

The Substitution Principle

Uncertainty in risk-risk consideration and decision making in the case of substituting Thiacloprid with Tau-fluvalinate

ANNA LARSSON 2015

MVEK02 BACHELOR DEGREE THESIS 15 HP

ENVIRONMENTAL SCIENCE | LUND UNIVERSITY





LUNDS
UNIVERSITET

WWW.CEC.LU.SE
WWW.LU.SE

Lund university
Supervisor: Ullrika Sahlin
Environmental education
CEC - Centre for environmental
and climate research
Ecology Building
223 62 Lund

Abstract

The “Substitution Principle” gives the direction to substitute hazardous substances to less dangerous ones when possible. The idea of substituting substances to less dangerous alternatives is currently of concern and the “Substitution Principle” is one of the tools used to do so. This has come into focus since polluted lakes, air and/or land areas has ended up as consequences of chemical emissions. For the substitution to be successful it needs to be preceded by consideration of the risk-risk tradeoff by the at the moment used chemical and its substitute. This study wants to show the problems when doing risk-risk tradeoffs under uncertainty and the challenge with this is illustrated with a case-study of the neonicotinoid Thiacloprid and a possible substitute, the pyrethroid Tau-fluvalinate. Different scenarios regarding the extent of substitution have been analyzed with respect to impact on freshwater and a hypothetical impact on pollinators. Estimated costs which are associated with these chemicals as well as the initial cost when doing a substitution have also been used as input. Impact score, that is how the substances affect the freshwater regarding toxicity which was derived from USEtox[®] assessment model, has been used to assess the impact of the two substances on freshwater. In this paper two treatments of uncertainty have been observed by applying two different decision theories, the “Expected Utility Theory” and the “Maximin Principle”.

It is concluded that Tau-fluvalinate is not a proper substitute to Thiacloprid regarding its effect on freshwater ecosystems. Tau-fluvalinate is a lot more hazardous to freshwater organisms. The utility differs when different factors are considered, in this case impact on pollinators and/or initial cost. It also differs looking

at the expected versus the maxmin utility. It can be concluded that the treatment of uncertainty in a risk-risk assessment affects which decisions will be made.

List of contents

Abstract 2

List of contents 4

1. Introduction 5

2. Methods and Materials 9

2.1 Decision theory 9

2.2 Substances 10

2.3 Substitution model 10

2.4 Emissions 12

2.5 Characterization Factors 12

2.6 Ecotoxicological information 15

2.7 Uncertainty analysis 17

3. Results 19

3.1 $AvlogEC_{50}$ 19

3.2 Characterization Factors 21

3.3 Risk-risk tradeoff 23

4. Discussion 25

5. Conclusion 29

6. Acknowledgments 30

7. References 31

8. Appendix 35

1. Introduction

A risk-risk tradeoff, i.e. losing one aspect and gaining another one occurs when a decision is made that in either way end up in something adverse. A development of a more safe production and use of chemicals requires consideration of these risk-risk tradeoffs. Substituting substances with less dangerous alternatives is possible when different substances which are available to choose from exist. One group of such chemicals is pesticides which are toxic substances used on agricultural land which cause environmental impacts that are more or less severe. For example these pesticides have ended up as reasons for polluted lakes, air and/or land areas and important pollinators, plants etc. has been affected which gives a domino effect (Bonmatin et al., 2014). This further states that risk-risk considerations for pesticides is continuously current. An early definition of the so called “Substitution Principle” is as a principle that supports

...the substitution of dangerous by less dangerous substances where suitable alternatives are available. (Commission of the European Communities, 2001,5)

The substitution principle is a part of REACH which is the Regulation on Registration, Evaluation, Authorization and Restriction of Chemicals (SOU, 2007). REACH was developed by the European Union (EC 1907/2006). A goal of REACH is to guarantee a high level of protection for the human health and the environment and for substances to be able to circulate freely on the inner market. Another goal is to support a development in competitiveness and innovations. Thus risk-risk tradeoffs are an inherent part of chemical regulation for a more safe production and use of

chemicals but even so, there are challenges with conducting risk-risk tradeoff in practice.

One such challenge is the complexity that arises when doing risk-risk tradeoffs under uncertainty. If everything was certain there would be clear which strategies to survive would be the best but the world we live in isn't certain, there is a lot of uncertainties in choosing what is best. Therefore a selection of options and approaches to deal with this uncertainty as well as a way to choose between them is needed (Kinzig & Starrett, 2012). It is a delicate matter to choose between a risk which we have reliable knowledge and little uncertainty about and a risk which there isn't much information about and uncertainty is large as well. It also seems to be difficulties when communicating this uncertainty to politicians and other decision makers. Even though given the identical information, the decisions may vary from one decision maker to another due to the differences regarding their values but also on how the uncertainty is treated. Differences in how hazardous a chemical is considered can also be seen between countries, in one country it can be considered as a big risk and in another as an unacceptable risk and this will affect the decision as well (Lofstedt, 2013). An unwillingness to act when facing complex decision problems which contain uncertainty may consequence in an obstacle for preventing risks but also to enhance the opportunities of innovation (Walport & Craig, 2014).

A discussion and demonstration of alternative treatments of uncertainty in risk-risk tradeoffs can be used to support development of principles to manage uncertainty in complex decision problems where the knowledge bases are of varying strength. The objective of this thesis is to describe two treatments of uncertainty in relation to risk-risk consideration when applying the substitution principle. The description will be illustrated by the risk-risk tradeoff between a neonicotinoid to its substitute.

Neonicotinoids are a group of insecticides commonly used in agricultural pest management. It is and has been one of the most important classes of insecticides and was in 2010 registered globally in 120 countries (Jeschke, et al. 2010).

New information regarding effects on ecosystem, organisms and the overall environment reveal that neonicotinoids may have negative impacts and a change in its use is promoted. In many countries including USA, France and Germany dating from 1999 and with the last case in 2013 atypical losses of honeybee has been explored and it is suggested that the use of neonicotinoid seed treatments is the cause (Bonmatin et al., 2014). It was suggested since the hive of the dead or dying bees' stored pollen containing neonicotinoids used in seed treatments (Bonmatin et al., 2014). Though there is studies which tell otherwise e.g. the Canadian study by Cutler and Scott-Dupree. In this field-study honeybee colonies exposed to canola treated with the neonicotinoid clothianidin shows that the colonies in the long-term will be unaffected (Cutler & Scott-Dupree, 2007). The study by Rundlöf shows that neonicotinoid has a negative effect on wild bees but not for honey bees which further confirms the earlier studie on honey bees (Rundlöf et al., 2015). This is an example which shows uncertainty on the effects of neonicotinoid. In the last decades, pyrethroid insecticides has because of the possible negative effects of neonicotinoids been the dominant spray insecticide whilst neonicotinoid treatments has been reduced and some even got banned (Hughes et al., 2014). Pyrethroid insecticides are used as foliar sprays while neonicotinoids are used as seed treatments. When banning the most common seed treatments more foliar sprays will be needed to keep control over pests (Hughes et al., 2014). Important to know is that neither neonicotinoids nor pyrethroid insecticides are good for the environment, pyrethroid insecticides may just not be as bad as neonicotinoids at certain points of evaluation. For example some pests are resistant to pyrethroids (Hughes et al., 2014).

