed that for surface water, the field sensitivity to runoff and drift plays a major role in comparison with pesticide properties (DT50 variable). In all components 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 of I-PHY was based on the inverse scale between 0 (no risk) and 1 (maximum risk), which is also used in some recent applications (Sadok et al., 2007).

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



**Fig. 3: Decision tree of the groundwater component of I-PHY (source: Bockstaller et al. (2008))**

In the last five years, the I-PHY indicators were implemented in more than 100 cases in France by advisers mainly working on assessment of risks on field and farm 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.

### 2.1.5. PRZM-USES

The method of pesticide risk and impact assessment developed by Mamy et al. (2007a&b) 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 (see also 2.1.7).



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 a 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 amount 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.

### 2.1.6. SYNOPSIS

Since published in 1997 (Gutsche and Rossberg, 1997), the model SYNOPSIS 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 data on pesticide use 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 georeferenced databases for land use, soil conditions and climate data and to a dataset of regionalised surveys of pesticide application. SYNOPSIS 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 Strasse Meyer, 2007). The model is integrated in the national action plan for pesticide risk reduction.

Besides the national and landscape functionality, SYNOPSIS can be run on field level to assess the environmental risk of pesticide applications under different environmental conditions. Within the sub-activity RA3.4 mainly the field based functionality of the model is 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 edge-biotopes and *Daphnia*, algae and fish for surface water.

SYNOPSIS 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.

Loads and *PEC*'s of an a.i. in the soil are caused directly by a 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 the 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 content. The considered exposure pathways into the surface water are drift, run-off, and drainage (Fig. 4).

From the time-dependent concentration curves, the short-term (*sPEC*) and long-term environmental concentrations (*IPEC*) are derived. The maximum concentration over a

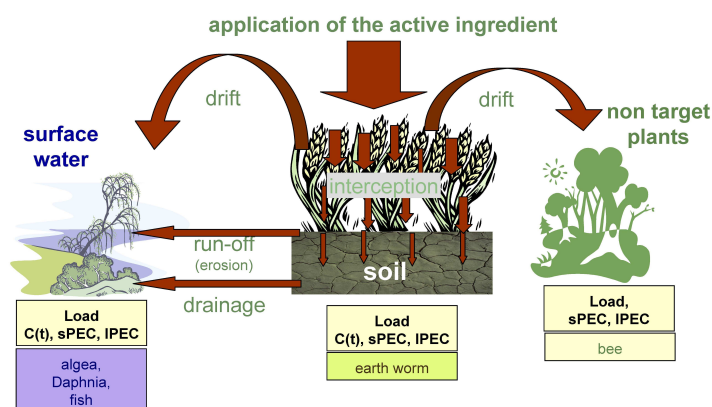
vegetation period ( $sPEC$ ) is used to calculate the acute risk potential. To estimate the chronic risk potential an integral over a time interval, equal to the time period of the  $NOEC$  standard test ( $t_{NOEC}$ ), is calculated on a daily basis. The maximum of these integrals over the vegetation period ( $IPEC$ ) is then considered for the chronic risk potential.

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

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 potentials.

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

All necessary physicochemical and ecotoxicological parameters of the applied active ingredients (n=350) are summarised in a database which is continuously updated at JKI.



**Fig. 4: Exposure pathways considered in SYNOPS (source, Gutsche and Strassemeyer, 2007)**

### 2.1.7. USES-LCA

The USES-LCA model is based on Uniform System for the evaluation of Substances 2.0 (USES 2.0) and was developed in the Netherlands (RIVM, 1998; Huijbregts et al., 2000). The model calculates the toxicity potentials for the impact categories aquatic, sediment and terrestrial ecotoxicity as well as human toxicity for substances emitted to air, fresh water, sea water, industrial soil and agricultural soil. The dispersion of the emitted substance is calculated by local fate models and the model Simplebox 2.0 which has five spatial scales (the arctic, tropic and moderate zone of the northern hemisphere, whereby the moderate zone is divided into a regional, continental and global scale). Human exposure through the environment is estimated on the predicted environmental concentration on regional and local scale. In the assessment module the PNEC is calculated for aquatic, terrestrial, sediment ecosystems and for fish and worm eating predators. If available, the PNEC's are derived from ecotoxicological data. If this data is missing for terrestrial and/or sediment systems, the PNEC's are estimated from the PNEC for aquatic ecosystems using the equilibrium-partitioning method. For the assessment of human toxicological effects the NOAEL or the LOAEL for inhalation and oral intake are estimated from available data. If neither could be calculated for a given substance, a route-to-route extrapolation from absorption rates or acute toxicity for inhalation and oral uptake can be conducted. In a last step the results of exposure and affect assessments are combined to

calculate the Risk Characterisation Ratios (RCR) for the protection targets on regional and local scale. These RCR's are compared to the RCR's of the reference substance 1,4-dichlorobenzene resulting in a toxicity potential in 1,4-DCB equivalents. Toxicity potentials are calculated for Aquatic fresh water – (AETP<sub>fresh</sub>), Aquatic salt water – (AETP<sub>salt</sub>) terrestrial – (TETP), Sediment fresh water (SETP<sub>fresh</sub>), Sediment salt water ecosystem (SETP<sub>salt</sub>) and Humans (HTP), each for an initial emission of the substance to the compartment air, fresh water, sea water, industrial soil and agricultural soil. For the evaluation performed in this report, AETP<sub>fresh</sub>, TETP and HTP for an initial emission of the substance to agricultural soil are first considered.

## 2.2. Summary of DR3.4 “Multicriteria evaluation of RA and LCA assessment methods considering pesticide application”

DR3.4 summarises the results of the evaluation of several risk assessment (RA) and life cycle assessment (LCA) methods (EDIP97, EI99, IMPACT2002+, I-PHY, PRZM-USES, SYNOPS, and USES-LCA) to calculate the environmental impacts of pesticide use. The evaluation scheme is mainly based on the work of the ITADA project COMETE (Bockstaller et al., 2006). It is divided into the three dimensions scientific soundness (with eleven criteria), practical feasibility (six criteria) and stakeholder utility (three criteria), similarly to the OECD-Report on environmental indicators (OECD, 1999). Most of the sub-themes for the dimensions practical feasibility and stakeholder utility are divided into three user groups (extension services, authorities and scientists); going from the fact that their demands are different from each other.

The assessment resulted in the following conclusions:

Considering the dimension “scientific soundness, the method PRZM-USES shows the best results for the coverage of environmental issues, human health and exposition pathways, followed by the LCA methods EI99, USES and Impact2002 and the risk assessment methods SYNOPS and I-PHY, which both do not consider human health. But the last two mentioned are advantageous regarding coverage of agricultural branches and production factors and finally the method SYNOPS has strengths in geographical application, because very detailed data sets for field surroundings and climate can be used. Looking at the other criteria sets such as the depth of analysis, the integration of processes, the avoidance of incorrect conclusions and transparency, no differences between the methods are observed. They all cover these aspects adequately.

Regarding the aspects of practical feasibility and stakeholder utility the methods SYNOPS and I-PHY are advantageous compared to the other methods (Tab. 2 and Tab. 4). Both methods are working with a graphical user interface, which facilitates the handling and allows a presentation of the results. This reduces the risk of misinterpreting and simplifies the communicability of the results. A second point is that both methods are working with an implemented pesticide database, which reduces the time to fill in. Regarding the other methods, the differences are only minimal, because in all of them it's much more time consuming to include new pesticides or to change the characterisation factors when new data are available.

As a result of this assessment, it emerged that none of the methods covers all aspects satisfactorily. Each method has some strong, but also some weak points. For a detailed description of the theoretical evaluation see DR3.4 Multicriteria evaluation of RA and LCA assessment methods considering pesticide application (Kägi et al. 2008<sup>2</sup>). The criteria used in

<sup>2</sup> [https://workspaces.inra-transfert.fr/QuickPlace/endure/PageLibraryC1257324005BE62D.nsf/h\\_80C07B6C3F3919D0C1257325002FDCCD/973654FEEED09426C12574DB003663CF/?OpenDocument](https://workspaces.inra-transfert.fr/QuickPlace/endure/PageLibraryC1257324005BE62D.nsf/h_80C07B6C3F3919D0C1257325002FDCCD/973654FEEED09426C12574DB003663CF/?OpenDocument)

DR3.4 to evaluate the practical feasibility and stakeholder utility are summarised in section 7 (Tab. 9-Tab. 23).

**Tab. 2 : Results of the theoretical comparison for the Criterion “practical feasibility”: list of criteria to score on a scale between 1 and 5 (1 = low accordance, 5 = high accordance). Average for the user groups extension service, authorities and scientists. For detailed results and description of the decision rules see Appendix (Section 7).**

Practical feasibility	score (1 to 5)							
	I-PHY	PRZM-USES	SYNOPS	EDIP97	EI99	Imp02	USES-LCA	average
Accessibility of input data	4.0	4.5	5.0	3.8	N/A	3.7	3.7	<b>2.7</b>
Qualification requirements (user)	3.0	1.0	2.3	1.9	N/A	2.1	1.9	<b>1.4</b>
External services	3.3	2.7	2.3	3.3	N/A	2.0	3.3	<b>1.8</b>
User-friendliness	3.0	1.0	3.0	1.0	N/A	1.0	1.0	<b>1.0</b>
Support	4.0	3.0	3.0	4.0	N/A	4.0	4.0	<b>2.5</b>
Time needed (to calculate/ fill in)	5.0	1.7	5.0	3.0	N/A	3.0	3.0	<b>2.3</b>
Average	<b>3.7</b>	<b>2.3</b>	<b>3.4</b>	<b>2.8</b>	<b>N/A</b>	<b>2.6</b>	<b>2.8</b>	<b>2.3</b>

**Tab. 3 : Results of the theoretical comparison for the Criterion “stakeholder utility”. List of criteria to score on a scale between 1 and 5 (1 = low accordance, 5 = high accordance). Average for the user groups extension service, authorities and scientists. For detailed results and description of the decision rules see Appendix (Section 7). Changed values compared to DR3.4 are marked in bold italics.**

Stakeholder utility	score (1 to 5)							
	I-PHY	PRZM-USES	SYNOPS	EDIP97	EI99	Imp02	USES-LCA	average
Coverage of needs	4.0	4.0	4.0	4.0	N/A	4.0	4.0	<b>4.0</b>
Unambiguousness of results	3.7	1.0	2.7	1.0	N/A	1.0	1.0	<b>1.7</b>
Communicability of results	3.7	1.0	3.0	1.0	N/A	1.0	1.0	<b>1.8</b>
Average	<b>3.8</b>	<b>2</b>	<b>3.2</b>	<b>2</b>	<b>N/A</b>	<b>2</b>	<b>2</b>	<b>2.5</b>

### 3. Material and Methods.

During a RA3.3 and RA3.4 workshop in Berlin in January 2009 it was decided to use the wheat and pomefruit case studies for the practical test of the feasibility and stakeholder utility in the method evaluation due to the data availability in these studies. Especially for the risk assessment in RA3.3 detailed data for the environmental conditions are needed. Because of this fact for most of the data collected within the case studies only worst case scenario based on MARS-climate database as monthly averages on 50 km<sup>2</sup> grids could be analysed. RA3.3 decided to base the comparison of SYNOPS, I-PHY and PRZM-USES on a set of data from Saxony-Anhalt (wheat) and the German side of Lake Constance (pomefruit), as for these regions geo-referenced field specific data (soils, climatic conditions and field surroundings) and surveyed plant protection strategies are available. Since the results of RA3.3 are partly included in this deliverable, RA3.4 decided to use these data sets for the comparison of the RA and LCA methods too.

Within this deliverable only a short overview of the surveyed plant protection strategies and eco-toxicological data used is given, because a detailed description of the used datasets and a comparison of the eco-toxicological values within the databases from SYNOPS, I-PHY and the FOOTPRINT PPDB database is included in deliverable DR3.3 “Report on environmental risk and benefits assessment” from RA3.3<sup>3</sup> and the geo-referenced field specific data and climatic data are not used for the calculation of characterisation factors for the pesticides according to the LCA methods.

### 3.1. Data used for the Analysis

#### 3.1.1. Surveyed Plant protection strategies

##### Saxony-Anhalt

The strategies were recorded within the German repetitive surveys on the pesticide use (NEPTUN). For wheat the data were assessed in 2000. In Saxony-Anhalt 29 farmers producing wheat take part in the study. Their wheat growing area (9007 ha) represent 3 % of the total wheat production area in Saxony-Anhalt. All the farmers produce according to the good plant protection practice. In total 112 different strategies were applied. The treatment frequency index (TFI) of all pesticides ranges between 0.72 and 8.7 with a mean of 3.77 and a standard deviation of 1.61.

In total 71 products were applied including 55 different active ingredients. For all active ingredients the required physico-chemical and eco-toxicological data for the risk assessment calculations were available within the SYNOPS and FOOTPRINT PPDB databases. With some exceptions for all the active ingredients the characterisation factors could be calculated with the LCA methods EDIP97 and USES-LCA. For Impact2002 the characterisation was possible for the aquatic toxicity with one exception but for the human toxicity only a few and for the terrestrial eco-toxicity none of the active ingredients could be characterised. The missing values were replaced by medians of the respective pesticide class defined in Nemecek & Kägi (2007) for all methods and categories with the exception of the terrestrial eco-toxicity and the human toxicity according to Impact2002 which were excluded from the analysis.

##### German side of Lake Constance

The strategies were also surveyed within the NEPTUN studies, but they are related to the year 2004. In the region Lake Constance 50 farmers with 268 ha of orchards, representing 4.3 % of the regions production area, were surveyed. All farmers produce according to the regulations of labelled production. Fifty different application strategies were used in the labelled apple production of these farmers. The TFI ranges between 14.4 and 59 with a mean of 30.5 and a standard deviation of 8.8.

In total 60 different products including 39 active ingredients were applied. For all active ingredients the required physico-chemical and eco-toxicological data for the risk assessment calculations were available within the SYNOPS<sup>4</sup> and FOOTPRINT PPDB<sup>5</sup> databases. With some exceptions for all the active ingredients the characterisation factors could be calculated with the LCA methods EDIP97 and USES-LCA. For Impact2002 the characterisation was possible for the aquatic toxicity with one exception but for the human toxicity only a few and for the terrestrial

<sup>3</sup> [https://workspaces.inra-transfert.fr/QuickPlace/endure/PageLibraryC1257324005BE62D.nsf/h\\_Toc/a4fbf4ded67e5f2dc1257325002fca37/?OpenDocument&Start=43&Count=20](https://workspaces.inra-transfert.fr/QuickPlace/endure/PageLibraryC1257324005BE62D.nsf/h_Toc/a4fbf4ded67e5f2dc1257325002fca37/?OpenDocument&Start=43&Count=20) (under review 10.12.2009)

<sup>4</sup> Short description about SYNOPS <http://www.jki.bund.de/> (10.12.2009)

<sup>5</sup> <http://www.eu-footprint.org/ppdb.html> (10.12.2009)

eco-toxicity none of the active ingredients could be characterised. The missing values were replaced by medians of the respective pesticide class defined in Nemecek & Kägi (2007) for all methods and categories with the exception of the terrestrial eco-toxicity and the human toxicity according to Impact2002 which were excluded from the analysis.

### 3.1.2. Physico-chemical- and toxicity data for the active ingredients

An evaluation of the different methods should be based on a consistent chemical dataset to avoid differences due to input data. RA3.3 and RA3.4 decided to use the database of SYNOPS as a reference and FOOTPRINT PPDB for data gaps or missing active ingredients. Both databases are actively managed and continuously updated. For both databases the EU review monographs are used as preferential data source. If EU monographs are not available alternative sources are used for example documents from national legislation processes, pesticide manuals, IVA-datasheets or publications.

### 3.1.3. Calculation of the characterisation factors

For the LCA methods EDIP97 (Hauschild and Wenzel, 1998), IMPACT2002 (Jolliet et al., 2003) and USES-LCA (Guinée et al., 2001) the characterisation factors had to be calculated, because there were only a few pesticides already characterised for each of the methods. The characterisation was based on the method descriptions and in case of IMPACT2002 and USES-LCA on calculation spreadsheets provided by the method developers. For EDIP97 there is no calculation tool available therefore the characterisation factors were calculated in EXCEL following the method description.

### 3.1.4. Calculation of the TFI

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

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

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:

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

### 3.1.5. Data from RA3.3

All risk assessment calculations included in this deliverable were calculated within the sub activity RA3.3 by Christian Bockstaller (I-PHY), Laure Mamy (PRZM-USES) and Jörn Strassemeier (SYNOPS). With the geo-referenced data set of environmental conditions described in DR3.3 a total of 784368 risk evaluations can be assessed (5028 wheat fields \* 156 strategies). For the region of Lake Constance 191800 (3836 orchards \* 50 strategies) risk potential calculations are possible. As I-PHY and PRZM-USES are not able to handle this number of calculations, because they have to be parameterised manually, the number of scenarios was already decreased in RA3.3 to 48 scenarios in wheat (7488 possible risk assessments) and 18 scenarios in the region of Lake Constance (900 possible risk assessments). For a description of these scenarios see DR3.3. Also the TFI index has already been calculated in RA3.3



### 3.2. Analysis

The first goal of this deliverable is to test if the theoretical assessment of the two dimensions feasibility and stakeholder utility can be confirmed in practise. To verify this for each method the above described number of scenarios should be calculated for the risk assessment methods in RA3.3 and the LCA Methods in RA3.4. The results of this test were not evaluated statistically as the information (time demand and number of calculations performed) are single values without repetitions. Therefore the analysis shown in Chapter 4.1 is more an experiential report describing the advantages and disadvantages of each single method. Nonetheless the results can be used for a comparison of the methods amongst themselves and with the TFI to test:

- if the methods classify the environmental impacts of the plant protection in the same way and
- if the TFI may be used as an estimator of the environmental impact of a pesticide application pattern.

For this purpose the spearman rank correlation was chosen for the comparison, because:

- it is more robust regarding normal distribution and outliers
- it does not assume a special relationship between the variables (e.g. linear) and
- one of the goals of all methods is a ranking of given set of pesticide application schemas.

