Fraunhofer IME

Study Report

Predicted Environmental Concentrations in Groundwater of Nitrate after fertilization using FOCUSPEARL

Simulations in oil seed rape (winter), potatoes, and cabbage

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Statement of compliance

This study "*Predicted Environmental Concentrations in Groundwater of Nitrate after fertilization using FOCUSPEARL - Simulations in oil seed rape (winter), potatoes, and cabbage*" was conducted according to the procedures described herein. This report is a true and accurate record of the results obtained. There were no circumstances that may have adversely impacted the quality or integrity of the study.
The GLP-regulation is not applicable. However, the study was performed in accordance with the Codex of "Good Modelling Practices" (Görlitz 1993 und Travis 1995)

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1. Simulation model

The simulation model FOCUS-PEARL 4.4.4 was used for the calculation of the predicted environmental concentrations in groundwater (PECgw) of nitrate. Solute transport was calculated with the Convection-Dispersion-Equation (CDE). Non-linear sorption was implemented using a Freundlich isotherm. Depth-dependent sorption and transformation parameters were considered according to the common approach in FOCUS (2000) and FOCUS (2009).

2. Scenarios

Soil and climate scenarios of the FOCUS simulation models

The soil and climate scenarios defined by FOCUS 2000 were selected to represent a vulnerability approximating the 90th percentile for each scenario (realistic worst-case). Soils were selected by expert judgment whereas the weather data sets were obtained from the MARS meteorological database (MARS = Monitoring Agricultural ResourceS). The nine locations cover all climatic regions of agricultural relevance in Europe (Figure 1) and are briefly characterized in Table 1. For all scenarios, daily weather data are available for a period of 20 years.

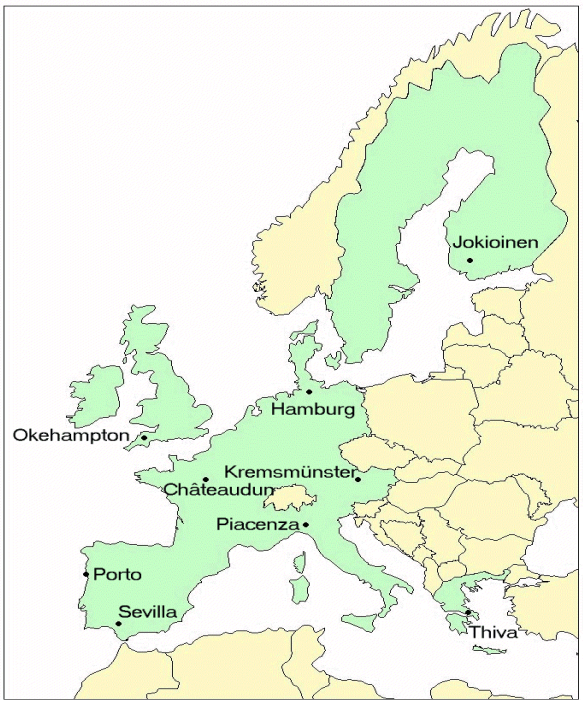

Figure 1: Locations of the nine FOCUS groundwater scenarios

Table 1: Characteristics of the nine weather and soil scenarios created by FOCUS

Location	Soil type (USDA)	Organic Matter [%]	Annual average air temperature [°C]	Annual sum of precipitation [mm]
Châteaudun	silty clay loam	2.4	11.3	648+ I*
Hamburg	sandy loam	2.6	9.0	786
Jokioinen	loamy sand	7.0	4.1	638
Kremsmünster	loam/silt loam	3.6	8.6	900
Okehampton	loam	3.8	10.2	1038
Piacenza	loam	2.2	13.2	857 + I*
Porto	loam	2.5	14.8	1150
Sevilla	silt loam	1.6	17.9	493 + I*
Thiva	loam	1.3	16.2	500 + I*

*irrigation

Crop scenarios

For the simulations a single variation (continuous cropping of oil seed rape (winter), potatoes, and cabbage) over a period of 26 years is taken into account according to the recommendations of FOCUS [FOCUS 2000].