The two substances which this study will be looking at is the neonicotinoid Thiacloprid and the pyrethroid Tau-fluvalinate and their effect on freshwater. The substitute Tau-fluvalinate was compared to Thiacloprid regarding effects on the environment and costs for the society. These substances were chosen since both are used on similar plants e.g. fruit plants (New York State Department of Environmental Conservation, 2006 and ADAMA, 2015). Thiacloprid is used on a

variety of chewing and sucking pests. Since Thiacloprid has high water solubility and fairly low K_{ow} it will possibly contaminate surface water during and after rainfall (Beketov & Liess, 2008). Tau-fluvalinate is a broad-spectrum insecticide used commercially both in residential and agriculture. By contrast to Thiacloprid, Tau-fluvalinate isn't soluble in water and the possibility to reach freshwater during or after rainfall is therefore low (Thurston County Health Department, 2013). The choice to look at an aquatic environment is because pyrethroids tend to have low toxicity to birds and mammals but are acute toxic to aquatic animals (UK Government, 2015). To limit the effect evaluation it was therefore chosen to look at the effect in freshwater.

There is a lot of different theories on how to decide in different situations and with different backgrounds. Also on how to do risk-risk considerations under uncertainty.

The objective of this thesis is to describe two different ways of taking into regard uncertainty in relation to risk-risk consideration when applying the substitution principle. The description will be illustrated by the risk-risk tradeoff between a neonicotinoid to its substitute.

The purpose of the case-study is to evaluate the knowledge uncertainty of aquatic values from a sample of references for one specific neonicotinoid, Thiacloprid and one specific substitute, Tau-fluvalinate. More specifically the case-study aims to 1) Compare the risks of Thiacloprid (neonicotinoid) and Tau-fluvalinate (pyrethroid) in an aquatic environment with exposure from agricultural land, 2) Explore the knowledge gap regarding a neonicotinoid and its substitute and 3) Demonstrate how the treatment of uncertainty and the cost for an alternative substance influence the decision in risk-risk considerations. A simplified risk-risk consideration analysis will be performed.

2. Methods and Materials

2.1 Decision theory

In this thesis two treatments of uncertainty in risk-risk tradeoffs are illustrated using two decision theories. These are the “Expected Utility Theory” (Kinzig & Starrett, 2012) and the “Maximin Principle” (Richland Community College, 2015).

The “Expected Utility Theory” is a Bayesian decision theory where uncertainty is treated with certainties. For each action the possible outcomes are identified as well as the likelihood that they will happen. Utilities are assigned with the outcomes and the action which maximizes expected utility will then be chosen (Kinzig & Starrett, 2012 and Troffaes, 2007). The utility varies depending on what the action is.

The “Maximin Principle” theory is not as precise as the “Expected Utility Theory” since it won’t use a mean value but will compare the “worst case” that is the minimum values to each other. The alternative which is the best is then defined as the alternative with the best worst case i.e. the maximal minimum utility. This is where the name “maximin” has its source. The “Maximin Principle” is therefore more sensitive to uncertainty compared to the “Expected Utility Theory” because of not using any mean values but rather only picking the worst case values (Richland Community College, 2015 and Troffaes, 2007).

2.2 Substances

Through risk analyses reports and fact sheets information about the substances was collected. Risk analyses reports were collected from a systematic search with neonicotinoid, substitutes/alternatives, substitution principle, decision theory, USEtox®, Thiachloprid, Tau-fluvalinate and Species Sensitivity Distributions (SSD) as search words on Web of Science, Google Scholar, Google and LUB Search.

Information regarding the proportion applied Thiachloprid versus Tau-fluvalinate was found for the two insecticides Calypso® which contain Thiachloprid and Mavrik® which contain Tau-fluvalinate.

2.3 Substitution model

A simplified risk-risk model was used to derive the utility for each level of substitution (x). This model was weighting the impacts on freshwater and pollinators with costs for the two substances respectively according to

$$utility(x) = -impact_{Aqua}(x) - impact_{poll}(x) - cost(x) \quad 1.$$

The impact on the aquatic environment was evaluated as

$$impact_{Aqua}(x) = (1 - x) \cdot CF_{ecoA} \cdot emission_A - x \cdot CF_{ecoB} \cdot emission_B \quad 2.$$

$CF_{ecoA} \cdot emission_A$ is the impact score for substance A that is how much substance A affect the freshwater given a recommended application on the farmland. The same for substance B in $CF_{ecoB} \cdot emission_B$. In this case substance A is Thiachloprid and substance B is Tau-fluvalinate. The calculation for impact score is described in more detail below.

Since Thiocloprid has been shown to have possible effects on pollinators i.e. bees (Bonmatin et al., 2014, Cutler & Scott-Dupree, 2007 and Rundlöf et al., 2015) the impact on pollinators was included as

$$impact_{poll} = (1 - x) \cdot impact_{pollA} + x \cdot impact_{pollB} \quad 3.$$

The substance which the decision will favor are influenced by the cost since a more expensive substance is less attractive than a less expensive substance. When substituting from one substance to another a high initial cost may be a consequence (Innovation Center Iceland, 2015). This could for example be if a new type of equipment needs to be installed or a renovation is needed. Therefore the initial cost was included as a negative factor of the utility according to the equation below.

$$cost(x) = (1 - x) \cdot cost_A + x \cdot cost_B + I(x > 0) \cdot initial\ cost \quad 4.$$

Here $I(x > 0)$ represent an indicator function which when the substitute is to be used is taking the value of 1.

Three different cases were evaluated regarding the utility. The first case looked at the utility when both the impact on pollinators and an initial cost was present i.e. not 0. The second case looked at the utility with no initial cost but with the impact on pollinators and in the last case the initial cost was present but the impact on pollinators was set to 0 to see how utility differ when taking no consideration of this impact.

2.4 Emissions

It isn't always 100 % of the substances which get substituted. Therefore different levels of exchange between the two substances Thiacloprid and Tau-fluvalinate was analyzed. This exchange was stated as x which is the level of substitution and the levels can be seen in Table 1. The choice to use these levels of exchange was to get an overview of the outcome for the whole range of exchange. In this case a higher amount of Tau-fluvalinate than Thiacloprid was needed to get the same toxic effect on pests and the ratio between them was found to be 5,84:1 (New York State Department of Environmental Conservation, 2006 and ADAMA, 2015). The calculated amounts can be seen in Table 1.

Table 1. The table shows how much Tau-fluvalinate which will be needed to replace Thiacloprid for each of the scenarios/levels of substitution. 5,84 g/ha of Tau-fluvalinate will be needed to replace 1 g/ha of Thiacloprid (New York State Department of Environmental Conservation, 2006 and ADAMA, 2015).

Scenario	Level of substitution (x)	Emissions Thiacloprid (g/ha)	Emissions Tau-fluvalinate (g/ha)
1	0	96	0
2	0,1	86,4	56,064
3	0,2	76,8	112,128
4	0,3	67,2	168,192
5	0,4	57,6	224,256
6	0,5	48	280,32
7	0,6	38,4	336,384
8	0,7	28,8	392,448
9	0,8	19,2	448,512
10	0,9	9,6	504,576
11	1	0	560,64

2.5 Characterization Factors

The Characterization Factors symbolize a substance's potency to do damage to the environment. It was calculated using Equation 5 by multiplying the Fate Factor (FF), the Exposure Factor (XF_{eco}) and the Effect Factor (EF_{eco}). FF is the Fate Factor and represents the persistence of a chemical in the environment presented in days for example. The Exposure Factor (XF_{eco}) is connected with FF and symbolizes the

bioavailability of a chemical presented in fraction of the chemical dissolved. EF_{eco} , the Effect Factor describes the effect on species in the way of how many which is affected and symbolizes the change in Potentially Affected Fraction (PAF) due to change in concentration (Huijbregts et al., 2010).

$$CF_{eco} = FF \cdot XF_{eco} \cdot EF_{eco} \quad 5.$$

When comparing two different chemicals differences in FF, XF_{eco} and EF_{eco} can tell important changes between the chemicals. These differences can be a part in why one of the chemicals are better for the environment.