The rank correlation analysis according to spearman is calculated as.

$$\rho = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)}$$

Where:

$d_i = x_i - y_i$  = the difference between the ranks of corresponding values  $X_i$  and  $Y_i$ , and  
 $n$  = the number of values in each data set (same for both sets).

Since the LCA models do not regard different environmental conditions on a field level it was decided in RA3.4 to base the method comparison on the strategies (156 applied in wheat and 50 in apple production). Therefore for the methods I-PHY, PRZM-USES and SYNOPS the mean of the risk potential for the different scenarios was calculated, to compare this mean with the results from the LCA methods. Nevertheless to check if this procedure influences the correlation results the rank correlation analysis was also performed for each of the scenarios.

## 4. Results for the two case studies wheat and pomefruit

### 4.1. Evaluation of the practical feasibility and stakeholder utility with a set of plant protection strategies.

The goal of the evaluation is to validate the theoretical comparison of the practical feasibility and stakeholder utility assuming that one of the main tasks for the methods will be to compare a large number of strategies and to select the ones with the lowest risk potential or toxicity potential. The risk assessment methods also should be able to include a wide spectrum of environmental conditions. The comparison of the risk assessment methods was conducted within RA3.3 using the geo-referenced data-set briefly described in 3.1.5. As the LCA toxicity models do not regard the different environmental conditions, because the models work on a regional and continental level, they could not be included in this part of the analysis. The calculations for the LCA models based on the 206 strategies were performed in RA3.4. The analyses carried out in RA3.3 and RA3.4 showed:

- that the total number of risk assessments based on the two geo-referenced datasets could only be performed with SYNOPS.
- for the other methods a reduced set of environmental conditions for Saxony-Anhalt (48) and the German side of Lake Constance (18) has to be created.
- PRZM-USES is even for the reduced set of scenarios not feasible, because of the manual parameterisation of the model.
- that the LCA toxicity models do not include the environmental conditions at all.

According to this experience the theoretical comparison described in DR3.4 was checked whether the values assigned to the methods in the theoretical comparison have to be changed. Regarding the dimension practical feasibility mainly the criteria user friendliness and time needed (to calculate/to fill in) were concerned (see Tab. 2). Because of the qualitative definition of the evaluation criteria user friendliness described in Tab. 15 the PRZM-USES evaluation for this criterion was not changed. Also the values for the criterion time needed to fill in although quantitative (Tab. 17) are not changed, because the time needed was adequately estimated. Already in the theoretical evaluation for these criteria the performance of the method PRZM-USES was rated to be lower compared to the other methods and so no further adaptations are made after the practical test.

**Tab. 4 : Results of the theoretical comparison for the Criterion “stakeholder utility” changed after the calculations performed in RA3.3 and RA3.4 (changed values compared are marked in bold italics). For detailed results and description of the decision rules see Appendix (Section 7).**

Stakeholder utility	score (1 to 5)							
	I-PHY	PRZM-USES	SYNOPS	EDIP97	EI99	Imp02	USES-LCA	average
Coverage of needs	4.0	<b>2.0</b>	4.0	<b>2.0</b>	N/A	<b>2.0</b>	<b>2.0</b>	<b>2.7</b>
Unambiguousness of results	3.7	1.0	2.7	1.0	N/A	1.0	1.0	<b>1.7</b>
Communicability of results	3.7	1.0	3.0	1.0	N/A	1.0	1.0	<b>1.8</b>
Average	<b>3.8</b>	<b>1.3</b>	<b>3.2</b>	<b>1.3</b>	N/A	<b>1.3</b>	<b>1.3</b>	<b>2.1</b>

However for the dimension stakeholder utility (Tab. 20 - Tab. 23) the evaluation in practice shows that for PRZM-USES as well as the LCA methods the theoretical evaluation is too optimistic. Especially when assuming that one of the main tasks for the methods will be to compare a large number of strategies on a field, farm, regional watershed and country level and

to assess the efficacy of environmental protection policies. For all the mentioned models the criteria coverage of needs is set to Low (2) instead of Strong (4) assessed in the theoretical evaluation.

## 4.2. Correlation results for the plant protection strategies in the two case study regions

The calculations performed in RA3.3 and RA3.4 could be used to assess whether the results for the plant protection strategies in terms of their environmental impacts are the same or comparable across the methods. The following chapter gives an overview of the ranking of the strategies according to the methods described in 2.1 for each case study region. First the results are compared with the ranking according to the TFI followed by a comparison across the methods for the aquatic eco-toxicity, the terrestrial eco-toxicity and the human toxicity. The method PRZM-USES is excluded from the analysis, because of the few strategies which could be analysed with this method. Finally the LCA results are compared with the RA results for the single scenarios to check if the comparison of the LCA results with the mean of the scenarios calculated with the RA method influences the results of the correlation analysis.

### 4.2.1. Results comparing the TFI with the RA and LCA methods

The treatment frequency index TFI is also included in the analysis, because often the TFI is not only used to describe the intensity of plant protection, but also as an indicator for the environmental impact, which might not be feasible. The TFI is calculated as the number of applied plant protection products (PPP) related to the fraction of the area the product was applied on ( $f_{\text{area}} = A_{\text{applied}}/A_{\text{field}}$ ) and related to the percentage of the used application rate to the maximum allowed application rate ( $f_{\text{rate}} = AR/AR_{\text{ma}}$ ). For each application of a PPP a sub-index ( $TFI_x$ ) is calculated as:

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

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:

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

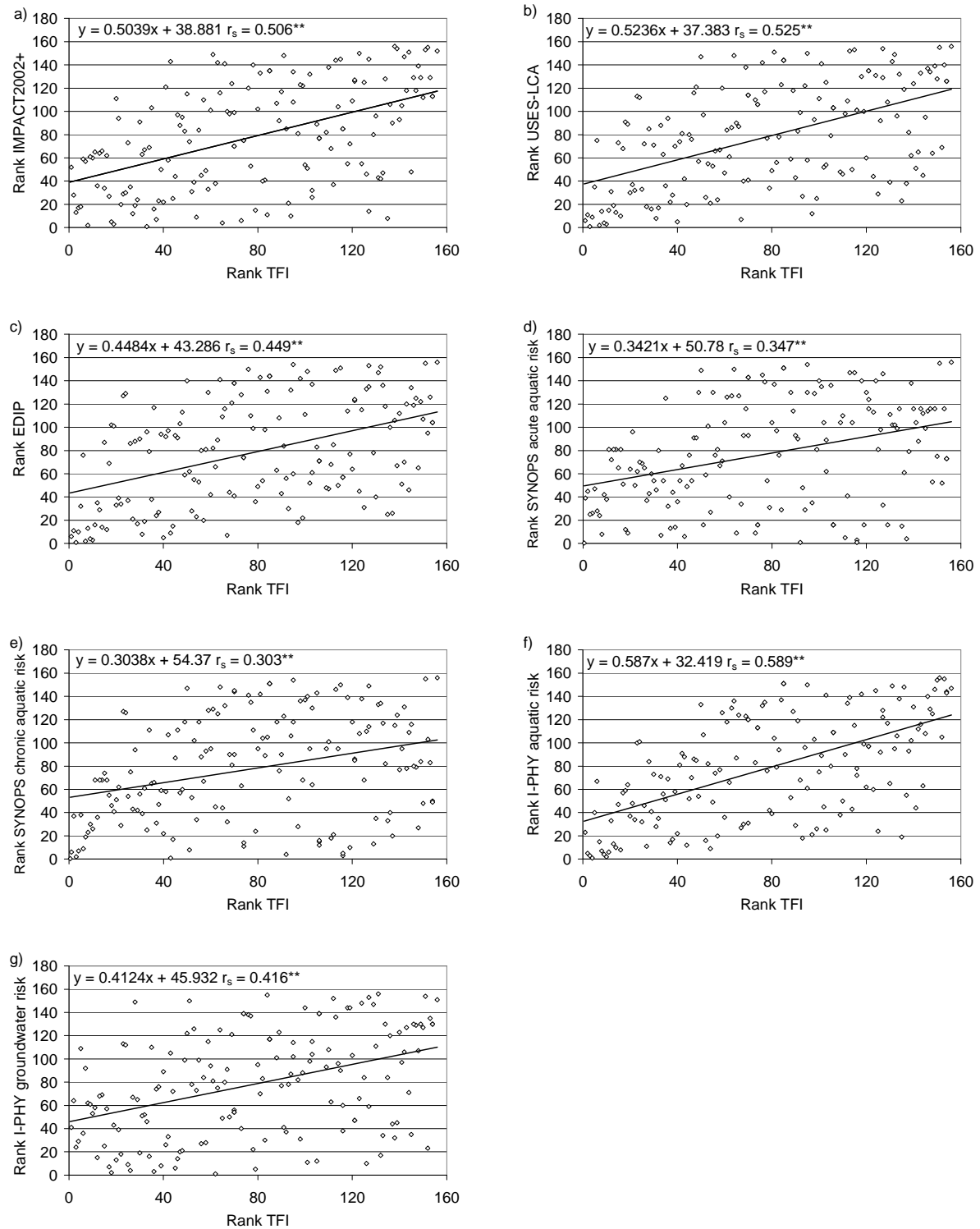
First the correlations between the TFI and the results of the 206 strategies for the aquatic ecosystem are presented including the toxicity according to the methods Impact2002+, USES-LCA, EDIP97 and the risks indicators calculated with SYNOPS (acute and chronic risk) and I-PHY (aquatic risk) the I-PHY groundwater risk was only included in the wheat case study, because no values were calculated for the case study pomefruit. In this second part the correlation between the TFI and the results for the terrestrial ecosystem are shown. The method I-PHY is not included in this part, because it calculates no risk for the terrestrial ecosystem. The chapter is completed with the results for the human health. This part only includes the methods EDIP97 and USES-LCA, as for IMPACT2002 the human toxicity factors are not available and the RA methods do not regard the human health.

The rank correlations between the TFI and the aquatic toxicity or aquatic risk according to the methods are very weak to weak for both case studies (Fig. 5 & Fig. 6). The correlation coefficient ranges between 0.30 (SYNOPS chronic aquatic risk) and 0.59 (I-PHY aquatic risk) for the case study wheat and between 0.12 (I-PHY aquatic risk) and 0.56 (EDIP97) for the comparison in the pomefruit case study. Although most of the correlations are significant at a  $p < 0.01$  there is no visible coherence between the results of a single method and the TFI. And also there is no evidence that one of the methods correlate better with the TFI than the others. The correlations

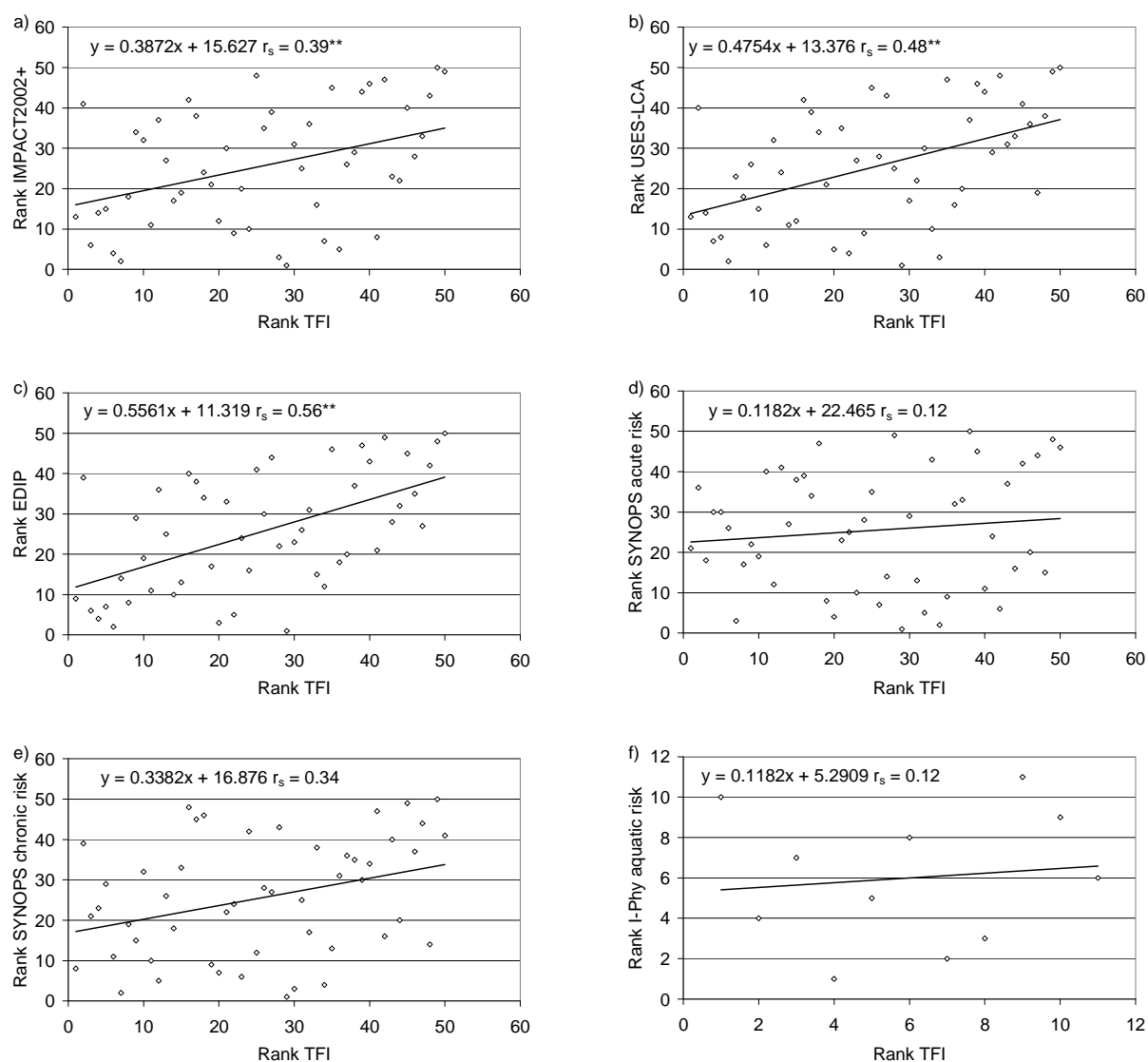
between the LCA methods and the TFI are slightly higher than between the RA methods and the TFI with the exception of I-PHY aquatic risk in the wheat case study which has the highest correlation at all. But on the other hand the correlation between I-PHY aquatic risk and the TFI is very weak for the strategies applied in the case study wheat.

Similar to the aquatic eco-toxicity the rank correlation between the TFI of the applied strategies and the terrestrial eco-toxicity and the terrestrial risk are on a very weak to weak level in both case studies (Fig. 7). But in both case studies the difference between the lowest and highest correlation coefficient is much smaller compared to the results for the aquatic ecosystem. In the case study wheat the lowest rank correlation between TFI and SYNOPSIS chronic terrestrial risk ( $r_s = 0.47$ ) is nearly as high as the highest one between the TFI and EDIP97 ( $r_s = 0.57$ ). Also in the pomefruit case study the difference is small ( $r_s$  TFI/SYNOPSIS acute terrestrial risk = 0.29 and  $r_s$  TFI/USES-LCA = 0.39). In contrast to the aquatic ecosystem the LCA methods and SYNOPSIS show a comparable correlation with the TFI.

Like for the other categories for both case studies the relation between TFI and the indicators are on a weak niveau. Both the lowest and highest rank correlations are calculated between the TFI and EDIP97<sub>soil</sub>, but for the different case studies. The lowest correlation is assessed for the 50 plant protection strategies in the pomefruit case study ( $r_s$  TFI/EDIP97 soil = 0.41) and the highest for the 156 applied in wheat ( $r_s$  TFI/EDIP97 soil = 0.64).