Table 2: Considered scenarios for the simulation of single variation of nitrate in ground water

Scenario	Crop	Application	App. Type	Dosage in kg/ha	Date	Time period
1a	Oil seed rape	1st	To the soil surface	45	30/08/1901	August/September
1b	Oil seed rape	1st	To the soil surface	215.1	28/02/1901	February/march
		2nd	To the soil surface	258.7	01/04/1901	April
2	Potatoes	1st	To the soil surface	273.1	01/04/1901	begin of April
		2nd	To the soil surface	279.8	30/06/1901	end of June/begin of July
3	Cabbage)	1st	To the soil surface	262.2	01/05/1901	May
		2nd	To the soil surface	335.7	01/06/1901	May/June
		3rd	To the soil surface	335.7	01/07/1901	July
		4th	To the soil surface	335.7	01/08/1901	August

3. Physico-chemical and Degradation Data

Nitrate

Ammonium nitrate degrades to ammonium and nitrate in soil. In order to simulate the fate of nitrate realistically the sorption constant in soil KOC of nitrate was set to zero and the water was set to an artificial value of 10000 mg/L at 20°C.

Nitrate

Molecular Mass:	62 g/mol
Vapour pressure:	0
Water solubility:	10 000 mg/L at 20 °C
Adsorption	0 L/kg (Koc)
	0 L/kg (Kom)
Freundlich Exponent.	0.9 (default)
Diffusion coefficient in water:	4.3 10-5 m² d-1 (FOCUS default)
Diffusion coefficient in air:	0.43 m² d-1 (FOCUS default)
Degradation:	DT50: 1000 d at 20 °C
Plant uptake factor:	0.0 (worst case)
Application mode:	annual application

4. Results

The global maximum concentrations are summarised in the following tables. Four simulations using different crops and application patterns are performed:

- Scenario 1a: Oil seed rape (winter), 45 kg/ha in August/September
- Scenario 1b: Oil seed rape (winter), 215.1 kg/ha in February/March, 258.7 kg/ha in April
- Scenario 2: Potatoes, 273.1 kg/ha in begin of April, 279.8 kg/ha in end of June/begin of July
- Scenario 3: Cabbage, 262.2 kg/ha in May, 335.7 kg/ha in May/June, 335.7 kg/ha in July, 335.7 kg/ha in August

The highest concentration of nitrate in leachate for the oil seed rape scenario (1a, 1b) are obtained in Châteaudun. For potatoes (scenario 2), the highest concentrations are predicted in Thiva. In Jokioinen the highest nitrate concentrations are found for cabbage.

Table 3: 80th percentile of annual leaching concentration for nitrate of scenario 1 (oil seed rape)

Scenario	1a: Oil seed rape (winter), 45 kg/ha in August/September	1b: Oil seed rape (winter), 215.1 kg/ha in February/March, 258.7 kg/ha in April
Location	80^{th} percentile of concentration in leachate (µg NO3 /L)	80^{th} percentile of concentration in leachate (µg NO3 /L)
CHATEAUDUN	53200.3691	543061.53
HAMBURG	24134.7502	250791.419
KREMSMUENSTER	13936.6333	141753.74
OKEHAMPTON	13255.8316	134466.351
PIACENZA	18512.5227	189279.942
PORTO	16390.4251	162046.403

Table 4: 80th percentile of annual leaching concentration for nitrate of scenario 2 (potatoes)

Scenario	2: Potatoes, 273.1 kg/ha in begin of April, 279.8 kg/ha in end of June/begin of July
Location	80th percentile of concentration in leachate (µg NO3 /L)
CHATEAUDUN	335617.5851
HAMBURG	292349.6938
JOKIOINEN	369525.1315
KREMSMUENSTER	185514.3181
OKEHAMPTON	149220.097
PIACENZA	239289.3722
PORTO	121735.34
SEVILLA	420744.0245
THIVA	539480.0475

Table 5: 80th percentile of annual leaching concentration for nitrate of scenario 3 (cabbage)

Scenario	3: Cabbage, 262.2 kg/ha in May, 335.7 kg/ha in May/June, 335.7 kg/ha in July, 335.7 kg/ha in August
Location	80th percentile of concentration in leachate (µg NO3 /L)
CHATEAUDUN	670070.9644
HAMBURG	648717.8676
JOKIOINEN	886762.5166
KREMSMUENSTER	401065.5267
PORTO	262669.438
SEVILLA	**********
THIVA	659263.4098

********** Simulation failed

5. Conclusion

Three different crops are considered to calculate the concentration of nitrate in the leachate. Nitrate reaches groundwater by leaching (Table 3, Table 4 and Table 5).

6. References

FOCUS (2000). FOCUS groundwater scenarios in the EU plant protection product review process. Report of the FOCUS Groundwater Scenario Workgroup, EC Document Reference Sanco/321/2000.

