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National Scenarios - Norway

Introduction of national scenarios for approval of new pesticides in Norway

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Sammendrag:

Dette er en samlerapport for prosjektet Norske Scenarier for periodene 1999-2002 og 2005-2008, med hovedvekt på modelleringsarbeidet som er gjort vha. modellene MACRO og PRZM. Målet med prosjektet har vært å forbedre risikovurderingsarbeidet i Norge ved å utvikle overflate- og grunnvannsscenarier som kan være representative for norske forhold, og for senere kunne bruke disse ved godkjenning av nye plantevernmidler. Dette har vært et samarbeid mellom Bioforsk Plantehelse, Universitetet for miljø og biovitenskap (UMB) og Mattilsynet.

Summary:

This is a final report for the project Norwegian Scenarios from the periods 1999-2002 and 2005-2008, mainly focusing on the simulations done with the models MACRO and PRZM. The aim of this project was to improve the risk assessment work in Norway by establishing surface- and groundwater scenarios which could be representative for Norwegian conditions and to later use these for approval of new pesticides. This project has been a cooperation between Bioforsk Plantehelse, Norwegian University of Life Sciences and the Norwegian Food Safety Authority.

Approved	Project leader
Børge Holen	Ole Martin Eklo
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Preface

The main goal of the project was to improve the risk assessment work by using pesticide leaching models for approval of new pesticides. A part of the project was therefore to establish scenarios from experimental fields which could be representative for Norwegian conditions. In order to calibrate and validate the risk assessment models, it was necessary to do field experiments and laboratory studies to achieve data for the models. This project started in 1999 and has, after an assignment from the Norwegian Food Safety Authority, been funded by the “Action plan on reducing risk connected to the use of pesticides”.

The project has been a cooperation between Bioforsk, Plant Health and Plant Protection Division (Ole Martin Eklo (project leader), Randi Bolli, Marit Almvik and Marianne Stenrød), Norwegian University of Life Sciences (Lars Egil Haugen, Gunnhild Riise, Helge Lundekvam and Trond Børresen) and the Norwegian Food Safety Authority (Terje Haraldsen and Roger Holten). The Norwegian Food Safety Authority has been an important partner actively participating in both development of scenarios and model simulations. Kjell Wærnhus at Bioforsk performed the pesticide sprayings of the fields.

Contents

1. Summary

The aim of this project was to improve the risk assessment of pesticides in Norway by establishing scenarios from experimental fields which could be representative for Norwegian conditions. To calibrate and validate the risk assessment models, field experiments and laboratory studies were performed. Dissipation studies were carried out at the field sites Heia and Rustad, while runoff studies were carried out at the experimental fields Bjørnebekk and Syverud. All sites are located in the South East of Norway.

The models MACRO and PRZM were calibrated and validated using results from laboratory studies and field experiments. The results obtained by the simulations from Heia and Rustad indicated high concentrations of pesticides in the drainage water. Water and solute fluxes were not included in the first experiments (Heia and Rustad), but in the field plot at Bjørnebekk and Syverud flow and concentration in runoff and drainage water were measured. Both models predicted the total water flow adequately from all experimental sites. PRZM tend to overpredict the water flow during small rainfall events and underpredict during heavy rainfall events. Both MACRO and PRZM had problems to predict the fate of the strong sorbed pesticide propiconazole, while the simulations for the much more mobile pesticide metalaxyl showed a better adaptation according to observed values. The simulations also indicated that PRZM is not a good model tool regarding pesticides in the drainage water, which probably is due to the lack of macropore transport in the model.

To evaluate and compare the Norwegian groundwater scenarios with other scenarios, simulations with FOCUS-MACRO were performed for the FOCUS scenario Châteaudun and the national scenarios from Sweden and Denmark. Norwegian endpoints (data from field studies) and endpoints agreed upon in EU were used either combined with a Norwegian climate file or climate files belonging to each scenario. The simulating results for the pesticides propiconazole, metalaxyl and isoproturon showed in general that Norwegian climate resulted in a higher pesticide leakage for most scenarios, but with relatively small effects. Metalaxyl was the pesticide most affected by the climate files. Different pesticide input values for degradation and sorption gave larger effects on pesticide leaching. Pesticide parameters are dependent on soil properties and climate and will vary with different sites. These simulations have showed that it is not the climate itself which gives the largest effect on pesticide leaching, but the climate dependent parameters like degradation and sorption.

PRAESS (Pesticide Risk Assessment Exposure Simulation Shell) was tested according to earlier simulations with PRZM and FOCUS-MACRO. The simulations indicated that PRAESS predicted both the water balance and the concentration of pesticides satisfactorily for both groundwater and surface water simulations. For the groundwater simulations, PRAESS predicted the amount of pesticides in the leachate at the same level as FOCUS_MACRO especially for propiconazole and metalaxyl. The results achieved with the PRAESS simulations, showed that it is a good and user friendly tool for predicting the exposure of pesticides in surface- and groundwater resources.

2. Sammendrag

Målet med prosjektet har vært å forbedre risikovurderingsarbeidet i Norge ved å utvikle scenarier som kan være representative for norske forhold. For å kalibrere og validere modellene var det nødvendig å utføre feltforsøk og laboratoriestudier. Studier på forsvinningsbildet av utvalgte plantevernmidler ble utført på forsøksfeltene Heia og Rustad, mens avrenningsmålinger ble gjennomført fra forsøksarealer på Bjørnebekk og Syverud. Alle forsøksfeltene er lokalisert i sørøstlig deler av Norge.

Modellene MACRO og PRZM ble kalibrert og validert ved hjelp av resultater fra laboratoriestudiene og feltforsøkene. Resultater fra simuleringene gjort på feltene Heia og Rustad, indikerte høye konsentrasjoner av plantevernmidler i drensvannet. Målinger av vann- og pesticidfluks var ikke inkludert i det første feltforsøket (Heia and Rustad), men i feltforsøkene på Bjørnebekk og Syverud ble vannmengde og konsentrasjon av plantevernmidler i drens- og overflatevann målt. Begge modellene viste god tilpasning av den totale vannbalansen fra alle feltene. PRZM hadde en tendens til å overpredikere vannavrenningen ved små nedbørsepisoder og underpredikere ved store nedbørsepisoder. Begge modellene hadde problemer med å predikere konsentrasjonen av propikonazol, som er et plantevernmiddel med stor grad av binding til jordpartikler, i drens- og overflatevann. Resultatene for det mer mobile plantevernmiddelet metalaksyl viste en bedre sammenheng mellom simulerte og observert verdier. Simuleringene indikerte også at PRZM ikke er et egnet modellverktøy for beregning av mengde plantevernmiddel i drensvannet, noe som kan skyldes mangelen på en rutine for makropore transport i modellen.

For å evaluere og sammenligne de norske grunnvannsscenariene med andre scenarier ble simuleringer med FOCUS-MACRO utført for FOCUS scenariet Châteaudun og de andre nasjonale scenariene fra Sverige og Danmark. Norske data (data fra feltstudier) og data man har blitt enige om i EU ble brukt i kombinasjon med norsk klimafil eller stedsspesifikke klimafiler. Modelleringsresultatene for propikonazol, metalaksyl og isoproturon viste generelt høyere utlekking for de fleste scenariene, men med relativt små effekter. Metalaksyl ble mest påvirket av endret klima. Ulike verdier for nedbryting og sorpsjon ga en ganske stor effekt på utlekking til drensvannet. Plantevernmiddel parameterne er avhengig av jordtype og klima og vil variere fra sted til sted. Disse simuleringene har vist at det ikke er klimaet i seg selv som påvirker avrenningsmønsteret til pesticidene, men de klimaavhengige parameterne som nedbryting og sorpsjon.

PRAESS (Pesticide Risk Assessment Exposure Simulation Shell) ble testet i forhold til tidligere simuleringer med PRZM og FOCUS-MACRO. Simuleringene indikerte at PRAESS predikerte både vannbalansen og plantevernmiddelkonsentrasjonen for både grunnvann og overflatevann tilfredsstillende. Mengde plantevernmiddel i drensvannet predikert ved hjelp av PRAESS lå på samme nivå som simuleringene med FOCUS-MACRO, spesielt for propikonazol og metalaksyl. Resultatene som ble oppnådd ved hjelp av PRAESS, viste at dette er et godt og brukervennlig verktøy for å beregne eksponering av plantevernmidler i overflate- og grunnvannsressurser.

3. Introduction

The Forum for the Co-ordination of Pesticide Fate Models and their Use (FOCUS) have developed “realistic worst case scenarios” of a tier 1 European Union (EU) level assessment of leaching potential. The scenarios are lists of properties and characteristics (soil, plant, and climate) independent of simulation models. Nine groundwater scenarios have been implemented in the models PEARL, PELMO, PRZM and MACRO (Fig. 1a). The ten surface water scenarios have been developed for use with the simulation models MACRO, PRZM and TOXSWA (Fig. 1b). The models MACRO and PRZM are always combined with the fate model TOXSWA. For drainage scenarios (D) MACRO provides the input file while for runoff scenarios (R) PRZM provides the input files for TOXSWA.

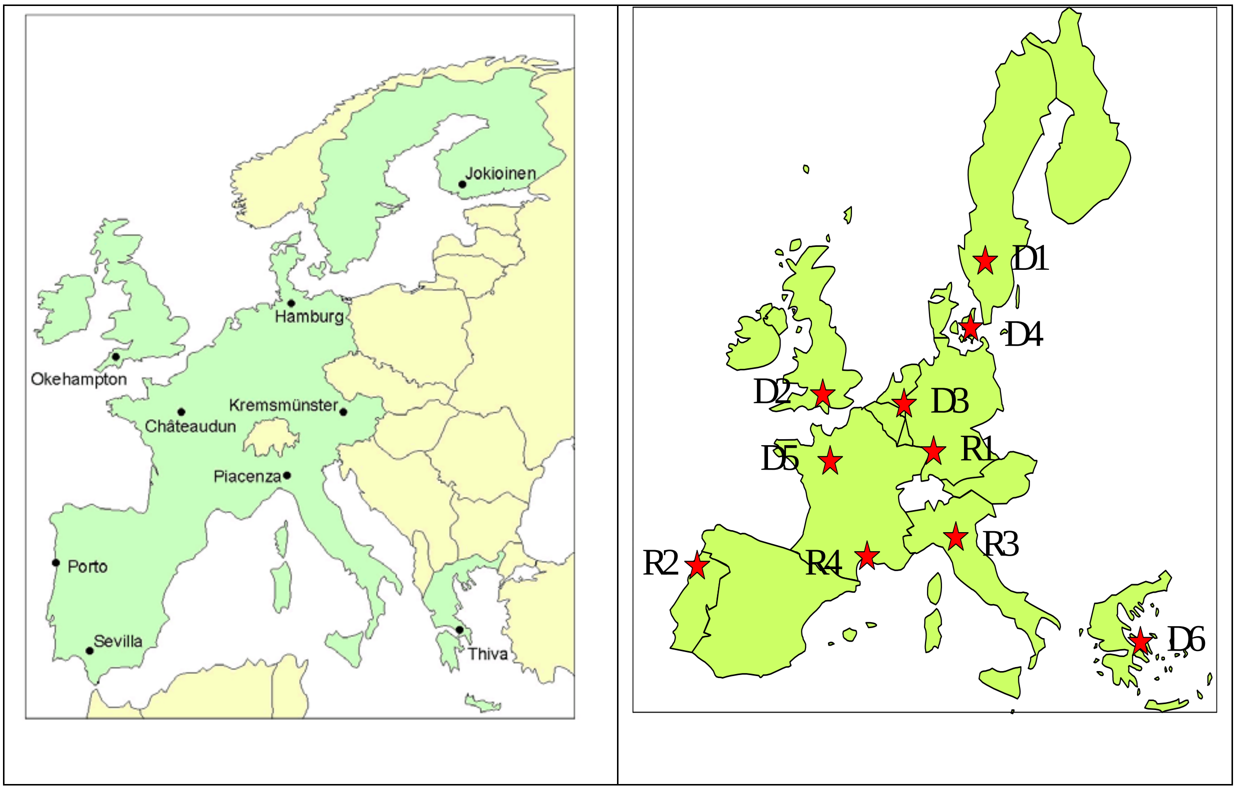

Figure 1a and 1b. Official FOCUS scenarios
a) (left) Sites for groundwater scenarios
b) (right) Sites for surface water scenarios (D=Drainage, R=Runoff)

Regardless of water solubility or affinity for solid surfaces, pesticides that are applied at agricultural fields are frequently found in brooks and rivers (Ludvigsen and Lode, 2005). Concentrations and total losses of pesticides are, however, heavily dependent on climatic conditions. Especially, precipitation events shortly after application and melting-freezing episodes during winter are of great concern with respect to runoff of pesticides (Riise et al., 2006). It has been stated from a member of the FOCUS group that the EU FOCUS scenarios do not cover the climatic conditions of Norway (Jarvis 2005, Appendix III) and experiences from field studies have showed that Norwegian climate, soil types and topography might be different from rest of Europe.
Typical climatic conditions for the Norwegian sites compared to other European sites are the combination of long periods in winter with low temperatures and snow covered ground, which usually leads to large water flow during snow melt.

The aim of this the project was to establish scenarios from experimental fields which could be representative for Norwegian conditions, and later to use these at the risk assessment work in Norway. In order to calibrate and validate the risk assessment models, it was necessary to do field experiments and laboratory studies to gather data for the models. The dissipation studies were performed in the period 1999 – 2002 at the field sites Heia and Rustad, while runoff studies in the period 2005-2008 were performed at the field sites Bjørnebekk and Syverud. Laboratory studies were carried out in soils sampled from the experimental fields. Both Sweden and Denmark have developed own national scenarios, and this work has led to three national groundwater scenarios in Sweden (Önnestad, Krusenberg and Näsbygård) and two national groundwater scenarios in Denmark (Karup and Langvad).

3.1 Climate

When the selection of the FOCUS scenarios was made, Europe was classified in different regions according to precipitation and temperature. The classification of Northern Europe is shown in Figure 2.

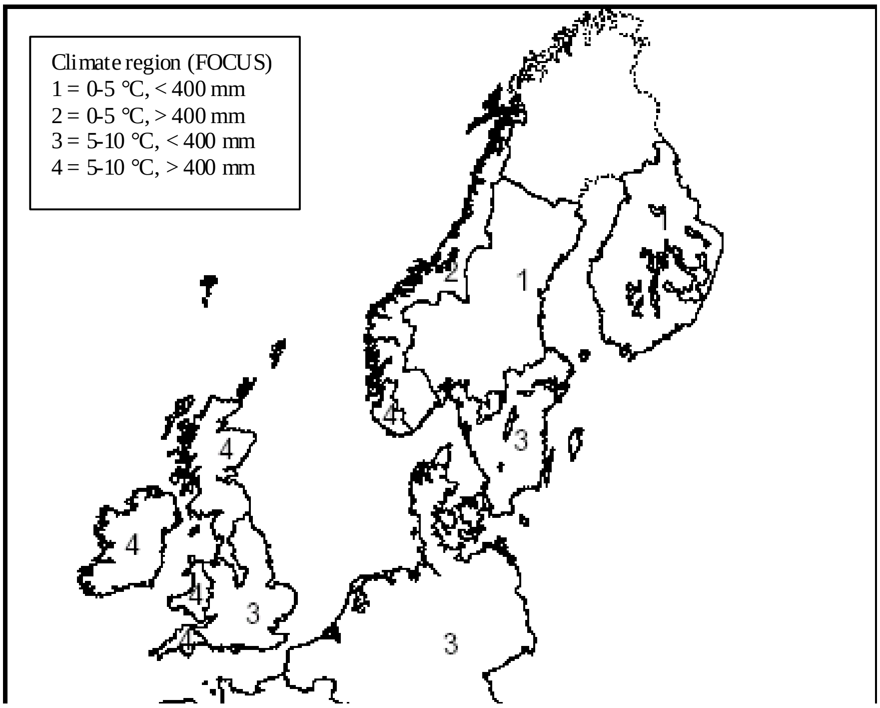

Figure 2. Climate regions based on air temperature and precipitation. The average annual air temperature and average annual precipitation are shown in the legend (Lars Egil Haugen, personal communication)

Figure 2 shows that the eastern part of southern Norway is in the same region as the mid part of Sweden and the main part of Finland (climate region 1), which has a relatively dry and cold climate. The southern part of southern Norway is closely to climate region 3 which covers Denmark and the southern parts of Sweden. The main part of Norway is in region 2, which is characterised as a cold and humid climate. This is a region we do not find in other parts of Europe. The south-west part of Norway is placed in region 4, a mild and wet climate which is typical for England. Typical climatic conditions for the Norwegian sites compared with others is the combination of long periods in winter with low temperatures and snow covered ground, which usually leads to large water flow during snow melt in spring.

Figure 2 is inaccurate for the climatic conditions in the southeast of Norway (climate region 1). Table 1 shows the annual mean temperature and annual mean precipitation for four locations in this region. All these places are located in region 1 in the figure, but have an annual mean precipitation which indicates that they should be located in region 2 (>400 mm). An annual mean precipitation of less than 400 mm in the southeast of Norway is unusual.

Table 1. Annual mean temperature and annual mean precipitation for four locations in the eastern part of southern Norway (Meteorologisk institutt, http://met.no/)

Locations	Annual mean temperature (°C)	Annual mean precipitation (mm)
Hamar	3.9	575
Roverud	3.8	660
Rygge	5.3	785
Ås	5.6	829

3.2 Soil

The Norwegian Forest and Landscape Institute has mapped about half of the agricultural land in Norway, which is approximately 3 % of the total area. The Norwegian sites included in this project represent three different soil types. The soil from Heia is classified as *Mollic Stagnosol* (THd) according to the World Reference Base for Soil Resources (IUSS Working Group WRB, 2006). Stagnosols are soils which periodically are saturated by stagnating water, and who often have problems with the drainage. This soil type represents about 0.7 % of the mapped agricultural area. The soils from Rustad and Syverud are classified as *Epistagnic Albeluvisol* (ERk) and they represents about 12.2 % of the mapped agricultural land. Albeluvisols are clayey soils where the clay content increases with soil depth. These soils often have a good soil structure and a high content of nutrients. Bjørnebekk is an artificially levelled silty clay loam which is not classified according to the Reference Base for Soil Resources (IUSS Working Group WRB, 2006). These soils are not very productive and are prone to cracking during dry conditions, and represents about 5.1 % of the mapped agricultural area in Norway. The soil textural classes (USDA) for different sites are shown in Figure 3.

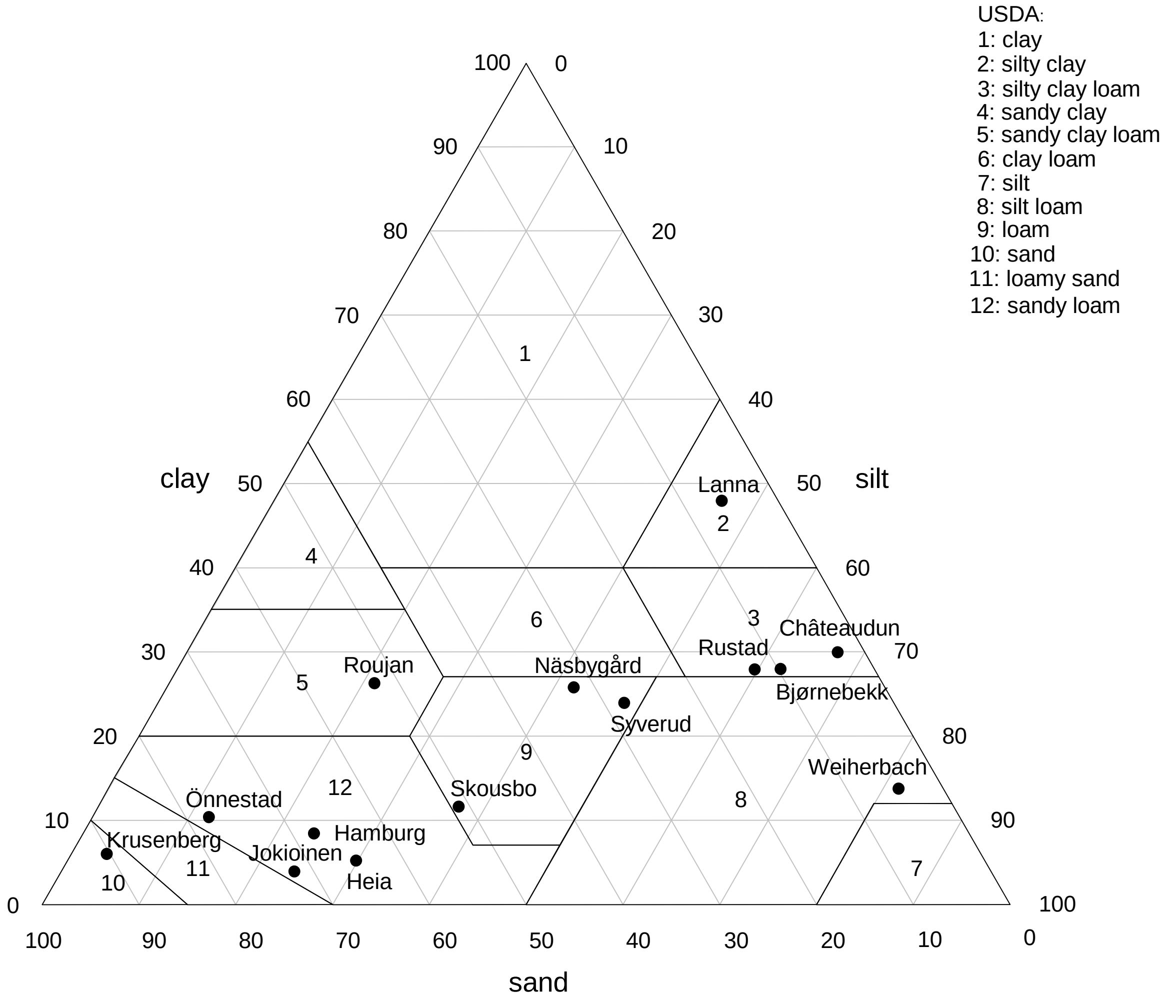

Figure 3. Soil textural classes in the top layer (0-20 cm) for different sites, according to USDA

The Norwegian site Rustad and Bjørnebekk have almost the same texture as Châteaudun and have the same clay content as the Swedish scenario Näsbygård (Figure 3). The Norwegian site Syverud has almost the same texture as Näsbygård. Heia has approximately the same soil texture as Jokioinen and Hamburg. The Swedish scenarios, Krusenberg and Önnestad, have a higher content of sand and a lower content of silt than the site at Heia. The surface runoff scenario Roujan has approximately the same clay content as Rustad, Bjørnebekk and Syverud, but has a lower content of silt and a higher content of sand. Weiherbach has almost the same sand content as Rustad and Bjørnebekk, but with a lower content of clay and a higher content of silt. The figure shows that there are small differences between the Norwegian soil types compared to the other soil types in the FOCUS scenarios. Soil types in combination with climate play an important role in pesticide leaching. Even small differences in texture between soil types might give large effects on the simulation results, since the pesticide parameters like degradation and sorption are important when simulating pesticide loss.

4. Materials and methods

4.1 The pesticides

The pesticides used in this project were isoproturon, metalaxyl and propiconazole. Isoproturon and metalaxyl in the period 1999-2002 and metalaxyl and propiconazole in the period 2005-2008. Values for the pesticides are achieved from the IUPAC Footprint database.