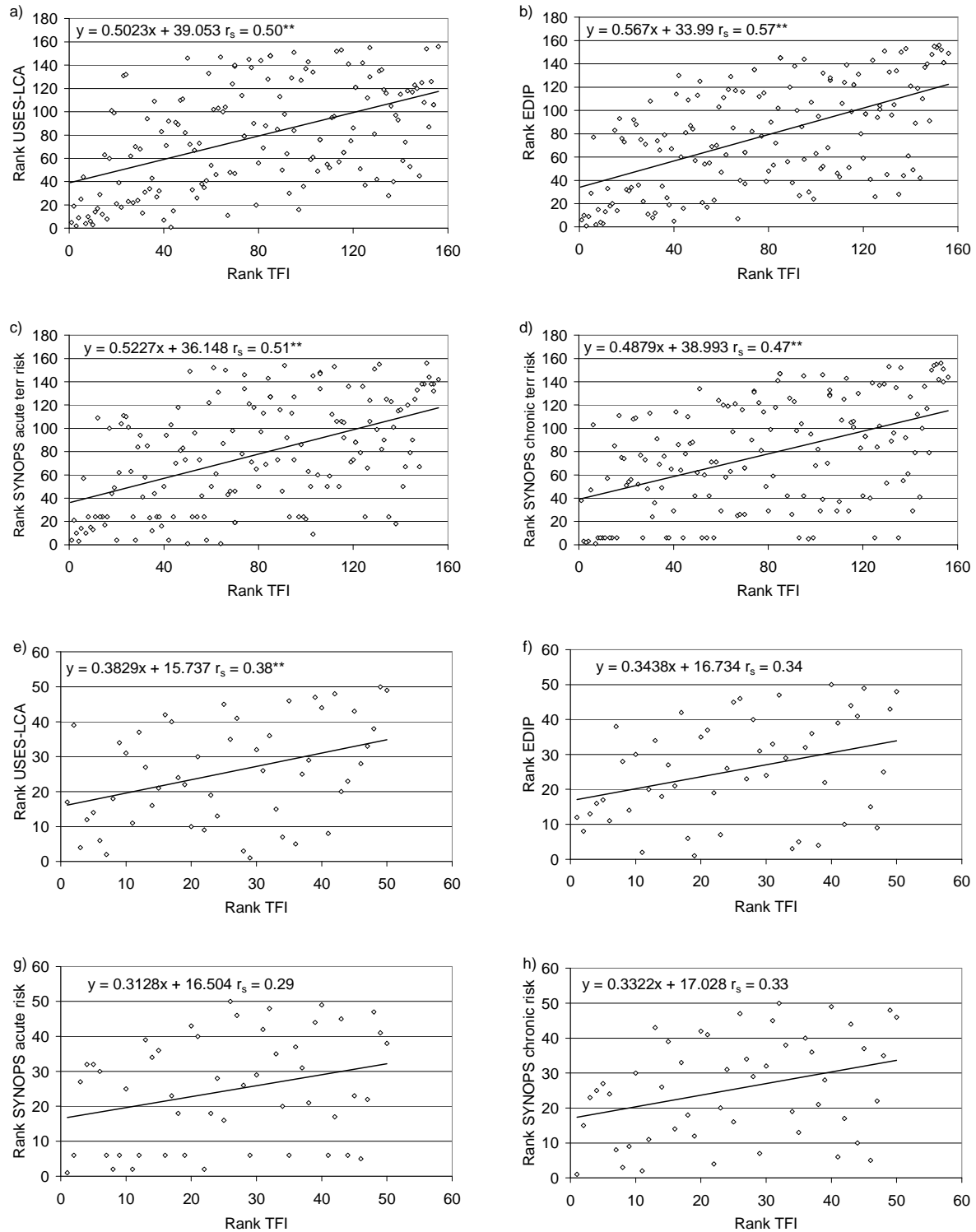


**Fig. 5:** Correlation between the TFI and the aquatic eco-toxicity of the strategies used in the wheat case study region calculated with a) Impact2002+, b) USES-LCA, c) EDIP, and the indicators d) SYNOPS acute aquatic risk, e) SYNOPS chronic aquatic risk, f) I-PHY aquatic risk and g) I-PHY groundwater risk;  $r_s$  = Spearman rank correlation coefficient;  $n = 156$ ,  $^{**}$  = significant at  $p < 0.01$

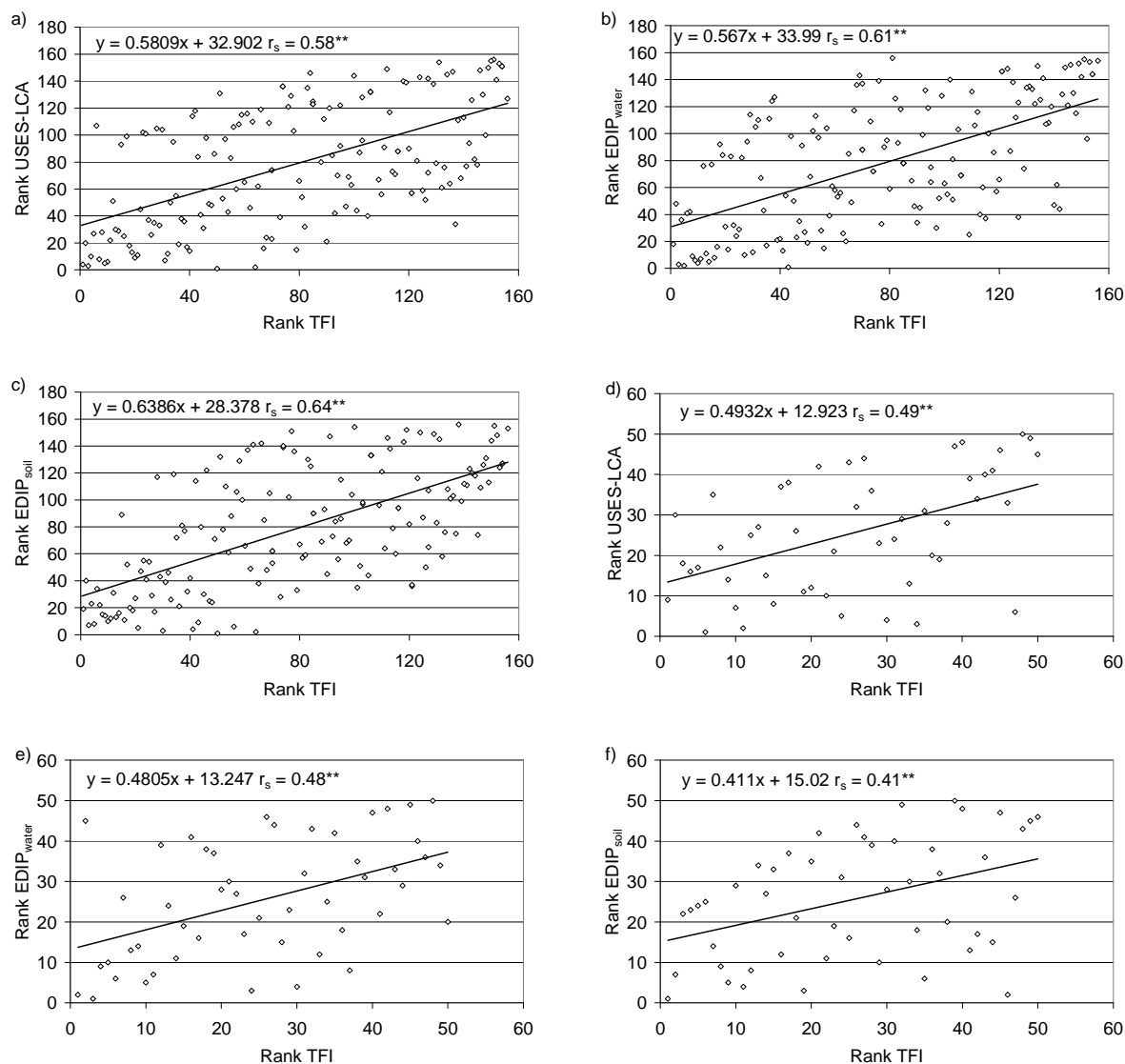


**Fig. 6 :** Correlation of to the TFI and the aquatic eco-toxicity of the strategies used in the pomefruit case study calculated with a) Impact2002+, b) USES-LCA, c) EDIP97, and the risk indicators d) SYNOPS acute aquatic risk, e) SYNOPS chronic aquatic risk, e) I-PHY aquatic risk and f) I-PHY groundwater risk;  $r_s$  = Spearman rank correlation coefficient;  $n = 50$  ( $n = 11$  for I-PHY);  $^{**}$  = significant at  $p < 0.01$





**Fig. 7 :** Correlation between the TFI and the terrestrial eco-toxicity of the strategies used in the wheat and pomefruit case study according to USES-LCA a (e), EDIP b (f), and the terrestrial risk indicators SYNOPS acute risk c (g) and SYNOPS chronic d (h);  $r_s$  = Spearman rank correlation coefficient;  $n = 50$  plant protection strategies;  $^{**}$  = significant at  $p < 0.01$



**Fig. 8 :** Correlation between the TFI and the human toxicity of the strategies calculated with a) USES-LCA, b) EDIP<sub>water</sub>, c) EDIP<sub>soil</sub> for the case study wheat (n=156) and with d) USES-LCA, e) EDIP<sub>water</sub>, and EDIP<sub>soil</sub> (f) for the case study pomefruit (n=50).  $r_s$  = Spearman rank correlation coefficient; \*\* = significant at  $p < 0.01$

## 4.2.2. Comparison of the Methods

### 4.2.2.1. Aquatic toxicity

#### Case study wheat (Saxony-Anhalt)

In total 156 application strategies applied in Saxony Anhalt in wheat are included in the comparison of the ranking across methods. As for the RA methods SYNOPSIS and I-PHY for each strategy 48 risk assessments with different environmental conditions were calculated in RA3.3 here the mean risk out of these evaluations for each strategy is used for the comparison.

In contrast to the comparisons described in 4.2.1 the rank correlation for the 156 strategies is much better for some methods (Tab. 5). Within the LCA methods the methods EDIP97 and USES-LCA are highly correlated with an  $r_s = 0.94$  (Fig. 9 a) whereas for the comparison of Impact2002+ and USES-LCA ( $r_s = 0.31$ ) and Impact2002+ and EDIP ( $r_s = 0.24$ ) the correlation is much lower. Between the RA methods only weak correlations are found based on the analysis of the 156 strategies. The highest accordance is calculated for the indicators SYNOPSIS chronic risk and I-PHY aquatic risk ( $r_s = 0.47$ ) and the lowest is found comparing SYNOPSIS chronic risk and I-PHY groundwater risk ( $r_s = 0.15$ ). Both RA methods SYNOPSIS and I-PHY calculate two indicators related to the aquatic ecosystem. For SYNOPSIS the correlation between the acute and the chronic risk is high ( $r_s = 0.82$  Fig. 9 d), whereas for I-PHY the correlation between the aquatic and the groundwater risk is lower ( $r_s = 0.49$ ). Comparing the accordance in ranking the pesticide strategies over the border RA/LCA the highest correlations are found between the aquatic risk indicator of I-PHY and the methods USES-LCA ( $r_s = 0.91$ ) and EDIP97 ( $r_s = 0.85$ ) as shown in Fig. 9 b and c. For the other comparisons between RA and LCA the correlations are much weaker with a correlation coefficient between 0.22 and 0.65.

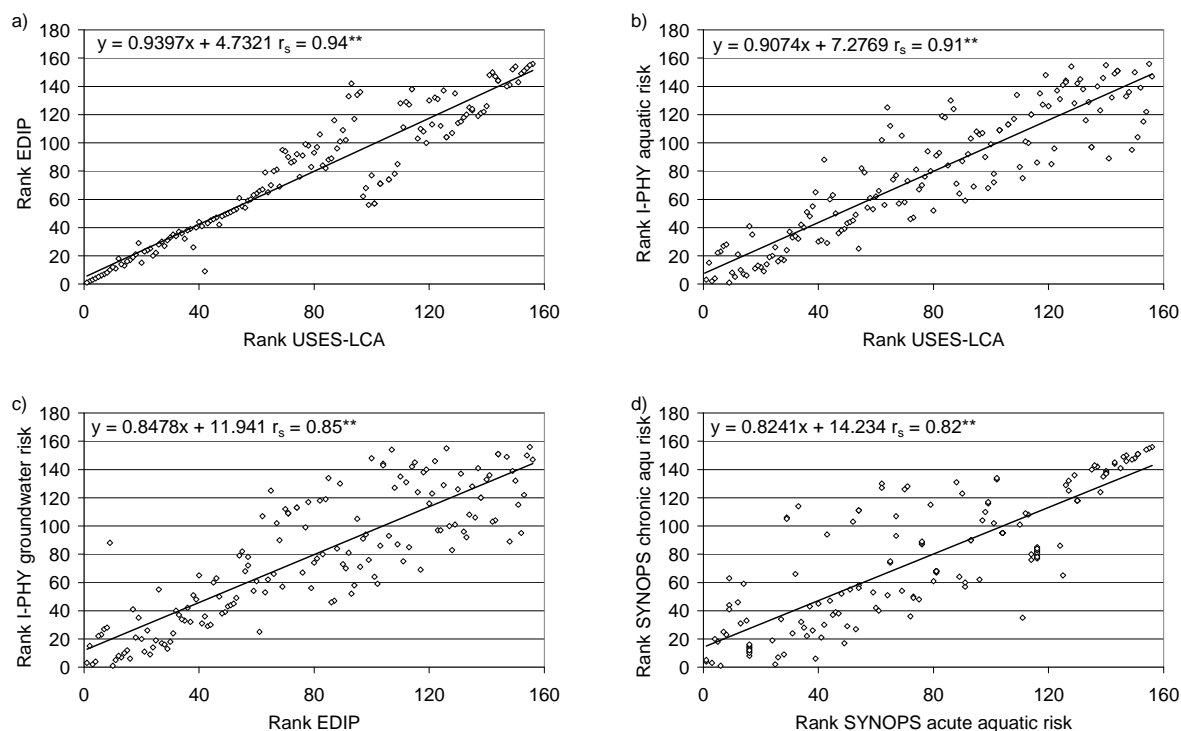
#### Case study pomefruit (German side of Lake Constance)

50 different plant protection strategies applied in orchards on the German side of Lake Constance are available for the comparison of the ranking across methods. For the comparison in RA3.3 18 different environmental scenarios were defined. Due to technical reasons for I-PHY only 11 strategies and 6 environmental conditions and only the aquatic risk indicator could be calculated. As a consequence the comparisons including I-PHY were based on these 11 strategies and the groundwater risk indicator from I-PHY couldn't be included. For the comparison described here again the mean risk is used.

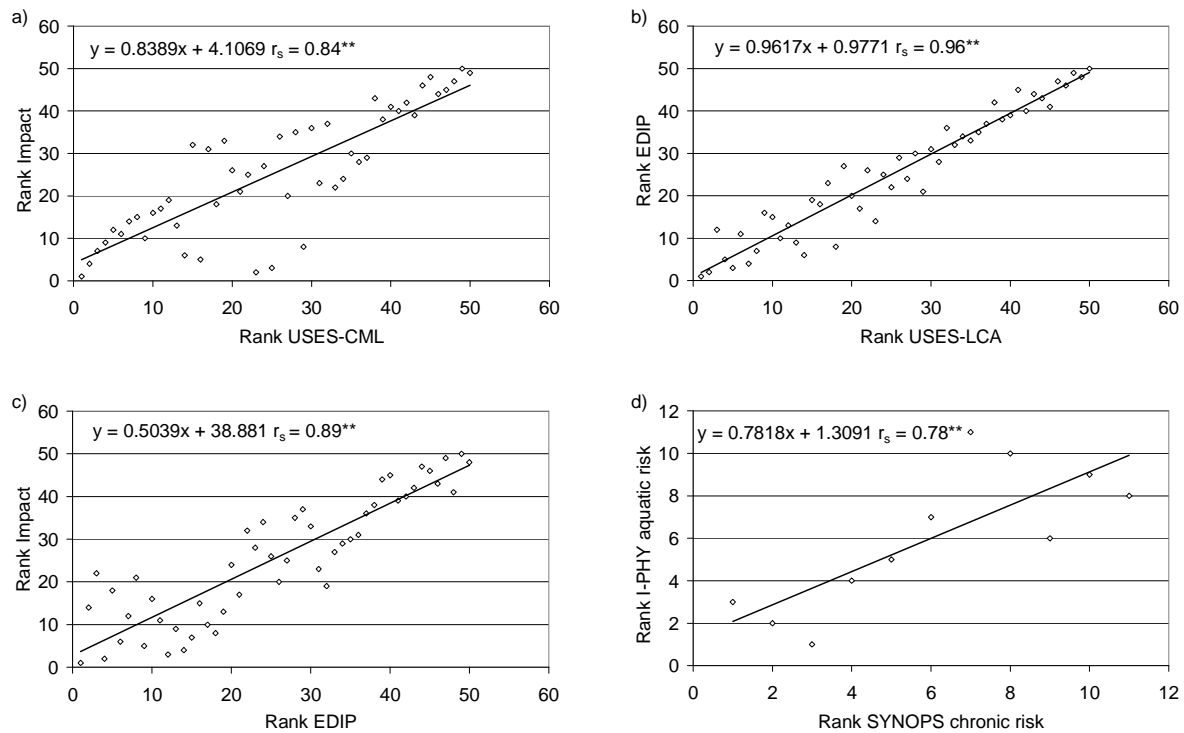
Like in the wheat case study there are much higher correlations for the ranking of the 50 strategies between some methods than between a single method and the TFI (Fig. 10 and Tab. 5). But mostly high correlations are found for other method comparisons than in the wheat case study and the high correlations found for the 156 strategies applied in wheat couldn't be validated with the results of this case study. Only for the ranking according to the methods USES-LCA and EDIP97 a high correlation is found again ( $r_s = 0.96$ ). For the other method comparisons with a high rank correlation in the wheat case study the coincidence is lower (Tab. 5) in the pomefruit case study compared to the wheat case study. For about 50 % of the comparisons the correlation is higher and for 50 % the correlation is lower compared to the wheat case study. Within the LCA methods rank correlations are high with a  $r_s$  from 0.84 (Impact2002+/EDIP97) to 0.96 (USES-LCA/Edip97) as shown in Fig. 10 a-c. The correlation for the different RA indicators ranged from weak ( $r_s = 0.15$  for SYNOPSIS acute aquatic risk/I-PHY aquatic risk) to fairly good for the indicators SYNOPSIS chronic aquatic risk and I-PHY aquatic risk ( $r = 0.78$ ; Fig. 10 d). Looking at the comparison of RA and LCA results the highest correlations are found between EDIP97 and Impact2002+ and I-PHY aquatic risk ( $r_s = 0.75$ ) the correlation between USES-LCA and the aquatic risk calculated with I-PHY is with a  $r_s$  of 0.59 clearly lower than in the wheat case study ( $r_s = 0.91$ ).

**Tab. 5 : Spearman rank correlation coefficients between the RA and LCA methods for aquatic risk/toxicity and the two case studies wheat and pomefruit; bold values indicate significance at  $p < 0.01$**

Indicator	Case study wheat						Case study pomefruit					
	USES-LCA	EDIP97	SYNOPSIS		I-PHY		USES-LCA	EDIP97	SYNOPSIS		I-PHY	
			acute	chronic	aquatic	gw			acute	chronic	Aquatic	gw
IMPACT2002+	<b>0.31</b>	<b>0.24</b>	<b>0.58</b>	<b>0.39</b>	<b>0.41</b>	<b>0.23</b>	<b>0.84</b>	<b>0.89</b>	0.15	0.27	<b>0.75</b>	N/A
USES-LCA		<b>0.94</b>	<b>0.41</b>	<b>0.50</b>	<b>0.91</b>	<b>0.38</b>		<b>0.96</b>	0.18	<b>0.37</b>	0.59	N/A
EDIP97			<b>0.47</b>	<b>0.65</b>	<b>0.85</b>	<b>0.22</b>			0.21	<b>0.38</b>	<b>0.75</b>	N/A
SYNOPSIS acute				<b>0.82</b>	<b>0.41</b>	<b>0.25</b>				<b>0.68</b>	0.15	N/A
SYNOPSIS chronic					<b>0.47</b>	0.15					<b>0.78</b>	N/A
IPHY aquatic						<b>0.49</b>						N/A



**Fig. 9 :** Relation of the strategy ranking for the method pairs a) USES-LCA/EDIP97, b) USES-LCA/I-PHY aquatic indicator; EDIP97/I-PHY aquatic risk indicator (c) and the both aquatic risk indicators of SYNOPSIS (d).  $r_s$  = Spearman rank correlation coefficient;  $n = 156$  plant protection strategies;  $^{**}$  = significant at  $p < 0.01$



**Fig. 10 :** Relation of the strategy ranking for the method pairs a) USES-LCA /Impact2002+, b) USES-LCA/EDIP97; c) EDIP97/Impact2002+ and the risk indicators Synops chronic aquatic risk and I-PHY aquatic risk (d).  $r_s$  = Spearman rank correlation coefficient.  $n = 50$  plant protection strategies;  $^{**}$  = significant at  $p < 0.01$

#### 4.2.2.2. Terrestrial toxicity

The analysis for the terrestrial eco-toxicity includes the methods USES-LCA, EDIP97 and the two indicators acute - and chronic terrestrial risk from SYNOPSIS. The method PRZM-USES, I-PHY and IMPACT2002+ are not included, because of the small number of calculations (PRZM-USES) the method calculates no terrestrial risk (I-PHY) or because the characterisation factors could not be calculated (IMPACT2002+).