Below equations describe the toxicity impact score (IS_{ecotox}) that is to say how much the different substances affect the freshwater regarding toxicity. Equation 6 was used to calculate IS_{ecotox} for Thiacloprid only and Equation 7 for Tau-fluvalinate only. Equation 8 was used to calculate IS_{ecotox} for the different mixes of the two substances which can be seen in Table 1. The toxicity impact score was calculated by multiplying the mass emitted of the substance in a specific compartment, in this case freshwater, with the corresponding CF_{eco} . Since two different decision theories was examined in this case-study a calculation of IS_{ecotox} with the average CF_{eco} ($avCF_{eco}$) was done for the “Expected Utility Theory”. To calculate IS_{ecotox} for the “Maximin Principle” calculations using the CF_{eco} with the minimum and maximum $avlogEC_{50}$ was done respectively.

$$IS_{ecotox} = CF_{eco \text{ thiacloprid, freshwater}} \cdot M_{thiacloprid, freshwater} \quad 6.$$

$$IS_{ecotox} = CF_{eco \text{ tau-fluvalinate, freshwater}} \cdot M_{tau-fluvalinate, freshwater} \quad 7.$$

$$IS_{ecotox} = CF_{eco \text{ thiacloprid, freshwater}} \cdot M_{thiacloprid, freshwater} \quad 8. \\ + CF_{eco \text{ tau-fluvalinate, freshwater}} \cdot M_{tau-fluvalinate, freshwater}$$

To be able to calculate CF_{eco} and further on IS_{ecotox} substance data stated in USEtox® were collected from risk analysis reports. The collected values can be seen in Appendix 1.

To calculate the degradation rates needed for the simulation EPI Suite™ (Estimation Program Interference) was used. EPI Suite™ is developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Collaboration (SRC) and uses physical/chemical properties and environmental fate estimation programs to estimate different properties (US EPA, 2013). In EPI Suite™ values from Appendix 1, as described in the program was in case of need transformed and then used as input. To be able to use the value outcome of EPI Suite™ in USEtox® a number of transformations were needed. To calculate $kdeg_A$ the Overall OH Rate Constant in tab AOPWIN was used. The Overall OH Rate Constant stands for hydroxyl radical rate constant in units of $cm^3/molecule\cdot sec$. It was then multiplied with the default OH that is the hydroxyl radical concentration in units of molecules or radicals per cm^3 which is $1,5E6$ molecules (radicals) per cm^3 per 12 hours of daylight. The calculated value was then derived by 2 assuming that this removing pathway only affects half of the day (USEtox® Org., 2013).

To calculate the remaining factors $kdeg_w$, $kdeg_{SI}$, $kdeg_{Sd}$ and $kdeg_P$ the tab named BIOWIN in EPI Suite™ was used. Starting with degradation rate in water the BioWin3-value was multiplied with its assigned half-life in days for the unit of output, in this case months or recalcitrant. Since the half-life was in days the value was converted to seconds by multiplying with $24 \cdot 3600$. Calculating $\ln(2)/half\ life(sec)$ the outcome was the value which was then used in USEtox®. The relationship between $kdeg_w$, $kdeg_{SI}$ and $kdeg_{Sd}$ was found to be 1:2:9 and therefore $kdeg_{SI}$ and $kdeg_{Sd}$ was acquired by multiplying with 2 and 9 respectively. $kdeg_P$ is assumed to be a factor of 10 lower than $kdeg_{SI}$ which was calculated (USEtox® Org., 2013 and Huijbregts et al., 2010). All the calculated degradation rates can be seen in Appendix 2.

The cells in USEtox® which were analyzed were Fate Factor (FF), Available Fraction XF_{eco} and Ecotoxicity Effect Factor EF_{eco} . Beyond these three Ecotoxicity potentials expressed in comparative toxic units CTU_e was also examined to lay weight on the comparative nature of the characterization factors (Huijbregts et al., 2010).

USEtox® was chosen since it is a well-established model to assess environmental impacts of chemicals. USEtox® is an environmental model to look at human and ecotoxicological impacts in Life Cycle Impact Assessment (LCIA) and Comparative Risk Assessment (CRA). The model describes the fate, exposure and effects of chemicals and has been developed by a group of researchers. LCIA wants to put the emissions in a life cycle in a bigger picture where the emission's potential impacts on the environment are characterized. The impacts extent from local impacts from land use to regional impacts due to e.g. toxic substances or acidification to global impacts like climate change (Huijbregts et al., 2010).

2.6 Ecotoxicological information

When measuring effects in water $avlogEC_{50}$ was used. $avlogEC_{50}$ describes the average of $logEC_{50}$ for different groups of species to capture the effect in an aquatic ecosystem (USEtox®, 2015). EC_{50} -values for four different groups of species were collected for both of the substances and $logEC_{50}$ was calculated for each of the values (see Table 2). As can be seen some values have greater-than or less-than symbols but in the calculations the stated value was used not considering these symbols.

Table 2. Collected EC₅₀-values for Thiocloprid and Tau-fluvalinate and the calculated logEC₅₀-values. The values are collected from Rayfull (2012), FAO (2005), Gilbert & Gill (2010), Beketov & Liess (2008), Bayer CropScience (2013), NRA (2001), NCBI (2015), EFSA (2010), Sigma Aldrich (2004), Champeau & Tremblay (2013) and Asker (2013).

Substance	Species	Group of species	EC ₅₀ (mg.L ⁻¹)	logEC ₅₀ (mg.L ⁻¹)	Ref.
Thiocloprid	Daphnia magna	D	85,1	1,93	Rayfull 2012
Thiocloprid	Scenedesmus subspicatus	algae	97	1,99	Rayfull 2012
Thiocloprid	Pseudokirchneriella subcapitata	algae	>100	>2	Rayfull 2012
Thiocloprid	Daphnia magna	D	>85,1	>1,93	FAO 2005
Thiocloprid	Daphnia magna	D	>85,1	>1,93	Gilbert & Gill 2010
Thiocloprid	Daphnia magna	D	>0,085	>-1,07	Beketov & Liess 2008
Thiocloprid	Daphnia magna	D	>=85,1	>=1,93	Bayer CropScience 2013
Thiocloprid	Hyalella azteca	crustacean	0,0245	-1,61	Bayer CropScience 2013
Thiocloprid	Rainbow trout /Bluegill sunfish	fish	<9,77	<0,99	NRA 2001
Thiocloprid	Amphipods	crustacean	0,0245	-1,61	NRA 2001
Thiocloprid	Rainbow trout	fish	<5,0	<0,70	NRA 2001
Thiocloprid	Bluegill sunfish	fish	<6,2	0,79	NRA 2001
Tau-fluvalinate	Daphnia magna	D	0,0004	-3,4	NCBI 2015
Tau-fluvalinate	Daphnia magna	D	0,001	-3	NCBI 2015
Tau-fluvalinate	Daphnia magna	D	0,074	-1,13	NCBI 2015
Tau-fluvalinate	Daphnia magna	D	0,325	-0,49	NCBI 2015
Tau-fluvalinate	Mysidopsis bahia	crustacean	0,000021	-4,7	EFSA 2010
Tau-fluvalinate	Scenedesmus subspicatus	algae	>2,2	>0,34	Sigma Aldrich 2004
Tau-fluvalinate	Daphnia	D	0,001	-3	Sigma Aldrich 2004
Tau-fluvalinate	Daphnia magna	D	0,0089	-2,05	Champeau & Tremblay 2013
Tau-fluvalinate	Scenedesmus subspicatus	algae	>42,0	>1,62	Champeau & Tremblay 2013
Tau-fluvalinate	Daphnia magna	D	0,000021	-4,7	Asker 2013
Tau-fluvalinate	Fish	fish	7,94E-05	-3,1	EFSA 2010
Tau-fluvalinate	Bluegill	fish	6,60E-04	-3,2	NCBI 2015

AvlogEC₅₀ was used to get an average of different species to be able to get an effect on the whole ecosystem since some species are more sensitive than others. The source to avlogEC₅₀ is Species Sensitivity Distribution (SSD) which are models of the sensitivity variation between different species due to a specific stressor

(US EPA, 2012). As can be seen in Table 2 some of the $\log EC_{50}$ -values are inequalities and in the calculations below they were treated as if it was that value.