<u>Isoproturon</u>
The phenylurea herbicide isoproturon (IPU) was earlier used for pre- and post-emergence control of annual grasses and broadleaved weeds in spring and winter cereals. The manufacturer of this pesticide withdrew the commercial product in 2003 because of concern about its health- and environmental properties with a potential risk for cancer and groundwater pollution. The pesticide is fairly soluble in water (70.2 mg/L), is only weakly retained by sorption (Koc = 122) and could therefore reach ground- and surface waters via leaching through the soil profile. Typical half-life for isoproturon in soil at 20°C is 12 days. The major degradation product is monodesmethyl-isoproturon (MMU).

<u>Metalaxyl</u>
Metalaxyl is a systemic fungicide with high water solubility (7100 mg/L), and is stable to both aquatic photolysis and hydrolysis at pH 7. Metalaxyl shows low sorption to soils (Koc = 500 ml/g) and can be rapidly leached from sandy soils that are low in organic matter. It is usually moderately persistent in soil with common half-lives of approx. 42 days at 20°C.

<u>Propiconazole</u>
Propiconazole is a systemic fungicide with moderate water solubility (150 mg/L), and is stable to aqueous photolysis, but may be hydrolyzed with a half-life of 54 days at pH 7. In soil propiconazole is slightly mobile (Koc = 1086 ml/g). Typical half-life for propiconazole in soil at 20°C is 90 days.

4.2 Laboratory studies

Degradation and sorption studies were performed with topsoil and subsoil from all experimental fields.

4.2.1 Degradation study

<u>Isoproturon</u>
Fresh samples were sieved to pass a 2 mm screen and pre-incubated for 1 week at 20°C and at 50 % water holding capacity. Isoproturon was applied at a rate of 5 µg/g to 50 g/g of soil in separate beakers bringing the soils to a water holding capacity of 60 %. Triplicate samples of loosely capped beakers were incubated in the dark at 20°C for eight incubation periods (Eklo et al., 2002).

<u>Metalaxyl and propiconazole</u>
The soils were sieved and stored at 4°C for six weeks before the pre-incubation started. Before application of pesticides, the sieved soils were pre-incubated for one week at 20°C at 40 % of their water holding capacity. Water was added to bring the soils to a water holding capacity of 60 %. The soils were incubated in the dark at 20°C and water was added weekly to restore losses. Triplicate samples were run for seven incubation periods: 0, 1, 2, 4, 6, 9 and 12 weeks (Eklo et al., 2008). The degradation study were performed according to the OECD guideline 307 “Aerobic and Anaerobic Transformation in Soil” (OECD, 2002).

4.2.2 *Sorption study*

Isoproturon, metalaxyl and propiconazole

The soil samples were air dried and sieved before use in the sorption experiments. The sorption isotherms were determined according to the OECD guideline 106 “Adsorption/desorption using a batch equilibrium method” (OECD, 1997), in 0.01 M $CaCl_2$ and at room temperature (20°C ± 1°C). The duration of the sorption experiments was 24 hours, which is sufficient for reaching apparent sorption equilibrium according to previous kinetics measurements for propiconazole by Thorstensen et al. (2001) and for metalaxyl by Olsen-Ingerø (1999). For more information see Eklo et al., 2008 and Wu and Riise, 2001.

4.3 Field experiments

The project has been divided into two phases;

1. Dissipation studies with isoproturon and metalaxyl at the field sites Heia and Rustad (1999-2002). In 1999, the only field experiment with isoproturon was at the Rustad field. Modelling was performed from the period using MACRO and PRZM, mainly to compare these two models regarding groundwater modelling (Haugen et al., 2002).

2. Propiconazole and metalaxyl in surface and drainage water from the field sites Syverud and Bjørnebekk (2005-2008). Modelling was performed from the period with MACRO and PRZM (Eklo et al., 2008 and Eklo et al., 2009).

A preliminary conclusion from the first field experiments (phase 1) was that the lack of comparison with measured water and solute fluxes made parameterisation uncertain. The simulations indicated relative high concentrations of the pesticides in the drainage water, and this had to be evaluated further. This was the reason for extending the investigations to include small field plots equipped with systems for sampling drainage and surface runoff.

4.3.1 *Dissipation studies at the field sites Heia and Rustad*

The field sites at Heia and Rustad are located in respectively Råde (Østfold) and Ås (Akershus) in the South East of Norway.

Experimental sites

Heia

The experimental field are situated in an area close to the coastline and has mild winters and early springs compared to the general climate in Norway. Because of the early spring and suitable soil for agriculture, production of vegetables and potatoes are important and beside cereals the most frequently grown crops in the area. This region represents one of the most intensively cultivated areas in Norway and the use of pesticides and nutrients are important.

Figure 4. A field with cabbage in the area

Normal annual precipitation is approximately 800 mm, while the normal annual mean temperature is about 5.6°C. The normal temperature is below zero in the winter months December, January and February. July is the warmest month with a mean temperature of about 15°C.

The dissipation studies were carried out in a sandy loam soil; for soil characterisation, see Table 2.

Table 2. Soil characterisation of the field site Heia

Layer	Depth	Sand	Silt	Clay	Tot C	Tot N	pH		Soil density
	cm		%		%	%	H_2O	$CaCl_2$	g cm^{-3}
Ap	0-30	64.9	29.9	5.2	2.2	0.05	6.4	5.6	1.39
Eg/Bt	30-40	55.7	40.3	4.0	0.3	0.05	6.1	5.4	1.69
Bt	40-60	46.3	40.5	11.1	0.1	0.05	6.1	5.5	1.68
BCg	60+	51.4	38.4	10.2	0.1	0.05	6.4	5.9	1.73

Rustad

The total catchment area where the field site Rustad is located is approximately 450 ha. The main land use is agriculture with a total area of 272 ha in addition to a forested area of 129 ha.

Figure 5. Overview of the area where the field site Rustad are situated

Figure 6. The farm Rustad

Cereal crops are the main crops in the catchment area and constitute about 80 - 90 % of the arable land. Other crops are potatoes and meadow.

The average annual temperature for Ås is 5.3°C, with a minimum of –4.8°C in January/February, and a maximum of 16.1°C in July. The normal annual precipitation is 785 mm, with a minimum of 35 mm in February and a maximum of 100 mm in October. Winters are usually relatively unstable, with alternating periods of freezing and thawing

The dissipation studies were carried out in a silty clay loam soil; for soil characterisation see Table 3.

Table 3. Soil characterisation of the field site Rustad

Layer	Depth	Sand	Silt	Clay	Tot C	Tot N	pH		Soil density
	cm		%		%	%	H_2O	$CaCl_2$	g cm^{-3}
Ap	0-26	12.7	60.1	27.4	1.9	0.15	6.6	5.8	1.32
Eg/Bt	26-34	9.5	57.3	33.2	0.4	0.05	5.7	4.9	1.75
Bt	34-71	6.3	55.3	38.5	0.3	0.05	6.6	5.6	1.62
BCg	71+	8.8	53.2	38.1	0.3	0.05	7.1	6.1	1.75

Treatment of sites, sampling procedure and analysis

The experimental design was a split-plot randomised block with four replicates. Three replicate samples were sampled at each sampling time. These replicate soil samples were bulked and mixed. None of the subplots were sampled twice in order to avoid side effects of the sampling. The field dissipation studies were performed with the pesticides isoproturon and metalaxyl together with potassium bromide (KBr) to follow the transport of water. The sampling was carried out five times during a season, and it was sampled at four depths: 0-20 cm, 20-40 cm, 40-60 cm and 60-80 cm. Isoproturon, metalaxyl and their metabolites were extracted from soil, concentrated by solid phase extraction and analysed by HPLC.

4.3.2 Runoff studies from the experimental fields at Bjørnebekk and Syverud

The sites Bjørnebekk and Syverud are located approximately 5 km apart, both in a distance of 4-5 km from Ås, 30-35 km South to South East of Oslo.

Experimental sites

Bjørnebekk

The plots were 22 m long and 8 m wide with a slope of 13 %. The soil is artificially levelled silty clay loam with poor aggregate stability. Below the plough layer the soil at Bjørnebekk is especially rich in clay (Table 4). In general, the soil at Bjørnebekk is not very productive and prone to cracking during dry conditions. Both surface runoff and erosion are quite extensive. The site is, however, representative for levelled soil rich in clays typically found in several counties in the South East of Norway (Eklo et al., 2008).

Figure 7. Bjørnebekk 12th of May 2005

Figure 8. Bjørnebekk 16th of June 2005

Table 4. Soil characterisation of the field site Bjørnebekk

Layer	Depth cm	Sand	Silt %	Clay	Tot C %	Tot N %	pH H_2O
Ap	0-10	9	64	26	1.5	0.2	5.95
A/B	10-13	14	64	23	0.6	0.1	5.98
Cg1	13-50	1	57	42	0.3	0.1	7.08
Cg2	50+	1	54	45			7.64

Syverud

The experimental plots are 27 m long and 7 m wide with a slope of 13 %. The soil at Syverud is loam/silt loam with a higher content of nutrients, richer in coarser size fractions, better aggregate stability, higher infiltration rate (drainable pore volume 16 %) and less susceptible to erosion compared to the soil at Bjørnebekk (Lundekvam & Skøien, 1998). Soil loss from the fields is generally less than 1/30 of the loss at Bjørnebekk. Crop productivity is approximately 50 % higher at Syverud compared to Bjørnebekk. The soil at Syverud was tile drained more than 40 years ago, so changes in physical conditions are well stabilized. Soil characterisation from the experimental field at Syverud is shown in Table 5.

Figure 9. Syverud 12th of May 2005

Figure 10. Syverud 16th of June 2005

Table 5. Soil characterisation of the field site Syverud

Layer	Depth cm	Sand	Silt %	Clay	Tot C %	Tot N %	pH H_2O
Ap1	0-10	26	47	27	3.1	0.29	5.45
Ap2	10-22	25	48	27	2.9	0.28	5.47
Eg	22-48	25	57	18	0.4	0.05	5.59
Btg	50-70	17	53	30	0.3	0.05	6.00
Cg	70+	13	48	39			6.67

Treatment of sites, sampling procedure and analysis

Plots at Bjørnebekk were subject to autumn ploughing and spring ploughing, while plots at Syverud only were subject to autumn ploughing. All plots were subject to harrowing in spring. The pesticides, metalaxyl and propiconazole, were applied in June and the tracer KBr was applied at the same time to follow the transport of water.

The individual plots were separated by soil mounds and a ditch in the upper end. At the lower end of the field was a perforated pipe that collected surface runoff from the plot (Figure 11). Water that drained through the pipes entered a tilting bucket that recorded the amount of water (Figure 12). The number of tilts was recorded continuously by data loggers with 5 min. resolution. Water proportional samples were collected from surface runoff from Bjørnebekk and surface runoff and drainage water from Syverud. The sampling frequency varied from few days to several weeks depending on amount of runoff. The water samples were analysed according to an accredited multi method for water (Holen and Christiansen, 2005).

Figure 11. Perforated pipe that collects surface water

Figure 12. Container which contains the tilting bucket sampler

4.4 The models

4.4.1 MACRO

MACRO is a physically-based one-dimensional numerical model of water flow and reactive solute transport in field soils (Jarvis, 1994). The model calculates coupled unsaturated-saturated water flow in cropped soil, including the location and extent of perched water tables, and can also deal with saturated flow to field drainage systems. The model accounts for macropore flow, with the soil porosity divided into two flow systems or domains (macropores and micropores) each characterised by a flow rate and solute concentration. Richards' equation and the convection-dispersion equation are used to model soil water flow and solute transport in the soil micropores, while a simplified capacitance type-approach is used to calculate fluxes in the macropores. Exchange between the flow domains is calculated using approximate, physically-based, expressions based on an effective aggregate half-width. Additional model assumptions include first-order kinetics for degradation in each of four "pools" of pesticide in the soil (micro- and macropores, solid/liquid phases), together with an instantaneous sorption equilibrium and a Freundlich sorption isotherm. A more detailed description of the model can be found in the MACRO user's manual (Stenemo & Jarvis, 2003).

Parameter estimation

The first parameterisation of MACRO was performed with measurements from the field experiment at Rustad together with degradation studies of the pesticides (see chapter 5.1.1). These data were used for the main parameterisation. The degradation studies of the pesticides were only performed for the upper 40 cm of the soil. The decrease in degradation as a function of depth recommended in FOCUS (2000) was as follow; 50 % of $DT_{50\ topsoil}$ in the 40-60 cm, 30 % of $DT_{50\ topsoil}$ in the 60-100 cm and no degradation below 100 cm depth. The Q_{10} – value was set to 2.2 and the Freundlich exponent was set to 0.9. The soil physical parameters were adjusted using the measured values of bromide in the 20 cm layer, and thereafter the soil chemical and biological parameters using the measured values of the pesticides in the soil layers.

The measured soil characteristics included water retention measurements and saturated hydraulic conductivity of undisturbed soil samples from a nearby soil profile. Soil water retention was measured at the following matrix potentials: 0, -0.8, -2, -5, -10, -50, - 100 and -1500 kPa. For the soil surface layer some measurements of the unsaturated hydraulic conductivity with a tension infiltrometer were included. Plant development was estimated from the air temperature ("degree-days approach"). Total depth of the simulated soil profile was 190 cm containing 22 layers with a thickness of 3-4 cm down to 60 cm depth. The same parameterisation was also made for Heia. For more information regarding parameters, see appendix I.

Syverud

The file which gave the best results for the transport of bromide from Rustad was used as the starting point for parameterisation at Syverud. Some soil characteristics for the site are shown in Table 5. The following changes were performed according to scenario specific data and recommendation for FOCUS-MACRO parameterisation:

- Soil profile
  - number of layers reduced to 15 from 22 (according to guidelines for FOCUS-MACRO)
- Start conditions
  - soil water content set according to drainage depth and measured field capacity
- Soil physical characteristics
  - according to measured soil water retention for three depths at the site
- Site specific data
  - the snow melting function changed from 2 to 4.5 mm per degree
  - drainage depth changed from 10 to 8 m. Drainage depth 1, 0 m is the same
- Solute transport
  - used recommended values for dispersivity (5 cm) and mixing depth (0.1 mm)
  - anion exclusion set to 0

- Plant growth
    - spring barley
    - deep root system
    - critical water potential set to -100 kPa

4.4.2 PRZM

PRZM (**P**esticide **R**oot **Z**one **M**odel) is a one-dimensional, dynamic compartment model which can be used to simulate chemical movement in unsaturated soil systems within and below the root zone (Carsel et al., 2006). The original version of the PRZM model was released in 1984 (Carsel et al., 1984), but it has been continuously improved since then. The version PRZM 3.21ß is used in the FOCUS surface water scenarios (FOCUS, 2001) for runoff and erosion modelling. The model uses a SCS curve number technique to estimate runoff and the Universal Soil Loss Equation (USLE) to estimate erosion. Evapotranspiration is estimated directly from pan evaporation or based on an empirical formula. Evapotranspiration is divided among evaporation from crop interception, evaporation from soil and crop transpiration. Water movement is simulated by the use of generalized soil parameters, including field capacity, wilting point and saturation water content. The chemical transport component can simulate pesticides or organic and inorganic nitrogen species. For pesticides, the transport components can simulate pesticide application on the soil or on the plant foliage. Dissolved, adsorbed and vapour-phase concentrations in the soil are estimated by simultaneously considering the processes of pesticide uptake by plants, surface runoff, erosion, decay, volatilization, foliar wash off, advection, dispersion and retardation.

A more detailed description of the model can be found in Carsel et al. (2006).

Parameter estimation

The parameter estimation was performed at two stages: an uncalibrated simulation followed by a simulation with calibration using the sensitive parameters. The hydrology module is always calibrated first and the pesticide module last. This is important, as water is the carrier of pesticides through the soil. Knowledge of the water flow is therefore a prerequisite of a valid description of the movement of pesticides in soil. This is a suggested procedure of Good Modelling Practice (GMP) obtained in the Cost Action 66 project (Vanclooster et al., 2000). There were three main sources of information that the parameter estimations were based on: measurements or calculation based on measurements, the PRZM3 manual or other literature sources and expert judgements. After calibration the next step was validation. In the validated simulations it is not allowed, according to Good Modelling Practice, to change parameters except data which is dependent on the climate and pesticide properties if new pesticides are introduced in the experimental field. An overview of the parameters from Syverud and Bjørnebekk can be found in appendix II. For Heia and Rustad, parameters can be found in Eklo and Haraldsen, 2002 A and 2002 B.

4.4.3 Model prediction

In the first phase of the project (1999-2002), the relation between measured and predicted values was considered by using following statistical approaches:

Modelling efficiency (ME) consider the relation between measured and predicted values for all observations.

$$ME = 1 - \frac{\sum (O_i - P_i)^2}{\sum (O_i - \overline{O})^2}$$

O = observed and P = predicted. There is a good correlation between observed and predicted values when ME is close to 1. Negative results imply that a mean value for the measurements gives a better approach than the model prediction.

Coefficient of residual mass (CRM) looks at the prediction of the amount of pesticide in the profile relative to that observed. A value close to 0 shows a good correlation between measured and simulated residues in the soil (a perfect degradation fit).

$$CRM = \frac{\sum (P_i - O_i)}{\sum O_i}$$

Coefficient of shape (CS) reflects the similarity in the shape of the predicted and observed curves. A value close to 1 indicates a perfect shape of the curves.

$$CS = \frac{\sum (O_i - \overline{O})^2}{\sum (P_i - \overline{P})^2}$$

5. Results

5.1 Laboratory studies

5.1.1 Degradation studies

Heia and Rustad

The degradation rate of isoproturon and metalaxyl was studied in topsoil and subsoil from Heia and Rustad. Table 6 shows the half-lives of isoproturon and metalaxyl in soil from the two sites.

Table 6. Half-lives (days) of isoproturon and metalaxyl in soil from Heia and Rustad

Pesticide	Rustad		Heia	
	Topsoil (0-20 cm)	Subsoil (20-40 cm)	Topsoil (0-20 cm)	Subsoil (20-40 cm)
Isoproturon	13	13	13	14
Metalaxyl	21	34	46	68

The half-life for isoproturon in topsoil and subsoil from both sites were similar. Even though the degradation rate of isoproturon was similar in the two layers, the production of monodesmethyl-isoproturon (MMU) was less pronounced in the subsoil layer from Heia. The amount of MMU reached a maximum after four weeks in the Heia subsoil, at most representing 3.2 % of the herbicide applied. Such a trend was not observed in the Rustad subsoil, as the production of MMU followed the same pattern in both soil layers, only at a lesser extent in the subsoil.

In the silty clay loam from Rustad, the transformation of metalaxyl was twice as fast in the Heia soil which implies that there were different modes of microbial degradation of the pesticides in the two soils. In the Rustad topsoil, the content of the acid-metabolite of metalaxyl was measured during the entire experimental period. After 12 weeks incubation the metabolite represented 12 % of the initial metalaxyl amount applied.

Bjørnebekk and Syverud

A degradation study was carried out with the pesticides metalaxyl and propiconazole in topsoil (0-20 cm) and subsoil (20-40 cm) from the experimental fields at Bjørnebekk and Syverud. Table 7 shows the results from the degradation study.

Table 7. Half-lives (days) of the pesticides in the topsoil and subsoil from Syverud and Bjørnebekk

Soil	Depth	Metalaxyl ($t_{1/2}$)	Propiconazole ($t_{1/2}$)
Syverud	0-20 cm	38	281
	20-40 cm	32	389
Bjørnebekk	0-20 cm	107	144
	20-40 cm	546	172

The degradation rates for metalaxyl show a faster degradation in Syverud than in Bjørnebekk, as expected from measurements of the microbial activity (Eklo et al., 2008). The degradation of metalaxyl was particularly slow in the Bjørnebekk soil ($100<t_{1/2}<550$ days) probably owing to low microbial activity. Sorption processes could influence the degradation, as metalaxyl appears to be preferentially sorbed on soil mineral surfaces (Sukop & Cogger, 1992). Despite higher microbial activity in the soils from Syverud, propiconazole had a faster degradation in the Bjørnebekk soils compared to the Syverud soils. This is probably due to stronger sorption in the Syverud soil, as organic matter plays a dominant role in the sorption of propiconazole. A Danish degradation study with propiconazole in different topsoils (0-20 cm) gave half-lives from 106-444 days, which are in accordance with our study.

5.1.2 Sorption study

A sorption study was carried out with the pesticides metalaxyl and isoproturon in topsoil and subsoil from the experimental fields at Heia and Rustad (Wu & Riise, 2001). Sorption experiments were also carried out for metalaxyl and propiconazole in top- and subsoil from the fields at Syverud and Bjørnebekk (Eklo et. al., 2008).

Sorption of isoproturon was in general higher in the topsoil compared to subsoil for both Heia (K_d=2.2 and 0.5, respectively) and Rustad (K_d=2.9 and 1.1, respectively). This can be attributed to the higher organic carbon content in the topsoil, as the organic matter is an important sorbent for hydrophobic pesticides such as isoproturon.

Metalaxyl is a mobile pesticide and the sorption of metalaxyl was higher in the soil from Rustad (K_d=1.8 and 1.2) than in the soil from Heia (K_d=0.9 and 0.6), and somewhat stronger in the topsoil compared to the subsoil. In the soil from Bjørnebekk and Syverud the sorption was in general low (K_d<1), but somewhat stronger in Bjørnebekk soil compared to Syverud soil. The results show a higher sorption in the topsoil compared to the subsoil at Syverud, corresponding with a higher organic carbon content. The results also indicated a slightly stronger sorption in Bjørnebekk subsoil compared to topsoil, which might indicate sorption to other compounds in soil than organic matter.

Propiconazole is a pesticide which generally shows a high degree of sorption to organic matter in soil. The studies indicated a connection between the sorption and the content of organic matter in soil. The strongest sorption appeared in the Syverud topsoil (K_d=25.7) followed by the Syverud subsoil (K_d=17.3) and the Bjørnebekk topsoil (K_d=20.9), and also the weakest sorption in the Bjørnebekk subsoil (K_d=5.7). Distribution coefficients adjusted for the content of organic matter in the soil showed high values for propiconazole (K_{oc}: 791-1536).

5.2 Field experiments

5.2.1 Dissipation studies at the experimental fields Heia and Rustad

Heia

In the Heia field the dissipation of isoproturon was fast, nearly 80 % of the isoproturon applied was lost during the first 22 days (Figure 13). Only minor amounts leached below 20 cm depth during the experiment, due to low precipitation in the first period after spraying. The isoproturon front reached a depth of 80 cm 40 days after application to the field, which is in accordance with the bromide analysis. The analysis showed that the bromide front had reached a depth of 80 cm 40 days after application. The dissipation half-life of isoproturon was calculated to be 16 days in the 0-20 cm layer and 22 days in the 0-80 cm layer. The appearance of the degradation product MMU was monitored during the entire experimental period. The highest concentration of MMU represents 13 % of the initial herbicide concentration at Heia.