##### Case studies wheat and pomefruit

All rank correlations between the methods are stronger than between a single method and the TFI with the exception of USES-LCA/SYNOPSIS acute terrestrial risk ( $r_s = 0.57$ ). The results of the methods are especially highly correlated with the chronic risk indicator of SYNOPSIS (Fig. 11 and Tab. 6) with a  $r_s$  of 0.77 to 0.93. In addition the methods EDIP97 and USES-LCA show a strong correlation ( $r_s = 0.8$ ) for the 156 strategies analysed.

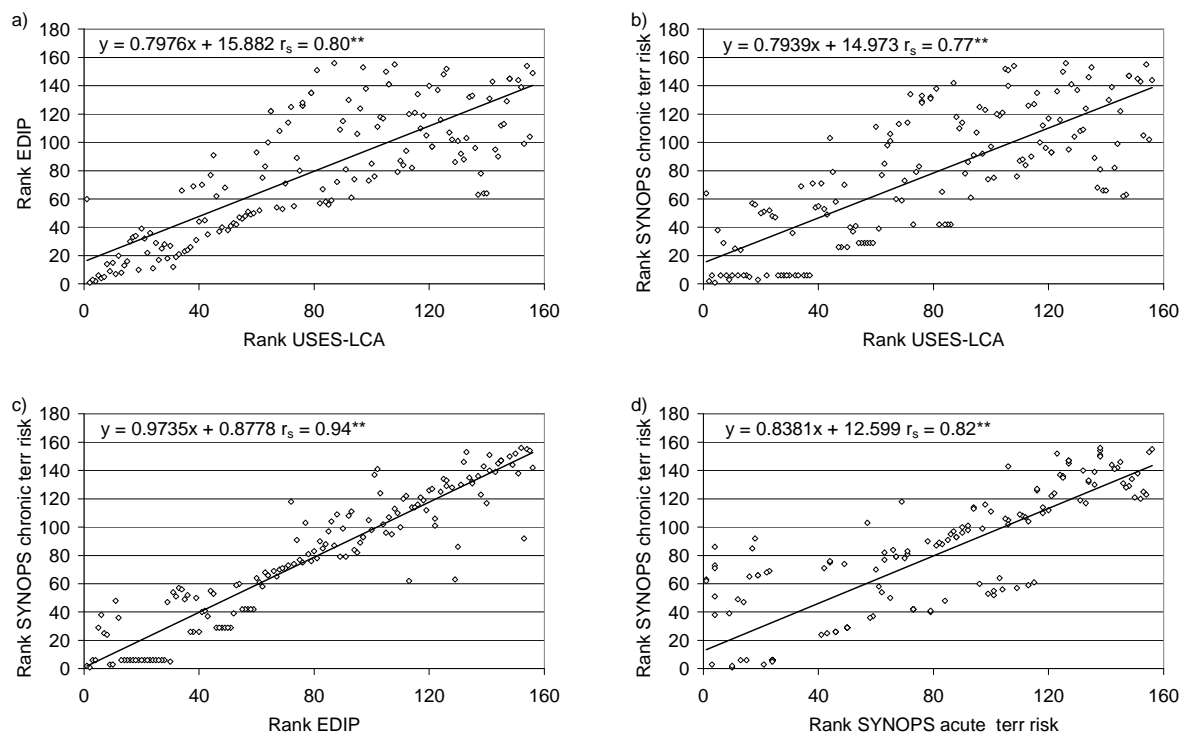
Like for the aquatic eco-toxicity the accordance between the methods are much weaker for the strategies applied in the case study pomefruit than for the case study wheat (Tab. 6). The only exceptions are the both indicators from SYNOPSIS with a  $r_s$  of 0.93. For the other method comparisons the correlation coefficient ranges between 0.19 and 0.58.

#### 4.2.2.3. Human toxicity

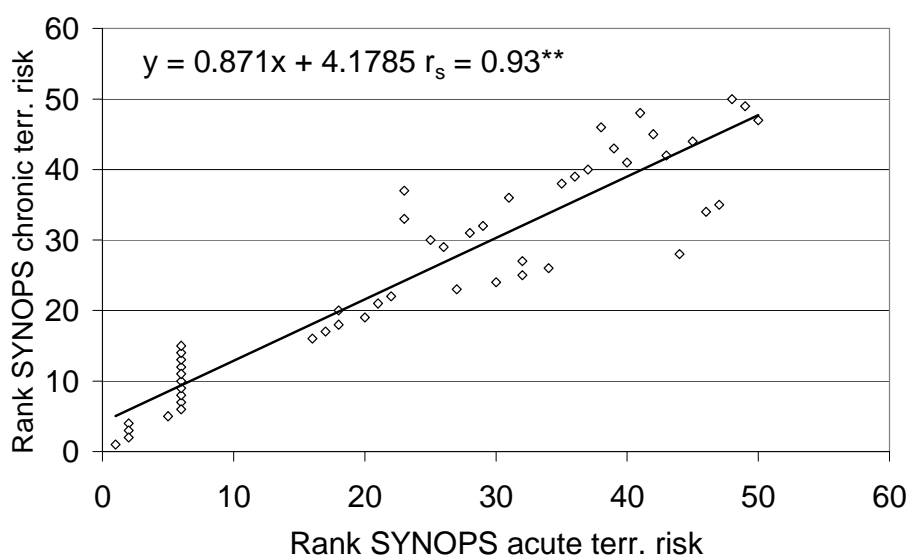
The human toxicity is only assessed by the LCA methods and PRZM-USES, but because of the low number of calculations performed with PRZM-USES this method is excluded from the analysis. Furthermore the method Impact2002+ has to be excluded, because the characterisation factors couldn't be calculated as data on ED (effect doses for cancer and non cancer effects for inhalation and oral uptake) and DALYs (Disability Adjusted Life Years) per incidence are not included in the SYNOPSIS and FOOTPRINT PPDB database. Within the method EDIP97 several indicators for human health are calculated regarding the different compartments and routes of exposure (air, soil and water). These indicators can't be summarised to a single one, because of the different unit's  $m^3$  soil, - air or - water needed to dilute the emission to a value which has no consequence on human health. The indicators for human toxicity via soil and water are presented here.

Comparing the ranking of the strategies according to the human toxicity the highest correlation is given between EDIP97<sub>soil</sub> and USES-LCA for the strategies applied in wheat ( $r_s = 0.8$ ). The two other method comparisons EDIP97<sub>soil</sub>/EDIP97<sub>water</sub> ( $r_s = 0.41$ ) and EDIP97<sub>water</sub>/USES-LCA ( $r_s = 0.29$ ) show an obviously lower accordance. For the pomefruit case study the picture is turned around, and the correlation is highest for the comparison EDIP97<sub>water</sub>/USES-LCA ( $r_s = 0.61$ ) followed by EDIP97<sub>soil</sub>/USES-LCA ( $r_s = 0.4$ ) and EDIP97<sub>soil</sub>/EDIP97<sub>water</sub> ( $r_s = 0.17$ ).





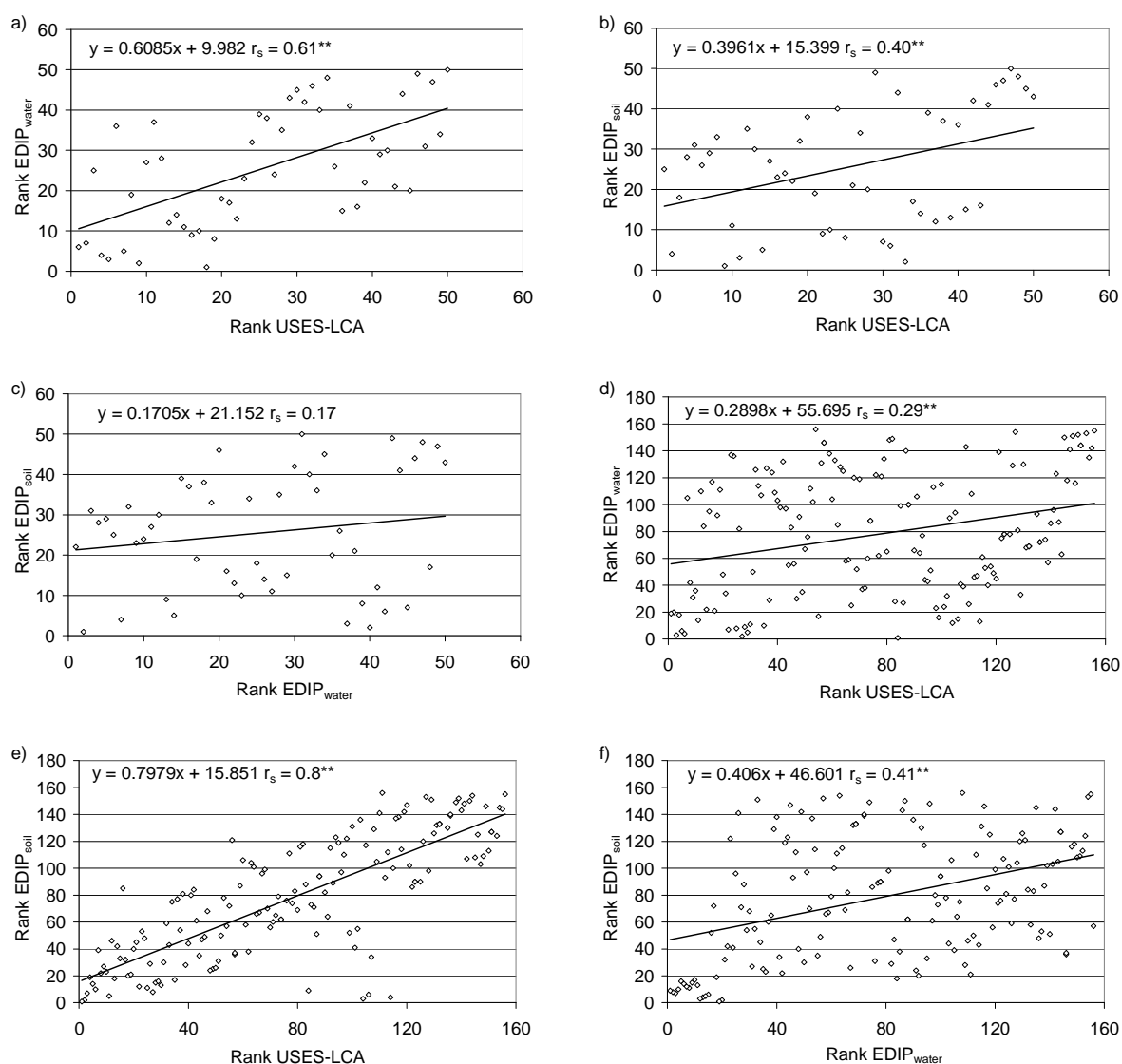
**Fig. 11 :** Relation of the strategy ranking for the method pairs USES-LCA/EDIP97 (a), USES-LCA/SYNOPSIS chronic risk, EDIP97/SYNOPSIS chronic risk (c) and EDIP97/SYNOPSIS acute terrestrial risk (d).  $r_s$  = Spearman rank correlation coefficient;  $n$  = 156 plant protection strategies



**Fig. 12 :** Ranking of the strategies according to the SYNOPSIS acute terrestrial risk in relation to the ranking according to SYNOPSIS chronic terrestrial risk.  $r_s$  = Spearman rank correlation coefficient;  $n$  = 50 plant protection strategies

**Tab. 6 : Spearman rank correlation coefficients between the RA and LCA methods for terrestrial risk/toxicity and the two case studies wheat and pomefruit; bold values indicate significance at  $p < 0.01$**

Indicator	Case study wheat			Case study pomefruit		
	EDIP97	SYNOPS acute terr. risk	SYNOPS chronic terr. risk	EDIP97	SYNOPS acute terr. risk	SYNOPS chronic terr. risk
USES-LCA	<b>0.80</b>	0.56	<b>0.77</b>	0.19	0.20	0.28
EDIP97		<b>0.74</b>	<b>0.94</b>		<b>0.46</b>	<b>0.58</b>
SYNOPS acute terr. risk			<b>0.82</b>			<b>0.93</b>



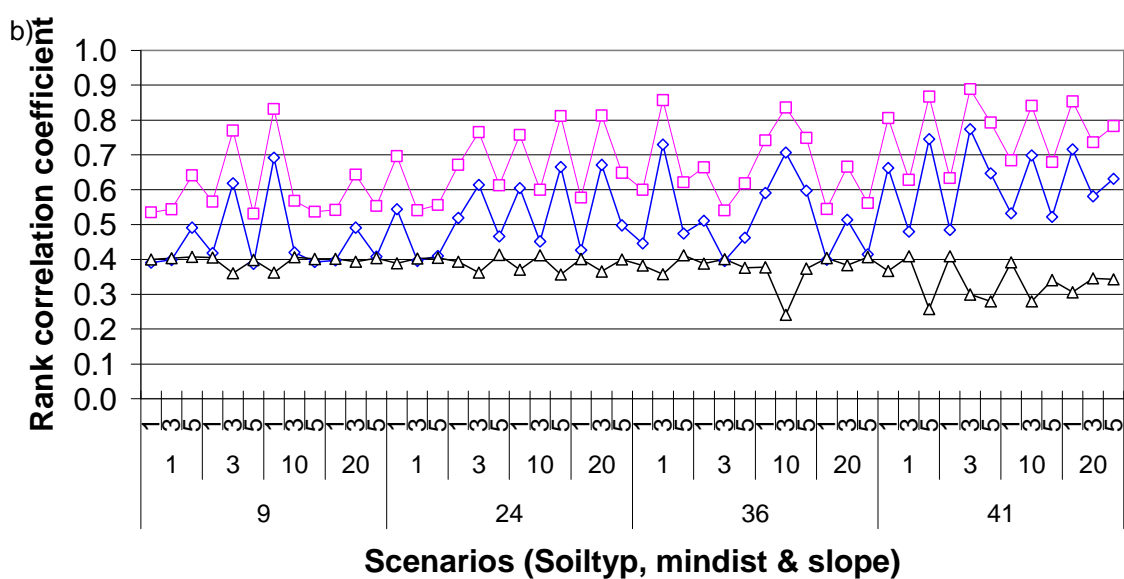
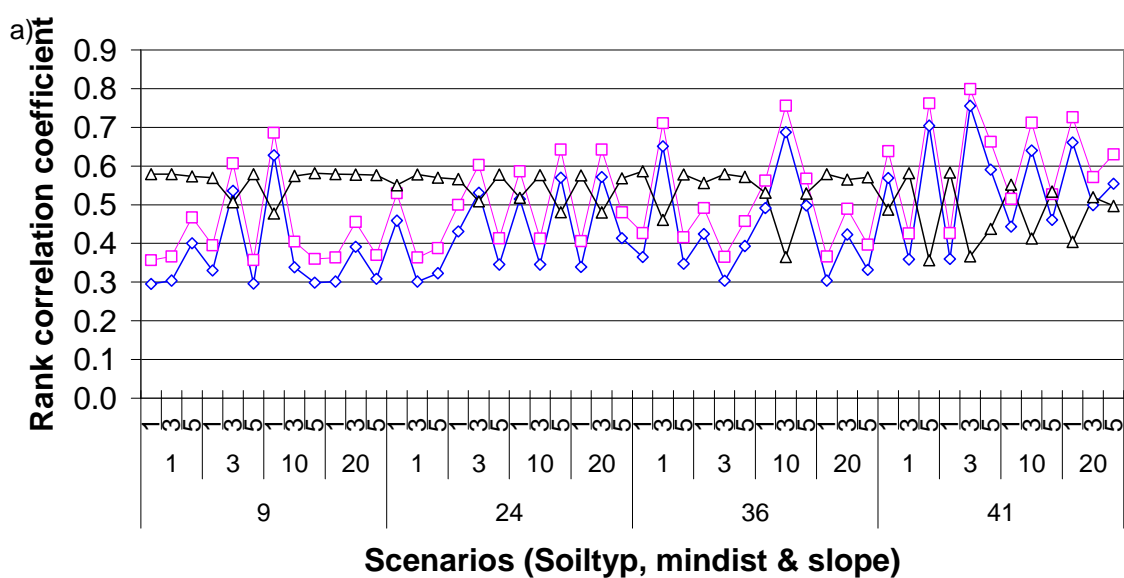
**Fig. 13 : Relation of the strategy ranking according to the human toxicity for the method pairs USES-LCA/EDIP97<sub>water</sub> (a), USES-LCA/EDIP97<sub>soil</sub> (b), and between EDIP97<sub>water</sub> and EDIP97<sub>soil</sub> (c) for the case study pomefruit (n=50) and USES-LCA/EDIP97<sub>water</sub> (d), USES-LCA/EDIP97<sub>soil</sub> (e), EDIP97<sub>water</sub> and EDIP97<sub>soil</sub> (f) for the case study wheat (n=156).**