To calculate $av\log EC_{50}$ a quantification of uncertainty for $av\log EC_{50}$ was made by quantifying uncertainty for each of the four groups of species. This was done separately for the different groups of species and thereafter sample from these generated a sample of $av\log EC_{50}$ -values. This process was done for both Thiocloprid and Tau-fluvalinate. The Bayesian quantification of uncertainty was made by assigning a prior distribution which was normally distributed with a prior mean and prior variance of 0 and 100 respectively to $\log EC_{50}$ -values for a group of species. The values for $\log EC_{50}$ was then updated by applying Bayes rule. Updating by Bayes rule means in practice to weight the prior mean with the sample mean according to the relation between the prior variance and sample variance based on the experimental information. This updated distribution is called a posterior distribution (Jacobs, 2008 and Sahlin, Personal communication, 2015). Random numbers were drawn from the respective posterior distribution of $\log EC_{50}$ and $av\log EC_{50}$ was calculated for each of them. This resulted as a distribution of $av\log EC_{50}$.

Uncertainty for the use of the “Maximin Principle” was treated by quantifying an upper and lower bound on $av\log EC_{50}$ -values. This was made by basing the averages on the most extreme values from all groups of species. The most extreme values, minimum and maximum for each group of species was picked from Table 2 and an average for all the minimum values and an average for all the maximum values was calculated. The minimum value for $av\log EC_{50}$ significate the average of the most sensitive species while the maximum $av\log EC_{50}$ significates the average of the most tolerant species.

2.7 Uncertainty analysis

The model for risk-risk consideration made with an uncertainty of knowledge was used to illustrate the variety of outcome with using different treatments of uncertainty by

applying two types of decision theories. The uncertainty analysis was made by driving USEtox® several times with different input for avlogEC₅₀. It was analyzed by comparing the output of using avlogEC₅₀ or minimum and maximum avlogEC₅₀ and the results regarding utility.

3. Results

3.1 AvlogEC₅₀

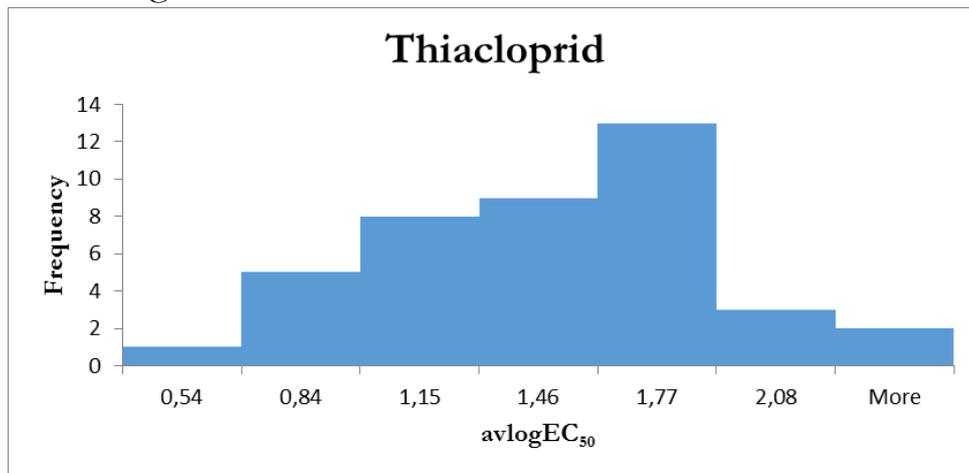


Figure 1. Calculated avlogEC₅₀ for Thiocloprid showing the distribution of avlogEC₅₀.

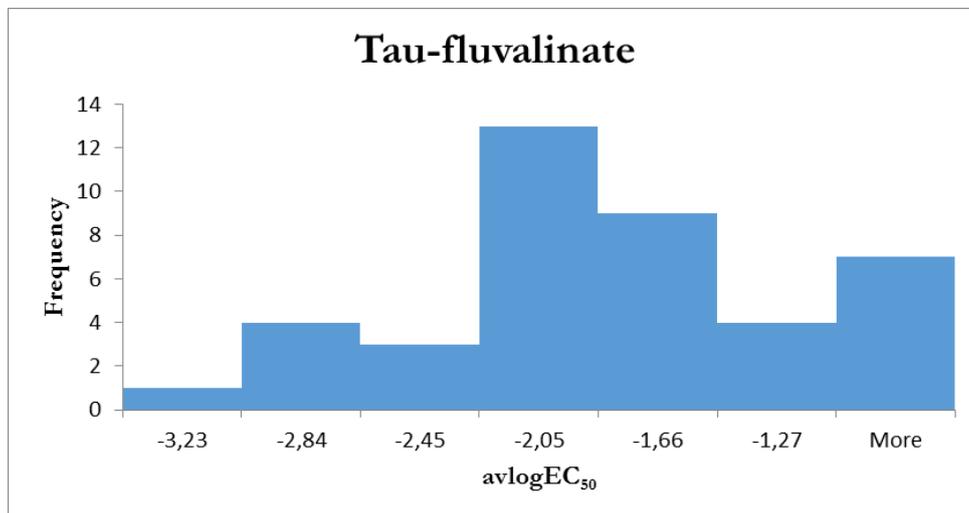


Figure 2. Calculated avlogEC₅₀ for Tau-fluvalinate showing the distribution of avlogEC₅₀.

Figures 1 and 2 show the distribution of the calculated avlogEC_{50} -values for Thiacloprid and Tau-fluvalinate using the “Expected Utility Theory”. The calculated minimum and maximum avlogEC_{50} using “Maximin Principle” for Thiacloprid was 0,025 and 1,6625 respectively and -3,04 and -1,6925 for Tau-fluvalinate.

As can be seen comparing Figure 1 and the minimum and maximum avlogEC_{50} for Thiacloprid the lowest value in Figure 1 is higher than the minimum avlogEC_{50} as well as the highest value in Figure 1 is higher than the maximum avlogEC_{50} . The maximum avlogEC_{50} is almost the mean in Figure 1. When doing the same analyze of Figure 2 and the minimum and maximum avlogEC_{50} for Tau-fluvalinate it can be seen that the lowest value in Figure 2 is lower than the minimum avlogEC_{50} and the highest value in Figure 2 is higher than the maximum avlogEC_{50} . Just like for the above comparison between Figure 1 and the minimum and maximum avlogEC_{50} for Thiacloprid the maximum avlogEC_{50} for Tau-fluvalinate is almost the mean in Figure 2.

3.2 Characterization Factors

In Figure 3 and 4 the “Expected Utility Theory” was used to calculate a mean value for CF_{eco} for Thiocloprid and in Figure 5 and 6 for Tau-fluvalinate. As can be seen comparing Figure 3 and 5 CF_{eco} for Tau-fluvalinate is a lot larger than CF_{eco} for Thiocloprid. The mean value for CF_{eco} is $7,12E+01$ for Thiocloprid and $2,5E+05$ for Tau-fluvalinate. Since FF and XF_{eco} are constant and not affected by $avlogEC_{50}$ the factor EF_{eco} is the determining factor for CF_{eco} . To compare with CTU_e , ecotoxicity potentials in comparative toxic units, it can be seen in Figure 4 and 6 that the overall distribution of the values for CTU_e doesn't differ from the distribution of the CF_{eco} -values in a big way neither for Thiocloprid nor for Tau-fluvalinate.