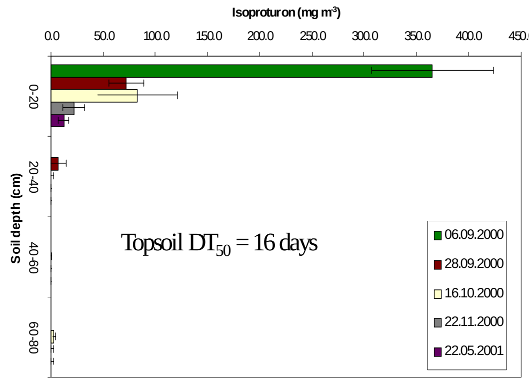

Figure 13. Distribution of isoproturon (mg/m^3) at Heia, 2000-2001

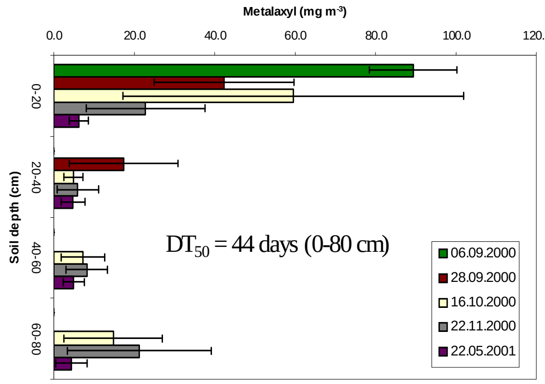

Figure 14. Distribution of metalaxyl (mg/m^3) at Heia, 2000-2001

Whereas very little of isoproturon could be recovered from the deeper layers, metalaxyl was readily found below the plough layer (Figure 14). Forty days after application, metalaxyl was found in the bottom layer, representing 16.5 % of the initial amount applied. This corresponds well with the lower sorption and higher water solubility of metalaxyl compared to isoproturon. Metalaxyl showed a dissipation half-life of 44 days in the topsoil and 169 days in the entire profile.

Rustad

Isoproturon was rapidly degraded in the silty clay loam from Rustad and was not particularly susceptible to leaching below 20 cm soil depth. Less than 10 % of isoproturon applied, leached below 20 cm depth. Figure 15 shows the distribution of isoproturon in 2000-2001. Isoproturon showed a dissipation half-life of 16 days in the topsoil and 22 days in the entire profile. Appearance of the major degradation product MMU in the field was monitored during the entire experimental period, at most representing 6 % of the initial herbicide concentration at Rustad.

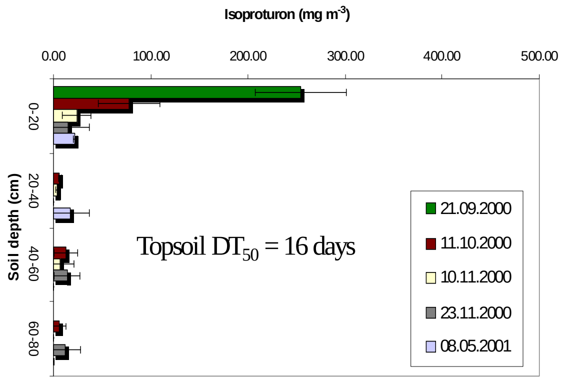

Figure 15. Distribution of isoproturon (mg/m^3) at Rustad, 2000/2001

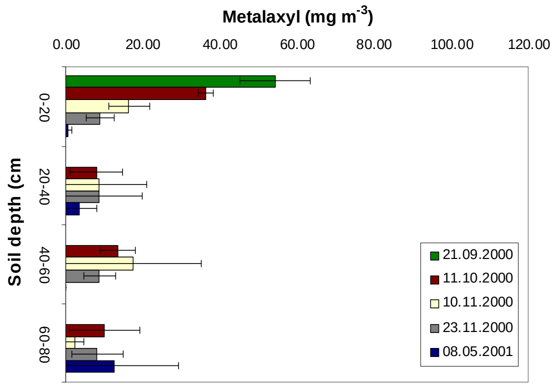

Figure 16. Distribution of metalaxyl (mg/m^3) at Rustad, 2000/2001

Compared to isoproturon metalaxyl leached at a higher extent in the Rustad profile (Figure 16). Twenty days after application of metalaxyl to the field, all of the applied metalaxyl could be recovered from the profile and the amount in the 60-80 cm layer constituted of 18 % of the applied amount. Metalaxyl showed a dissipation half-life of 25 days in the topsoil and 86 days in the entire profile. The dissipation half-lives of metalaxyl at Heia (DT_{50} = 169 days) were about twice as large as those found at Rustad (DT_{50} = 86 days). Table 8 shows a summary of the dissipation half-lives of isoproturon and metalaxyl for both fields.

Table 8. Dissipation half-lives (days) for isoproturon and metalaxyl at Heia and Rustad for the period 2000-2001

Pesticide	Rustad		Heia	
	Topsoil (0-20 cm)	Profile (0-80 cm)	Topsoil (0-20 cm)	Profile (0-80 cm)
Isoproturon	16 days	22 days	13 days	21 days
Metalaxyl	25 days	86 days	44 days	169 days

5.2.2 Runoff studies from the experimental fields at Bjørnebekk and Syverud

There are several advantages with small scale field experiments. The plots are subject to ordinary agricultural practices and natural variations in weather conditions. At the same time the experimental conditions can be more easily controlled compared to large scale catchment studies. Seasonal, annual and areal variations in runoff of pesticides are to a large extent related to differences in properties of the pesticide, the soil, soil treatment and the climate conditions. In these study two pesticides with different mobility characteristics, metalaxyl and propiconazole, were applied at two Norwegian fields with different soil erodibility and water flow pattern.

Climatic conditions and runoff pattern

For the period 2005-2006 the area received 798 mm precipitation, which is rather close to normal (785 mm). Mean temperature during the period June 2005 to May 2006 was 5.8°C, which is 0.5°C above normal (5.3°C). The cold period, February and March 2006, was colder than normal and the winter 2006 had rather high amounts of snow protecting the soil against frost. For the period 2007-2008 the area received 1066 mm precipitation which is nearly 300 mm above the normal value (176 mm in January). The average temperatures were, except for June 2007, generally above normal values, resulting in a higher mean temperature than normal. For the investigated period the mean temperature was 7.1ºC, which is 1.8ºC above the normal value.

Bjørnebekk

The soil at Bjørnebekk is more susceptible to erosion and surface runoff compared to Syverud which has a rather high infiltration capacity. For the Bjørnebekk site, higher amounts of runoff were observed during the period 2007-2008 compared to the period 2005-2006, as the runoff values for the autumn ploughing (APL) and spring ploughing (SPL) plots were 290 mm and 115 mm in the period 2005-2006 compared to 440 mm (APL) and 340 mm (SPL) in 2007-2008.

Syverud

During the period 2005-2006, 513 mm water left the field in total as surface and drainage water. During the period 2007-2008, totally 615 mm of water was transported as drainage and surface water, divided into 499 mm as drainage and 115 mm as surface runoff. The major difference between the two investigated periods is the amount of surface runoff. Surface runoff made up 115 mm in 2007-2008 and only 25 mm in 2005-2006. Increased winter temperatures and precipitation in 2008 were the major reasons for the differences in surface runoff.

Loss of pesticides

Special climate conditions promoted high loss of pesticides in the period 2007-2008. Higher loss in 2007-2008 compared to the period 2005-2006, was due to high precipitation in summer and high precipitation and temperatures in the winter of 2007-2008 (see Tables 9 and 10).

Table 9. Runoff of water (mm), loss (g/ha) and average concentrations (µg/L) of the pesticides metalaxyl and propiconazole during the period: 31.05.2005-07.10.2006. The ranges (max-min) are given in parentheses. Results are given for surface runoff (S) at Bjørnebekk (BJ) and surface runoff (S) and drainage (D) at Syverud (SY). The plots at Syverud are subject to autumn ploughing (APL), while the plots at Bjørnebekk are subject to both autumn (APL) and spring ploughing (SPL)

Plot	Runoff-type	Treat.	Runoff	Loss		Concentration	
				Metalaxyl	Propiconazole	Metalaxyl	Propiconazole
			(mm)	g/ha	g/ha	µg/L	µg/L
BJ	S	APL	290	1.546 (0.03-0.57)	0.383 (0.010-0.12)	0.53 (0.04-5.9)	0.13 (0.03-0.76)
BJ	S	SPL	115	0.593 (0.006-0.35)	0.162 (0.006-0.05)	0.51 (0.11-1.9)	0.14 (0.10-0.33)
SY	S	APL	33	0.0248 (0-0.021)	0.0265 (0-0.022)	0.075 (0-0.19)	0.080 (0-0.20)
SY	D	APL	569	0.275 (0-0.081)	0.179 (0-0.040)	0.048 (0-0.17)	0.032 (0-0.08)

Table 10. Runoff of water (mm), loss (g/ha) and average concentrations (µg/L) of the pesticides metalaxyl and propiconazole, during the period 01.06.2007- 04.04.2008. The ranges (max-min) are given in parentheses. Results are given for surface runoff at Bjørnebekk (BJ) and surface runoff (S) and drainage water (D) at Syverud (SY). The plots at Syverud are subject to autumn ploughing (APL), while the plots at Bjørnebekk have two different treatments, autumn ploughing (APL) and spring ploughing (SPL)

Plot	Runoff-type	Treat.	Runoff	Loss		Concentration	
				Metalaxyl	Propiconazole	Metalaxyl	Propiconazole
			(mm)	g/ha	g/ha	µg/L	µg/L
BJ	S	APL	444	3.579 (0.01-2.11)	1.047 (0.01-0.52)	0.81 (0.04-18)	0.24 (0.03-2.5)
BJ	S	SPL	340	1.463 (0.01-0.62)	0.380 (0-0.09)	0.43 (0.10-7.0)	0.11 (0.07-0.70)
SY	S	APL	115	0.061 (0-0.042)	0.068 (0-0.026)	0.053 (0-3.0)	0.059 (0-0.3)
SY	D	APL	499	0.385 (0-0.32)	0.079 (0-0.022)	0.077 (0-2.4)	0.016 (0-0.07)

For the mobile pesticide metalaxyl, the highest loss occurred at Bjørnebekk APL plots, next to Bjørnebekk SPL plots for both the investigated periods. At Syverud, more metalaxyl was passing through the drains than the surface runoff due to high infiltration capacity for both the investigated periods. With respect to propiconazole a relatively larger amount (%) was lost through the surface runoff from both the Syverud and the Bjørnebekk field in 2007-2008 compared to the previous period. More extensive periods with water saturated conditions leading to higher surface runoff and transport of particles are the most probable reason for the enhanced transport of propiconazole through surface runoff. Similar amount of propiconazole was lost through the drains at Syverud and through the surface runoff from the SPL plots at Bjørnebekk in 2005-2006 (0.07 %). For the period 2007-2008 the surface runoff of propiconazole from the SPL plots at Bjørnebekk was much higher than the transport trough the drains at Syverud (Table 10).

5.3 Simulations with MACRO and PRZM

National scenarios in the Nordic countries have mainly been developed for the simulation model MACRO and the scenarios are a combination of using MACRO as a groundwater model and a drainage model. In the first phase of this project, also PRZM was used for groundwater modelling even if this usually is used as a surface water model in EU. The main goal was to compare these two models and to see if they can be used for risk assessment modelling in Norway. This part of the project was carried out with a dissipation study at Heia and Rustad with no measurements of the water flux. The lack of comparison with measured water and solute fluxes made parameterisation uncertain, which was the reason for extending the investigations to include small field plots at Bjørnebekk and Syverud, equipped with systems for sampling drainage and surface runoff. The main purpose was to use PRZM to make national surface water scenarios and MACRO to make groundwater scenarios.

5.3.1 *Heia and Rustad*

The statistical approach is described in chapter 4.4.3 for the model parameters: Model efficiency (ME), coefficient of residual mass (CRM) and coefficient of shape (CS). The following limits have been used:

ME>0.6 -0.2<CRM<0.2 CS close to 1

Water flow

Potassium bromide (KBr) was applied to each field site together with the pesticides to follow the transport of water. Figure 17 and 18 shows the measured and simulated values for bromide in different soil layers at the field sites Heia and Rustad, respectively, simulated with MACRO and PRZM.

A B

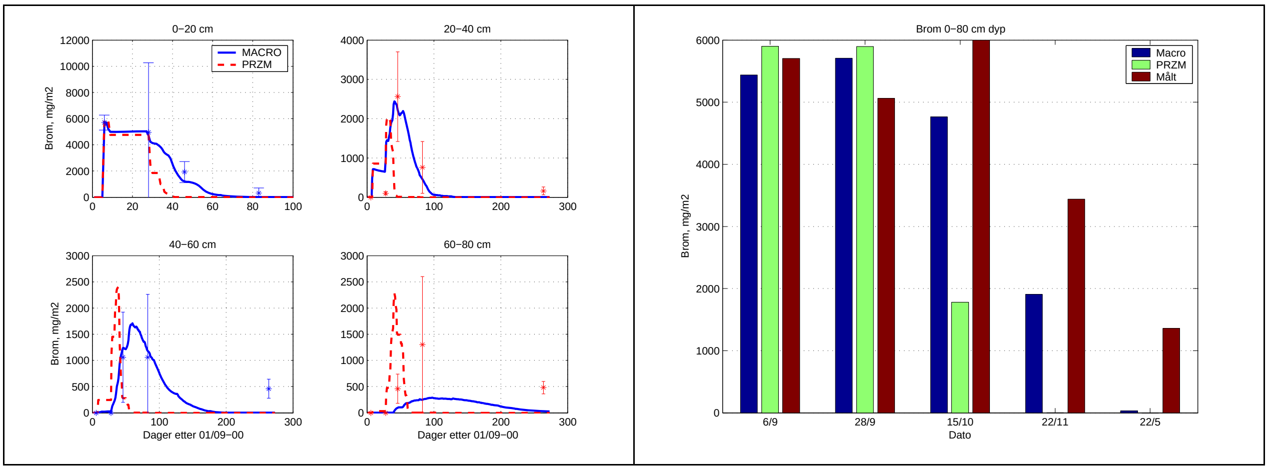

Figure 17. Measured and simulated values for bromide in soil at Heia, 2000/2001. Simulated with MACRO and PRZM.

A. *Measured and simulated values from different soil depths as a function of time*
B. *Measured and simulated mass balance from the 0-80 cm depth as a function of time*

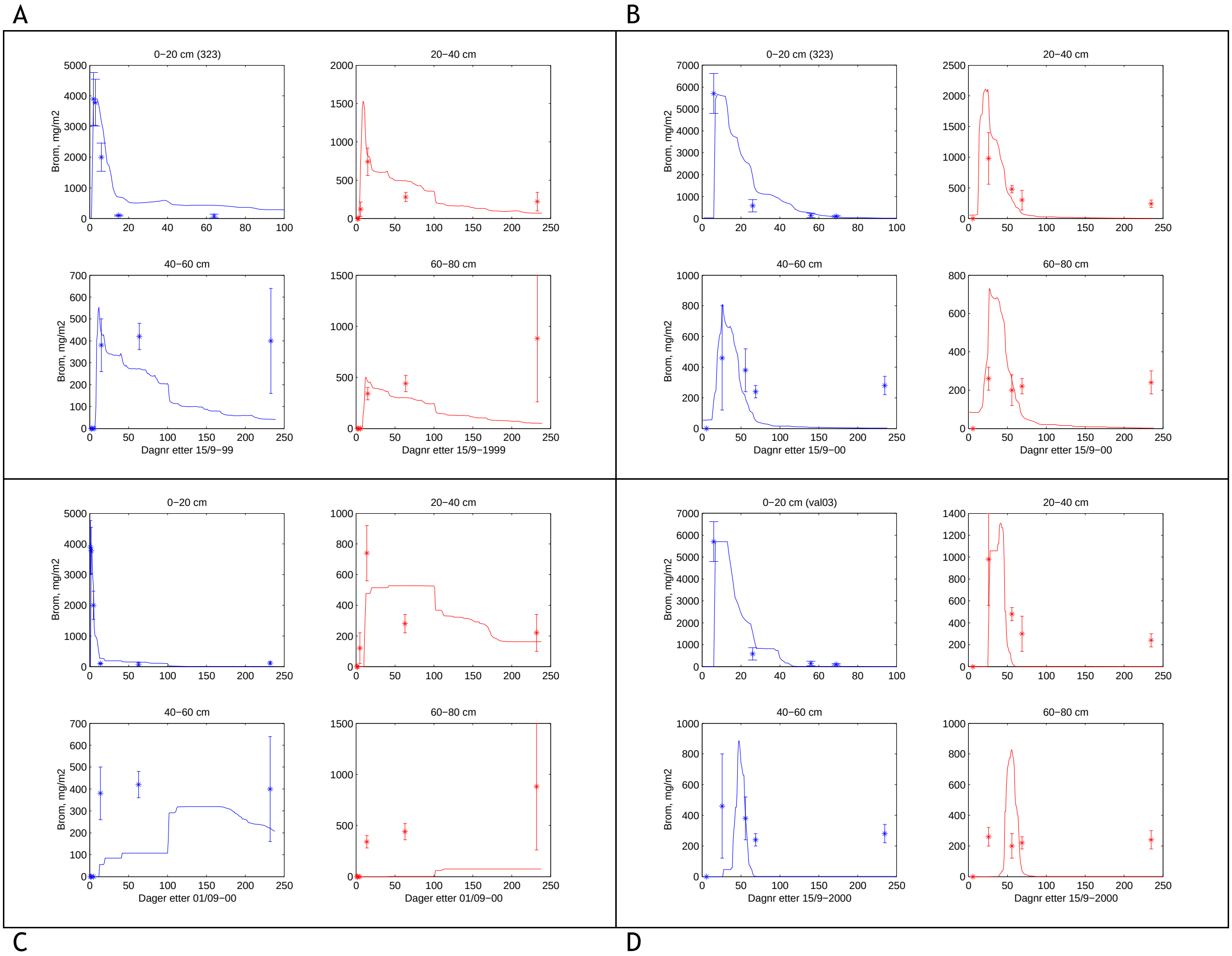

Figure 18. Measured and simulated values for bromide in soil at Rustad, 1999/2000 and 2000/2001. Simulated with MACRO and PRZM.

A. Measured and simulated values from different soil depths as a function of time – MACRO 1999/2000
B. Measured and simulated values from different soil depths as a function of time – MACRO 2000/2001
C. Measured and simulated values from different soil depths as a function of time – PRZM 1999/2000
D. Measured and simulated values from different soil depths as a function of time – PRZM 2000/2001

The measurements of bromide for 1999 from Rustad (Figure 18) indicated a faster downward transport of bromide than simulated from the upper layers in the MACRO simulations. PRZM gives a good simulation of the water movement in the upper layer. The opposite trend was found for the deeper layers, where the simulations showed a faster decline than the measurements. Table 11 shows the different statistical calculations for the water transport (bromide) for the fields Heia and Rustad in the years 1999 and 2000. The statistical values show that there is a good adaptation between measured and predicted values regarding the model efficiency (ME) for both models in 1999. The calculation of the coefficient of residual mass (CRM) show a good adaptation for the data from 1999, especially for MACRO, but PRZM under-predicts the residual masses. The index CS (coefficient of shape) shows good results for both models.

Table 11. Different statistical indices for model prediction of bromide

		1999			2000		
		ME	**CS**	**CRM**	**ME**	**CS**	**CRM**
Heia	MACRO				0.34	1.12	0.03
	PRZM				0.60	0.88	0.30
Rustad	MACRO	0.77	0.73	0.16	-3.80	> 100	1.32
	PRZM	0.87	1.00	-0.25	-1.30	0.34	-0.40

The results for 2000 show a poorer fit for Rustad with negative values of ME. Negative results imply that a mean value for the measurements might give a better approach than the model prediction. For Heia the results were somewhat better. Regarding the prediction of residual mass (CRM) for Rustad, PRZM under-predicts while MACRO over-predicts. For Heia the models simulate the residual mass much better. It seems, statistically, that the simulation results achieved for Rustad in 2000 was poorer than the results from 1999. However, by studying the simulations graphical it seems that the simulations fit well with the measured values. One of the reasons for the poorer statistical fit is few measurements, especially at the peak values where small deviations in time give large differences in concentrations. The overall impression is that the water transport is fairly well simulated for both models, especially from the upper soil layer (0-20 cm). Results from both fields show that MACRO gives a better prediction of the water balance, especially for deeper layers, than PRZM. In 2000, PRZM predict a very quick leaching of bromide from deeper layers for both fields. A mass balance calculation for Heia also showed that the simulated leaching is much faster than the measured disappearance of bromide from the upper layer.

Pesticides

Isoproturon, a moderately sorbed pesticide, was sprayed both years while metalaxyl, a weakly sorbed pesticide was sprayed only in the autumn 2000. The parameter file which gave the best fit for bromide was used for the pesticide simulations. Only values of sorption and degradation rate were changed according to measurements.

Isoproturon

Figure 19 and 20 show the measured and simulated values for isoproturon in different soil layers at the field sites Heia and Rustad, respectively, simulated with MACRO and PRZM.

A B

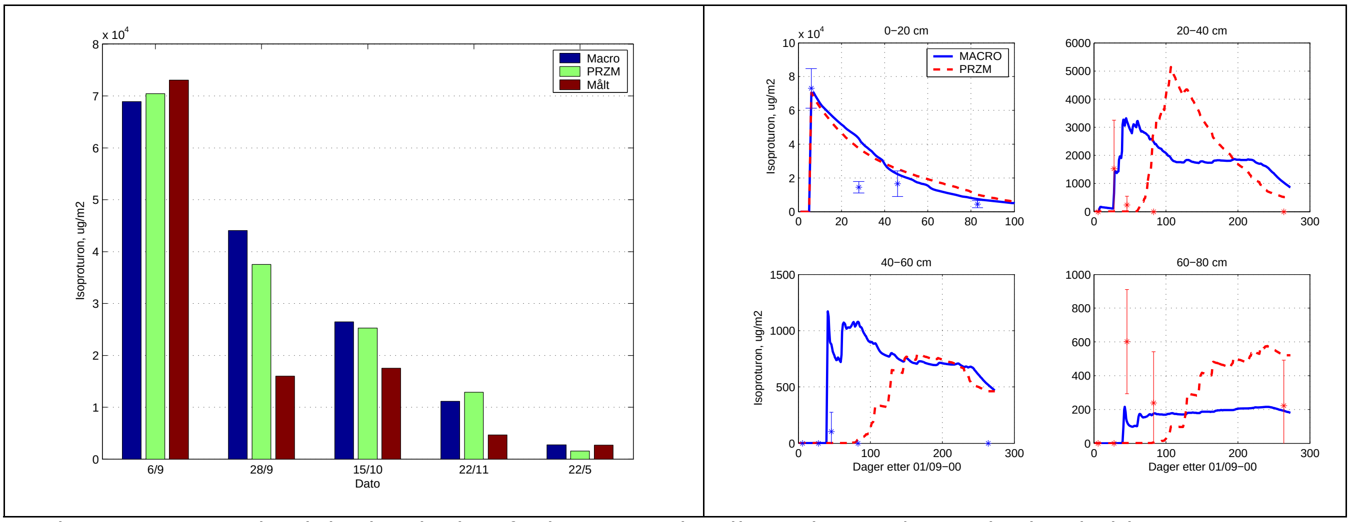

Figure 19. Measured and simulated values for isoproturon in soil at Heia, 2000/2001. Simulated with MACRO and PRZM.