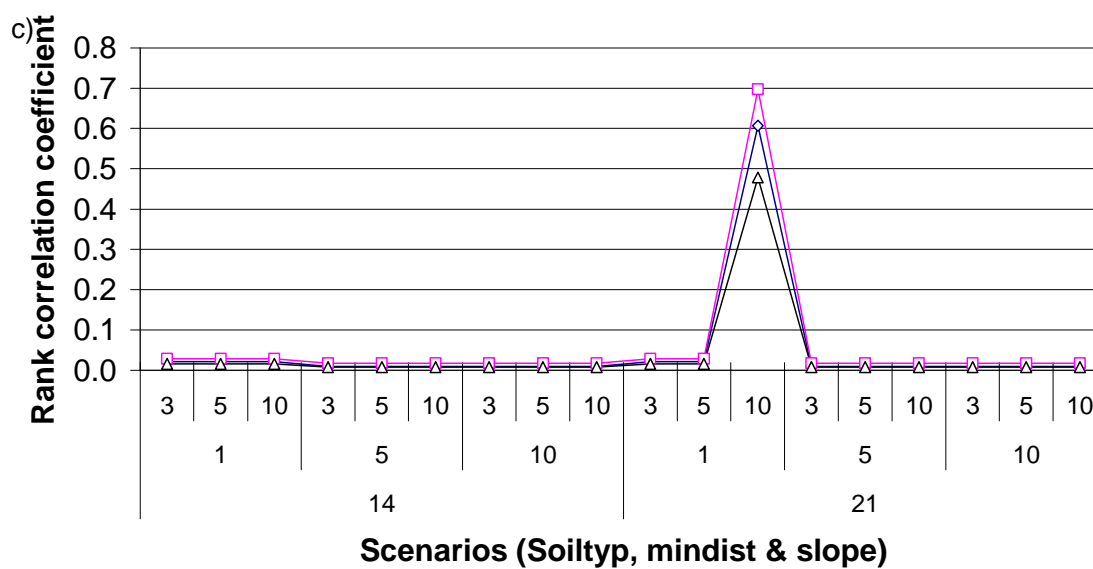
### 4.2.3. Influence of the scenarios

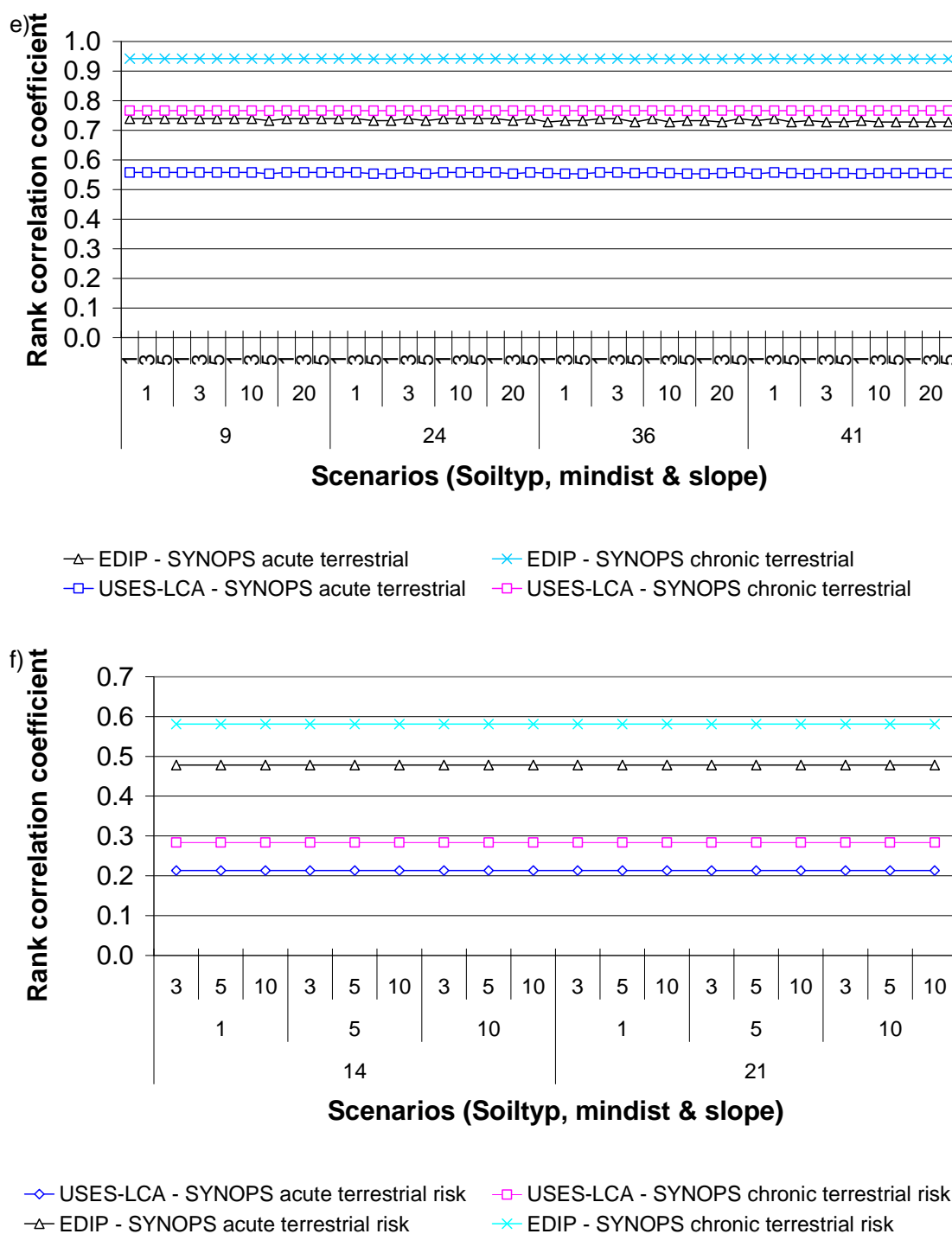
The results described in chapter 4.2.2 might be influenced by the fact that the LCA methods do not regard different environmental scenarios and that for I-PHY and SYNOPS the mean risks out of 48 different environmental scenarios for the case study wheat and 18 for the case study pomefruit are used for the comparison. To analyse the effects of single scenarios or factors (soiltyp, minimal distance to surface water (mindist), or slope of the field) on the correlation results the analysis was extended and a rank correlation was calculated between the LCA results and the RA results for each of the 48 environmental scenarios.

The analysis shows that in the case study wheat for the aquatic ecosystem between the acute and chronic risk indicators SYNOPS for water and the methods EDIP97 and USES-LCA there is a wide range of variation in the rank correlation coefficients across the environmental scenarios (Fig. 14 a & b and Tab. 7), whereas the variation of the correlation coefficients between Impact2002+ and SYNOPS are much smaller. But for none of the indicator combinations there is a factor with a consistent trend of higher or lower correlations for one of the method comparisons. For all the LCA methods the pattern of the correlation coefficients over the scenarios are comparable for the two indicators, but EDIP97 and USES-LCA show slightly higher correlations with the chronic risk, whereas IMPACT2002 correlates much better with the acute indicator of SYNOPS. For the pomefruit case study the results give a completely different picture. In general the correlations between the LCA methods and the chronic indicator are much higher than with the acute indicator with which all three methods hardly correlate. Also the variation of the rank correlation coefficient calculated for the different scenarios is very small compared to the wheat case study for all method combinations (Fig. 14 c & d) and in addition there is one scenario (Soiltyp 21, mindist 1 and slope 10) for which all correlations show a peak. For EDIP97 and USES-LCA the correlation with the chronic and acute risk indicator of SYNOPS are slightly higher respectively much higher for this scenario, whereas for IMPACT2002 the correlation with the chronic indicator is slightly lower but much higher with the acute indicator for this scenario. The correlations between the indicators concerning the terrestrial ecosystem are more uniform over the scenarios for both case studies. The ranges of the coefficients are much smaller for the correlation between the LCA methods and the acute indicator compared to the results for the aquatic ecosystem and for the chronic indicator there is no difference at all between the scenarios. Like for the aquatic system the methods EDIP97 and USES-LCA correlate better with the chronic indicator of SYNOPS in both case studies.

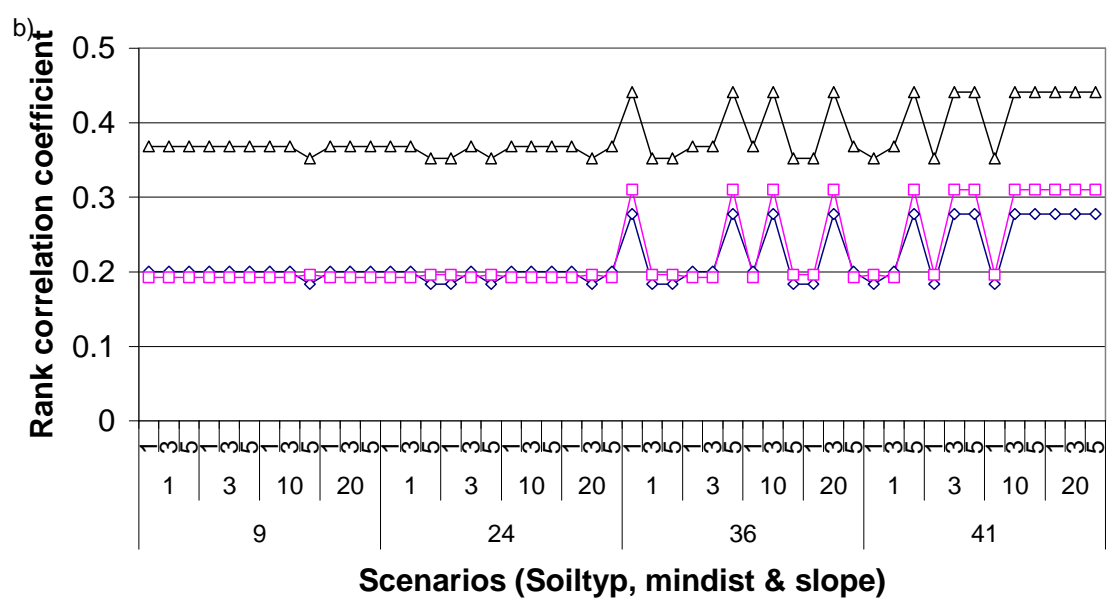
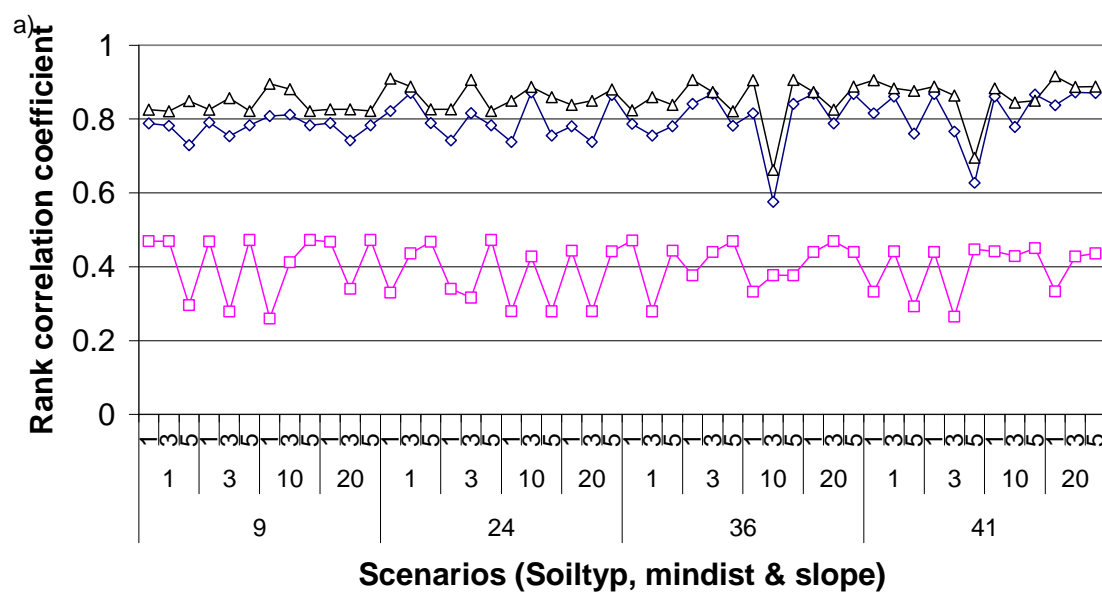
Comparing the correlations between the LCA results and the aquatic and groundwater indicator of I-PHY for the environmental scenarios in the wheat case study some points emerge (Fig. 15 a & b). Again the correlations between EDIP97 and USES-LCA and risk assessment indicators show comparable changes across the scenarios. Furthermore also the changes in the correlation between IMPACT2002 and the groundwater indicator follow the same pattern than for the other LCA methods. A second point is that for the relation between the groundwater indicator of I-PHY and the LCA methods there are only three different values for the correlation for each of the methods, whereas for the aquatic indicator the correlation results are more differentiated. The results for the pomefruit case study are only shown in Fig. 15 c, because of the few scenarios calculate with I-PHY and the fact that only 11 instead of 50 plant protection strategies were used a classification is difficult.

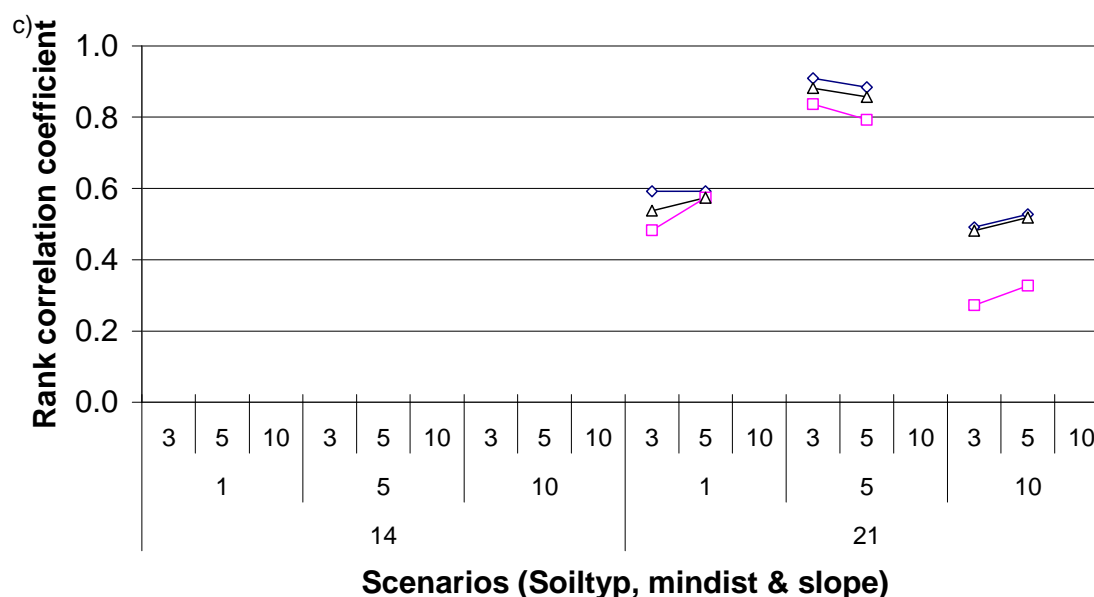






**Fig. 14 :** Rank correlation coefficients between the aquatic and terrestrial eco-toxicity calculated with the LCA methods USES-LCA, EDIP97, and Impact2002+ and the indicators SYNOPSIS acute aquatic risk (a, c), SYNOPSIS chronic aquatic risk (b, d) and the SYNOPSIS acute and chronic terrestrial risk (e, f) for the wheat case study (a, b, e) with 48 different environmental scenarios and the pomefruit case study (c, d, f) with 18 scenarios; n = 156 plant protection strategies in the wheat case study and 50 in the pomefruit case study





**Fig. 15 :** Rank correlation coefficients between the aquatic and terrestrial eco-toxicity calculated with the LCA methods USES-LCA, EDIP97, and Impact2002+ and the indicators I-PHY aquatic risk (a, c), I-PHY groundwater risk (b) for the wheat case study (a, b) with 48 different environmental scenarios and the pomefruit case study (c) with 6 scenarios; n = 156 plant protection strategies in the wheat case study and 11 in the pomefruit case study

**Tab. 7 :** Range of the Spearman rank correlation coefficient between the risk assessment indicators and the LCA toxicity results for the environmental scenarios used in the RA calculations in both case studies. n = number of strategies used for the calculation of the coefficient; values in italics indicate that for the LCA methods the terrestrial eco-toxicity was used

Case study	Risk Indicator	n	aquatic/terrestrial eco-toxicity		
			EDIP97	USES-LCA	Impact2002
wheat (48 scenarios)	SYNOPS acute aquatic risk	156	0.36-0.80	0.30-0.76	0.36-0.59
	SYNOPS chronic aquatic risk	156	0.53-0.84	0.39-0.77	0.24-0.41
	SYNOPS acute terrestrial risk	156	<i>0.73-0.74</i>	<i>0.55-0.56</i>	N/A
	SYNOPS chronic terrestrial risk	156	<i>0.94-0.942</i>	<i>0.661-0.668</i>	N/A
	I-PHY aquatic risk	156	0.58-0.87	0.66-0.92	0.26-0.47
	I-PHY groundwater risk	156	0.18-0.28	0.35-0.44	0.19-0.31
Pomefruit (18 scenarios)	SYNOPS acute aquatic risk	50	0.02-0.70	0.01-0.61	0.01-0.48
	SYNOPS chronic aquatic risk	50	0.34-0.39	0.34-0.37	0.25-0.31
	SYNOPS acute terrestrial risk	50	<i>0.48</i>	<i>0.21</i>	N/A
	SYNOPS chronic terrestrial risk	50	<i>0.58</i>	<i>0.28</i>	N/A
	I-PHY aquatic risk (6 scenarios)	11	0.48-0.88	0.27-0.84	0.49-0.91



## 5. Discussion and Conclusion

The main goal of task TR3.4a LCA methodological work in the 3 JPA was to extend the theoretical method comparison started in the 2 JPA and described in DR3.4 with a test of the practical feasibility and stakeholder utility using a set of plant protection strategies. Based on the time demand and the number of strategies which could be analysed with the single methods it was planned to change some values for the two dimensions in the deliverable DR3.4, if the calculations show that the theoretical assessment has to be adapted. Testing the methods (see section 4.1) showed, that a theoretical comparison could give a good overview of the performance of several methods, but also that a practical test is needed to cover all aspects. Especially the definition of the objective has a major influence on the results of the practical testing, whereas in the theoretical comparison not all aspect can be included in the analysis. For example it was defined, that the practical feasibility and stakeholder utility are determined by the methods ability to calculate a large number of risk or toxicity assessments and that the risk assessment methods have to be able to include a wide range of environmental conditions. These assumptions give an advantage to the methods I-PHY and SYNOPS compared to PRZM-USES, as they are created to handle a large number of assessments. If the assumption had been that practical feasibility and stakeholder utility were defined by the ability that the fate of a few substances should be calculated as accurate as possible on a field level with a limited number of different scenarios, then the method PRZM-USES would have been possibly the best one. But also for the LCA methods the assumptions are disadvantageous, because the models Impact2002+ and USES-LCA are created to assess the toxicity on a European or northern hemisphere level, and so small scale environmental conditions can't be included in the calculations. The results of the comparison have to be analysed with the above mentioned points in mind. It emerged that the theoretical and practical comparison of the methods should be completed by a list with the positive and negative features and the most suitable field of applications for each of the models (Tab. 8). However under the given assumptions, the practical test shows that the models SYNOPS followed by I-PHY are the most appropriate ones to compare a large number of strategies including several environmental scenarios for each strategy. The model PRZM-USES is the most feasible for a detailed fate modelling, and the LCA methods are the best ones if the toxicity of the whole agricultural production including the production and use of other inputs should be regarded. Nevertheless for PRZM-USES, EDIP97, Impact2002+ and USES-LCA the values for the criteria user friendliness and time to fill in are not changed, because the methods fulfil the qualitative (user friendliness) and quantitative (time needed) criteria defined in DR3.4 (see also Tab. 15 and Tab. 17 in the appendix). For the criterion coverage of needs in the dimension stakeholder utility the values for the four methods have to be changed from strong (4) to low (2) as the applicability defined in the theoretical part of this analysis (Tab. 21) are not met by PRZM-USES, EDIP97, Impact2002+ and USES-LCA.