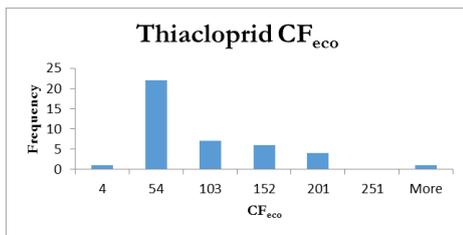


Figure 3. Calculated values for CF_{eco} for Thiocloprid using $avlogEC_{50}$.

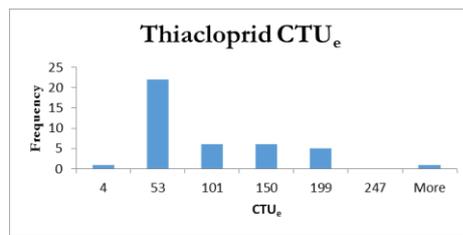


Figure 4. Calculated values for CTU_e for Thiocloprid using $avlogEC_{50}$.

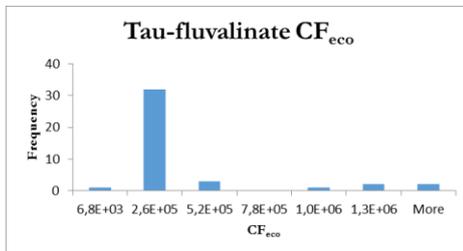


Figure 5. Calculated values for CF_{eco} for Tau-fluvalinate using $avlogEC_{50}$.

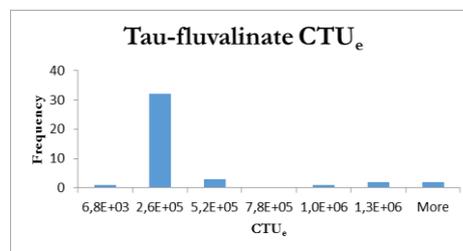


Figure 6. Calculated values for CTU_e for Tau-fluvalinate using $avlogEC_{50}$.

CF_{eco} for Thiocloprid and Tau-fluvalinate were also calculated using the minimum and maximum avlogEC₅₀. The minimum and maximum CF_{eco} for Thiocloprid was 9,6E+02 and 2,2E+01 respectively and the same values for Tau-fluvalinate was 9,9E+05 and 4,5E+04 respectively. As can be seen Tau-fluvalinate has a higher CF_{eco} both using the minimum and maximum avlogEC₅₀.

The impact score for the different scenarios 1-11 was calculated using Equation 6, 7 and 8. The result using avCF_{eco} versus minimum and maximum CF_{eco} can be seen in Table 3. As can be seen the relation for IS_{ecotox} for the different scenarios is the same regardless if avCF_{eco} or CF_{eco} with minimum and maximum avlogEC₅₀ was used. Scenario 11 has the largest IS_{ecotox} and scenario 1 has the smallest. It can be seen that the more Tau-fluvalinate in the mixture the higher IS_{ecotox}.

Table 3. Results from calculation of Impact Score IS_{ecotox} using avCF_{eco} and CF_{eco} with the min and max logEC₅₀ for the different scenarios.

Scenario	1	2	3	4	5	6
Level of substitution	0	0,1	0,2	0,3	0,4	0,5
IS _{ecotox} (using avCF _{eco})	6,84E+03	1,40E+07	2,80E+07	4,21E+07	5,61E+07	7,01E+07
IS _{ecotox} (using CF _{eco} minlogEC ₅₀)	9,22E+04	5,56E+07	1,11E+08	1,67E+08	2,22E+08	2,78E+08
IS _{ecotox} (using CF _{eco} maxlogEC ₅₀)	2,11E+03	2,52E+06	5,05E+06	7,57E+06	1,01E+07	1,26E+07
Scenario	7	8	9	10	11	
Level of substitution	0,6	0,7	0,8	0,9	1	
IS _{ecotox} (using avCF _{eco})	8,41E+07	9,81E+07	1,12E+08	1,26E+08	1,40E+08	
IS _{ecotox} (using CF _{eco} minlogEC ₅₀)	3,33E+08	3,89E+08	4,44E+08	5,00E+08	5,55E+08	
IS _{ecotox} (using CF _{eco} maxlogEC ₅₀)	1,51E+07	1,77E+07	2,02E+07	2,27E+07	2,52E+07	

3.3 Risk-risk tradeoff

Using Equation 1 the utility was calculated for the different scenarios. In Figure 7 the factor impact on pollinators per emission as well as the initial cost has been put into the calculation. The initial cost was estimated to a value which would be a meaningful factor in the calculation. Different values of initial cost was examined to find one which had an impact on the results since the purpose of this study was to show how different treatments of uncertainty affect decisions in risk-risk consideration. Since there is no initial cost for scenario 1 (0 % substitution) the utility is bigger at that part of the curve. It can be seen that the expected utility is maximized for 0 % substitution while for the “Maximin Principle” a substitution of 100 % is the most optimal.

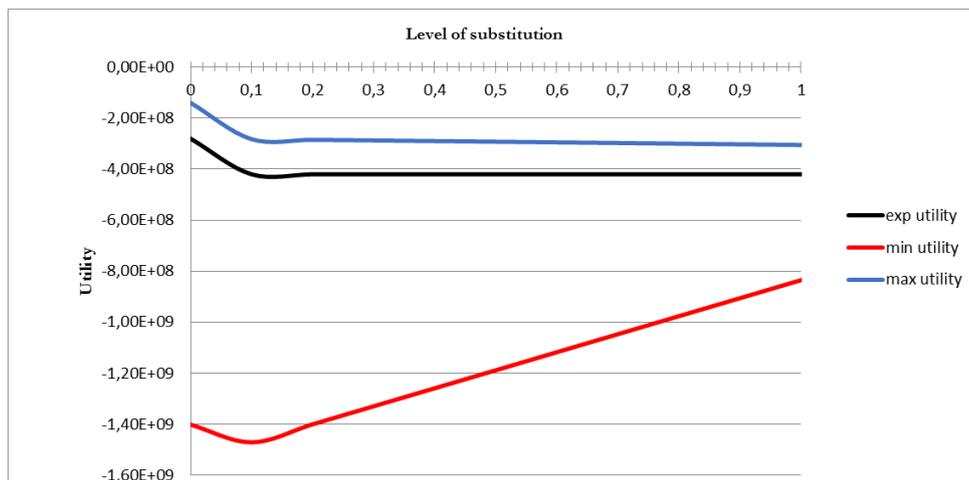


Figure 7. Utility for the different levels of substitution. In this figure both impact on pollinators per emission and the initial cost has been put into the calculation.

In Figure 8 the initial cost is put as 0 while the impact on pollinators per emission is the same as for the figure above. As can be seen the expected utility is equal for the whole range of substitution while the “Maximin Principle” has its optimum at a substitution of 100 %.