- *A. Measured and simulated mass balance from the 0-80 cm depth as a function of time*
- *B. Measured and simulated values from different soil depths as a function of time*

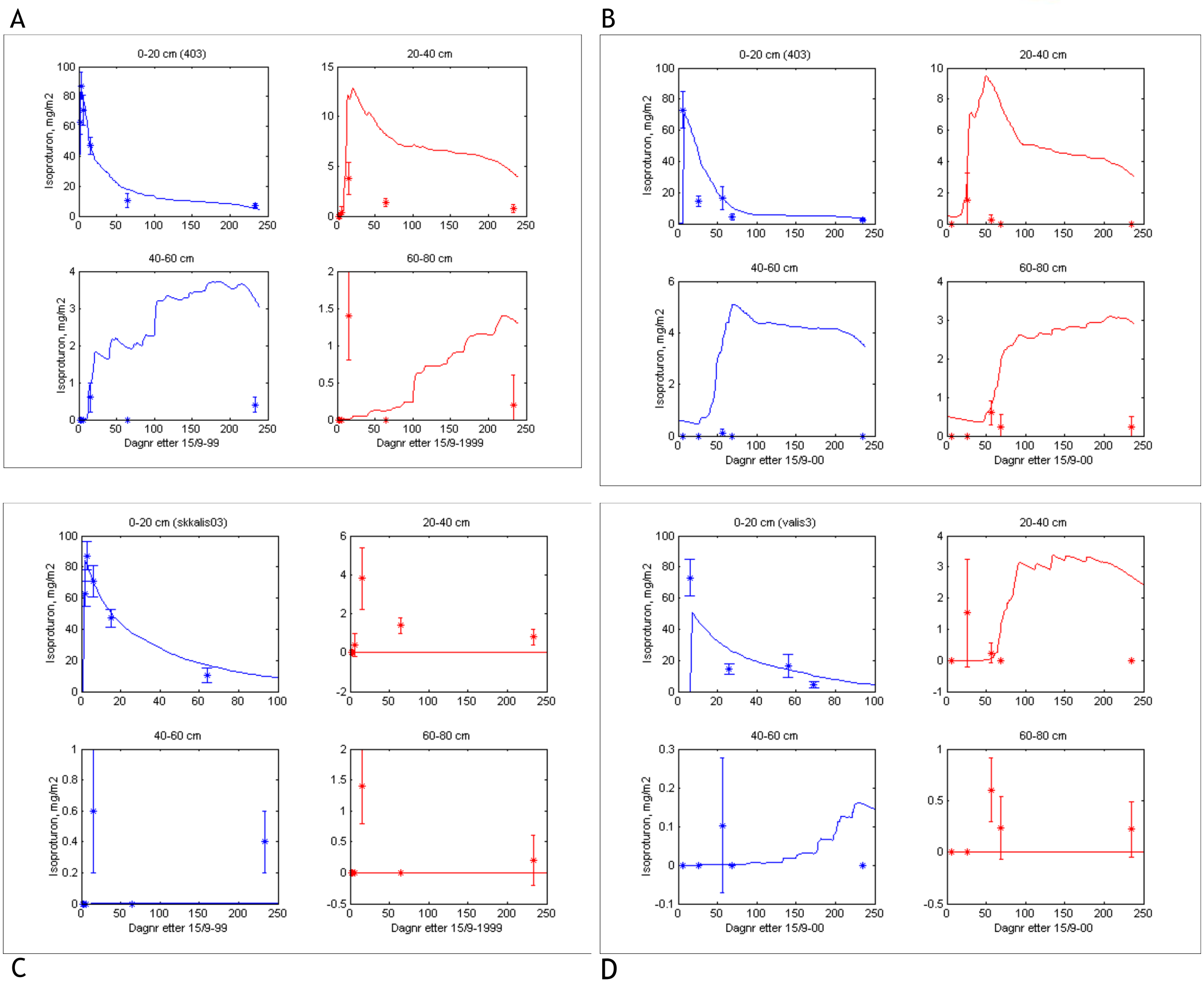

Figure 20. Measured and simulated values for isoproturon in soil at Rustad, 1999/2000 and 2000/2001. Simulated with MACRO and PRZM.

A. Measured and simulated values from different soil depths as a function of time – MACRO 1999/2000
B. Measured and simulated values from different soil depths as a function of time – MACRO 2000/2001
C. Measured and simulated values from different soil depths as a function of time – PRZM 1999/2000
D. Measured and simulated values from different soil depths as a function of time – PRZM 2000/2001

For the upper layer (0-20 cm) there is a good adaptation between simulated and measured values for both fields and both models, especially for the year 1999. The statistical calculations showed in table 12 also confirm this consideration even if there is some graphical disagreement between simulated and measured values below 20 cm. The statistical values are not so good for year 2000 with negative values for the modelling efficiency, except simulations from Heia with PRZM.

Table 12. Different statistical indices for model prediction of isoproturon

		1999			**2000**		
		ME	**CS**	**CRM**	**ME**	**CS**	**CRM**
Heia	MACRO				-1.58	0.19	0.94
	PRZM				0.87	0.88	0.30
Rustad	MACRO	0.98	1.02	0.14	-2.3	0.21	1.41
	PRZM	0.98	1.01	-0.06	-0.4	0.26	0.20

The autumn 2000 was a very special year with precipitation close to 500 mm for the months October, November and December. The mass balance, showed for Heia in Figure 19A, indicates that a large part of the pesticide is leached below 80 cm. For the silty clay loam soil at Rustad there is a tendency that the MACRO simulations generate more leaching of isoproturon below 20 cm than PRZM. Since PRZM showed a quicker transport of bromide to deeper soil layers than MACRO, this difference might be caused by the different approach the models have regarding adsorption/desorption. There are fewer disagreements between the models for the sandy loam at Heia, but the use of MACRO gives some better adaptation between predicted and measured values.

Metalaxyl
Figure 21 and 22 shows the measured and simulated values for metalaxyl in different soil layers at the field sites Heia and Rustad, respectively, simulated with MACRO and PRZM.

A B

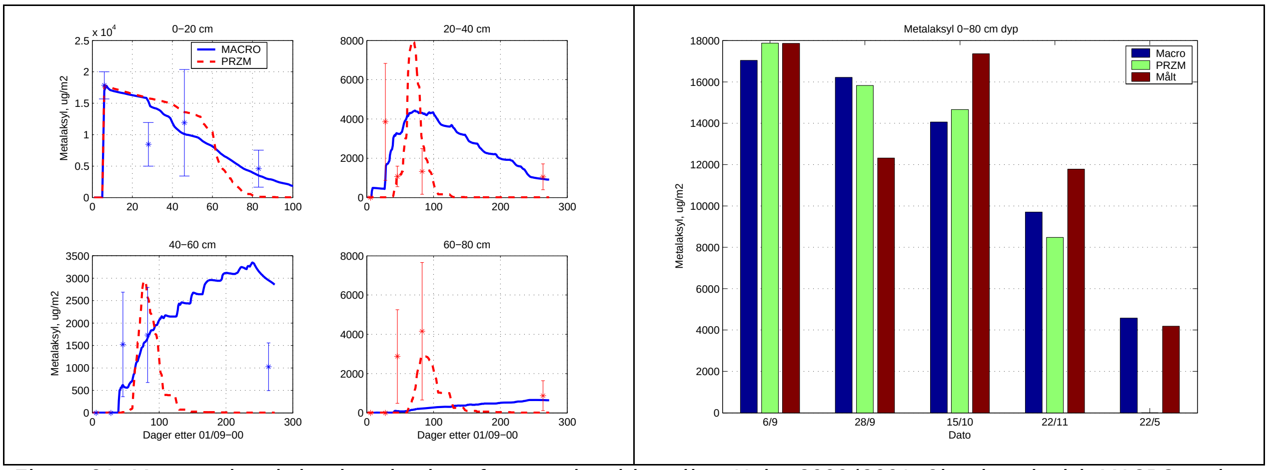

Figure 21. Measured and simulated values for metalaxyl in soil at Heia, 2000/2001. Simulated with MACRO and PRZM.

A. Measured and simulated values from different soil depths as a function of time
B. Measured and simulated mass balance from the 0-80 cm depth as a function of time

A B

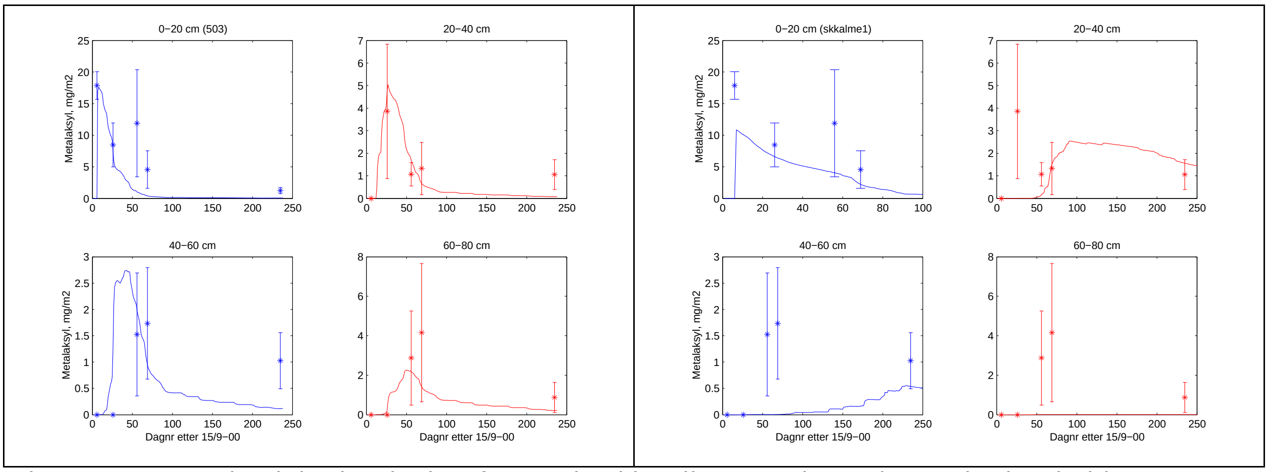

Figure 22. Measured and simulated values for metalaxyl in soil at Rustad, 2000/2001. Simulated with MACRO and PRZM.

A. Measured and simulated values from different soil depths as a function of time – MACRO 2000/2001
B. Measured and simulated values from different soil depths as a function of time – PRZM 2000/2001

The results from Heia show a relatively good agreement between measurements and simulations, see Figure 21A. The statistical calculations in Table 13 also give a good adaptation between predicted and measured values for Heia for both models. The mass balance for the last sampling date (22/5) results in a good agreement between measured and simulated concentrations with MACRO. The simulations with PRZM result in very small amounts left in the soil on this specific sampling date.

Table 13. Different statistical indices for model prediction of metalaxyl

		2000		
		ME	**CS**	**CRM**
Heia	MACRO	0.26	0.55	-0.02
	PRZM	0.67	0.60	-0.10
Rustad	MACRO	-0.09	2.32	-0.49
	PRZM	0.03	0.89	-0.49

For Rustad, the MACRO simulations give a quite good agreement between measurements and simulations see Figure 22A. The PRZM simulations are not so good, especially for the deeper layers (Figure 22B).

Both models give acceptable prediction for bromide, isoproturon and metalaxyl in the upper soil layer (0-20 cm), but for the deeper soil layers the prediction is more variable. It seems that MACRO gives a better description of the water balance (transport of bromide). For the deeper soil layers PRZM describes the fate of pesticides which sorbs moderately (isoproturon) better than MACRO, while MACRO simulates the more mobile pesticide (metalaxyl) better than PRZM. As a preliminary conclusion from the field experiments, lack of comparison with measured water and solute fluxes make parameterisation uncertain. The simulations indicated relatively high concentration of the pesticides in the drainage water which had to be evaluated further. This was the reason for extending the investigations to include small field plots equipped with systems for sampling drainage and surface runoff. The field sites at Bjørnebekk (surface water) and Syverud (surface and drainage water) were therefore introduced in the project.

5.3.2 Simulations from Syverud with MACRO

Model simulations from Heia and Rustad indicated high concentrations of the pesticides isoproturon and metalaxyl, but this could not be verified from the results collected from the field experiments. Measurements from the small field plot at Syverud gave the opportunity to examine if the high concentrations of pesticides in drainage water/groundwater from earlier simulations were real. Syverud is not a part of the national groundwater scenarios for Norway.

Water flow

Measurements of water flow from both the drainage system and surface runoff were measured at the plot. The calibration of the water flow was performed on data from the first period, 2005 to end of 2006, where daily runoff values existed. For the second period, only accumulated values of runoff between sampling dates were available. During the first simulation period there were three episodes with measured surface runoff. As expected, the MACRO simulation did not simulate surface runoff in these episodes. Measured and simulated drainage flow is shown in Figure 23 for the period 2005-2006. The correlations, both as daily fluxes and accumulated values, were very good. There is only a minor tendency to underestimation of the peaks in the model simulations. The results show that the water balance was well simulated.

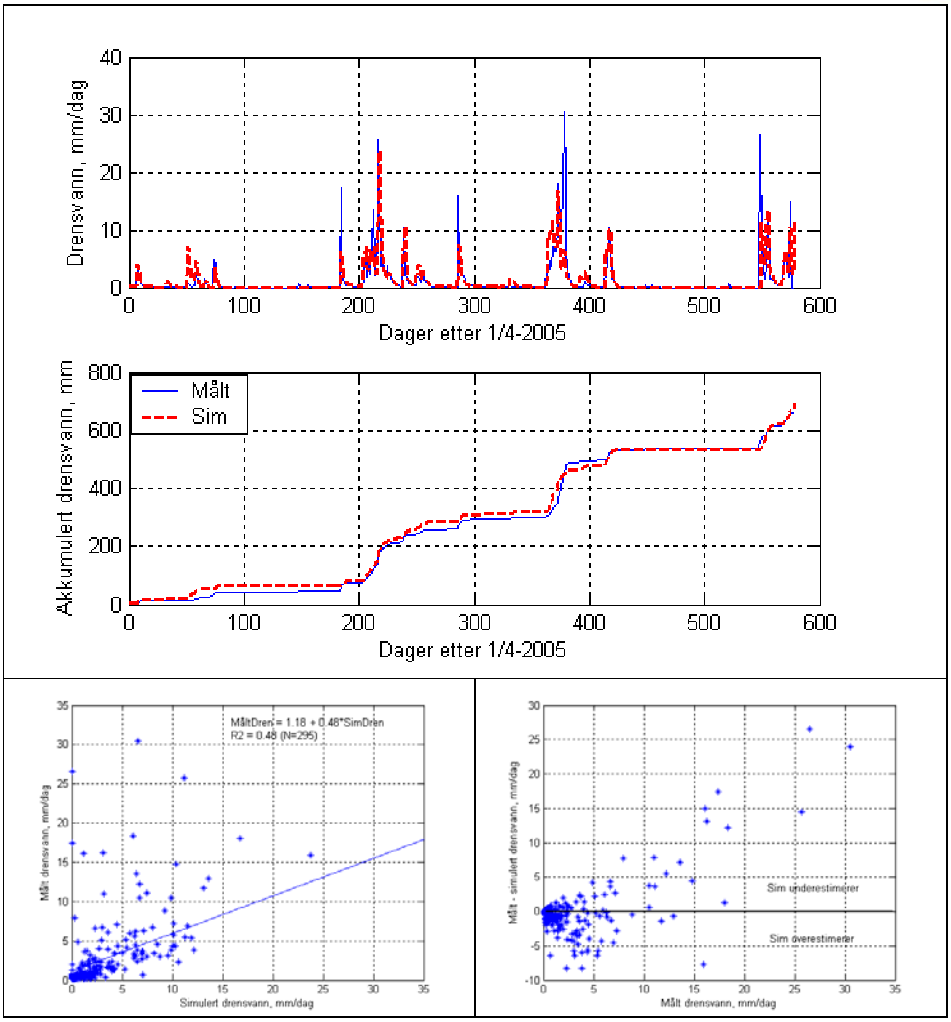

Figure 23. Measured and simulated drainage flow rate (mm/day (upper), accumulated drain flow (mm) (middle), measured versus simulated (lower left) and measured (x) versus difference between measured and simulated (lower right) from 2005-2006

Measured and simulated values of accumulated drainage for 2007-2008 also shows a good fit, but there is some deviation in early June probably due to local showers (Figure 24). Measured surface runoff during snowmelt was about 100 mm in 2008 and is the main reason for the increased deviation during late winter 2008.

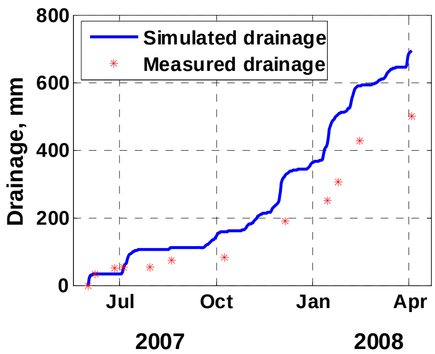

Figure 24. Measured and simulated accumulated drainage flow (mm), 2007-2008

Measured and simulated concentration of bromide in the drainage water showed larger disagreement, see Figure 25. The measurements showed that bromide reached the drainage system faster than simulated both years. The highest concentration was measured in the early autumn drainage episode in 2005 and in the end of June 2007. Different parameterisations were tried, including anion-exclusion, but none of them were able to simulate the fast transport. The accumulated loss of bromide to drainage water until the spring next year was about the same in 2007-2008 as for the measurements and simulations in 2005-2006.

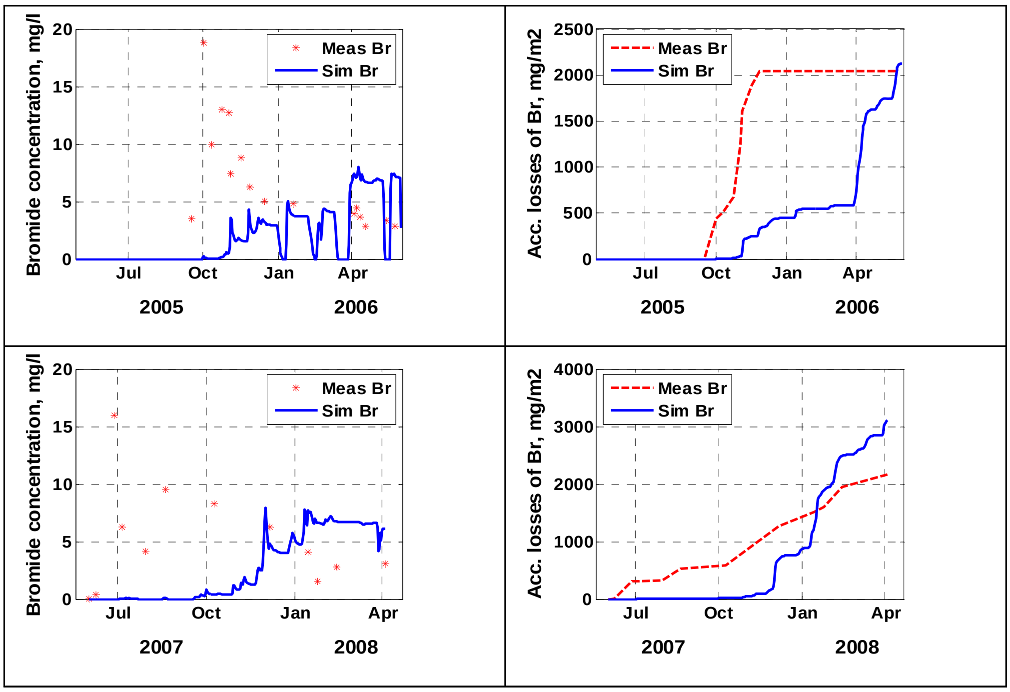

Figure 25. Measured and simulated bromide concentration and accumulated losses. The measured concentrations are in volume-weighted water samples for the periods between sampling

Pesticides

Propiconazole, a stronger sorbed pesticide ("immobile") and metalaxyl, a weaker sorbed pesticide ("mobile") were sprayed in the spring 2005 and 2007. The parameter file which gave the best fit for water flow (drainage water) was used for the pesticide simulation. Only values of sorption and degradation rate were changed according to measured values in the laboratory. Propiconazole was chosen instead of isoproturon to test how MACRO works for stronger sorbed pesticides, because the models often have problems with those pesticides.

Propiconazole

Low concentration of the pesticide was measured in the drainage water, < 0.1 µg/L. The simulated concentration and the accumulated amount of propiconazole in the drainage water were close to zero. Turbidity, which also was measured in the drainage water, indicated that there could be a relationship between concentration of propiconazole and the amount of particles in the drainage water. The disagreement between model simulations and field measurements indicates that other processes than ionic transport is important for stronger sorbed pesticides. Model simulations, with irrigation simulating rainfall, indicated that an ionic transport of stronger sorbed pesticides most probably would occur in connection with heavy rainfall just after spraying.

Metalaxyl

The concentrations of metalaxyl are of the same order of magnitude for the measurements and model simulation in 2005-2006. The accumulated amount of metalaxyl is close to the simulated the first year, but thereafter there is an increase in simulated values while the measurement curve levels out. Both the measured and simulated concentrations are below 1 µg/L in the drainage water. For 2007-2008 the measured concentrations are close to zero when metalaxyl reaches the drainage water according to the simulations. The accumulated values show that the simulated leaching of metalaxyl continues after the end of the measurement period and reaching 4-5 times higher amounts. The only way to reduce this seems to be a decrease in half-life of the pesticide, which is not investigated further here.

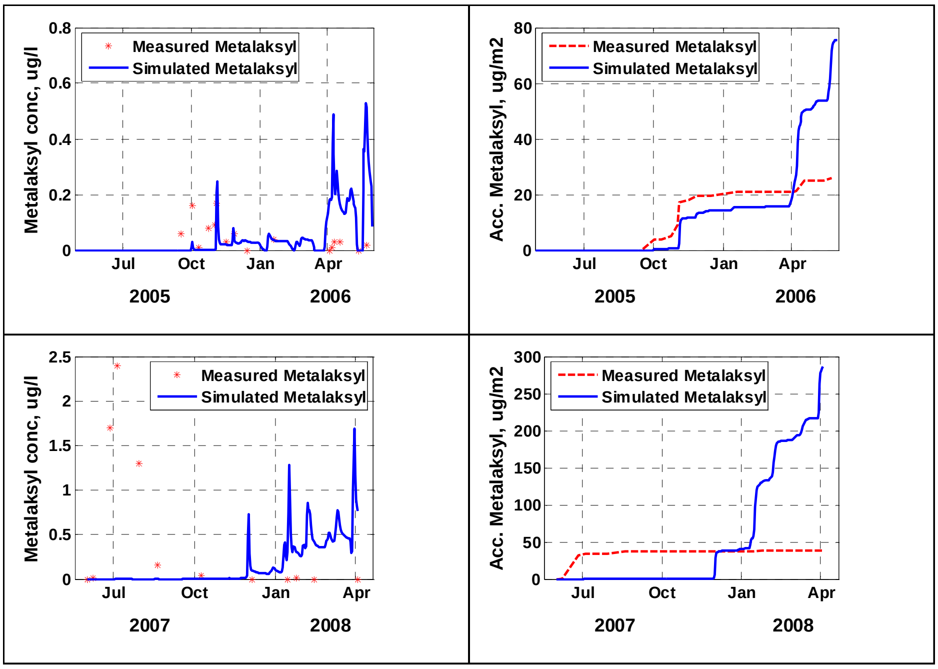

Figure 26. Measured and simulated concentration and accumulated losses of metalaxyl in 2007-2008. The measured concentrations are for volume-weighted water samples for the periods between sampling

5.3.3 Simulations from Bjørnebekk and Syverud with PRZM

The main purpose for PRZM in the second phase of the project was to make Norwegian surface water scenarios, and it was decided to make these scenarios from the fields Bjørnebekk and Syverud where flow and concentration in runoff and drainage water were measured.