As said before, the method comparison is influenced by the assumptions made for the analysis because not all aspects can be covered in a theoretical comparison, but from the theoretical and practical comparison together with a list of the advantages and disadvantages for each method the most appropriate fields of application can be outlined. The method SYNOPS is most appropriate for a GIS based evaluation of a large number of plant protection strategies including detailed environmental data. The usage of spatial modelling allows the comparison of strategies at a field- farm- watershed and regional level and an efficiency assessment of environmental protection policies. The GUI gives the user the opportunity the present the results and to compare them visually. The same is true for the method I-PHY but with some limitations compared to SYNOPS. As no GIS modelling is used, the comparison in a spatial context is restricted and the practical test showed that SYNOPS is able to calculate a higher number of risk assessments. The method PRZM-USES is the least user friendly risk assessment method, but with the most detailed fate modelling. This method is less usable for a spatial comparison of

strategies or policies but more for an accurate calculation of the fate of the active ingredients used. The LCA toxicity models can't be compared with the risk assessment methods, because of different targets. For the LCA methods the goal is an assessment of the toxicity of a given substance on a European level and so the environmental surrounding and conditions on a field level are not included. But the strength of these models is that the results are expressed in units which can be compared to the toxicity of other substances emitted in other steps of the production, other regions and other compartments e.g. hydrocarbons or heavy metals to air during the production of inputs (machinery, fertiliser...). This comparability allows an evaluation of scenarios which are not assessable with the risk assessment methods. For example a herbicide application is replaced by a hoeing: The toxicity linked with the production, application of the pesticide and to the active ingredient in the environment itself is avoided, but on the other hand the hoeing is also linked with the release of toxic substances (from extracting of minerals for the machine to the higher diesel consumption for the hoeing compared to the application of a herbicide). With the LCA these two options can be compared. In addition to that the analysis can be extended to other impacts for example the mineralization effects of the hoeing which might have positive or even negative environmental impacts (higher availability - or losses of nitrogen) or the energy consumption.

**Tab. 8 : List of positive and negative aspects of the methods I-PHY, PRZM-USES, SYNOPS, EDIP97, Impact2002+ and USES-LCA**

<p><b>I-PHY</b></p> <ul style="list-style-type: none"> <li>+ scientific soundness, applicable for a large set of strategies, GUI, environmental conditions included</li> <li>- terrestrial ecosystem not included, human health partly included</li> </ul> <p><b>PRZM-USES</b></p> <ul style="list-style-type: none"> <li>+ scientific soundness, most detailed fate modelling, environmental condition included</li> <li>- no GUI, parameterisation is time consuming, applicability for a large data set</li> </ul> <p><b>SYNOPS</b></p> <ul style="list-style-type: none"> <li>+ scientific soundness, GUI, environmental condition included, best applicability for a large dataset, including of GIS datasets</li> <li>- human health not included</li> </ul> <p><b>EDIP97</b></p> <ul style="list-style-type: none"> <li>+ aquatic- and terrestrial eco-toxicity and human toxicity included, unit comparable to toxicity from other means of the production</li> <li>- environmental conditions not included, simplest fate modelling, no GUI</li> </ul> <p><b>Impact2002+</b></p> <ul style="list-style-type: none"> <li>+ aquatic- and terrestrial eco-toxicity and human toxicity included, unit comparable to toxicity from other means of the production</li> <li>- environmental conditions not included, no GUI, least good documentation</li> </ul> <p><b>USES-LCA</b></p> <ul style="list-style-type: none"> <li>+ aquatic- and terrestrial eco-toxicity and human toxicity included, unit comparable to toxicity from other means of the production</li> <li>- environmental conditions not included, no GUI</li> </ul>
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One benefit of the test in practise is that not only the practical feasibility and stakeholder utility can be assessed, but also the accordance of the ranking of several strategies assessed with different methods can be compared. This work has not been carried out for different risk

assessment methods and LCA methods up to now. The models EDIP97, Impact2002+ and USES-CML were already compared in the project OMNIITOX described in Rosenbaum & Margni (2004), but they used 35 substances (including some pesticides) and compared the absolute mid point characterisation factors. The rank correlation of several plant protection strategies each including several active ingredients with different application rates performed here is to our opinion more useful, because this analysis shows if the final results of the different methods are comparable.

The TFI is included in the correlation analysis to show if this indicator describing the intensity of crop protection is useful to illustrate the environmental impacts. The rank correlations between the TFI and the methods results for both case studies and the toxicity/risks for the aquatic and terrestrial ecosystem and the human toxicity are quite weak to medium. As the methods are developed for an assessment of the environmental impact this result might indicate that the TFI is not useful to describe environmental impacts of plant protection. Unfortunately also between the methods the rank correlation for the strategies is mostly weak to medium with some exceptions. The modified EDIP97 and USES-LCA correlate highly ( $r_s$  between 0.8 and 0.96) except for the terrestrial toxicity in the case study pomefruit where the correlation is very weak ( $r_s = 0.19$ ). Also the correlations between EDIP97 and SYNOPSIS chronic risk for the aquatic and terrestrial ecosystem and the case study wheat are on a high level ( $r_s$  0.85 and 0.96) but on the other hand the correlations in the case study pomefruit are much lower (0.38 respectively 0.46). As mentioned before the weak to medium strong correlations between the TFI and the method results might imply that the TFI is not useful as an estimator of the environmental impacts. Looking at the different approaches this is even more obvious. All the methods compared in this analysis use several physico-chemical (dt50, KOC...) and toxicological criteria (LC50, NOEC...) to estimate the toxicity of a given active ingredient, whereas the TFI only uses the fraction of the area on which the active ingredient is applied and the used application rate related to the maximum allowed application rate. This shows that the idea of the TFI is not to assess the toxicity of plant protection. But on the other hand the correlations between the method results are in many cases weak. But in these cases methodological differences especially the fate modelling of the active ingredients cause the low relation. For example the risk assessment methods use a detailed fate model which includes the drift and runoff, whereas for the LCA methods used here the assumption was made that the initial emission is the soil compartment. This might explain the lower correlations between the risk assessment and life cycle assessment methods for the aquatic eco-toxicity in the case study pomefruit compared to the case study wheat, because for applications in pomefruit the drift plays a higher role. But as the main goal of this analysis is to evaluate the practical feasibility and stakeholder utility a deeper analysis of the models is not part of the task in RA3.4 and would have been a too large effort. Under these circumstances the correlation analysis is a first step to understand if the results from the different methods are comparable. Unfortunately the results of the analysis indicate that the comparability is limited. The developers of the LCA methods already created a consensus model based on EDIP, USES and IMPACT which was published in 2008 (Rosenbaum et al., 2008). But there was no calculation tool available to characterise active ingredients which were not characterised by the authors of this method and because of that the method couldn't be included in this analysis. A next step in the analysis would be to include a larger number of plant protection strategies and compare the result on the basis of each active ingredient and to analyse the methods results for the active ingredients which contribute mainly to the difference between the methods. Across the border risk and life cycle assessment a really high accordance in the ranking of pesticide applications is not probably, because of the different targets and the different methodologies and the high correlations found for some comparisons are surprising.

The rank correlation analysis for the different environmental scenarios used for the risk assessment shows an indifferent picture. Only for the comparison between the SYNOPSIS acute indicator for the aquatic ecosystem and the LCA results there is one scenario with a major

impact on the results of the correlation analysis (Fig. 14 c). In all other comparisons the correlation coefficient varies, but there is no factor (mindist, soiltyp or slope) which explains the variation.

Regarding the suitability of the different methods for consideration of pesticides in the agricultural LCA the method USES-LCA is to our opinion the most feasible. On the one hand the method is well known and used and on the other hand the results of the theoretical evaluation are as good or better than for the other LCA methods and with the given databases (SYNOPS and Footprint) the calculation of characterisation factors is possible for more than 300 active ingredients and the categories aquatic and terrestrial eco-toxicity and human toxicity. Disadvantages of Impact2002+ are that the documentation of the method is little expressive and that the characterisation for the human toxicity of active ingredients is difficult, because the ED and the DALY are not available for many active ingredients. The limitation of the method EDIP97 is the simple fate model, although with the fate modelling in SYNOPS and the subsequent assessment of the toxicity following the methodology of EDIP97 results comparable to USES-LCA could be achieved. The new method USETOX described in Rosenbaum et al. (2008) and created as a consensus model by the developers of EDIP, USES, Impact and some other methods might be an option for future LCA toxicity assessments regarding pesticides. But up to now there are only some pesticides characterised and so it is a step back compared to the 300 active ingredients characterised with USES-LCA.

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## 7. Appendix 1: Results and descriptions from DR3.4

In this Appendix the results for the scientific soundness are not included, because they are not concerned by the test in practise. For a description of this dimension see DR3.4.

### Criterion “practical feasibility”

The criterion practical feasibility is divided into three user groups (Tab. 9 - Tab. 10), going from the fact that these user groups have different requirements. The detailed results and the decision rules for the subcategories are summarised in Tab. 12 - Tab. 17. In practice it is very difficult to estimate the practical feasibility for the single groups. The calculation tool used in the method EI99 was not available and therefore all values are set to 1.

In general the methods are most suitable for scientists followed by authorities and extension services.

#### Accessibility of input data

This criterion assesses the availability of data for different data groups (Meteorological data, overview of field characteristics, pesticide properties and field specific data). For the methods SYNOPS, I-PHY and PRZM-USES, the data are easier to access than for the methods EDIP, USES and Impact2002, because they have databases implemented. The data accessibility is worst for the user group extension services, because, for this group, pesticide properties and field specific data are less available than for authorities or scientists.

#### Qualification requirements

For extension services the main problem is the qualification requirement. For all methods an advanced training is needed for data collection, calculation or programming the input files and interpretation. The PRZM-USES method has the highest requirements (more than one week is needed to learn how to use the models). The methods SYNOPS and I-PHY have the lowest requirements, because they are software-based with predefined input options.

#### External service

This category considers the necessity of an external service for using the method. The assessment strongly varies according to the target group designated and the assumption that we have to take about the technical and scientific self-sufficiency. All methods show the same trend. The lowest rates are achieved for the target group “authorities” and the highest for the one “scientists”.

#### User-friendliness

The methods SYNOPS and I-PHY are most user-friendly, because they use a graphical user interface with predetermined input options and illustrated results. All other methods are lacking these options.

#### Support

The support of SYNOPS is suboptimal to the one offered by the other methods, because only an example is available, whereas for all other methods also a handbook is present.

#### Time needed to calculate/fill in

For SYNOPS and I-PHY the least time is needed to fill in and calculate because a database for the active ingredients is implemented in the software. The longest time is needed for the PRZM-USES, because the models of the method have to be parameterized. The time needed to calculate the other methods is in between, because no parameterization has to be done, but also no database is implemented.



**Tab. 9 :** Criterion “practical feasibility”: list of themes to score on a scale between 1 and 5 (1 = low accordance, 5 = high accordance).

Practical feasibility User Group (extension services)	score (1 to 5)							average
	SYNOPS	I-PHY	EDIP	EI99	USES	Imp02	PRZM-USES	
Accessibility of input data	5	4	3	1	3	3	4	<b>3.3</b>
Qualification requirements (user)	1	2	1	1	1	1	1	<b>1.1</b>
External services	3	4	2	1	2	2	2	<b>2.3</b>
User-friendliness	3	3	1	1	1	1	1	<b>1.6</b>
Support	3	4	4	1	4	4	3	<b>3.3</b>
Time needed (to calculate/ fill in)	5	5	3	1	3	3	1	<b>3.0</b>
Average	3.3	3.7	2.3	1	2.3	2.2	2.0	

**Tab. 10 :** Criterion “practical feasibility”: list of themes to score on a scale between 1 and 5 (1 = low accordance, 5 = high accordance).

Practical feasibility User Group (authorities)	score (1 to 5)							average
	SYNOPS	I-PHY	EDIP	EI99	USES	Imp02	PRZM-USES	
Accessibility of input data	5	3	4	1	4	4	4.7	<b>3.7</b>
Qualification requirements (user)	3	3	2.3	1	2.3	2.3	1	<b>2.1</b>
External services	1	3	3	1	3	1	1	<b>1.9</b>
User-friendliness	3	3	1	1	1	1	1	<b>1.6</b>
Support	3	4	4	1	4	4	3	<b>3.3</b>
Time needed (to calculate/ fill in)	5	5	3	1	3	3	1	<b>3.0</b>
Average	3.3	3.5	2.9	1	2.9	2.6	2.0	

**Tab. 11:** Criterion “practical feasibility”: list of themes to score on a scale between 1 and 5 (1 = low accordance, 5 = high accordance).

Practical feasibility User Group (scientists)	score (1 to 5)							average
	SYNOPS	I-PHY	EDIP	EI99	USES	Imp02	PRZM-USES	
Accessibility of input data	5	5	4.5	1	4	4	4.7	<b>4.0</b>
Qualification requirements (user)	3	4	2.3	1	2.3	3	1	<b>2.7</b>
External services	3	3	5	1	5	3	5	<b>3.6</b>
User-friendliness	3	3	1	1	1	1	1	<b>1.6</b>
Support	3	4	4	1	4	4	3	<b>3.3</b>
Time needed (to calculate/ fill in)	5	5	3	1	3	3	3	<b>3.3</b>
Average	3.7	4	3.3	1	3.2	3.0	3.3	

**Tab. 12: The sub-theme “accessibility of input data” is subdivided into accessibility of input data for three groups of users (extension services (1), authorities (2) and scientist (3). For data provided by model developers the score is always 5 (for example pesticide properties in databases of SYNOPS and I-PHY)**

## SYNOPS

Accessibility of input data Data group	User group		
	1	2	3
Meteorological data	5	5	5
Overview of field characteristics			
Pesticides properties <ul style="list-style-type: none"> <li>Name</li> <li>Physicochemical properties</li> <li>Retention properties</li> <li>Degradation rates</li> <li>Exposure</li> <li>Effect assessment</li> </ul>	5	5	5
Field specific data: <ul style="list-style-type: none"> <li>dose</li> <li>detailed spraying or application programme</li> <li>data on sprayer</li> <li>additional data (incorporation of pesticides, etc.)</li> </ul>	4	4	4
Average	5	5	5
Min	4	4	4
Max	5	5	5

## I-PHY

Accessibility of input data Data group	User group		
	1	2	3
Meteorological data			
Overview of field characteristics (soil, surrounding)	4	3	5
Pesticides properties <ul style="list-style-type: none"> <li>Name</li> <li>Physicochemical properties</li> <li>Retention properties</li> <li>Degradation rates</li> <li>Exposure</li> <li>Effect assessment</li> </ul>	5	5	5
Field specific data: <ul style="list-style-type: none"> <li>dose</li> <li>detailed spraying or application programme</li> <li>data on sprayer</li> <li>additional data (incorporation of pesticides, etc.)</li> </ul>	4	2	4
Average	4	3	5
Min	4	2	4
Max	5	5	5

**EDIP**

<b>Accessibility of input data</b> <b>Data group</b>	<b>User group</b>		
	<b>1</b>	<b>2</b>	<b>3</b>
Meteorological data			
Overview of field characteristics (soil, surrounding)			
Pesticides properties <ul style="list-style-type: none"> <li>• Name</li> <li>• Physicochemical properties</li> <li>• Retention properties</li> <li>• Degradation rates</li> <li>• Exposure</li> <li>• Effect assessment</li> </ul>	3	4	5
Field specific data: <ul style="list-style-type: none"> <li>• dose</li> <li>• detailed spraying or application programme</li> <li>• data on sprayer</li> <li>• additional data (incorporation of pesticides, etc.)</li> </ul>	3	4	4
Average	3	4	4.5
Min	3	4	4
Max	3	4	5

**USES**

<b>Accessibility of input data</b> <b>Data group</b>	<b>User group</b>		
	<b>1</b>	<b>2</b>	<b>3</b>
Meteorological data			
Overview of field characteristics (soil, surrounding)			
Pesticides properties <ul style="list-style-type: none"> <li>• Name</li> <li>• Physicochemical properties</li> <li>• Retention properties</li> <li>• Degradation rates</li> <li>• Exposure</li> <li>• Effect assessment</li> </ul>	3	4	4
Field specific data: <ul style="list-style-type: none"> <li>• dose</li> <li>• detailed spraying or application programme</li> <li>• data on sprayer</li> <li>• additional data (incorporation of pesticides, etc.)</li> </ul>	3	4	4
Average	3	4	4
Min	3	4	4
Max	3	4	4

**Imp02**

<b>Accessibility of input data</b> <b>Data group</b>	<b>User group</b>		
	<b>1</b>	<b>2</b>	<b>3</b>
Meteorological data			
Overview of field characteristics (soil, surrounding)			
Pesticides properties <ul style="list-style-type: none"> <li>• Name</li> <li>• Physicochemical properties</li> <li>• Retention properties</li> <li>• Degradation rates</li> <li>• Exposure</li> <li>• Effect assessment</li> </ul>	3	4	4
Field specific data: <ul style="list-style-type: none"> <li>• dose</li> <li>• detailed spraying or application programme</li> <li>• data on sprayer</li> <li>• additional data (incorporation of pesticides, etc.)</li> </ul>	3	4	4
Average	3	4	4
Min	3	4	4
Max	3	4	4

**PRZM-USES**

<b>Accessibility of input data</b> <b>Data group</b>	<b>User group</b>		
	<b>1</b>	<b>2</b>	<b>3</b>
Meteorological data	4	5	5
Overview of field characteristics (soil, surrounding)			
Pesticides properties <ul style="list-style-type: none"> <li>• Name</li> <li>• Physicochemical properties</li> <li>• Retention properties</li> <li>• Degradation rates</li> <li>• Exposure</li> <li>• Effect assessment</li> </ul>	4	5	5
Field specific data: <ul style="list-style-type: none"> <li>• dose</li> <li>• detailed spraying or application programme</li> <li>• data on sprayer</li> <li>• additional data (incorporation of pesticides, etc.)</li> </ul>	4	4	4
Average	4	4.7	4.7
Min	4	4	4
Max	4	5	5

<b>decision rules for the sub-theme “accessibility of input data”</b>	
Data not available	1
Data partly available	2
Data half-and-half available and not available	3
Data mostly available	4
Data completely available	5

**Tab. 13 :** The sub-theme “qualification requirements” is subdivided into three groups of users (extension workers (1), authorities (2) scientists (3)). For SYNOPS and I-PHY the data on pesticides are part of the model (program). Therefore, the collection refers to active ingredients or products which are not included in the databases.