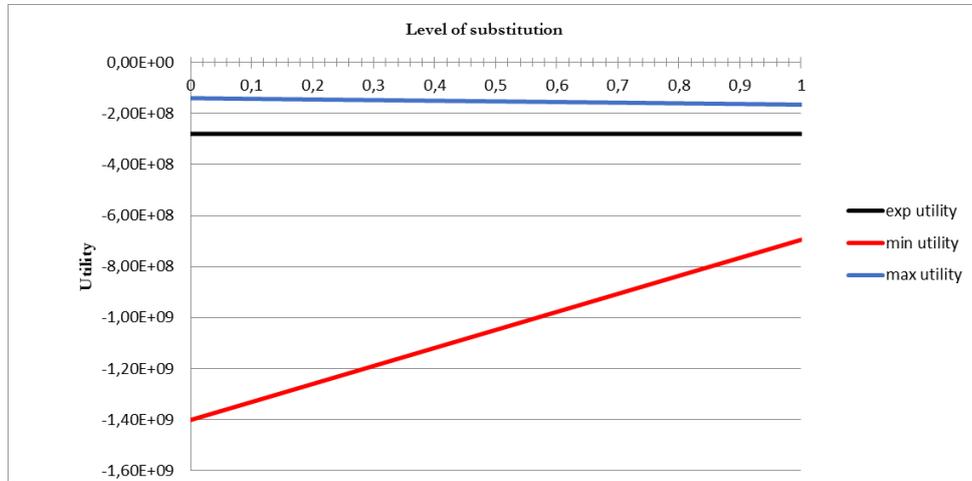


Figure 8. Utility for the different levels of substitution. In this figure impact on pollinators per emission has been put into the calculation. The initial cost is 0.

In Figure 9 the initial cost is put into the calculation as the same value used in Figure 7 but the impact on pollinators per emission is set as 0. Therefore the only impact which is looked at is the impact on freshwater. As can be seen in Figure 9 the result is a declining utility the more Tau-fluvalinate is used in the mixture. This relationship is regardless if the “Expected Utility Theory” or the “Maximin Principle” were used to do the calculations.

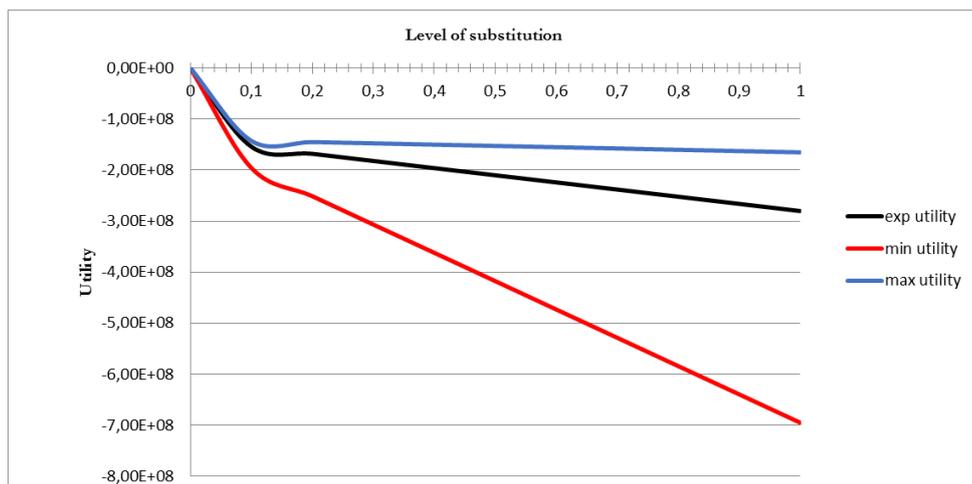


Figure 9. Utility for the different levels of substitution. In this figure an initial cost is present but the impact on pollinators per emission is set as 0.

4. Discussion

This case-study has shown that Tau-fluvalinate is more hazardous to freshwater ecosystems than Thiacloprid. This has been concluded since it has a higher CF_{eco} (Figure 5 versus Figure 3) and also needs to be applied in a higher volume than Thiacloprid (Table 1). The utility has been seen to vary depending on which factors are weighed in and this caused differences in optimum substitution between expected utility and maximum utility.

This study focuses on the effects of Thiacloprid and Tau-fluvalinate in aquatic environments with exposure from farmland. Therefore, the results will not tell how the effects are on terrestrial organisms. In this case, Thiacloprid is more likely to end up in freshwater but has a lower CF_{eco} , which is the potency to cause damage to the environment than Tau-fluvalinate. This means that if Tau-fluvalinate were to reach freshwater, it would be a lot more hazardous than Thiacloprid would be. Since both Thiacloprid and Tau-fluvalinate have a low toxicity for birds and mammals, it should not be an important difference between them regarding their effects on land (Gilbert & Gill, 2010). Even so, the possible negative effects of neonicotinoids on bees may give another result (Bonmatin et al., 2014; Cutler & Scott-Dupree, 2007; Rundlöf et al., 2015). Though a similar case-study as this one should be done with a focus on effects on terrestrial environments to be able to conclude this theory.

When searching for information regarding the two substances, it seems there are more papers and studies on Thiacloprid than for Tau-fluvalinate, which further supports the theory of a larger gap of knowledge regarding the substitute to the neonicotinoid. Another reason can be that because of the lower probability for Tau-fluvalinate to reach freshwater, not so many studies on this environment have been done. As has been stated earlier, more studies need to be done on Tau-fluvalinate and

other possible substitutes to minimize and seal this gap. More studies are also necessarily on Thiacloprid to reduce the uncertainty regarding its effects on especially pollinators.

The different levels of substitution used in this case-study represented the whole range of substitution from fully substituted to not substituted at all which give a good insight in the possibilities for substitution and how much impact score and utility varies due to the levels. By looking at Table 3 it seems that the most hazardous scenario is when the substitution is 100 % (Scenario 11). This is independent whether the “Expected Utility Theory” or the “Maximin Principle” has been used in the calculation. The best scenario is in scenario 1 when the substitution is 0 % (100 % Thiacloprid) which further supports that Tau-fluvalinate is a lot more hazardous to freshwater than Thiacloprid.

More EC_{50} -values and values for a greater number of species was found for Thiacloprid than for Tau-fluvalinate which once again indicates that there is more knowledge about the neonicotinoid than for its substitute, the pyrethroid. The same number of groups of species was needed to achieve a reliable result and therefore only four groups were looked at in this case-study. Since both fish and Daphnia which is sensitive to these pollutants which can be seen in Table 2 was used in the calculation it should be an enough range of groups of species to get a good result. Some of the EC_{50} -values had greater-than or less-than symbols and the value which were stated was then picked regardless if it said greater-than or less-than. This isn't the most correct way and therefore the outcome may have been incorrect in the estimation of $avlogEC_{50}$. With using values which had a greater-than sign in front of them may have lowered the $avlogEC_{50}$ and therefore also increased CF_{eco} as well as the impact score. With using values which had a less-than symbol in front of them the $avlogEC_{50}$ may have increased which gives a lower CF_{eco} and impact score. Since the total outcome regarding IS_{ecotox} ended in a big difference between substituting and not substituting I don't think that these greater-than and less-than values have had an important impact and could have changed the outcome in a meaningful way.

When using the “Expected Utility Theory” to calculate avlogEC_{50} it seems that the range is bigger between the minimum and maximum compared to the range of using the “Maximin Principle”. It seems that the maximum avlogEC_{50} (“Maximin Principle”) is almost a mean of avlogEC_{50} using the “Expected Utility Theory”. The same situation was found for both substances. Since the mean was calculated for CF_{eco} this shouldn’t have given any big consequences.

The calculation and variation of CF_{eco} was dependent on the factor EF_{eco} since the other factors were constant. Since this factor is the only one of FF , XF_{eco} and EF_{eco} which depends on the EC_{50} for species this variation affected the CF_{eco} . Looking at the factor Ecotoxicity potentials expressed in comparative toxic units CTU_e the differences to CF_{eco} wasn’t big which confirms the results which have been acquired for CF_{eco} .