Bjørnebekk and Syverud

The results from the field experiments in 2005 – 2006 have been used to calibrate the model. Data achieved from experiments done in 2007 – 2008 was used to validate the model by using the same soil type and pesticide properties, but different meteorological data.

Simulation of water flow

Various strategies were attempted in order to get a good adaptation of the runoff. The parameter which had the biggest influence on the water flow was the curve number. Figure 27 and 28 show the calibrated and validated simulations of surface water from the experimental field at Bjørnebekk.

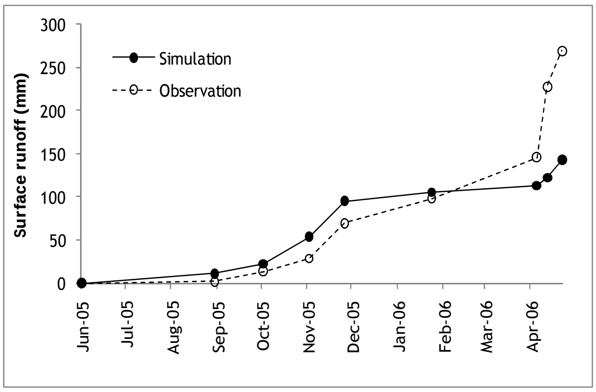

Figure 27. Cumulative calibrated simulation of surface water at Bjørnebekk, 2005-2006

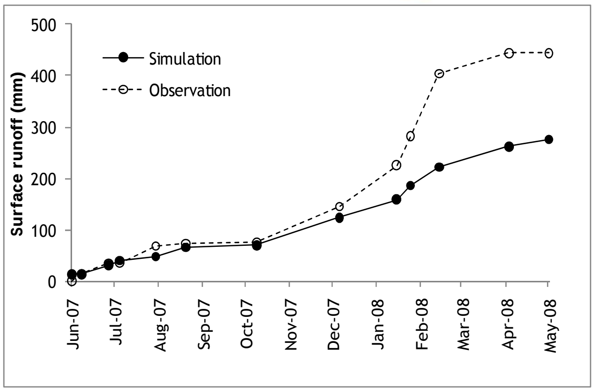

Figure 28. Cumulative validated simulation of surface water at Bjørnebekk, 2007-2008

Figure 27 show the result after calibration. The difference between the total amount of simulated water and observed values were about 47 %. For validated data, the difference was 38 % (Figure 28).

Figure 29 and 30 show the calibrated simulations of surface water and drainage water from the experimental field at Syverud.

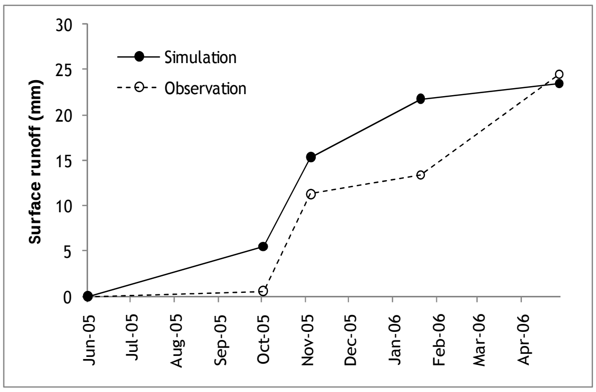

Figure 29. Cumulative calibrated simulation of surface water at Syverud, 2005-2006

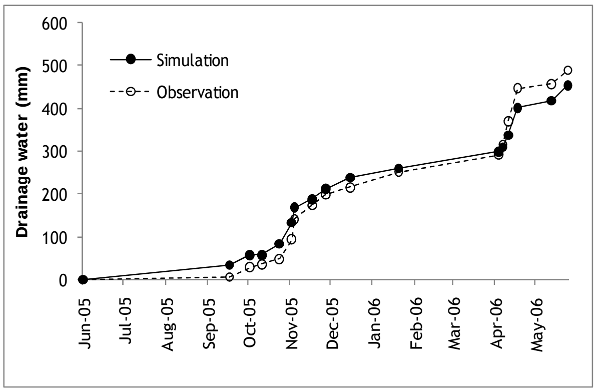

Figure 30. Cumulative calibrated simulation of drainage water at Syverud, 2005-2006

The total amount of simulated surface water was about 4 % lower than the observed values. According to Resseler et al. (1996) a satisfactory simulation occurs when the difference between the simulated and the observed amount of water do not exceed 25 % during a year. For drainage water there is good accordance between the simulated and the observed values. The difference is only 7 % between the total amount of predicted and observed drainage water.

Figure 31 and 32 show the validated simulation of surface water and drainage water. For surface water the difference between the total amount of simulated and observed values was 34 %, while the difference for drainage water was 19 %.

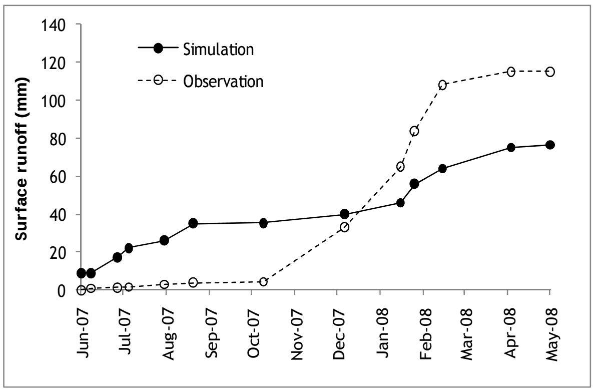

Figure 31. Cumulative validated simulation of surface water at Syverud, 2007-2008

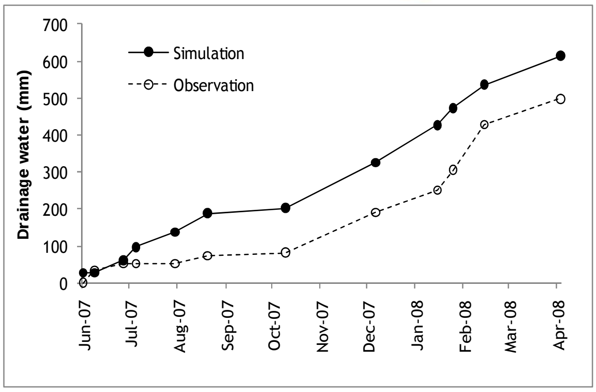

Figure 32. Cumulative validated simulation of drainage water at Syverud, 2007-2008

The cumulative amount of water simulated from both Syverud and Bjørnebekk was within a factor of 10 from the measurements. Reichenberger (2005) have done some considerations about the acceptability limit for the deviation between simulated and measured values. According to these considerations the acceptability limit for surface runoff was set to a factor of 10.

PRZM predicts the water flow (both surface runoff and drainage water) from Syverud and Bjørnebekk adequately. The timing of runoff events was simulated satisfactory in most cases, but there were some problems in periods characterised by frozen soil, freezing and thawing cycles, and high surface runoff during snowmelt events. PRZM considers the effect of snowmelt in the runoff equation, but the curve numbers are not adjusted to account for the effects of snowpack or frozen ground on runoff generation (Reichenberger, 2005). The model also tends to over-predict the water flow for low-intensity rainfalls and small runoff events and to under-predict for high-intensity rainfalls and large runoff events, which is in accordance with Reichenberger (2005). This is probably due to the daily calculation step of PRZM and the non-consideration of actual rainfall intensities. Meteorological data used for environmental fate modelling generally consists of daily values for precipitation, temperature and evapotranspiration. The daily resolution of weather data is used primarily because daily data is easier to obtain than data with finer temporal resolution. For environmental processes such as leaching, which occur over time scales of weeks to years, daily weather data provides adequate resolution to describe the driving force of infiltration with a reasonable degree of accuracy. For more transient processes such as runoff and erosion, which have time scales of minutes to days, the use of daily weather creates significant uncertainties (FOCUS, 2001).

Simulation of the pesticides propiconazole and metalaxyl

To simulate the movement of the pesticides, pesticide parameters are implemented in the calibrated hydrology module. Figure 33 and 34 shows the calibrated and validated values for the total amount of propiconazole in surface runoff from Bjørnebekk.

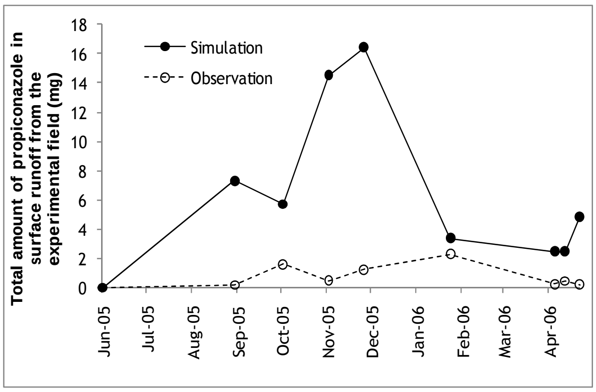

Figure 33. Calibrated values for the total amount of propiconazole in surface runoff from Bjørnebekk, 2005-2006

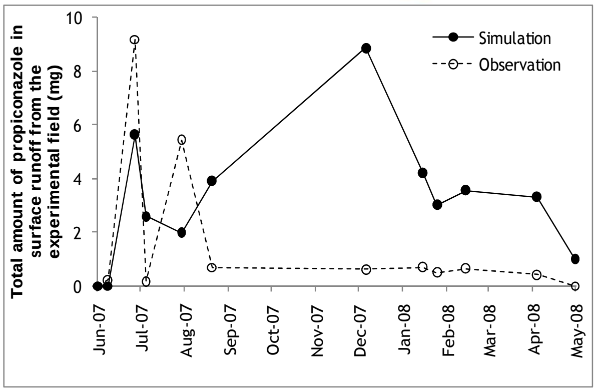

Figure 34. Validated values for the total amount of propiconazole in surface runoff from Bjørnebekk, 2007-2008

The model estimates to high concentration of propiconazole in the surface water compared to the observed values. It seems, especially for this catchment, that propiconazole is distributed in two runoff events for both the periods 2005-2006 and 2007-2008.

Figure 35 and 36 show the calibrated and validated values for the total amount of metalaxyl in surface runoff from Bjørnebekk.

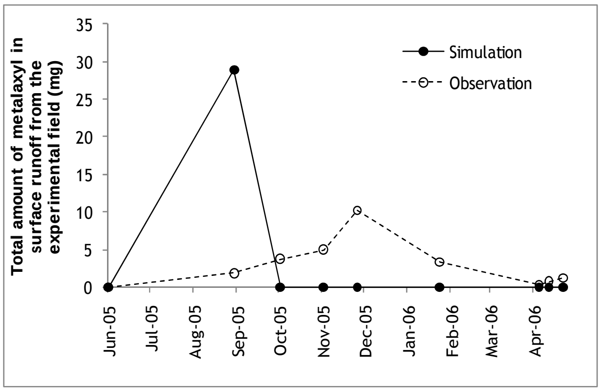

Figure 35. Calibrated values for the total amount of metalaxyl in surface runoff from Bjørnebekk, 2005-2006

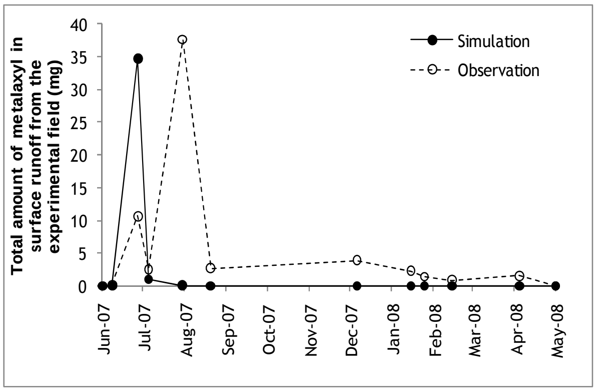

Figure 36. Validated values for the total amount of metalaxyl in surface runoff from Bjørnebekk, 2007-2008

The model estimates to high runoff for metalaxyl in surface water compared to the observed values. Simulated and observed concentrations of the pesticide follows the same pattern, but with a tendency for metalaxyl to give a high simulated concentration at the beginning of the period.

Figure 37 and 38 show the calibrated and validated values for the total amount of propiconazole in surface runoff from Syverud.

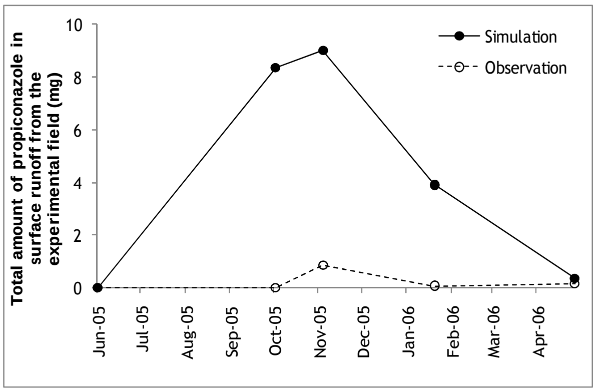

Figure 37. Calibrated values for the total amount of propiconazole in surface runoff from Syverud, 2005-2006

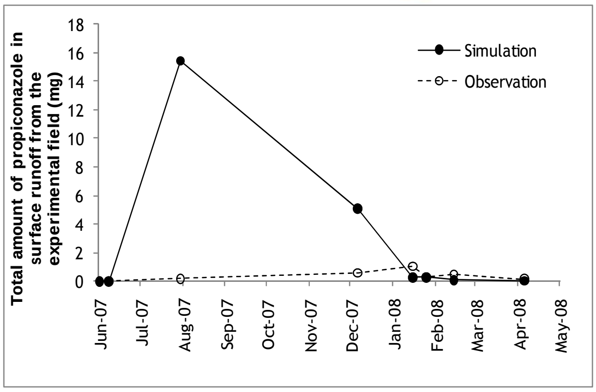

Figure 38. Validated values for the total amount of propiconazole in surface runoff from Syverud, 2007-2008

In general, the model estimates to high concentration of propiconazole in the surface water compared to observed values. In drainage water the model under-predict the concentrations of propiconazole. Propiconazole is a pesticide which sorbs relatively strong to soil and dissolved soil particles in water. Observed values from drainage water show that sorbed propiconazole might be released by thawing in the spring.

Figure 39 and 40 show the calibrated and validated values for the total amount of metalaxyl in surface runoff from Syverud.

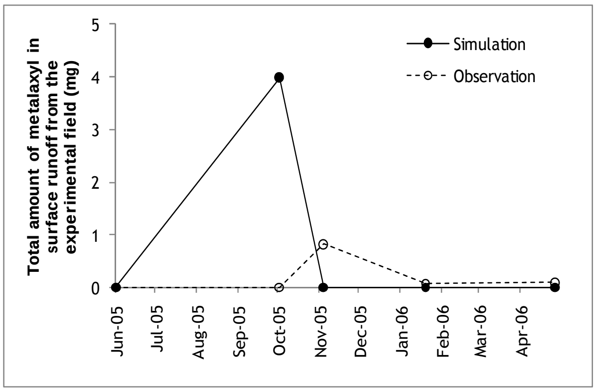

Figure 39. Calibrated values for the total amount of metalaxyl in surface runoff from Syverud, 2005-2006

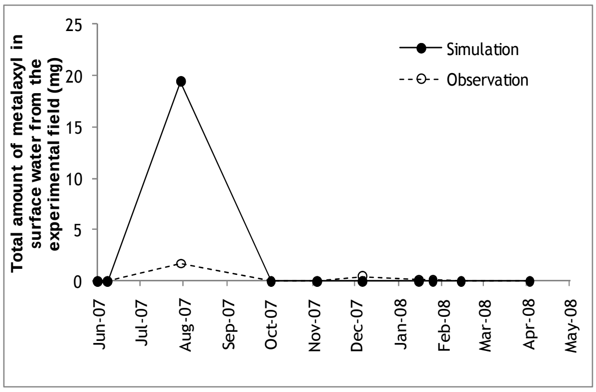

Figure 40. Validated values for the total amount of metalaxyl in surface runoff from Syverud, 2007-2008

The model also estimates to high concentration of metalaxyl in surface water compared to the observed values. Simulated and observed concentrations of the pesticide follows the same pattern, but with a tendency to give a high simulated concentration at the beginning of the period.

As for the water flow, the model tends to over-predict pesticide runoff for low-intensity rainfalls and small runoff events and to under-predict for high-intensity rainfalls and large runoff events (Reichenberger, 2005).

Calculations of the annual mean concentrations
Table 14 and 15 show the annual mean concentration of propiconazole and metalaxyl from Syverud and Bjørnebekk in the periods 2005-2006 and 2007-2008, respectively. The results from 2005-2006 are calibrated simulations while the results from 2007-2008 are validated simulations.

Table 14. Annual mean concentrations for metalaxyl and propiconazole in surface runoff and drainage water from Syverud in the periods 2005-2006 and 2007-2008

		Total amount of water (mm)		**Total amount of pesticides (mg)**		**Annual mean concentration (µg/L)**	
		Simulated	Observed	Simulated	Observed	Simulated	Observed
2005-2006	**Surface runoff**	23.4	24.5				
	Metalaxyl			3.99	0.98	*0.424*	*0.100*
	Propiconazole			21.6	1.07	*2.296*	*0.109*
	Drainage water	454	489				
	Metalaxyl			0.0025	10.4	*1.4E-05*	*0.053*
	Propiconazole			2.5E-18	4.65	*1.37E-20*	*0.024*
2007-2008	**Surface runoff**	76.5	115				
	Metalaxyl			19.4	2.46	*0.631*	*0.053*
	Propiconazole			21.1	2.72	*0.686*	*0.059*
	Drainage water	614	499				
	Metalaxyl			0.042	15.5	*0.0002*	*0.077*
	Propiconazole			2.18E-15	2.91	*8.8E-18*	*0.015*

Table 15. Annual mean concentrations for metalaxyl and propiconazole in surface runoff from Bjørnebekk in the periods 2005-2006 and 2007-2008

		Total amount of water (mm)		**Total amount of pesticides (mg)**		**Annual mean concentration (µg/L)**	
		Simulated	Observed	Simulated	Observed	Simulated	Observed
2005-2006	**Surface runoff**	143	269				
	Metalaxyl			28.9	26.5	*1.135*	*0.553*
	Propiconazole			57.1	6.7	*2.243*	*0.140*
2007-2008	**Surface runoff**	276	444				
	Metalaxyl			35.8	63.7	*0.729*	*0.806*
	Propiconazole			38.1	18.6	*0.776*	*0.235*

The simulated pesticide runoff losses are affected by uncertainty from both water transport and chemical transport simulation. According to Reichenberger (2005), the deviation between simulated and measured values can be expected to be higher for pesticide runoff than for the corresponding runoff water volumes. For doing do an aquatic risk assessment, an under or over prediction of pesticide input into a surface water body by more than a factor of 10 cannot be considered as acceptable. The acceptability limit was therefore also set to a factor of 10 between simulated and measured values.

For the surface runoff simulations from Syverud the model predicts the annual mean concentration for metalaxyl four times higher than the observed values for the calibrated simulations, and 12 times higher for the validated simulations. For propiconazole the model predicts the annual mean concentration 21 times higher than the observed values for the calibrated simulations, and 12 times higher for the validated simulations.

The model predicted the annual mean concentration for metalaxyl from Bjørnebekk twice as high as the observed value for the calibrated simulations. For the validated simulations the model predicts almost similar values for simulated and observed measurements. For propiconazole, the annual mean concentration was simulated 16 times higher than observed values for the calibrated simulations, and three times higher for the validated simulations.

According to Reichenbergers (2005) considerations, most of the results achieved of pesticide runoff from the experimental fields are acceptable. The simulations of metalaxyl in surface runoff are for both fields in good accordance with both calibrated and validated simulations. For propiconazole the simulations are good for Bjørnebekk, especially the validated simulations. For Syverud the calibrated simulations are not good but the validated simulations lies almost within the acceptability limit (factor of 12). In general, the results are somewhat better for the validated simulations than the calibrated simulations. The results also show that the model may have problems to predict runoff concentrations for pesticides which sorb strongly to soil.

The tables show that PRZM is not a good model tool for simulating the amount of pesticides in the drainage water. This is probably due to the lack of macropore transport in the model.

5.4 Testing of the simulation tools MACRO and PRAESS (Pesticide Risk Assessment Exposure Simulation Shell). Short comparison of modelling performed with Norwegian scenarios and other national scenarios.

5.4.1 MACRO

The FOCUS group has proposed nine European groundwater scenarios to be used for tier 1 registration of active substances under the EU directive 91/414 (FOCUS 2000). The groundwater leaching scenarios have been developed for four models: PRZM 3.2 (Carsel et al., 1998), PELMO 3.2 (Jene, 1998), PEARL 1.1 (Leistra et al., 2000) and MACRO 4.2 (Jarvis and Larsson, 1998). Only one FOCUS scenario, Châteaudun (France), was developed for MACRO 4.2.

The discussion about how representative the FOCUS scenarios was for Norwegian soils, climate and agriculture led to the initiation of the project "Norwegian Scenarios" and the development of two national scenarios (Heia and Rustad). The same thoughts were earlier reflected in the other Nordic countries and led to the development of three national scenarios in Sweden (Önnestad, Krusenberg and Näsbygård) and two scenarios in Denmark (Karup and Langvad). In Norway, MACRO was chosen to assess the leaching potential of active substances, especially in clay soils. To evaluate and compare the Norwegian groundwater scenarios, simulations with FOCUS-MACRO were performed for the FOCUS scenario Châteaudun and the national scenarios from Sweden and Denmark. Figure 41 gives an overview of the FOCUS scenarios including the Swedish and Norwegian sites.

Figure 41. An overview of the location of the different FOCUS scenarios and also the Swedish and the Norwegian sites

Climate

The climate plays an important role in the modelling of water flow and pesticide leaching. An overview of the annual air temperature and precipitation for different scenarios are summarised in Figure 42 and 43. The data from Hamburg and Jokioinen were collected from the document "Generic guidance for FOCUS groundwater scenarios" (FOCUS 2000). The other results were calculated from data used in the FOCUS MACRO routine (20 years average). Data from the Swedish and Danish scenarios were also included.