## SYNOPS

<b>Qualification requirement</b>	<b>User Group</b>		
	<b>1</b>	<b>2</b>	<b>3</b>
Data collection	1	3	3
Calculation	1	3	3
Interpretation	1	3	3
Average	1	3	3
Min	1	3	3
Max	1	3	3

Only true for single field application. Regional risk assessment can only be run at JKI

## I-PHY

<b>Qualification requirement</b>	<b>User Group</b>		
	<b>1</b>	<b>2</b>	<b>3</b>
Data collection	3	3	5
Calculation	1	3	3
Interpretation	1	3	3
Average	2	3	4
Min	1	3	3
Max	3	3	5

## EDIP

<b>Qualification requirement</b>	<b>User Group</b>		
	<b>1</b>	<b>2</b>	<b>3</b>
Data collection	1	3	3
Calculation	1	1	1
Interpretation	1	3	3
Average	1	2.3	2.3
Min	1	1	1
Max	1	3	3

**USES**

Qualification requirement	User Group		
	1	2	3
Data collection	1	3	3
Calculation	1	1	1
Interpretation	1	3	3
Average	1	2.3	2.3
Min	1	1	1
Max	1	3	3

**Imp02**

Qualification requirement	User Group		
	1	2	3
Data collection	1	3	3
Calculation	1	1	3
Interpretation	1	3	3
Average	1	2.3	3
Min	1	1	3
Max	1	3	3

**PRZM-USES**

Qualification requirement	User Group		
	1	2	3
Data collection	1	1	3
Calculation	1	1	3
Interpretation	1	1	3
Average	1	1	3
Min	1	1	3
Max	1	1	3

decision rules for the sub-theme “qualification requirements”	1	2	3
Advanced training (> 1 week)	1	1	1
Advanced training (2 days - ≤ 1 week)	1	1	1
Advanced training (≤ 2 days)	1	3	3
Graduated engineer (agronomist)	3	3	5
Apprenticeship (agriculturist)	5	5	5

**Tab. 14: The sub-theme “external services” is subdivided into three groups of users (extension workers (1), authorities (2) scientists (3)). Use table to fill in**

decision rules for the sub-theme “external services”	1	2	3
Necessary for survey, calculation and interpretation	1	1	3
Necessary for calculation and interpretation	2	1	3
Recommended for calculation and interpretation	3	3	5
Recommended for interpretation	4	3	5
Survey, calculation and interpretation without external services feasible	5	5	5

**Tab. 15 : The sub-theme “user-friendliness” is subdivided into three groups of users (extension workers (1), authorities (2) and scientists (3)). Use table to fill in**

<b>decision rules for “user-friendliness”</b>	<b>1</b>	<b>2</b>	<b>3</b>
Table <u>with</u> predetermined input options <u>with</u> illustration of results <u>with</u> recommendations for the analysis and <u>with</u> checking techniques	5	5	5
Table <u>with</u> predetermined input options <u>and obligatory with</u> illustration of results as well as recommendations for the analysis or with checking techniques	5	5	5
All other combinations with three features	3	4	4
Table <u>with</u> predetermined input options <u>with</u> illustration of results <u>without</u> recommendations for the analysis <u>and without</u> checking techniques	3	3	3
Table <u>with</u> predetermined input options <u>without</u> illustration of results <u>with</u> recommendations for the analysis and <u>without</u> checking techniques	2	3	3
All cases with two or one feature(s) not mentioned-above	1	2	2
None of the above-mentioned features available	1	1	1

**Tab. 16: The sub-theme “support”. The methods SYNOPS and I-PHY are working with an interface for data input and the product names instead of the active ingredients could be used. This should be mentioned in the text explanation.****SYNOPS**

<b>Support</b>	
Language	3
Explanations	3
Average	3

**I-PHY**

<b>Support</b>	
Language	3
Explanations	5
Average	4

**EDIP**

<b>Support</b>	
Language	5
Explanations	3
Average	4

**USES**

<b>Support</b>	
Language	5
Explanations	3
Average	4

**Imp02**

<b>Support</b>	
Language	5
Explanations	3
Average	4

**PRZM-USES**

<b>Support</b>	
Language	5
Explanations	3
Average	4

<b>Decision rules for the sub-theme “support”</b>	
Language	
• program and telephone or email support in English	5
• telephone or email support in English	3
Explanations	
• handbook and example	5
• handbook or example	3
• none of the above mentioned	1

**Tab. 17: The sub-theme “Time needed” is subdivided into three groups of users (extension workers (1), authorities (2) and scientists (3))**

**SYNOPS**

<b>Time needed for</b>	<b>1</b>	<b>2</b>	<b>3</b>
one crop protection strategy	5	5	5
per Farm	4	5	5
Average	5	5	5

**I-PHY**

<b>Time needed for</b>	<b>1</b>	<b>2</b>	<b>3</b>
one crop protection strategy	5	5	5
per Farm	4	5	5
Average	5	5	5

**EDIP**

<b>Time needed for</b>	<b>1</b>	<b>2</b>	<b>3</b>
one crop protection strategy	3	3	3
per Farm	3	3	3
Average	3	3	3



**USES**

<b>Time needed for</b>	<b>1</b>	<b>2</b>	<b>3</b>
one crop protection strategy	3	3	3
per Farm	3	3	3
Average	3	3	3

**Imp02**

<b>Time needed for</b>	<b>1</b>	<b>2</b>	<b>3</b>
one crop protection strategy	3	3	3
per Farm	3	3	3
Average	3	3	3

**PRZM-USES**

<b>Time needed for</b>	<b>1</b>	<b>2</b>	<b>3</b>
one crop protection strategy	1	1	3
per Farm	1	1	3
Average	1	1	3

<b>decision rules for the sub-theme “time needed (to calculate/ fill in)”</b>	<b>User group</b>		
	<b>1</b>	<b>2</b>	<b>3</b>
Crop protection strategy			
• 1 d	1	1	2
• 0.5 d < and ≤ 1 d	2	1	2
• 3 h < and ≤ 5 h	3	3	3
• 1 h < and ≤ 3 h	4	5	5
• ≤ 1 h	5	5	5
Farm			
• 3 d	1	1	2
• 1.5 d < and ≤ 3 d	2	1	2
• 10 h < and ≤ 15 h	3	3	3
• 5 h < and ≤ 10 h	4	5	5
• ≤ 5 h	5	5	5

**Criterion “stakeholder utility”**

Likewise for practical feasibility, the criterion stakeholder utility is divided into three user groups (Tab. 18 - Tab. 20). The decision rules for the subcategories are summarised in (Tab. 20 - Tab. 23). All methods meet the needs of all three user groups to a high degree, because all could be applied to different spatial areas and could be used to compare strategies policies and scenarios at different levels (farm, regional). The methods SYNOPS and I-PHY are more advantageous in terms of unambiguousness and communicability of results, since the results are presented with more details (for example graphical illustrations and reference values) than in EDIP, USES, Impact2002 and PRZM-USES.

**Tab. 18: Criterion “stakeholder utility”: list of themes to score on a scale between 1 and 5 (1 = low accordance, 5 = high accordance).**

Stakeholder utility User group (extension worker)	score (1 to 5)							average
	SYNOPS	I-PHY	EDIP	EI99	USES	Imp02	PRZM-USES	
Coverage of needs	4	4	4	4	4	4	4	<b>4</b>
Unambiguousness of results	2	4	1	1	1	1	1	<b>1.6</b>
Communicability of results	3	4	1	1	1	1	1	<b>1.7</b>
Average	3.3	4.0	2.0	2.0	2.0	2.0	2.0	

**Tab. 19: Criterion “stakeholder utility”: list of themes to score on a scale between 1 and 5 (1 = low accordance, 5 = high accordance).**

Stakeholder utility User group (authorities)	score (1 to 5)							Average
	SYNOPS	I-PHY	EDIP	EI99	USES	Imp02	PRZM-USES	
Coverage of needs	4	3	4	4	4	4	4	<b>3.9</b>
Unambiguousness of results	3	4	1	1	1	1	1	<b>1.7</b>
Communicability of results	3	3	1	1	1	1	1	<b>1.6</b>
Average	3.3	3.3	2.0	2.0	2.0	2.0	2.0	

**Tab. 20: Criterion “stakeholder utility”: list of themes to score on a scale between 1 and 5 (1 = low accordance, 5 = high accordance).**

Stakeholder utility User group (scientist)	score (1 to 5)							average
	SYNOPS	I-PHY	EDIP	EI99	USES	Imp02	PRZM-USES	
Coverage of needs	4	5	4	4	4	4	4	<b>4.1</b>
Unambiguousness of results	3	3	1	1	1	1	1	<b>1.6</b>
Communicability of results	3	4	1	1	1	1	1	<b>1.7</b>
Average	3.3	4.0	2.0	2.0	2.0	2.0	2.0	

**Tab. 21 : The sub-theme “Coverage of needs”. Use table to fill in Tab. 18-Tab. 20. See next table for demands.**

<b>Decision rules for the sub-theme “Accordance with user group needs”</b>		
None		1
Low		2
Medium		3
Strong		4
Completely		5

<b>User Group</b>	<b>Category</b>	<b>Demand</b>
Extension workers	Spatial area	field, farm region
	Applicability	Comparisons of strategies at field-, farm-, watershed, regional level
authorities	Spatial area	region, country(s)
	Applicability	assessment of efficacy of environmental protection policies, assessment of scenarios regarding plant protection
scientists	Spatial area	field, farm, region, country(s)
	Applicability	Comparisons at field-, farm-, regional-, country level, survey of environmental protection policies Ex ante assessment of pesticide risk of innovative crop protection strategies Assessment of pesticide risk within sustainability evaluation

**Tab. 22 : The sub-theme “Unambiguousness of results” is subdivided into three (four) groups of users (extension workers (2), authorities (3) scientists (4)). Use table to fill in Tab. 18-Tab. 20.**

Decision rules for the sub-theme “Unambiguousness of results” 1 = very bad, 5 = high accordance	User Group		
	extension workers	authorities	Scientists
Only results	1	1	1
Without detailed analysis with reduced graphical illustration	1	2	1
Without detailed analysis with graphical illustration	3	2	1
With detailed analysis but without recommendations without or with reduced graphical illustration	2	3	3
With detailed analysis without recommendations with graphical illustration	4	4	3
With detailed analysis with recommendations without or with reduced graphical illustration	2	3	5
With detailed analysis with recommendations with graphical illustration	5	5	5

**Tab. 23 : The sub-theme Communicability of results”. Use table to fill in Tab. 18-Tab. 20.**

<b>Decision rules for the sub-theme “Communicability of results” 1 = very bad, 5 = high accordance</b>	
Results in scientific units Without graphical illustration without target value (absolute)/ reference value (relative) without comments/ help for the interpretation	1
Results in scientific units with rating Without graphical illustration without target value (absolute)/ reference value (relative) without comments/ help for the interpretation	2
Results in scientific units with graphical illustration (single farms) without target value (absolute)/ reference value (relative)	2
Results in scientific units with rating Without graphical illustration with target value (absolute)/ reference value (relative) without comments/ help for the interpretation	3
Results in scientific units with graphical illustration (Ranking) without target value (absolute)/ reference value (relative) without comments/ help for the interpretation	3
Results in scientific units with rating with graphical illustration without target value (absolute)/ reference value (relative) with comments/ help for the interpretation	4
Results in scientific units with graphical illustration with target value (absolute)/ reference value (relative) with comments/ help for the interpretation	4
Results in scientific units with rating With graphical illustration With target value (absolute)/ reference value (relative) with comments/ help for the interpretation	5

## 8. Appendix 2:

**Tab. 24 :** 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 <sup>-1</sup> ]
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
	Quinoxifen	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
	Metribuzin	21087-64-9	2	70.0
	Pendimethalin	40487-42-1	1	600.0

HIF	Active ingredient	CAS_Nr	applications n	mean dosis [g ha-1]
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

**Tab. 25 :** 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
	Tolyfluanid	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
	Mecoprop-P	16484-77-8	2	24.0
	Fluazifop-P	79241-46-6	1	107.0

HIF	active ingredient	CAS_Nr	applications n	mean dosis [g ha-1]
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



Tab. 26 : PRZM input data: sorption coefficient Kd and degradation rates k

Pesticide	Soil 9												Soil 36							
	Kd (L/kg)						k (day <sup>-1</sup> )						Kd (L/kg)				k (day <sup>-1</sup> )			
	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
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
Quinoxifen	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

Tab. 27 : Summary of USES input data (Data from JKI database except when indicated)

Pesticide	ADI (mg/kg/d)	PNEC <sub>aq</sub> (µg/L)	PNEC <sub>terr</sub>	Mw (g/mol)	log K <sub>ow</sub>	Melting point (°C)	Pvap 25°C (Pa)	Sw 25°C (mg/L)	Koc (L/kg)	DT50 <sub>sw</sub> (days)	DT50 <sub>soil</sub> (days)	DT50 <sub>sed</sub> (days)	pKa
Azoxystrobin	0.1	1.5 10 <sup>-3</sup> *	EP ***	403.4	2.5	116 ****	1.1 10 <sup>-10</sup>	6.7	424	47.7	279	57.5	
Chloromequat	0.05 *	-	EP	158.1	-2.3	245 ****	1.01 10 <sup>-4</sup>	1200000	1.02	13.8	4	22.7	
Clodinafop	0.003	2.1 10 <sup>-3</sup> *	EP	311.7	3.9	48.2 ****	1.6 10 <sup>-4</sup>	4	1439	66.1	0.9	109.5	
Diflufenican	0.2	2.5 10 <sup>-5</sup> *	EP	394.3	4.9	160 **	3.1 10 <sup>-5</sup>	0.05	1989	39.4	141.6	151.9	
Epoxiconazol	0.008	1.0 10 <sup>-3</sup> *	EP	329.76	3.33	136.7 **	0.02	7.05	883	33	402.7	181.8	
Fenpropidin	0.02	1.2 10 <sup>-4</sup> *	EP	273.5	2.59	-	0.021	530	3798	6.3	69.3	21.2	10.5 *
Fenpropimorph	0.003 **	1.6 10 <sup>-5</sup> *	EP	303.5	4.06	-	2.3 10 <sup>-3</sup>	4.3	995	31.7	37.4	43.3	6.98 *
Fenvalerat	0.02 **	-	EP	419.9	6.42	-	1.92 10 <sup>-5</sup>	0.001	12805	7.6	42.4	23.1	
Florasulam	0.05	1.18 10 <sup>-4</sup> *	EP	359.3	-1.22	212 **	1 10 <sup>-5</sup>	6360	22	86.3	1.8	88.1	4.54 *
Fluquinconazol	0.005 **	-	EP	376.2	3.24	192.4 **	6.4 10 <sup>-9</sup>	1.15	857	33.5	377.8	257.6	
Flurtamone	0.03	9.9 10 <sup>-4</sup> *	EP	333.3	3.24	148.5 ****	1 10 <sup>-5</sup>	11.5	329	31.4	87.3	333.8	
Ioxynil	0.005 **	1.1 10 <sup>-3</sup> *	EP	370.9	3.51	207.8 **	2.04 10 <sup>-6</sup>	15	549	13.2	7	37.6	
Kresoxim-methyl	0.4	1.5 10 <sup>-2</sup> *	EP	313.3	3.4	101.6 ****	2.3 10 <sup>-6</sup>	2	308	131.8	5	64.6	
Metconazol	0.048	-	EP	319.8	3.85	104.2 **	1.3 10 <sup>-5</sup>	30.4	1001	17	350.5	279	1.5 *
Prochloraz	0.01 **	4 10 <sup>-3</sup> *	EP	376.7	4.12	48.3 **	4.5 10 <sup>-6</sup>	26.5	1062	15.4	99.2	1615.4	
Propiconazol	0.04 *	5.1 10 <sup>-3</sup> *	EP	342.2	3.72	-	5.6 10 <sup>-5</sup>	110	689	140.1	95.8	46.9	1.09 *
Quinoxifen	0.2	8 10 <sup>-4</sup> *	EP	308.14	4.66	103 **	2 10 <sup>-5</sup>	0.047	1906	22	322.7	222.7	3.56 *
Tebuconazol	0.03	1.2 10 <sup>-3</sup> *	EP	307.8	3.7	105 **	9.69 10 <sup>-7</sup>	32	906	21.9	117.8	46.7	
Tribenuron	0.01	-	EP	381.4	0.78	141 ****	5.3 10 <sup>-8</sup>	2040	31	70.1	4	67.4	4.7 *
Trinexapac	0.3	-	EP	224.2	-0.29	36 ****	2.16 10 <sup>-3</sup>	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