Looking at the utility the outcome is different dependent on which factors that have been weigh in. In Figure 8 where the initial cost is put as 0 it can be seen that the expected utility has the same value through the whole range of substitution. This can be explained by the impact on pollinators which weigh up the higher $\text{IS}_{\text{ecotox}}$ for Tau-fluvalinate as well as the missing initial cost. Therefore when the impact on pollinators isn’t weigh in i.e. Figure 9, the utility decreases the more substitution. This is the same reason for why min utility slightly increases in all cases but the one without impact on pollinators. In Figure 7 the curve looks the same as Figure 8 except for the part from 0 to 0,1 substitution. This is because for the 0 substitution there is no initial cost and therefore the utility is higher in this range. For maxmin the optimal substitution is never 0 which depends on the slightly increase for min utility. This slight increase is enough to make a fully substitution the optimal. This observations show that depending on which factors which is put into the calculation the outcome differs and in this case the outcome changes from the optimal to not be doing a substitution to be doing a full substitution.

In this case-study use of alternative treatments of uncertainty in risk-risk tradeoffs have shown to result in big differences depending on which factors are

put into the function. You should be aware of that in other cases other results may be found and only looking at one of these two treatments of uncertainty can lead to critical consequences. This depends among others on the fact that the “Maximin Principle” is more sensitive to uncertainties since the deviation using only the minimum and maximum can be very different from case to case. The availability to compare different approaches when dealing with uncertainty is an important tool to initiate a discussion by politicians and other decision makers on how to confront uncertainty in risk-risk tradeoffs. Therefore comparing different approaches should be used in a bigger range.

To continue with this study an interesting aspect to look at is synergistic effects of these substances. A synergistic effect means that one substance (A) increases the toxicity of another substance (B) when used together. Though if substance A is used alone it will have no toxic effect and will then be called a synergist (Walker et al., 2012). This is interesting since either Thiacloprid or Tau-fluvalinate may be a synergist or may be applied together with a synergist and therefore give or have an increased toxicity to the ecosystem applied.

When given more information about the chemicals which we are using in the society it is quite possible that more substances will be banned in the future. Therefore it is important to start observing possible substitutes before these bannings to not stand by the risk to be standing with big uncertainties for the substances which will then be used.

The “Substitution Principle” is a great tool for an improve of chemical-based accidents in the environment but uncertainty is a difficulty which are hard to work with. In this case the substitute was found to be more hazardous than the substance it was supposed to replace and therefore this case does not belong to the substitution principle. Though if we look at the same substitution but on impact on land the results could be different. This further verifies that it is important to gather as much information as possible before taking a decision. This thesis has shown an example of working with uncertainty and two different ways to approach it.

5. Conclusion

This study concludes that Tau-fluvalinate should not be used as a substitute to Thiacloprid considering the effects on aquatic life. The risk for Tau-fluvalinate to reach freshwater is lower than for Thiacloprid due to not being too soluble in water but because of the much higher CF_{eco} for Tau-fluvalinate it is a lot more hazardous to aquatic life. It is possible that it is the opposite situation for effects on land but to be able to conclude it a study on Thiacloprid and Tau-fluvalinate regarding their CF_{eco} and IS_{ecotox} on land is needed. The utility varies depending on which factors are weighed in in the assessment and in this case expected utility has different optimums than maximum utility. These differences further confirm that depending on how uncertainty is treated in risk-risk assessment various decisions will be made.

This case-study emphasizes the need for more studies and observations of Tau-fluvalinate and other substances which could be possible substitutes for the more hazardous substances we use in the society today. Data regarding synergistic effects of the possible substitutes is also required to be able to initiate a more safe use of these chemicals. It is quite possible that more substances will be banned in the future when they have been further studied regarding their effects on the environment. Therefore it is even more important to observe possible substitutes before the banning to not be standing with big uncertainties for the substances which will then be used.

6. Acknowledgments

I would like to thank Olof Berglund and my supervisor Ullrika Sahlin for making this bachelor degree thesis possible. Further I want to thank Ullrika Sahlin for her help and advice through the whole process and especially for her fast feedback.

At last but not least I want to thank everyone who has been beside me through the process, pushing me forward and answering my sometimes confused questions.

7. References

- ADAMA. (2015). *MAVRIK® Aquaflo Insecticide*. Nelson: ADAMA.
- Asker, I. (2013). *Evaluation of risk for aquatic organisms when realistic conditions of use are considered in risk assessments of plant protection products (PPPs) - A risk assessment of PPPs used in cultivation of spring rape (Brassica napus)*. Uppsala: Uppsala University.
- Bayer CropScience. (2013). *Bayer CropScience Safety Data Sheet Calypso® 480 SC Insecticide*. Bayer CropScience Pty Ltd.
- Beketov, M. a, & Liess, M. (2008). *Acute and delayed effects of the neonicotinoid insecticide thiacloprid on seven freshwater arthropods*. *Environmental Toxicology and Chemistry / SETAC*, 27(2), 461–470. <http://doi.org/10.1897/07-322R.1>
- Binder, T., Ceric, H., Hossinger, a., & Selberherr, S. (2002). *A strategy to enforce the discrete minimax principle on finite element meshes*. *International Conference on Simulation of Semiconductor Processes and Devices*, 183–186. <http://doi.org/10.1109/SISPAD.2002.1034547>
- Bonmatin, J. M., Giorio, C., Girolami, V., Goulson, D., Kreuzweiser, D. P., Krupke, C., Liess, M., Long, E., Marzaro, M., Mitchell, E.A.D., Noome, D.A., Simon-Delso, N., Tapparo, A. (2014). *Environmental fate and exposure; neonicotinoids and fipronil*. *Environmental Science and Pollution Research*, 35–67. <http://doi.org/10.1007/s11356-014-3332-7>
- Champeau, O., Tremblay, L. (2013). *Ecotoxicity review of 26 pesticides. Report No. 2357*. Nelson: Cawthron Institute.
- ChemSpider. (2015). *(Z)-thiacloprid*. (Electronic) Accessible: <http://www.chemspider.com/Chemical-Structure.103099.html> (2015-05-11)
- Commission of the European Communities. (2001). *Strategy for a future Chemicals Policy*. Brussels: Commission of the European Communities.

- Cutler, G.C., Scott-Dupree, C.D. (2007). *Exposure to Clothianidin Seed-Treated Canola Has No Long-Term Impact on Honey Bees*. *Journal of Economic Entomology*, 100(3), 765-772. [http://doi.org/10.1603/0022-0493\(2007\)100](http://doi.org/10.1603/0022-0493(2007)100)
- EFSA conclusion. (2010). *Conclusion on the peer review of the pesticide risk assessment of the active substance tau-fluvalinate*, 8(7), 1–75. <http://doi.org/10.2903/j.efsa.2010.1645>
- EPA. (2003). *EPA Fact Sheet for Thiacloprid*. United States Environmental Protection Agency. Washington: EPA.
- EPA. (2005). *Reregistration Eligibility Decision for Tau-fluvalinate*. United States Environmental Protection Agency, 259. Washington: EPA.
- European Commission. (2004). *Review report for the active substance thiacloprid*, 6(3), 1–63. Retrieved from European Commission <http://ec.europa.eu/food/plant/protection/evaluation/newactive/thiacloprid.pdf>.
- Food and Agriculture Organization of the United Nations FAO. (2005). *FAO Specifications and Evaluations for Agricultural Pesticides*, 50.
- Gilbert, L.I., Gill, S.S. (2010). *Insect Control: Biological and Synthetic Agents*. Elsevier, B.V.
- Hughes, J., Reay, G., Watson, J. (2014). *Insecticide use on Scottish oilseed rape crops: Historical use patterns and pest control options in the absence of neonicotinoid seed treatments*. *Proceedings Crop Protection in Northern Britain 2014*, 21-26.
- Huijbregts, M., Hauschild, M., Jolliet, O., Margni, M., McKone, T., Rosenbaum, R.K., van de Meent, D. (2010). *USEtox™ User Manual*. 18(1-2), 99–108. Retrieved from <http://www.ncbi.nlm.nih.gov/pubmed/10768541>
- Huijbregts, M., Margni, M., Meent, D. Van De, Jolliet, O., Rosenbaum, R. K., Mckone, T., & Hauschild, M. (2010). *USEtox™ - Chemical database: organic-*. http://www.usetox.org/sites/default/files/support-tutorials/database_organics.pdf
- Innovation Center Island. (2015). *Initial cost budget*. (Electronic) Accessible: <http://www.nmi.is/support/beginning/initial-cost-budget/> (2015-05-13)
- Jacobs, R. (2008). *Bayesian Statistics: Normal-Normal Model*. 1–3. New York, University of Rochester: Department of Brain & Cognitive Sciences.