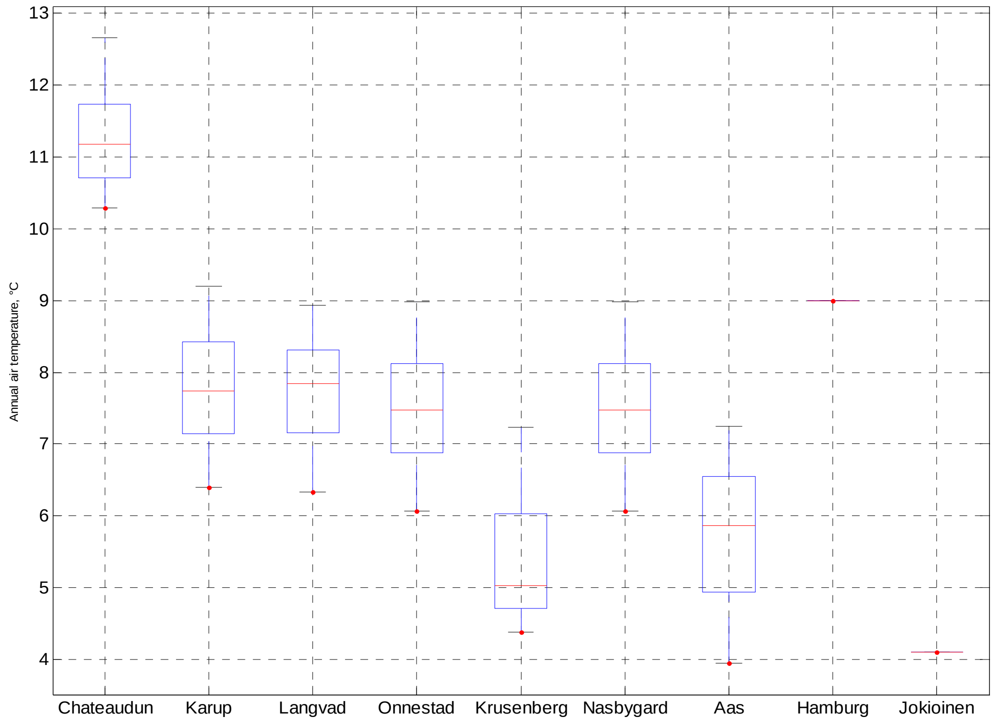

Figure 42. Average annual air temperature (20 years). Single values are shown for Hamburg and Jokioinen (FOCUS, 2002). The plots show the median, 25^{th} and 75^{th} percentile with non-outliers (length of line) and outliers as points

The annual air temperature ranges between 11°C (Châteaudun) and 4°C (Jokioinen). The Norwegian sites, Rustad and Heia (Aas), have an annual air temperature close to the Swedish site Krusenberg. Aas has a higher annual air temperature than Jokioinen, but lower than the other sites. Note that the two Norwegian sites have very similar climate so the same climate file has been used for both scenarios.

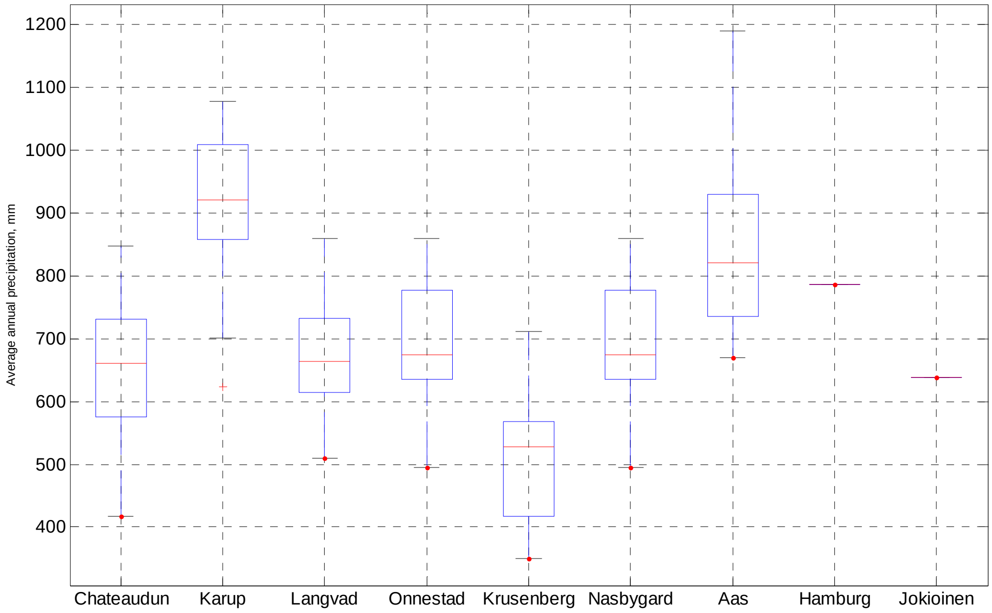

Figure 43. Average annual precipitation (20 years). Single values are shown for Hamburg and Jokioinen (FOCUS 2002). The plots show the median, 25th and 75th percentile with non-outliers (length of line) and outliers as points

The average annual precipitation ranges between 500 mm (Krusenberg) and 900 mm (Karup). The Norwegian sites, Rustad and Heia (Aas), have approximately 800 mm of precipitation per year which is a little lower than Karup and close to Hamburg.

Compared to the other sites the average climatic conditions for the Norwegian sites are low annual air temperature and relative high precipitation. The combination of long periods in winter with low temperature (decreased degradation) and snow covered ground (large water flow during snowmelt) initiated the work with the Norwegian scenarios.

Soils

The soil textural classes (USDA) at the different sites are summarised in Figure 3. The Norwegian site, Rustad, has almost the same texture as Châteaudun and the same clay content as the Swedish scenario Näsbygård. The other Swedish sites and one of the Danish sites have a content of 80 % or more of sand, and clay between 5 and 10 %. The official FOCUS-scenario Hamburg has about the same clay content, but lower sand content (about 70 %). The Danish site with highest clay content (Langvad) belongs to the class sandy loam.

Simulation results

To compare different scenarios, simulations with FOCUS-MACRO were performed for the FOCUS scenario Châteaudun and the Swedish, Danish and Norwegian scenarios. Norwegian endpoints (data from field studies) and endpoints agreed upon in EU (Table 16) (EU's pesticide database, EU's list of endpoints) have been used, either combined with a Norwegian climate file (covering the southeast of Norway) or climate files belonging to each scenario. The scenario from Châteaudun was only simulated with the scenario specific climate file, because of problems when using another climate file. The general parameters in the simulations like application rate, application date, interception and crop were the same for all scenarios. The chemical properties like molecular mass, vapour pressure and water solubility were also the same for all scenarios. Table 16 shows the Norwegian endpoints and the endpoints agreed upon in EU for the pesticide input parameters. These were the only input parameters which were changed in the simulations. For other parameters in the model, FOCUS default has been used. The results are summarised in the Tables 17 – 20.

Table 16. Input pesticide parameters for groundwater modelling for the estimation of Predicted Environmental Concentrations (PEC) for propiconazole, metalaxyl and isoproturon

	Norwegian endpoints	EU endpoints
Propiconazole		
$DT50_{soil}$ (d):	201 (geomean, n=2)	72
K_{foc}:	984	382
1/n:	1.13	0.90
Metalaxyl		
$DT50_{soil}$ (d):	64 (geomean, n=2)	36 (median, n=7)
K_{foc}:	20	162
1/n:	0.90	0.90
Isoproturon		
$DT50_{soil}$ (d):	13 (geomean, n=2)	11.9 (geomean, n=2)
K_{foc}:	95	104
1/n:	0.96	0.90

Table 17. Results from groundwater modelling with MACRO (4.4.2) for propiconazole, metalaxyl and isoproturon using the FOCUS scenario Châteaudun and the Swedish, Danish and Norwegian national scenarios. Data from Norwegian field studies and a Norwegian climate file have been used in the model

Substance	**Scenario**	**80^{th} percentile (µg/L)**
Propiconazole	Châteaudun (FOCUS)	
	Karup (DK)	1.08
	Langvad (DK)	0.75
	Önnestad (SE)	3.30
	Krusenberg (SE)	0.07
	Näsbygård (SE)	4.19
	Heia (NO)	1.83
	Rustad (NO)	1.93
Metalaxyl	Châteaudun (FOCUS)	
	Karup (DK)	7.14
	Langvad (DK)	6.95
	Önnestad (SE)	9.49
	Krusenberg (SE)	19.20
	Näsbygård (SE)	7.66
	Heia (NO)	6.26
	Rustad (NO)	7.19
Isoproturon	Châteaudun (FOCUS)	
	Karup (DK)	0.13
	Langvad (DK)	3.83
	Önnestad (SE)	2.69
	Krusenberg (SE)	0.13
	Näsbygård (SE)	6.26
	Heia (NO)	2.00
	Rustad (NO)	1.08

Table 18. Results from groundwater modelling with MACRO (4.4.2) for propiconazole, metalaxyl and isoproturon using the FOCUS scenario Châteaudun and the Swedish, Danish and Norwegian national scenarios. Data from Norwegian field studies and scenario specific climate files have been used in the model

Substance	**Scenario**	**80^{th} percentile (µg/L)**
Propiconazole	Châteaudun (FOCUS)	0.73
	Karup (DK)	0.83
	Langvad (DK)	0.38
	Önnestad (SE)	2.20
	Krusenberg (SE)	1.35
	Näsbygård (SE)	3.29
	Heia (NO)	1.83
	Rustad (NO)	1.93
Metalaxyl	Châteaudun (FOCUS)	3.30
	Karup (DK)	5.77
	Langvad (DK)	3.79
	Önnestad (SE)	9.29
	Krusenberg (SE)	7.20
	Näsbygård (SE)	4.58
	Heia (NO)	6.26
	Rustad (NO)	7.19
Isoproturon	Châteaudun (FOCUS)	0.12
	Karup (DK)	0.07
	Langvad (DK)	2.05
	Önnestad (SE)	1.08
	Krusenberg (SE)	0.08
	Näsbygård (SE)	5.67
	Heia (NO)	2.00
	Rustad (NO)	1.08

Table 19. Results from groundwater modelling with MACRO (4.4.2) for propiconazole, metalaxyl and isoproturon using the FOCUS scenario Châteaudun and the Swedish, Danish and Norwegian national scenarios. Endpoints agreed upon in EU and a Norwegian climate file has been used in the model

Substance	Scenario	80^{th} percentile (µg/L)
Propiconazole	Châteaudun (FOCUS)	
	Karup (DK)	$3.20e^{-5}$
	Langvad (DK)	0.02
	Önnestad (SE)	0.08
	Krusenberg (SE)	$4.20e^{-3}$
	Näsbygård (SE)	0.71
	Heia (NO)	0.08
	Rustad (NO)	$9.80e^{-3}$
Metalaxyl	Châteaudun (FOCUS)	
	Karup (DK)	$1.60e^{-3}$
	Langvad (DK)	0.09
	Önnestad (SE)	0.18
	Krusenberg (SE)	0.02
	Näsbygård (SE)	0.36
	Heia (NO)	0.10
	Rustad (NO)	0.04
Isoproturon	Châteaudun (FOCUS)	
	Karup (DK)	0.01
	Langvad (DK)	2.38
	Önnestad (SE)	0.72
	Krusenberg (SE)	0.02
	Näsbygård (SE)	4.62
	Heia (NO)	0.95
	Rustad (NO)	0.23

Table 20. Results from groundwater modelling with MACRO (4.4.2) for propiconazole, metalaxyl and isoproturon using the FOCUS scenario Châteaudun and the Swedish, Danish and Norwegian national scenarios. Endpoints agreed upon in EU and scenario specific climate files have been used in the model

Substance	Scenario	80^{th} percentile (µg/L)
Propiconazole	Châteaudun (FOCUS)	$9.70e^{-4}$
	Karup (DK)	$4.60e^{-5}$
	Langvad (DK)	$1.90e^{-3}$
	Önnestad (SE)	0.03
	Krusenberg (SE)	$8.50e^{-3}$
	Näsbygård (SE)	0.46
	Heia (NO)	0.08
	Rustad (NO)	$9.80e^{-3}$
Metalaxyl	Châteaudun (FOCUS)	$1.60e^{-3}$
	Karup (DK)	$9.50e^{-4}$
	Langvad (DK)	0.04
	Önnestad (SE)	0.07
	Krusenberg (SE)	$8.60e^{-3}$
	Näsbygård (SE)	0.25
	Heia (NO)	0.10
	Rustad (NO)	0.04
Isoproturon	Châteaudun (FOCUS)	0.02
	Karup (DK)	$1.64e^{-3}$
	Langvad (DK)	1.09
	Önnestad (SE)	0.16
	Krusenberg (SE)	$7.64e^{-4}$
	Näsbygård (SE)	4.43
	Heia (NO)	0.95
	Rustad (NO)	0.23

Propiconazole

The results from the different simulations are shown in Figure 44.

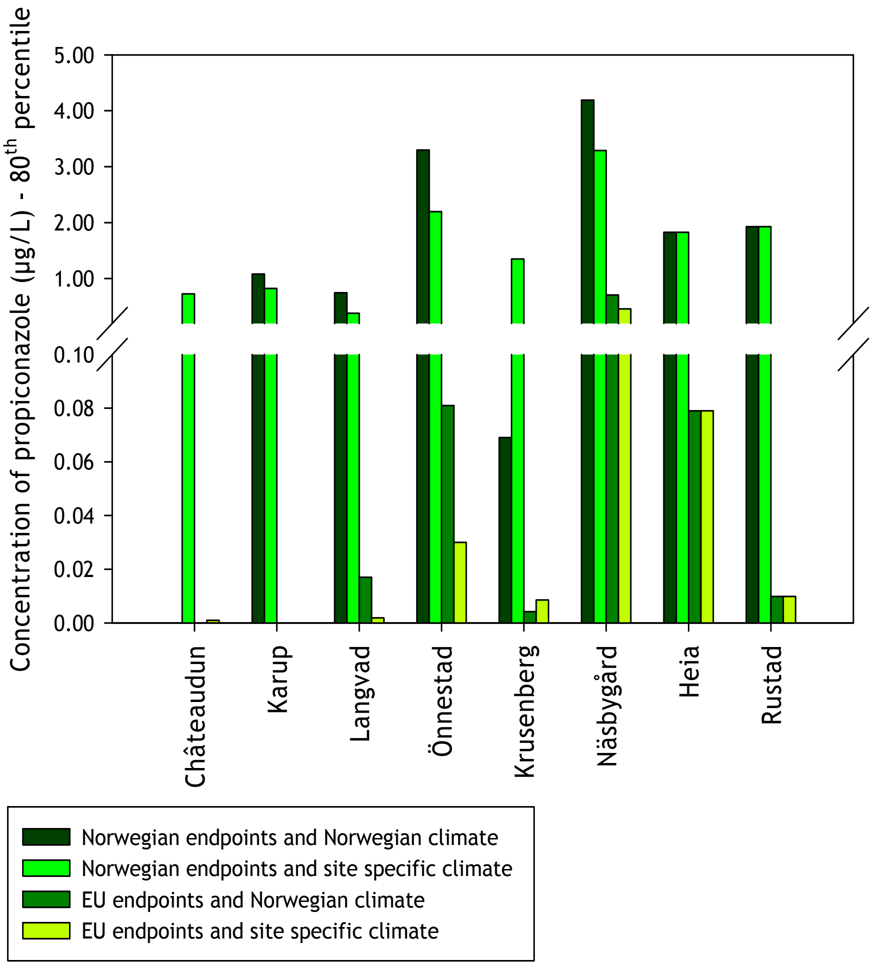

Figure 44. Leaching of propiconazole (80th percentile) from different scenarios, using Norwegian endpoints and EU endpoints together with Norwegian climate file and scenario specific climate files simulated with FOCUS-MACRO

For propiconazole, which sorbs stronger to soil particles than metalaxyl, the simulated concentrations (80th percentile) in the leachate were low compared to the simulations for metalaxyl (Fig. 45). Using Norwegian endpoints together with the Norwegian climate file and scenario specific climate files, the difference between the scenarios are small. The Swedish scenarios, especially Krusenberg, indicate that the climate might have an effect on leaching when using Norwegian input data. Simulations with EU endpoints together with Norwegian climate or scenario specific climate, gave quite large effects on the simulation results when changing the input data. Except for Önnestad, there were small differences between different climate files when using endpoints agreed upon in EU. The FOCUS scenario Châteaudun shows that the choice of input data might have a large effect according to leaching (Fig. 44, Tables 18 and 20).

Metalaxyl
The results from the different simulations are shown in Figure 45.

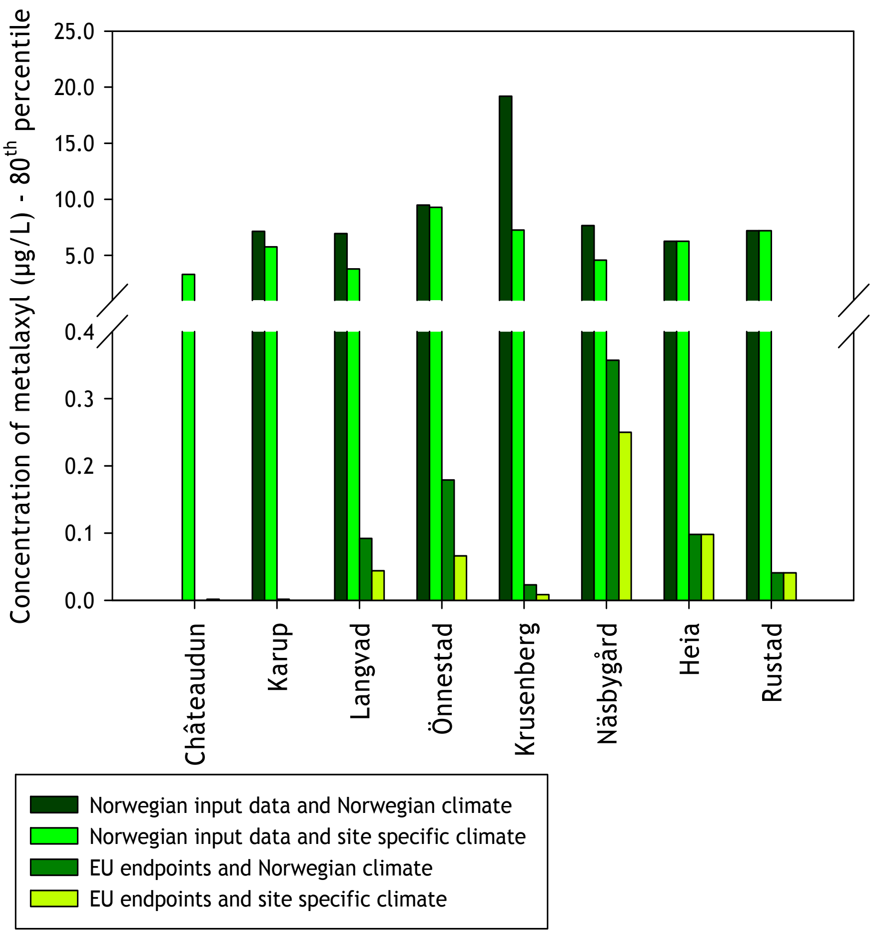

Figure 45. Leaching of metalaxyl (80th percentile) from different scenarios, using Norwegian endpoints and EU endpoints together with a Norwegian climate file and scenario specific climate files simulated with FOCUS-MACRO

The results show that there is a small difference in the 80th percentile between the scenarios when using Norwegian endpoints together with Norwegian climate or climate files which is specific for each scenario. The Swedish scenario Krusenberg, results in a higher degree of leaching of metalaxyl by using the Norwegian climate file than using the scenario specific climate file. When using EU endpoints in the simulations together with Norwegian climate or scenario specific climate files, the results show large differences compared to the simulations done with Norwegian input data. Simulations with the scenarios Önnestad and Näsbygård, result in some differences in leaching when using different climate files together with EU endpoints. Châteaudun shows the same tendency as for propiconazole, a quite large effect on the concentration of metalaxyl in the leachate when using different input data.

Isoproturon
The results from the different simulations are shown in Figure 46.

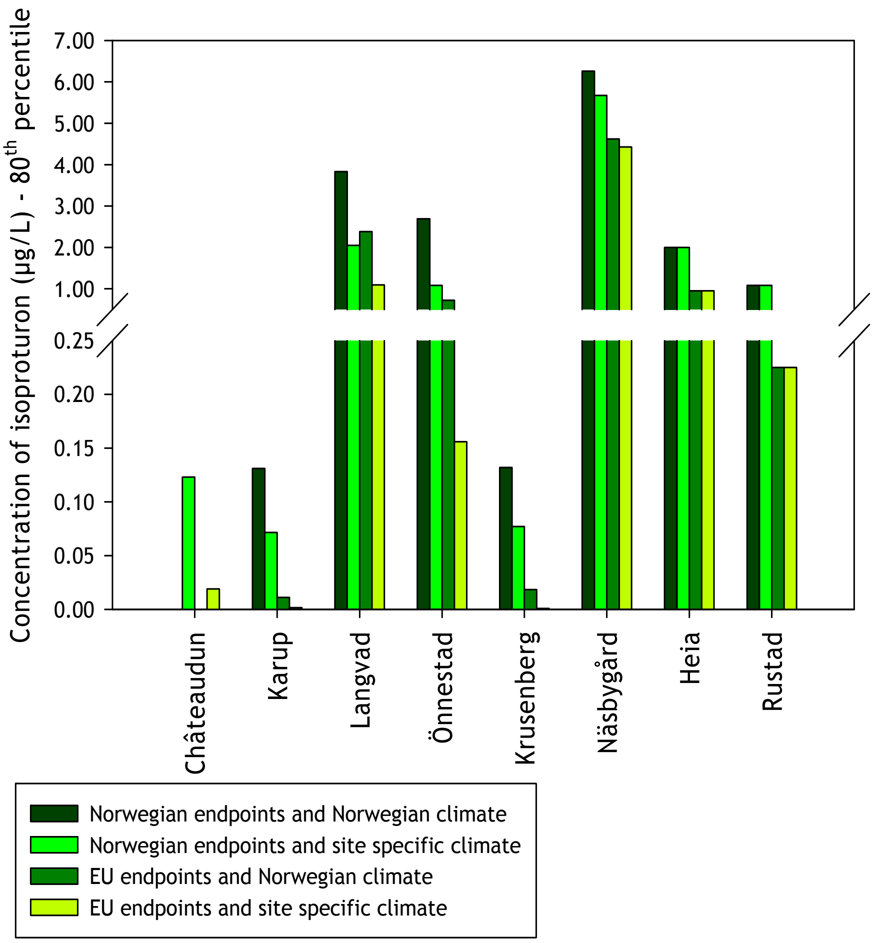

Figure 46. Leaching of isoproturon (80th percentile) from different scenarios, using Norwegian endpoints and EU endpoints together with a Norwegian climate file and scenario specific climate files simulated with FOCUS-MACRO

As for propiconazole and metalaxyl, the results show small differences for the 80th percentile between the scenarios when using Norwegian endpoints together with Norwegian climate or climate files which are specific for each scenario. The Swedish and Danish scenarios, except the scenario from Näsbygård, show some higher degree of leaching of isoproturon when using the Norwegian climate file. Dissimilarities between the use of endpoints agreed upon in EU and Norwegian endpoints are small compared to the simulations done with propiconazole and metalaxyl. This may be explained by small differences between the pesticide input parameters (see Table 16). Different climate files gave little effect on the concentration of leached isoproturon when using EU endpoints, except for Önnestad.