**Tab. 28 : Toxicities of the active ingredients according to the methods EDIP97, CML01 and Impact2002. Values in Italics are estimated.**

Case study	Active ingredient	CAS-Nr.	Group	EDIP				CML			IMPACT	
				ecotoxicity, chronic in water	ecotoxicity, chronic, in soil	human toxicity, via surface water	human toxicity, via soil	freshwater aquatic ecotoxicity	human toxicity	terrestrial ecotoxicity	aquatic ecotoxicity	human toxicity
apple	Amitrol	000061-82-5	Herbicide	5.3602	0.1198	0.0009	1.2300	1.3224	0.0482	92.6843	1629.6056	<i>0.0001</i>
apple	Bitertanol	055179-31-2	Fungicide	1.7265	0.1058	6.7679	0.3273	0.7601	0.0458	10.6211	235.1587	<i>0.0003</i>
apple	Captan	000133-06-2	Fungicide	40.6306	0.0498	4.3374	1.4616	0.0028	0.0144	0.1716	1.6716	0.0003
apple	Cyprodinil	121552-61-2	Fungicide	8.5150	1.0870	2.2377	0.3347	10.2263	0.4234	2.5781	852.7547	<i>0.0004</i>
apple	Dithianon	003347-22-6	Fungicide	7.7118	0.0800	0.1885	0.5719	0.0042	0.0074	0.0300	84.4059	<i>0.0004</i>
apple	Diuron	000330-54-1	Herbicide	207.4689	0.0387	0.8476	1.4111	485.9090	23.4466	148.3173	43955.7460	0.0028
apple	Ethephon	016672-87-0	Other	0.6952	0.0283	0.0000	0.3474	0.0117	0.0059	0.0935	151.5245	0.0001
apple	Fenarimol	060168-88-9	Fungicide	3.7467	0.3344	4.0213	0.3164	11.4406	0.6680	111.0506	255.8325	<i>0.0001</i>
apple	Fenoxycarb	079127-80-3	Insecticide	1.1291	0.0200	2.4607	0.3259	1.5381	0.0809	2.8946	3.7726	<i>0.0000</i>
apple	Fenpyroximat	134098-61-6	Insecticide	25.0507	1.4430	1.5249	1.1936	11.8894	4.5908	6.2353	6063.5814	<i>0.0001</i>
apple	Fluazifop-P	083066-88-0	Herbicide	0.1979	0.0050	2.4182	0.1278	0.0086	0.0005	0.6421	1.3154	<i>0.0000</i>
apple	Fluquinconazol	136426-54-5	Fungicide	100.8227	0.2000	2.0801	0.9789	36.9051	3.4576	38.5920	34436.9505	<i>0.0001</i>
apple	Flusilazol	085509-19-9	Fungicide	5.6268	0.1495	3.8688	0.3673	2.4398	1.2672	355.9640	5515.7149	0.0007
apple	Glufosinat	051276-47-2	Herbicide	0.1459	0.0050	0.0000	0.0004	0.0535	0.0017	1.2354	503.3677	<i>0.0012</i>
apple	Glyphosat	001071-83-6	Herbicide	0.0003	0.0125	0.0000	0.0037	0.0001	0.0000	0.0089	102.2796	0.0000
apple	Imidacloprid	138261-41-3	Insecticide	0.3130	10.0000	388.2805	238273.9406	1.2359	0.0437	48.0604	15.1848	<i>0.0001</i>
apple	Indoxacarb	173584-44-6	Insecticide	0.7350	0.0071	7.4576	0.3755	0.0499	0.0063	4.2040	4.8146	<i>0.0001</i>
apple	Kresoxim-methyl	143390-89-0	Fungicide	121.2709	0.0053	56.5068	5.4972	17.6359	0.9203	0.2620	2233.1177	<i>0.0064</i>
apple	Copperhydroxid	020427-59-2	Fungicide	1340.9098	<i>0.1051</i>	0.0005	<i>1.8665</i>	1665.9411	1007.0299	<i>7.0435</i>	2935036.0922	<i>0.0064</i>
apple	Copperoxychlorid	001332-40-7	Fungicide	239.9523	<i>0.1051</i>	0.0006	<i>1.8665</i>	224.8247	173.2695	<i>7.0435</i>	218414.3189	<i>0.0064</i>
apple	Mancozeb	008018-01-7	Fungicide	8.1898	0.2588	0.0176	6.2247	0.0006	0.0009	0.0108	6.8519	<i>0.0000</i>
apple	MCPA	000094-74-6	Herbicide	0.0139	0.0589	0.0008	1.2922	0.0072	0.0007	29.6599	200.3427	0.0003
apple	Mecoprop-P	016484-77-8	Herbicide	0.0772	0.1012	0.0187	5.6614	0.0212	0.0018	104.2540	82.0878	<i>0.0002</i>
apple	Methoxyfenozide	161050-58-4	Insecticide	1.1611	0.0687	16.0514	0.5167	9.9420	0.2057	26.7021	5023.4680	<i>0.0064</i>
apple	Metiram	009006-42-2	Fungicide	0.0057	0.0125	0.0000	6.4521	0.0000	0.0000	0.0000	15.1015	<i>0.0000</i>
apple	Myclobutanil	088671-89-0	Fungicide	2.1777	0.8091	1.7154	5.6866	3.6694	0.2081	44.6956	29481.7433	<i>0.0001</i>
apple	Oxydemeton-methyl	000301-12-2	Insecticide	137.1742	50.0000	0.8066	505.8329	24.2127	2.4025	1294.3254	214.9217	<i>0.0012</i>
apple	Penconazol	066246-88-6	Fungicide	0.3553	0.0833	41.5102	8.6116	0.6875	0.0578	11.6907	209.8194	<i>0.0001</i>
apple	Pirimicarb	023103-98-2	Insecticide	342.9355	0.1667	1.5553	79.2043	561.3270	23.6157	40.6852	203.6000	<i>0.0008</i>
apple	Prohexadion	127277-53-6	Other	<i>3.1964</i>	<i>0.1051</i>	0.0000	0.0056	<i>0.9608</i>	<i>0.0817</i>	<i>7.0435</i>	1.2914	<i>0.0064</i>
apple	Pyrimethanil	053112-28-0	Fungicide	33.8643	0.1600	1.8543	1.3761	102.5692	4.0317	8.4553	22602.6188	<i>0.0000</i>

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CS	A.I.	CAS-Nr.	Group	EDIP				CML			IMPACT	
				ecotoxicity, chronic in water	ecotoxicity, chronic, in soil	human toxicity, via surface water	human toxicity, via soil	freshwater aquatic ecotoxicity	human toxicity	terrestrial ecotoxicity	aquatic ecotoxicity	human toxicity
apple	Sulphur	007704-34-9	Fungicide	0.4840	0.1051	59.9940	1.8665	0.1048	0.0232	7.0435	156.5980	0.0064
apple	Tebufenozid	112410-23-8	Insecticide	16.4047	0.0833	26.1553	0.3344	20.7173	0.6785	31.3027	1472.9197	0.0064
apple	Tebufenpyrad	119168-77-3	Insecticide	3.7739	1.4706	21.7389	1.9685	1.6969	0.1719	11.4150	1718.9030	0.0001
apple	Thiacloprid	111988-49-9	Insecticide	0.9850	5.0000	0.1854	54.7627	0.0046	0.0010	1.3664	33.8723	0.0004
apple	Thiophanat-methyl	023564-05-8	Insecticide	4.8514	16.6667	0.1115	4.9474	0.2632	0.0244	2.1467	79.0062	0.0008
apple	Tolylfluanid	000731-27-1	Fungicide	7.1225	0.0158	1.5742	0.3118	0.0179	0.0178	0.0269	7.4953	0.0064
apple	Triadimenol	055219-65-3	Fungicide	3.7279	0.1250	2.6486	0.8611	12.3290	0.4957	25.6159	1048.1553	0.0002
apple	Trifloxystrobin	131929-60-7	Fungicide	61.6043	0.0150	5.7820	0.1278	5.7354	0.2375	0.4571	17.6831	0.0064
wheat	2,4-D	000094-75-7	Herbicide	0.1242	0.8532	0.0020	1.3853	0.0283	0.0016	4.8967	261.1510	0.0002
wheat	a-Cypermethrin	067375-30-8	Insecticide	82.2187	0.4545	0.8818	1.3179	8.0044	10.5881	2.0827	439.9952	0.0017
wheat	Amidosulfuron	120923-37-7	Herbicide	5.1414	0.0100	0.0678	0.5825	4.7803	0.1627	15.6323	2218.9431	0.0002
wheat	Azoxystrobin	131860-33-8	Fungicide	16.6135	0.0556	2.4689	8.3688	56.2497	2.3779	23.7954	27881.3590	0.0004
wheat	Bentazone	025057-89-0	Herbicide	4.4883	0.1429	0.0038	2.2336	6.7472	0.1875	8.7386	62.5926	0.0000
wheat	beta-Cyfluthrin	068359-37-5	Insecticide	108.3289	0.0125	523.5546	430.8785	8.8755	13.4909	13.5394	5648.6991	0.0017
wheat	Bifenox	042576-02-3	Herbicide	299.6255	0.0350	3.4969	0.2512	22.3915	2.5784	6.9462	1181.7889	0.0000
wheat	Carbendazim	010605-21-7	Fungicide	63.0955	4.5455	0.1275	6.2445	60.3633	3.6122	24.6771	37643.1432	0.0022
wheat	Carfentrazone	128621-72-7	Herbicide	67.0560	0.0061	2.0422	0.3398	0.1697	0.0160	0.0756	6.0729	0.0001
wheat	Chlormequat	007003-89-6	Other	1.8217	0.1051	0.0001	1.8665	0.4385	0.0408	7.0435	0.0000	0.0064
wheat	Cinidon-ethyl	142891-20-1	Herbicide	9.6476	0.0050	4.3433	0.1290	0.0328	0.0128	0.5747	0.1801	0.0001
wheat	Clodinafop	114420-56-3	Herbicide	1.3906	0.2381	4.7811	0.3130	0.0038	0.0016	1.4053	0.3351	0.0000
wheat	Cyproconazole	094361-06-5	Fungicide	32.5045	0.0800	1.4901	1.1338	131.4795	6.1957	259.2972	383718.3066	0.0001
wheat	Cyprodinil	121552-61-2	Fungicide	8.5150	1.0870	2.2377	0.3347	10.2263	0.4234	2.5781	852.7547	0.0004
wheat	Deltamethrin	052918-63-5	Insecticide	27.0035	0.2000	0.5733	3.8322	1.4341	0.8916	0.1302	23586.3869	0.0017
wheat	Dichlorprop-P	015165-67-0	Herbicide	0.1909	0.0417	0.0013	0.9265	0.0495	0.0045	8.1118	15.6348	0.0002
wheat	Difenoconazole	119446-68-3	Fungicide	13.4705	0.0164	2.4884	0.1847	63.6178	2.8973	55.9124	743.0590	0.0001
wheat	Diflufenican	083164-33-4	Herbicide	363.1102	0.0833	30.9682	0.8256	845.0963	42.9687	9.5706	14638.1725	0.0000
wheat	Dimethoate	000060-51-5	Insecticide	60.8717	0.1000	33.0947	6839.0500	23.4760	2.0726	1735.4926	8335.9615	0.1875
wheat	Dithianon	003347-22-6	Fungicide	7.7118	0.0800	0.1885	0.5719	0.0042	0.0074	0.0300	84.4059	0.0004
wheat	Epoxiconazole	106325-08-0	Fungicide	6.2686	0.0833	2.4961	0.8694	20.5050	1.0703	110.4460	33618.1831	0.0001
wheat	Esfenvalerate	066230-04-4	Insecticide	72295.6023	9.4340	104874.1147	2945.0109	32614.4533	6364.5537	589.3118	45609.3834	0.0002
wheat	Ethephon	016672-87-0	Other	0.6952	0.0283	0.0000	0.3474	0.0117	0.0059	0.0935	151.5245	0.0001
wheat	Fenoxaprop-ethyl ester	071283-80-2	Herbicide	0.4260	0.0310	2.5163	0.1401	0.0339	0.0033	1.9473	35.0801	0.0002

ENDURE – Deliverable DR3.10

CS	A.I.	CAS-Nr.	Group	EDIP				CML			IMPACT	
				ecotoxicity, chronic in water	ecotoxicity, chronic, in soil	human toxicity, via surface water	human toxicity, via soil	freshwater aquatic ecotoxicity	human toxicity	terrestrial ecotoxicity	aquatic ecotoxicity	human toxicity
wheat	Fenoxaprop-P ethyl ester	071283-80-2	Herbicide	0.4260	0.0310	2.5163	0.1401	0.0339	0.0033	1.9473	35.0801	0.0002
wheat	Fenpropidin	067306-00-7	Fungicide	74.6659	0.0167	0.0898	1.8749	16.3485	5.7293	0.9716	250351.1223	0.0001
wheat	Fenpropimorph	067306-03-0	Fungicide	0.9174	0.0377	2.3121	0.3268	0.6410	0.0450	22.5018	1904.9504	0.0001
wheat	Fenvalerat	051630-58-1	Insecticide	336.8274	0.6410	5258.9767	713.1249	105.7934	42.6916	258.8401	45.5900	0.0017
wheat	Florasulam	145701-23-1	Herbicide	8962.1153	0.0316	0.0011	0.4465	1418.0139	44.8686	3.3965	2559.9181	0.0000
wheat	Flufenacet	142459-58-3	Herbicide	4.0064	1.0000	2.3096	0.5065	7.9919	0.2093	140.2778	1464.5429	0.0000
wheat	Flupyrsulfuron	150315-10-9	Herbicide	840.3361	0.0050	0.0763	17.3149	82.2623	12.2207	28.3365	823.8072	0.0002
wheat	Fluquinconazole	136426-54-5	Fungicide	100.8227	0.2000	2.0801	0.9789	36.9051	3.4576	38.5920	34436.9505	0.0001
wheat	Fluroxypyr	069377-81-7	Herbicide	0.0539	0.0100	0.9340	3.8345	0.0563	0.0021	4.5282	200.0394	0.0002
wheat	Flurtamone	096525-23-4	Herbicide	199.4813	0.0056	1.7148	0.3263	332.4609	17.5062	40.7775	310.0553	0.0064
wheat	Glyphosat	001071-83-6	Herbicide	0.0003	0.0125	0.0000	0.0037	0.0001	0.0000	0.0089	102.2796	0.0000
wheat	Iodosulfuron	185119-76-0	Herbicide	498.2596	0.0050	0.0021	0.5581	182.9376	14.2517	51.2267	1368.4362	0.0003
wheat	Ioxynil	001689-83-4	Herbicide	0.7817	0.2500	18.1646	1.0566	0.0939	0.0091	35.4950	0.1515	0.0004
wheat	Isoproturon	034123-59-6	Herbicide	532.8218	3.3333	0.9797	1.3192	665.8932	16.3815	92.4437	4587.2313	0.0002
wheat	Kresoxim-methyl	143390-89-0	Fungicide	121.2709	0.0053	56.5068	5.4972	17.6359	0.9203	0.2620	2233.1177	0.0064
wheat	lambda-Cyhalothrin	091465-08-6	Insecticide	918.9420	0.1000	7417.9823	14896.4504	184.2393	122.5800	262.6731	3394.5121	0.0017
wheat	MCPA	000094-74-6	Herbicide	0.0139	0.0589	0.0008	1.2922	0.0072	0.0007	29.6599	200.3427	0.0003
wheat	Mecoprop-P	016484-77-8	Herbicide	0.0772	0.1012	0.0187	5.6614	0.0212	0.0018	104.2540	82.0878	0.0002
wheat	Metconazole	125116-23-6	Fungicide	27.7508	0.0833	8.0985	0.4989	56.8748	4.6219	17.8481	50767.0997	0.0001
wheat	Metribuzin	021087-64-9	Herbicide	2387.9457	0.0452	0.4232	4.8036	2686.6576	97.6212	407.5409	252.6459	0.0001
wheat	Metsulfuron	005585-64-8	Herbicide	83.9454	0.0100	0.0006	0.2863	117.2628	4.0131	5.4767	3926.7629	0.0003
wheat	Parathion	000056-38-2	Insecticide	33.1794	1.2500	25.8915	25.3581	7.3303	3.0642	6.9524	372.0634	0.0012
wheat	Pendimethalin	040487-42-1	Herbicide	3.0191	0.2165	8.4766	1.7248	6.7971	1.1438	5.6675	29253.6070	0.0002
wheat	Prochloraz	067747-09-5	Fungicide	253.5658	0.0625	5.8113	0.3640	274.9579	24.6776	31.3574	12007.6828	0.0097
wheat	Propiconazole	060207-90-1	Fungicide	25.6345	0.5587	5.0982	0.5278	18.9970	1.0534	4.4853	2714.1681	0.0000
wheat	Quinoxifen	124495-18-7	Fungicide	3.1113	0.0903	1.7587	0.5695	4.5732	0.5183	0.7107	119.8060	0.0001
wheat	Spiroxamine	118134-30-8	Fungicide	365.3902	0.0316	0.3291	1.5700	31.4872	21.4922	4.2834	16682.2138	0.0064
wheat	Tebuconazole	107534-96-3	Fungicide	25.4655	0.1000	6.8459	0.6376	39.5034	2.7125	18.2955	25493.5826	0.0001
wheat	Thifensulfuron	079277-67-1	Herbicide	459.1368	0.0208	0.0049	2.0527	54.2974	3.4948	23.0379	45.7715	0.0003
wheat	Tribenuron	106040-48-6	Herbicide	68.5166	0.0086	0.9819	94.9397	6.2161	0.5437	82.2396	56.4852	0.0003
wheat	Tridemorph	081412-43-3	Fungicide	2.5281	0.0250	2.2298	0.3273	0.9520	0.1274	3.8063	2209.3186	0.0001
wheat	Trinexapac	104273-73-6	Other	0.3046	0.0537	0.0004	1.4915	0.0161	0.0053	0.1351	53.9474	0.0064