- Jeschke, P., Nauen, R., Schindler, M., & Elbert, A. (2010). *Overview of the Status and Global Strategy for Neonicotinoids (dagger)*. *Journal of Agricultural and Food Chemistry*, (July), 1–7. <http://doi.org/10.1021/jf101303g>
- Kinzig, A., Starrett, D. (2012). *Coping With Uncertainty: A Call for a New Science-Policy Forum*. *Sciences-New York*, 32(5), 330–335.
- Lofstedt, R. (2013). *The substitution principle in chemical regulation: a constructive critique*. *Journal of Risk Research*, (November), 1–22. <http://doi.org/10.1080/13669877.2013.841733>
- National Center for Biotechnology Information NCBI. (2015). *FLUVALINATE*. (Electronic) Accessible: <https://pubchem.ncbi.nlm.nih.gov/compound/fluvalinate> (2015-05-05)
- National Registration Authority for Agricultural and Veterinary Chemicals NRA. (2001). *Evaluation of the new active THIACLOPRID in the new product Calypso 480 SC Insecticide*, (November). National Registration Authority for Agricultural and Veterinary.
- New York State Department of Environmental Conservation. (2006). *Re: Registration of the New Active Ingredient Thiacloprid Contained in the Pesticide Product Calypso® 4 Flowable Insecticide (EPA Reg. No. 264-806)*. New York, New York State Department of Environmental Conservation.
- Richland Community College. (2015). *Decision Theory*. (Electronic) Accessible: <https://people.richland.edu/james/summer02/m160/decision.html> (2015-05-13)
- Rundlöf, M., Andersson, G.K.S., Bommarco, R., Fries, I., Hederström, V., Herbertsson, L., Jonsson, O., Klatt, B.K., Pedersen, T., Yourstone, J., Smith, H.G. (2015). *Seed coating with a neonicotinoid insecticide negatively affects wild bees*. *Nature*, 521.
- Samson, A. (Ed.) (2014). *The Behavioral Economics Guide 2014 (With a Foreword by George Loewenstein and Rory Sutherland) (1st ed.)*.
- Sigma Aldrich. (2004). *Material Safety Data Sheet TAU-FLUVALINATE*. Version 1.4. 1-5.
- STATENS OFFENTLIGA HANDLINGAR SOU (2007). *Reach – genomförande och sanktioner SOU 2007:80*. Stockholm: Edita Sverige AB.

- Thurston County Health Department (2013). *Tau-fluvalinate*. Olympia, Thurston County Health Department.
- Troffaes, M. C. M. (2007). *Decision making under uncertainty using imprecise probabilities*. *International Journal of Approximate Reasoning*, 45(1), 17–29.
<http://doi.org/10.1016/j.ijar.2006.06.001>
- UK Government. (2015). *Alternatives to insecticides/neonicotinoids*. (Electronic) Accessible:
https://www.gov.uk/government/uploads/system/uploads/attachment_data/file/244128/RFI5741-121206- EAC- Key_brief.pdf (2015-04-30)
- US EPA. (2012). *Species Sensitivity Distributions (SSDs)*. (Electronic) Accessible:
http://www.epa.gov/caddis/da_advanced_2.html (2015-05-03)
- US EPA. (2013). *Estimation Program Interference (EPI) Suite*. (Electronic) Accessible:
<http://www.epa.gov/oppt/exposure/pubs/episuite.htm> (2015-05-11)
- US EPA. (2015). *Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11*. Washington DC: United States Environmental Protection Agency.
- USEtox® Org. (2013). *What is the relation between kdeg (s-1) and half-life (days/hrs)?* (Electronic) Tillgänglig: <http://www.usetox.org/forum/other-questions/what-relation-between-kdeg-s-1-and-half-life-dayshrs> (2015-05-11)
- USEtox®. (2015). 2015-04-06.
- Walker, C.H., Sibly, R.M., Hopkin, S.P., Peakall, D.B. (2012). *PRINCIPLES OF ECOTOXICOLOGY*. Boca Raton: Taylor & Francis Group.
- Walport, M., Craig, C. (2014). *Innovation: Managing Risk, Not Avoiding It*. London: The Government Office for Science.
- Zhejiang Rayfull Chemicals Co., Ltd. (2012). *Thiacloprid*. (Electronic) Accessible:
<http://www.rayfull.com/Productshows.asp?ID=644#.VUzETPntmkp> (2015-05-05)

8. Appendix

Appendix 1. Input values for Thiocloprid and Tau-fluvalinate where MW is Molecular weight, K_{OW} is Partitioning coefficient between octanol and water, K_{oc} is Partitioning coefficient between organic carbon and water, K_{H25C} is Henry law coefficient (at 25°C), P_{vap25} is Vapor pressure (at 25°C), Sol₂₅ is Solubility (at 25°C) and K_{DOC} is Partitioning coefficient between dissolved organic carbon and water. Values collected from European Commission (2004), FAO (2005), EPA (2003), Thurston County Health Department (2013), EPA (2005), NCBI (2015) and EFSA (2010).

CAS		111988-49-9		102851-06-9
		Thiocloprid		Tau-fluvalinate
MW	g.mol ⁻¹	2,53E+02		5,03E+02
K_{ow}	---	1,80E+01		1,82E+04
K_{oc}	L.kg ⁻¹	6,15E+02		2,40E+02
K_{H25C}	Pa.m ³ .mol ⁻¹	5,00E-10		1,20E-04
P _{vap25}	Pa	8,00E-12		5,25E-09
Sol ₂₅	mg.kg ⁻¹	1,85E-01		1,20E-02
K_{DOC}	L.kg ⁻¹	5,02		8,62E+05

Appendix 2. Calculated degradation rates and input values for Thiocloprid and Tau-fluvalinate where k_{deg_P} is Degradation rates in above-ground plant tissues, k_{deg_A} is Degradation rates in air, k_{deg_W} is Degradation rates in water, $k_{deg_{sd}}$ is Degradation rates in sediment and $k_{deg_{SI}}$ is Degradation rates in soil. Values are calculated with EPI Suite™ with values collected and transformed from ChemSpider (2015), European Commission (2004), EFSA (2010), EPA (2005) and values in Appendix 1.

CAS		111988-49-9		102851-06-9
		Thiocloprid		Tau-fluvalinate
k_{deg_P}	s ⁻¹	1,20E-08		7,10E-09
k_{deg_A}	s ⁻¹	6,70E-05		2,20E-05
k_{deg_W}	s ⁻¹	6,02E-08		3,55E-08
$k_{deg_{sd}}$	s ⁻¹	5,42E-07		3,20E-07
$k_{deg_{SI}}$	s ⁻¹	1,20E-07		7,10E-08