5.4.2 PRZM

PRAESS (Pesticide Risk Assessment Exposure Simulation Shell)

Waterborne Environmental Inc. has developed a modelling platform called PRAESS, based on PRZM, which is designed to evaluate the potential for pesticides to occur in surface- and groundwater resources (Ritter et al., 2010). The architecture of PRAESS allows seamless executions of several environmental fate and transport models in the Windows environment (i.e. WINPRZM, RICEWQ, EXAMS and ADAM). A shared model input structure provides the flexibility for the user to create, update maintain databases on pesticide environmental fate properties and exposure scenarios. The developed scenarios from Bjørnebekk and Syverud (cereals) are included in PRAESS and are ready to be used in surface water and groundwater assessments. PRAESS contains a number of features not available in similar modelling systems that are being used for pesticide exposure assessment in the EU or the United States including:

- The ability to conduct groundwater and surface water assessments within a single modelling system
- The inclusion of an aquifer model to estimate pesticide concentrations in leachate and in groundwater
- The flexibility for the user to add scenarios over time
- The flexibility to simulate up to five receiving water systems with each combination of crop-soil-weather condition
- Watershed simulations

Simulation results

PRAESS was tested according to earlier simulations with PRZM (Table 11 and 12) and according to the groundwater simulations done for Norwegian national scenarios with MACRO (chapt. 5.4.1). The same input parameters as for the MACRO simulations (Table 16), both Norwegian endpoints and EU endpoints, were used for the groundwater simulations together with a Norwegian climate file. The surface and drainage water simulations with PRAESS had the same input parameters as earlier PRZM simulations (chapt. 5.3.2 and appendix II). The simulations were run for 26 years.

Groundwater simulations

Results from earlier simulations with MACRO (Heia and Rustad) and results from the PRAESS simulations (Syverud) are summarized in the Tables 21 and 22. Simulations were performed at 1 m depth.

Table 21. Results from groundwater modelling for propiconazole, metalaxyl and isoproturon using the Norwegian national scenarios. Data from Norwegian field studies and a Norwegian climate file has been used in the model. Heia and Rustad are simulated with MACRO (4.4.2), while Syverud is simulated with PRAESS_GW

Substance	Scenario	80th percentile (µg/L)
Propiconazole	Heia	1.83
	Rustad	1.93
	Syverud	1.67
Metalaxyl	Heia	6.26
	Rustad	7.19
	Syverud	12.10
Isoproturon	Heia	2.00
	Rustad	1.08
	Syverud	0.17

Table 22. Results from groundwater modelling with for propiconazole, metalaxyl and isoproturon using the Norwegian national scenarios. Endpoints agreed upon in EU and a Norwegian climate file has been used in the model. Heia and Rustad are simulated with MACRO (4.4.2), while Syverud is simulated with PRAESS_GW

Substance	Scenario	80th percentile (µg/L)
Propiconazole	Heia	0.08
	Rustad	$9.80e^{-3}$
	Syverud	$2.00e^{-3}$
Metalaxyl	Heia	0.10
	Rustad	0.04
	Syverud	$8.10e^{-3}$
Isoproturon	Heia	0.95
	Rustad	0.23
	Syverud	$3.70e^{-3}$

Propiconazole

Results from the PRAESS simulation and earlier MACRO simulations for propiconazole are shown in Figure 47.

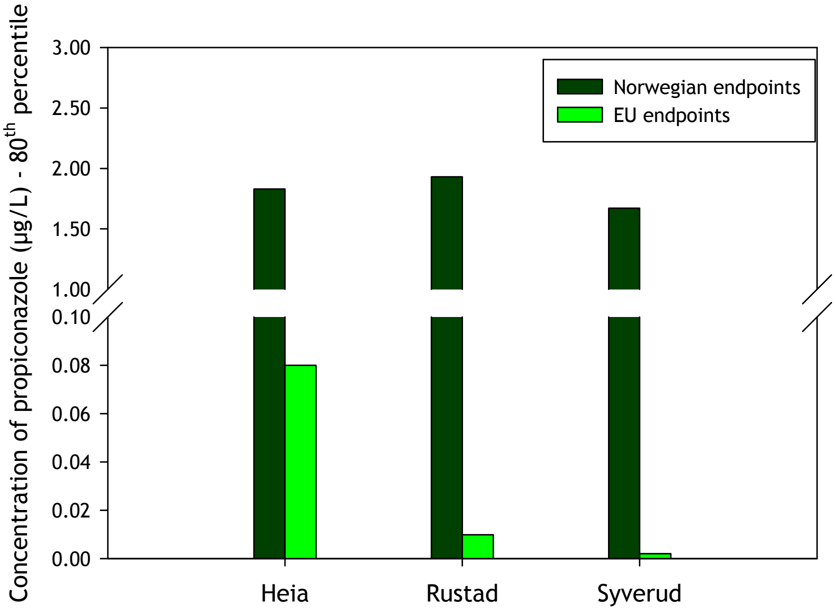

Figure 47. Leaching of propiconazole (80th percentile) from the Norwegian scenarios, using Norwegian endpoints and EU endpoints together with a Norwegian climate file. Heia and Rustad simulated with MACRO. Syverud simulated with PRAESS

PRAESS simulates the concentration of propiconazole in the leachate very good and in accordance with the simulations done with MACRO, especially with Norwegian input data. The results are also consistent with the simulations from Sweden and Denmark (Fig. 44).

Metalaxyl

Results from the PRAESS simulation and earlier MACRO simulations for metalaxyl are shown in Figure 48.

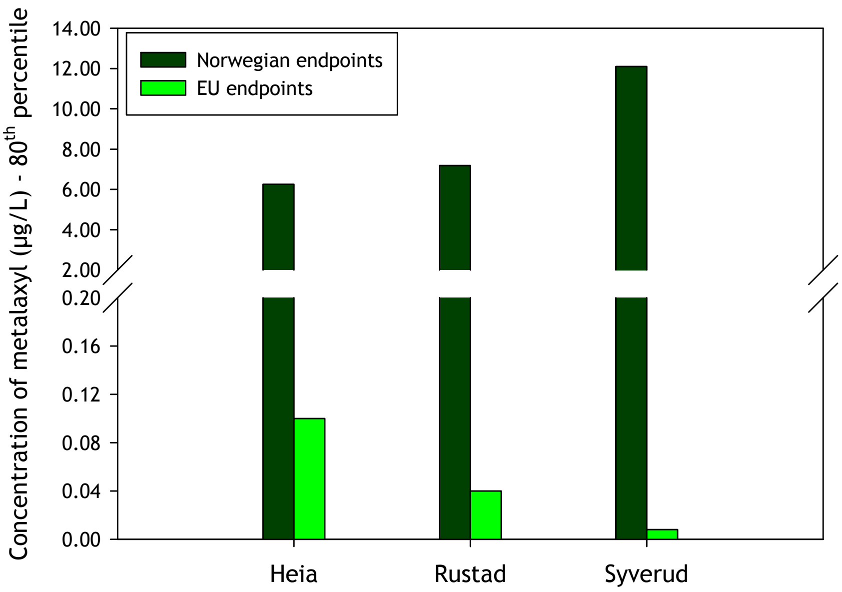

Figure 48. Leaching of metalaxyl (80th percentile) from the Norwegian scenarios, using Norwegian endpoints and EU endpoints together with a Norwegian climate file. Heia and Rustad simulated with MACRO. Syverud simulated with PRAESS

PRAESS simulates some more leaching of metalaxyl than the MACRO simulations using Norwegian endpoints. The 80th percentile for Syverud is 12.1 µg/L, while the value for Heia and Rustad is 6.3 and 7.2 µg/L respectively.

Isoproturon

Results from the PRAESS simulation and earlier MACRO simulations for isoproturon are shown in Figure 49.

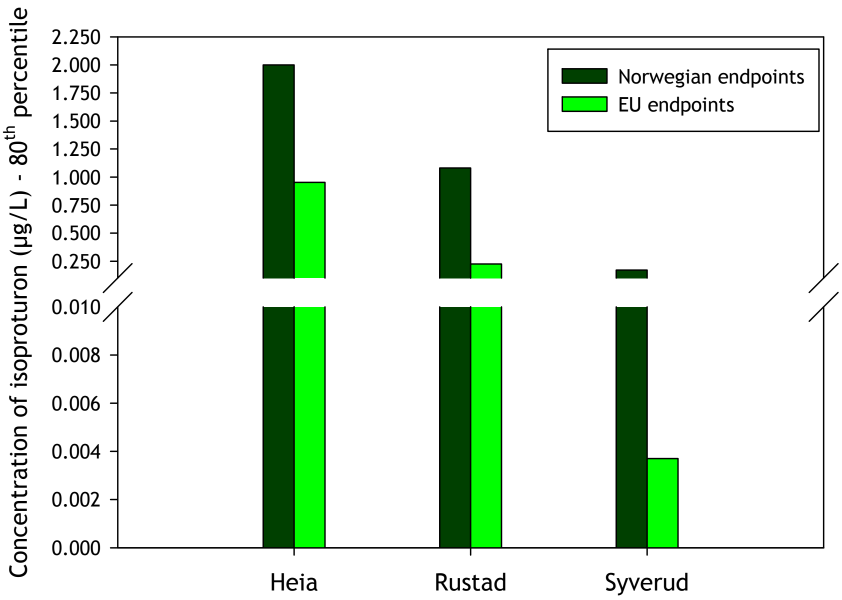

Figure 49. Leaching of isoproturon (80th percentile) from the Norwegian scenarios, using Norwegian endpoints and EU endpoints together with a Norwegian climate file. Heia and Rustad simulated with MACRO. Syverud simulated with PRAESS

For isoproturon, the 80th percentile was predicted to be 0.2 µg/L for Syverud, and 2.0 and 1.1 µg/L for Heia and Rustad, respectively. PRAESS predicts the concentration lower than the other scenarios which is simulated with MACRO, but the value is still within a factor of 10 compared to the others.

Surface water simulations

Water balance

The water balance, which is important for all modelling regarding pesticide exposure assessment, was also predicted well with PRAESS. The amount of surface runoff from Bjørnebekk was predicted to be 141 mm while the observed value was 143 mm (2005-2006) (Table 15). Surface runoff and drainage water from Syverud were predicted to 29 mm and 426 mm, respectively. The observed mean values were 23 mm (2005-2006) for the surface runoff and 454 mm (2005-2006) for the drainage water (Table 14).

Propiconazole

Figure 50 show the simulations done with PRAESS for propiconazole with the scenarios Syverud and Bjørnebekk.

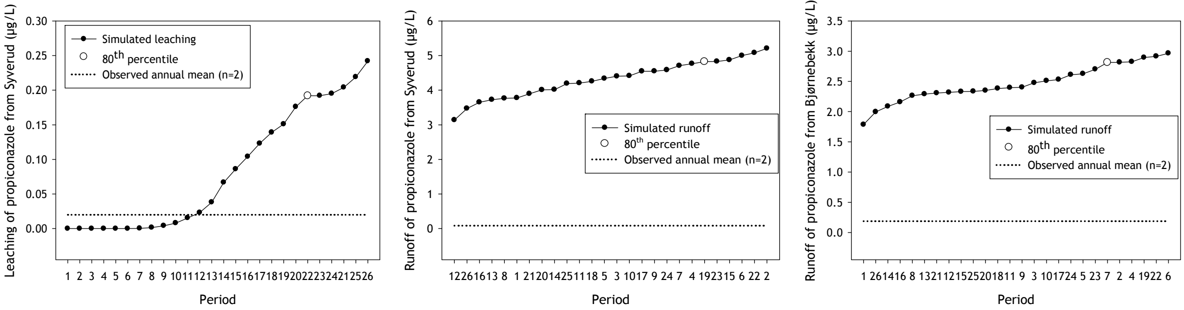

Figure 50. Leaching and runoff simulations of propiconazole with the scenarios Syverud and Bjørnebekk. The observed annual mean is obtained from the tables 11 and 12. Simulations with PRAESS

Simulated leaching of propiconazole from Syverud resulted in a concentration range from 7.90e^{-17} µg/L to 0.24 µg/L, with an 80th percentile of 0.19 µg/L. The observed annual mean value for propiconazole is 0.02 µg/L and within the simulated concentration range. The runoff simulations from Syverud varied from 3.14 – 5.21 µg/L, with an 80th percentile of 4.82 µg/L. The observed annual mean value for propiconazole is 0.08 µg/L. The simulated values with PRAESS are very high according to the observed value. The concentration of propiconazole in surface runoff from Bjørnebekk ranged between 1.79 – 2.97 µg/L, with an 80th percentile of 2.81 µg/L. The observed annual mean value is 0.19 µg/L. If we use Reichenberger's (2005) considerations according to an acceptability limit at 10, the observed mean value is within the simulated concentration range.

Metalaxyl

Figure 51 show the simulations done with PRAESS for metalaxyl with the scenarios Syverud and Bjørnebekk.

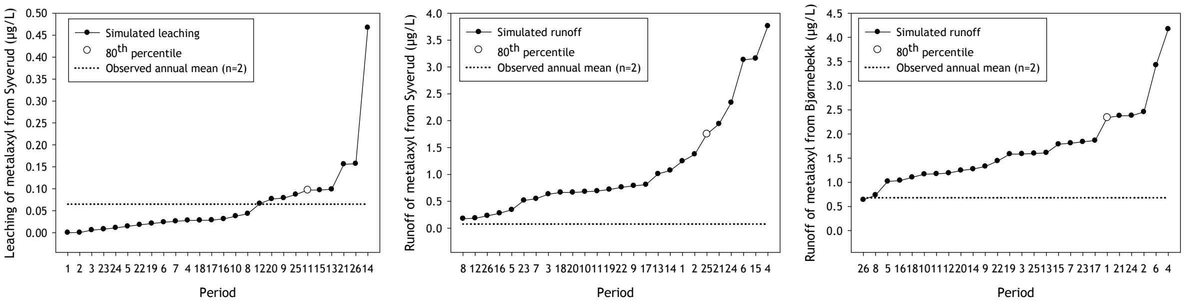

Figure 51. Leaching and runoff simulations of metalaxyl with the scenarios Syverud and Bjørnebekk. The observed annual mean is obtained from the tables 11 and 12. Simulations with PRAESS

Leaching of metalaxyl from Syverud resulted in simulated concentrations between 1.12e^{-7} µg/L and 0.47 µg/L, with an 80th percentile of 0.10 µg/L. The observed annual mean value for metalaxyl is 0.07 µg/L and within the simulated concentration range. The surface runoff simulations from Syverud varied from 0.23 – 3.76 µg/L, with an 80th percentile of 1.75 µg/L. The observed mean concentration of metalaxyl is 0.08 µg/L, which is lower than the simulated concentration range. If we consider an acceptability limit at 10, the observed mean value is within the simulated concentration range. Simulated runoff values from Bjørnebekk resulted in the concentration range 0.64 µg/L – 4.17 µg/L, with an 80th percentile at 2.34 µg/L. The observed annual mean concentration for metalaxyl is 0.68 µg/L and within the simulated values.

6. Discussion

Through work in the Forum for the Co-ordination of Pesticide Fate Models and their Use (FOCUS), EU has developed model scenarios for both groundwater and surface water. There have, however, been concerns whether these scenarios cover special Norwegian conditions such as high amount of precipitation in spring, strongly sloping fields, clayey soils and the occurrence of snowmelt on frozen ground. Concentrations and total losses of pesticides are heavily dependent on climatic conditions and especially precipitation events shortly after application and melting-freezing episodes during winter. Typical climatic conditions in Norway are the combination of long periods in winter with low temperatures and snow covered ground, which usually leads to large water flow during snowmelt in spring. Such conditions are not observed in many other countries in Europe, even though parts of Sweden, Finland and maybe Denmark might encounter similar conditions.

In Norway, approximately 3 % of the total area is agricultural land and about half of this area is mapped and digitalised. The sites used in this project represent three different soil types which totally covers only 18 % of the mapped area. However, other soil types with relative similar properties compared to the soil types used in this project, exists. The soil texture classes for the different sites in figure 2 shows that there is small differences in the texture comparing the Norwegian sites with the FOCUS and Swedish scenarios. Soil texture play an important role in water movement and pesticide leaching and even small differences in the texture might give large effects in the simulation results. Pesticide parameters like degradation and sorption are dependent on soil properties and climate, and other values than in southern parts of Europe might be expected.

National scenarios in the Nordic countries have mainly been developed with the simulation model MACRO and the scenarios using MACRO both as a groundwater and drainage model. In addition Norwegian surface runoff scenarios have been developed for the surface water model PRZM, even though the model also was tested regarding pesticide leaching. It is important that models used in risk assessment work simulate the water flow accurate. Many models often have problems regarding winter hydrology, especially in periods characterised by frozen soil, freezing and thawing cycles, and high surface runoff during snowmelt events. MACRO predicts the water flow, both daily fluxes and accumulated values, adequately. PRZM tends to over-predict the water flow for low-intensity rainfalls and small runoff events and under-predict for high-intensity rainfalls and large runoff events. The accumulated values are in general very good, especially for the drainage water. Meteorological data used for environmental fate modelling generally consist of daily values for precipitation, temperature and evapotranspiration. For environmental processes such as leaching, which occur over time scales of weeks to years, daily weather data provide adequate resolution to describe the driving force of infiltration with a reasonable degree of accuracy. For more transient processes such as runoff and erosion, which have time scales of minutes to days, the use of daily weather creates significant uncertainties (FOCUS, 2001).

Model simulations from the first field experiments at Heia and Rustad indicated high concentrations of pesticides in drainage water, but this could not be verified because data for measured water and solute fluxes was lacking. The investigations were therefore extended to include small field plots (Bjørnebekk and Syverud) equipped with systems for sampling drainage and surface runoff. The MACRO simulations showed a good adaptation for metalaxyl which is a weakly sorbed pesticide. MACRO had problems predicting propiconazole in the leachate, which indicates that other processes than ionic transport is important for stronger sorbed pesticides. For PRZM most of the results achieved for pesticide runoff from the experimental fields are acceptable. The results also show that PRZM, like MACRO, may have problems to predict runoff concentrations for pesticides which sorb strongly to soil. The results also indicate that PRZM is not a good model tool for simulating the amount of pesticides in drainage water, which probably is due to the lack of a macropore transport function in the model.

Waterborne Environmental Inc. has developed a modelling platform called PRAESS, based on PRZM, which has been designed to evaluate the potential for pesticides to occur in surface- and groundwater resources. PRAESS was tested according to earlier simulations with PRZM and according to the groundwater simulations done for Norwegian national scenarios with MACRO. The simulations indicated that the new modelling tool predicts the concentration of pesticides satisfactorily for both groundwater and surface water simulations. The water balance, which is important for all modelling regarding pesticide exposure assessment, was also predicted well. From the results obtained with these simulations, it seems that PRAESS is a good and user friendly tool for predicting the exposure of pesticides in both surface- and groundwater resources.

7. Conclusion

In order to evaluate the Norwegian groundwater scenarios, simulations were performed with MACRO for both the Norwegian scenarios and the Swedish and Danish national scenarios. Châteaudun was included as the only FOCUS groundwater scenario in MACRO. The main parameters controlling the fate and exposure of pesticides in soil and water are sorption, degradation and transport. These parameters are influenced by the properties of the pesticide, the soil, the climate and the agricultural practice which all will interfere with each other. Precipitation will directly influence the fate of pesticide especially by its effect on transport, and temperature affects degradation directly.

By running the different scenarios with endpoints agreed upon in EU with climate files from Norway, we were able to look at the direct effect of precipitation on transport and temperature on degradation. The 80^{th} percentile for almost all of the sites (locations) showed increased leaching for all pesticides tested (propiconazole, isoproturon and metalaxyl) when using Norwegian climate in comparison to simulations using site specific climate. However, the direct effect of the Norwegian climate file was relatively low especially for the mobile fungicide metalaxyl. The Swedish scenario Önnestad was the site where the Norwegian climate file affected the PECs most.

Climate will indirectly affect the exposure of pesticide by its effect on soil quality (properties) and moisture which influence degradation and especially microbial activity but also sorption and transport. The indirect effects of climate were expressed by using the specific Norwegian endpoints for sorption and degradation in the other scenarios. This increases the leaching for all sites. The leaching of metalaxyl was most affected by the Norwegian endpoints, while the leaching of isoproturon was less affected. When the Norwegian climate file and Norwegian endpoints were added, the leaching of all pesticides increased even more.

The intention behind the FOCUS scenarios is that they are supposed to cover all climatic regions in Europe. This is a rather ambitious goal. In Sweden and Denmark several national scenarios have been introduced and France has also developed separate scenarios for all regions. OECD has introduced an idea to divide North America and EU into Eco-regions, but so far this work has not been completed as it is hard to find relevant parameters for the selection of regions. The trend is to identify more site specific risk of exposure, and this might lead to the demand for more specific information in the future also within countries. For Norway important endpoint data will be available when results from degradation and sorption studies of several pesticides at four locations widespread in Norway have been obtained. These locations represent South-East (Ås), South-West (Særheim), Mid-West (Kvithamar) and North of Norway (Tromsø). These studies might help to verify whether climate and other factors, affecting the fate and behaviour of pesticides, are so different in the northern parts of Europe that there is a need for specific national groundwater and/or surface water scenarios.

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9. Appendixes

Summary of appendixes

No.	Subject
I	Parameters for different locations and soils, pesticides and plant growth parameters – MACRO
II	Input parameters for PRZM
III	Personal communication from Nick Jarvis, Member of the EU FOCUS Surface Water Scenarios Group

Appendix I Parameters for different locations and soils, pesticides and plant growth - MACRO

Climatic parameters which are used for all FOCUS scenarios are showed in Table 1. These values are also used in the Norwegian simulations.

Table 1. Climatic parameters in MACRO, reference values used for all FOCUS scenarios

Parameters	Description	Ref.value	Rustad	Heia
CONC	Pesticide concentration in rainfall (mg/m^3)	0	0	0
RAINCO	Rainfall correction factor	1	1	1
SNOWCO	Snowfall correction factor	1	1	1
RINTEN	Rainfall intensity (mm/h)	2	2	2
SNOWMF	Snowmelt factor (mm °C d^{-1})	4.5	2.0	2.0
ALBEDO	Albedo	0.25	0.25	0.25

According to soil characteristic, there are 11 reference parameters in the FOCUS scenarios. Table 2 show the reference values and chosen values for the Norwegian scenarios.

Table 2. Reference values for some soil characteristics in the FOCUS scenarios and values used in the Norwegian scenarios Rustad and Heia

Parameters	Description	Ref.value	Rustad	Heia
DV	Dispersivity (cm)	5	0.1	1
ZMIX	Mixing depth (mm)	0.1	1	1
ZP	Slope of shrinkage characteristics	0	0	0
ZM	Tortuosity factor (micropores)	0.5	0.5	0.5
ZA	Geometry factor	1	1	1
FRACMAC	Fraction of sorption sites in macropores	0.02	0.02	0.02
TEMPINI	Initial soil temperature	10	4	4
SOLINIT	Initial pesticide concentration (mg/m^3)	0	0	0
CONCIN	Pesticide concentration at bottom boundary	0	0	0
CRITAIR	Critical soil air content for transpiration reduction (m^3/m^3)	0.05	0.05	0.05
AEXC	Excluded pore volume (m^3/m^3)	0	10	0

Table 3, 4 and 5 shows scenario specific soil and site parameters for different horizons.

Table 3. Scenario-specific soil and site parameters for the Ap-horizon

Parameters	Description	Önnestad	Krusenberg	Heia	Näsbygård	Rustad	Châteaudun	Lanna	Skousbo	Bjørnebekk	Syverud
	Depth (cm)	0-20	0-20	0-30	0-25	0-18		0-30	0-25	0-20	0-20
	Sand (%)	78	91	65	33	13	3	7	51	11	28
	Silt (%)	12	4	30	42	60	67	46	37	62	49
	Clay (%)	10	5	5	25	27	30	47	12	27	23
	Organic carbon (%)	1.9	1.0	2.2	1.2	1.9	1.4	2.0	1.4	2.4	3.2
GAMMA	Bulk density (g/cm^3)	1.4	1.3	1.4	1.4	1.2	1.3	1.4	1.5	1.5	1.4
TPORV	Saturated water content	44.0	49.0	44.0	44.0	57.0	43.0	47.0	42.0	48.0	50.0
WILT	Wilting point	6.0	7.0	14.9	14.0	11.4	25.8	26.0	15.0	16.0	12.0
RESID	Residual water content	4.0	5.0	13.4	0.0	0.0	0.0	0.0	4.0	0.0	0.0
XMPOR	Water content at macro /micorpore boundary	42.0	43.0	40.5	40.0	49.9	41.0	40.0	40.0	44.0	47.8
CTEN	Water tension at macro /micropore boundary (cm)	20.0	18.0	11.0	10.0	6.0	20.0	10.0	10.0	10.0	20.0
ZLAMB	Pore size distribution index	0.484	0.407	0.133	0.142	0.081	0.070	0.070	0.150	0.205	0.271
ZM	Tortuosity factor micropores							0.5	0.5		
ZN	Tortuosity factor macropores	3.0	3.0		3.0			2.0	3.0		
ASCALE	Effective diffusion pathlength (mm)	1.0	1.0	4.0	90.0	5.0		150.0	55.0		
KSATMIN	Saturated hydraulic conductivity (mm/hr)	104.0	95.0	50.0	100.0	68.0	72.0	200.0	30.0	41.0	58.0
KSM	Conductivity at macro /micropore boundary (mm/hr)	3.7	2.2	4.9	0.4	1.4	0.3	0.1	0.5	1.0	1.0
DRAINDEP	Drain depth (m)		1.0	1.0	1.0	1.0		1.0	1.2	1.0	1.0
SPACE	Drain spacing		15.0	15.0	15.0	15.0		13.5	10.0	8.0	8.0
BGRAD	Transmission coefficient at bottom boundary (1/h)	0.4 BTEN	1.0e-05		1.0e-05			2.0e-06	3.0e-06		

Table 4. Scenario-specific soil and site parameters for the E/B-horizon

Parameters	Description	Önnestad	Krusenberg	Heia	Näsbygård	Rustad	Châteaudun	Lanna	Skousbo	Bjørnebekk	Syverud
	Depth (cm)	33-53	35-55	30-40	25-50	29-38	25-50	30-60	25-45	25	25
	Sand (%)	96	90	56	26	10	2	3	70	11	28
	Silt (%)	2	6	40	44	57	31	41	17	62	49
	Clay (%)	2	4	4	30	33	67	56	13	27	23
	Organic carbon (%)	0.2	0.3	0.3	0.4	0.4	0.9	0.8	0.8	0.7	0.8
GAMMA	Bulk density (g/cm^3)	1.6	1.5	1.7	1.5	1.7	1.4	1.4	1.7	1.6	1.7
TPORV	Saturated water content	40.0	42.0	41.3	41.0	34.2	44.0	46.0	36.0	42.0	47.0
WILT	Wilting point	4.0	5.0	6.9	15.0	12.9	23.7	29.0	13.0	16.0	12.0
RESID	Residual water content	3.0	3.0	1.9	0.0	0.0	0.0	0.0	4.0	0.0	0.0
XMPOR	Water content at macro/micorpore boundary	33.0	35.0	38.4	40.0	32.2	43.0	42.0	34.0	42.5	44.6
CTEN	Water tension at macro/micropore boundary (cm)	16.0	20.0	13.0	10.0	6.0	20.0	10.0	12.0	25.0	10.0
ZLAMB	Pore size distribution index	0.919	0.557	0.246	0.131	0.040	0.090	0.050	0.150	0.047	0.366
ZM	Tortuosity factor micropores							0.5	0.5		
ZN	Tortuosity factor macropores	3.0	3.0		3.0			2.0	3.0		
ASCALE	Effective diffusion pathlength (mm)	1.0	1.0	50.0	90.0	17.0		100.0	55.0		
KSATMIN	Saturated hydraulic conductivity (mm/hr)	295.0	40.0	3.5	20.0	163.0	108.0	50.0	15.0	8.1	25.0
KSM	Conductivity at macro/micropore boundary (mm/hr)	3.6	1.7	2.5	0.5	1.0	0.5	0.3	1.0	1.0	1.0

Table 5. Scenario-specific soil and site parameters for the B-horizon

Parameters	Description	Önnestad	Krusenberg	Heia	Näsbygård	Rustad	Châteaudun	Lanna	Skousbo	Bjørnebekk	Syverud
	Depth (cm)	40-60	50-100	30-40	50-75	38-58	60-100	60-100	75-120	50	50
	Sand (%)	94	12	47	36	6	30	2	33	4	23
	Silt (%)	4	32	41	39	55	26	37	39	60	56
	Clay (%)	2	56	12	25	39	44	61	28	36	21
	Organic carbon (%)	0.1	0.3	0.1	0.2	0.3	0.3	0.3	0.2	1.3	0.8
GAMMA	Bulk density (g/cm^3)	1.6	1.4	1.7	1.5	1.7	1.4	1.4	1.8	1.7	1.7
TPORV	Saturated water content	39.0	48.0	39.4	40.0	34.2	44.0	47.0	33.0	49.7	40.0
WILT	Wilting point	3.0	28.0	9.3	15.0	17.3	18.8	31.0	16.0	16.0	16.0
RESID	Residual water content	2.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0
XMPOR	Water content at macro/micropore boundary	32.0	45.0	36.5	39.0	32.2	43.0	45.0	32.0	49.5	38.2
CTEN	Water tension at macro/micropore boundary (cm)	16.0	10.0	13.0	10.0	6.0	40.0	10.0	16.0	35.0	10.0
ZLAMB	Pore size distribution index	0.943	0.056	0.202	0.121	0.046	0.140	0.050	0.150	0.035	0.058
ZM	Tortuosity factor micropores							0.5	0.5		
ZN	Tortuosity factor macropores	3.0	3.0		3.0			2.0	3.0		
ASCALE	Effective diffusion pathlength (mm)	1.0	50.0	25.0	100.0	20.0		300.0	55.0		
KSATMIN	Saturated hydraulic conductivity (mm/hr)	300.0	20.0	11.5	10.0	271.0	43.2	30.0	1.0	2.4	2.5
KSM	Conductivity at macro/micropore boundary (mm/hr)	3.5	0.3	2.6	0.4	1.0	1.0	0.2	0.1	1.0	1.0

Table 6 show the plant growth parameters for spring cereals for different sites

Table 6. Plant growth parameters for spring cereals

Parameters	Descriptions	Krusenberg	Önnestad	Näsbygård	Rustad	Heia	Châteaudun
BETA	Root adaptability factor (m)	0.2	0.2	0.2	0.2	0.2	0.1
CANCAP	Maximum water interception by the crop (mm)	2.0	2.0	2.0	2.0	2.0	2.0
CFORM	Form factor for the period from emergence to maturity	2.0	2.0	2.0	2.0	2.0	2.0
DFORM	Form factor for the period from maturity to harvest	0.3	0.3	0.3	0.3	0.3	0.3
IDSTART	The day of emergence of the crop	135	116	116	135	135	69
IDMAX	The day of maturity of the crop	172	165	165	172	172	161
IHARV	The day of harvest of the crop	247	238	238	247	247	201
LAIMAX	Leaf area index at maturity	4.0	4.0	4.0	4.0	4.0	5.0
LAIHARV	Leaf area index at harvest	1.0	1.0	1.0	1.0	1.0	5.0
ROOTMAX	Maximum root depth (m)	0.7	0.5	1.0	0.7	0.7	0.6
RPIN	Percentage of the root length in the top 25 % of the root depth	60	60	60	60	60	60
LAIMIN	The leaf area index at the date ZDATEMIN	0.01	0.01	0.01	0.01	0.01	0.01
ZHMIN	The crop height at the date ZDATEMIN	0.01	0.01	0.01	0.01	0.01	0.01
ROOTINIT	Root depth at the date ZDATEMIN (m)	0.01	0.01	0.01	0.01	0.01	0.01
ZDATEMIN	The day number corresponding at LAIMIN, ROOTINIT and ZHMIN	136	117	117	136	136	70
WATEN	Critical tension for root water uptake	1.9	1.4	5.1	1.9	1.9	2.0 (?)

Appendix II Input parameters for PRZM

Tables 1 – 3 show the parameters which were chosen to calibrate the model.

Table 1. Parameter descriptions for the scenarios Bjørnebekk and Syverud

PARAMETER AND DESCRIPTION	VALUE, SOURCE AND COMMENTS
Record 1 TITLE: label for simulation title	
Record 2 HTITLE: label for hydrology information title	
Record 3 PFAC: pan factor used to estimate the daily potential evapotranspiration (ET) from daily pan evaporation	Chosen value is 1.0 for both scenarios, because the meteorological file contents pot. ET
SFAC: snowmelt factor in cm/degrees Celsius above freezing	Chosen value is 0.20 for both scenarios. This value is also recommended from FOCUS.
IPEIND: pan factor flag	This is set to 0, indicating that daily pan evaporation data is read from the meteorological file
ANETD: minimum depth from which evaporation is extracted	ANETD is location specific and is highly correlated to climatic conditions. This value helps determine soil evaporative losses during fallow. Chosen value is 10 cm for both scenarios
INICRP: flag for initial crop	This is set to 1 for both scenarios, indicating initial crop
ISCOND: surface condition of initial crop	This is set to 1 for both scenarios, indicating fallow
Record 6 ERFLAG: flag to select simulation of erosion	This is set to 4 for both scenarios indicating use of MUSS equation, the soil loss equation appropriate for small watersheds
Record 7 USLEK: soil erodibility factor for MUSS	Scenario specific soil data, decided from manual. Set to 0.38 for Syverud and 0.35 for Bjørnebekk
USLELS: topographic factor for MUSS	Scenario specific soil data, decided from manual. Set to 1.9 for Syverud and 1.8 for Bjørnebekk
USLEP: practice factor for MUSS	Scenario specific soil data, decided from manual. Set to 1.0 for both scenarios
AFIELD: field area for MUSS	Scenario specific data, 0.0402 ha at Syverud and 0.0178 ha at Bjørnebekk
IREG: SCS rainfall distribution region	Data decided from manual, set to 3 for both scenarios (type 2)
SLP: land slope (%)	Scenario specific data. Slope set to 13 % for both scenarios
HL: hydraulic length (m)	Scenario specific data, set to 25 m for both scenarios
Record 8 NDC: number of different crops in simulation	Only one crop in simulation, set to 1 for both scenarios
Record 9 ICNCN: crop number	Set to 1 for both scenarios

CINTCP: maximum interception storage AMXDR: maximum rooting depth of crop COVMAX: maximum canopy coverage ICNAH: surface condition after harvest CN: runoff curve numbers for fallow, cropping and residue WFMAX: maximum dry weight of crop HTMAX: max canopy at maturation date	Crop specific data, decided from manual. Set to 0.16 for both scenarios Crop specific data decided from manual. Set to 30 cm for both scenarios Crop specific data. Set to 90 % for both scenarios This is ignored if ERFLAG>0, so no value for both scenarios Only used if erosion flag is off (ERFLAG = 0). CN values are read from Record 9E Only required if CAM = 3 (record 16). Set to 0.0 for both scenarios Set to 80 cm for both scenarios
Record 9A CROPNO: crop number NUSLEC: number of sets of erosion factors	 Set to 1 for both scenarios Set to 4 for both scenarios (emergence, maturation, harvest, fallow)
Record 9B (four dates) Dates for each set of erosion factors – emergence, maturation, harvest and fallow	 Crop and scenario specific data. Emergence 3/5, maturation 19/9, harvest 28/9 and fallow 19/10
Record 9C (four values) USLEC: universal soil loss cover management factors	 Crop specific data decided from manual. Set to 0.2 – 0.2 – 0.5 – 1.0 for both scenarios. Values correspond to dates in record 9B
Record 9D (four values) MNGN: Manning's roughness coefficient	 Scenario specific soil data decided from manual. Set to 0.17 – 0.17 – 0.17 – 0.17 for both scenarios. Values correspond to dates in record 9B
Record 9E (four values) CN: runoff curve numbers of antecedent moisture condition II for fallow, cropping and residue	 Crop and scenario specific data decided from manual. Set to 74 – 74 – 76 – 78 for Syverud and 84 – 84 – 88 – 94 for Bjørnebekk. Values correspond to dates in record 9B
Record 10 NCPDS: number of cropping periods	 Set to 1 for both scenarios, since it is only one cropping period in the simulations
Record 11 EMD, EMM, IYREM: crop emergence date MAD, MAM, IYRMAT: crop maturation date HAD, HAM, IYRHAR: crop harvest date INCROP: crop number associated with NDC	Crop and scenario specific data: 3/5 19/9 28/9 Set to 1 for both scenarios, only one crop
Record 13 NAPS: total number of applications occurring at different dates NCHEM: number of chemicals in simulation FRMFLG: flag for testing of ideal soil moisture conditions for application	 Set to 1 for both scenarios Set to 1 for both scenarios, parent only Set to 0 for both scenarios, PRZM soil moisture test not used

DKFLG2: flag to allow input of biphasic degradation half-life	Set to 0 for both scenarios, no biphasic half-life
Record 15 PSTNAM: name of chemical for output file	
Record 16 AP_DDMMYY: target application dates WINDAY: number of days in which to check soil moisture following target date CAM: flag to select application method DEPI: incorporation depth of application (cm) TAPP: target application rate (kg/ha) APPEFF: application efficiency (fraction) DRFT: spray drift (fraction)	16/6 – 2005 and 7/6 - 2007 Set to 0, option not used Selected chemical applications methods was CAM = 1 for both scenarios. This is the default for use with FOCUS scenarios Default application depth is 4 cm Propiconazole: 0.250 kg/ha (2005) 0.125 kg/ha (2007) Metalaxyl: 0.225 kg/ha (2005 and 2007) This is set to 1.0 for both scenarios This is set to 0 for both scenarios
Record 17 FILTRA: filtration parameter (for CAM 3) IPSCND: disposition of pesticide after harvest UPTKF: plant uptake factor	Set to 0, option not used for FOCUS This is set to 3, left alone, for both scenarios This is set 0.5 for both pesticides
Record 19 STITLE: label for soil properties title	
Record 20 CORED: total depth of soil core (cm) BDFLAG: bulk density flag THFLAG: filed capacity and wilting point flag KDFLAG: soil adsorption flag HSWZT: drainage flag MOC: method of characteristics flag IRFLAG: irrigation flag ITFLAG: soil temperature simulation flag IDFLAG: thermal conductivity and heat capacity flag BIOFLG: biodegradation flag	Set to 100 cm at Syverud and 50 cm at Bjørnebekk Set to 0, bulk density is entered directly Set to 0, soil moisture defined for each scenario Set to 2, normalized Freundlich equation Set to 0, free drainage assumed Set to 0, MOC not used Set to 0, no irrigation simulated Set to 2, soil temperature is simulated with the use of temperature and moisture corrected degradation Set to 1, model simulates temperature profile using default thermal conductivity and heat capacity Set to 0, microbial population degradation algorithms not used
Record 26 DAIR: molecular diffusion coefficient for the pesticides in air	Set to 4300 cm^2/day, FOCUS definition

HENRYK: normalized Henry's law constant of the pesticides – dimensionless ENPY: enthalpy of vaporization of the pesticides (kcal/mole)	Set to 1.6E-5 for metalaxyl and 9.2E-5 for propiconazole Set to 22.7 kcal/mole, FOCUS definition
Record 30A (only if KDFLAG = 2,3) FRNDCF: freundlich exponent 1/n (dimensionless)	 Set to 0.9 and 0.82 for metalaxyl in Syverud and Bjørnebekk, respectively. Set to 1.13 and 0.82 for propiconazole in Syverud and Bjørnebekk, respectively
Record 31 (only if ITFLAG = 1,2) ALBEDO: monthly values of soil surface albedo (12 values) EMMISS: reflectivity of soil surface to long wave radiation (fraction) ZWIND: height of wind speed measurement above the soil surface (m)	 Set to 0.6 - 0.6 - 0.3 - 0.3 - 0.18 - 0.1 - 0.1 - 0.1 - 0.1 - 0.15 - 0.18 - 0.6 for both scenarios Set to 0.96, average for natural surfaces at normal temperatures. FOCUS definition Set to 2 m
Record 32 (only if ITFLAG = 1,2) BBT: average monthly values of bottom boundary soil temperatures in degrees Celsius (12 values)	 Set to 4.1 - 3.8 - 3.4 - 3.8 - 7.8 - 8.4 - 9.9 - 10.6 - 9.2 - 8.9 - 7.4 - 6.3 for both scenarios
Record 32A (only if ITFLAG = 2) QFAC: Q10 – factor for determining degradation rate increase when temperature increases by 10 °C TBASE: reference temperature for degradation data	 Set to 2.2, FOCUS definition Set to 20 °C, which is standard temperature for degradation studies in laboratory
Record 32B (only if ITFLAG = 2) ABSREL: flag for type of reference soil moisture data B-VALUE: exponent for moisture correction REFMOIST: reference moisture correction for degradation data	 Set to 2, reference soil moisture entered relative to field capacity Set to 0.7 as default, FOCUS definition Set to 100 %
Record 33 NHORIZ: total number of horizons	 Syverud: 5 horizons, Bjørnebekk: 3 horizons
Record 34 (repeat records 34-38 up to NHORIZ) HORIZN: horizon number THKNS: thickness of the horizon BD: soil dry bulk density (g/cm^3)' THETO: initial soil water content (cm^3/cm^3) AD: soil drainage parameter (day^{-1}) DISP: pesticides hydrodynamic dispersion coefficient (cm^2/day) ADL: lateral soil drainage parameter (day^{-1})	 See soil parameters in table 2 See soil parameters in table 2 See soil parameters in table 2 Set to field capacity for scenario and horizon; see soil parameters in table 2 Set to 0, option not used Set to 0, parameter not used Set to 0, option not used
Record 36 (for DKFLG2 = 0) DWRATE: dissolved phase pesticides degradation rate for first phase of bi-phase reaction (day^{-1})	 See pesticide parameters in table 3

DSRATE: adsorbed phase pesticides degradation rate for first phase of bi-phase reaction (day^{-1}) DGRATE: adsorbed phase pesticides degradation rate for first phase of bi-phase reaction (day^{-1})	DSRATE is similar to DWRATE, FOCUS definition DGRATE is set to 0, FOCUS definition
Record 37 (for each horizon) DPN: thickness of compartments (cm) THEFC: field capacity (cm^3/cm^3) THEWP: wilting point (cm^3/cm^3) OC: organic carbon (%) KD: layer specific partition coefficient for each horizon (l/kg)	 Set to 0.1 cm for 0-10 cm depth and 5 cm for >10 cm depth, FOCUS definition See soil parameters in table 2 See soil parameters in table 2 See soil parameters in table 2 See pesticide parameters in table 3
Record 38 (for each horizon but only if ITFLAG = 1,2) SPT: initial temperature (Celsius) SAND: sand content (%) CLAY: clay content (%) THCOND: thermal conductivity (cal/cm day °C) VHTCAP: heat capacity per unit volume (cal/cm^3 °C)	 Set to 5 °C for each horizon See soil parameters in table 2 See soil parameters in table 2 Set to 0, default values used (IDFLAG = 1) Set to 0, default value used (IDFLAG = 1)
Record 40 ILP: flag for initial pesticide concentrations in soil before start of simulation	 Set to 0 (no initial pesticide concentration in soil profile)
Record 42 Output options	
Record 45 NPLOTS: number of time series plots STEP4: output time steps	 Set to DAY, these values create the daily time series output file (scenario filename.zts)

Table 2. Soil and site parameters

	Syverud					Bjørnebekk		
	0-10 cm	10-25 cm	25-50 cm	50-70 cm	70-100 cm	0-10 cm	10-20 cm	20-50 cm
Sand (%)	26	25	25	17	13	9	14	1
Silt (%)	47	48	57	53	48	64	64	57
Clay (%)	27	27	18	30	39	26	23	42
Organic carbon (%)	3.1	2.9	0.4	0.3	0.3	1.5	0.6	0.3
Bulk density (g/cm^3)	1.4	1.4	1.7	1.7	1.7	1.5	1.6	1.6
Field capacity (%)	40.7	40.7	33.0	31.1	31.1	36.2	38.2	38.2
Wilting point (%)	12.0	12.0	16.0	18.0	18.0	16.4	16.0	16.0

Table 3 show the decay rates and sorption coefficients for the pesticides propiconazole and metalaxyl.

Table 3. Decay rate (per day) and dissolved (DWRATE) and adsorbed (DSRATE) phase and Freundlich coefficients (K_F and $1/n^{ads}$) of propiconazole (P) and metalaxyl (M) for each horizon used in calibrated and validated simulations

Horizon	Parameter	Syverud	Bjørnebekk
1	DWRATE P	0.00247	0.00481
	DWRATE M	0.01824	0.00648
	DSRATE P	0.00247	0.00481
	DSRATE M	0.01824	0.00648
	K_F P	32.0	15.8
	K_F M	0.65	0.75
2	DWRATE P	0.00247	0.00481
	DWRATE M	0.01824	0.00648
	DSRATE P	0.00247	0.00481
	DSRATE M	0.01824	0.00648
	K_F P	32.0	15.8
	K_F M	0.65	0.75
3	DWRATE P	0.00178	0.00403
	DWRATE M	0.02166	0.00127
	DSRATE P	0.00178	0.00403
	DSRATE M	0.02166	0.00127
	K_F P	14.9	4.6
	K_F M	0.41	0.75
4	DWRATE P	0.00178	
	DWRATE M	0.02166	
	DSRATE P	0.00178	
	DSRATE M	0.02166	
	K_F P	14.9	
	K_F M	0.41	
5	DWRATE P	0.00178	
	DWRATE M	0.02166	
	DSRATE P	0.00178	
	DSRATE M	0.02166	
	K_F P	14.9	
	K_F M	0.41	
	$1/n^{ads}$ P	1.13	0.82
	$1/n^{ads}$ M	0.9	0.82

Appendix III Personal communication from Nick Jarvis, Member of the EU FOCUS Surface Water Scenarios Group, 2005

Swedish University of Agricultural Sciences
Department of Soil Sciences

12th January

To whom it may concern

This letter is to confirm that, in my considered opinion, the EU 'FOCUS' Surface Water scenarios for pesticide exposure assessments do not adequately address the major issues and concerns for surface water contamination by pesticides under Norwegian conditions.

From the point of view of climate, the FOCUS drainage scenario D1 (Lanna, Sweden) is definitely the only scenario that could possibly be considered representative for at least some parts of Norwegian agriculture. However, one of the major concerns for surface water contamination under Norwegian agricultural conditions is the occurrence of surface runoff, with often strongly sloping fields and high precipitation amounts during the pesticide application period in spring and early summer, and also the frequent occurrence of snowmelt on frozen ground. None of the EU FOCUS scenarios specifically dealing with surface runoff have a suitable (i.e. Scandanavian) climate.

Yours sincerely

NJarvis

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