FOCUS (2009): Technical advice on the Q10, agreed by the Commission Standing Committee on the Food Chain and Animal Health (provided by EFSA), available at FOCUS home page (http://viso.ei.jrc.it/focus/docs/Technical%20advice%20on%20the%20Q10.doc)

Görlitz G. (1993): Verfahrensregeln zur korrekten Durchführung und Auswertung von Modellrechnungen zur Simulation des Umweltverhaltens von Pflanzenschutzmitteln.

Travis K.Z. (1995): Recommendations for the correct use of models and reporting of modelling results.- in: 'Leaching Models and EU registration'. Final report of the FOCUS Group. Doc. 4952/VI/95

7. Appendix: PEARL FOCUS Summary Output file

Oil seed rape (winter), 45 kg/ha in August/September

RUN_ID	RESULT_TEXT	SUBSTANCE	NO3	LOCATION	APPLICATION_SCHEME	CROP_CALENDAR	SOIL_TYPE	METEO_STATION	IRRIGATION_SCHEME
100	Concentration closest to the 80th percentile (ug/L)	NO3	53200.3691	CHATEAUDUN	Nitrate_OSR1	CHAT-WOILSEED	CHAT-S_Soil	CHAT-M	No
101	Concentration closest to the 80th percentile (ug/L)	NO3	24134.7502	HAMBURG	Nitrate_OSR1	HAMB-WOILSEED	HAMB-S_Soil	HAMB-M	No
102	Concentration closest to the 80th percentile (ug/L)	NO3	13936.6333	KREMSMUENSTER	Nitrate_OSR1	KREM-WOILSEED	KREM-S_Soil	KREM-M	No
103	Concentration closest to the 80th percentile (ug/L)	NO3	13255.8316	OKEHAMPTON	Nitrate_OSR1	OKEH-WOILSEED	OKEH-S_Soil	OKEH-M	No
104	Concentration closest to the 80th percentile (ug/L)	NO3	18512.5227	PIACENZA	Nitrate_OSR1	PIAC-WOILSEED	PIAC-S_Soil	PIAC-M	No
105	Concentration closest to the 80th percentile (ug/L)	NO3	16390.4251	PORTO	Nitrate_OSR1	PORT-WOILSEED	PORT-S_Soil	PORT-M	No

Oil seed rape (winter), 215.1 kg/ha in February/March, 258.7 kg/ha in April

RUN_ID	RESULT_TEXT	SUBSTANCE	NO3	LOCATION	APPLICATION_SCHEME	CROP_CALENDAR	SOIL_TYPE	METEO_STATION	IRRIGATION_SCHEME
106	Concentration closest to the 80th percentile (ug/L)	NO3	543061.53	CHATEAUDUN	Nitrate_OSR2	CHAT-WOILSEED	CHAT-S_Soil	CHAT-M	No
107	Concentration closest to the 80th percentile (ug/L)	NO3	250791.419	HAMBURG	Nitrate_OSR2	HAMB-WOILSEED	HAMB-S_Soil	HAMB-M	No
108	Concentration closest to the 80th percentile (ug/L)	NO3	141753.74	KREMSMUENSTER	Nitrate_OSR2	KREM-WOILSEED	KREM-S_Soil	KREM-M	No
109	Concentration closest to the 80th percentile (ug/L)	NO3	134466.351	OKEHAMPTON	Nitrate_OSR2	OKEH-WOILSEED	OKEH-S_Soil	OKEH-M	No
110	Concentration closest to the 80th percentile (ug/L)	NO3	189279.942	PIACENZA	Nitrate_OSR2	PIAC-WOILSEED	PIAC-S_Soil	PIAC-M	No
111	Concentration closest to the 80th percentile (ug/L)	NO3	162046.403	PORTO	Nitrate_OSR2	PORT-WOILSEED	PORT-S_Soil	PORT-M	No

Potatoes, 273.1 kg/ha in begin of April, 279.8 kg/ha in end of June/begin of July

RUN_ID	RESULT_TEXT	SUBSTANCE	NO3	LOCATION	APPLICATION_SCHEME	CROP_CALENDAR	SOIL_TYPE	METEO_STATION	IRRIGATION_SCHEME
112	Concentration closest to the 80th percentile (ug/L)	NO3	335617.585	CHATEAUDUN	Nitrate_PO	CHAT-SPOTATOES	CHAT-S_Soil	CHAT-M	FOCUS
113	Concentration closest to the 80th percentile (ug/L)	NO3	292349.694	HAMBURG	Nitrate_PO	HAMB-SPOTATOES	HAMB-S_Soil	HAMB-M	No
114	Concentration closest to the 80th percentile (ug/L)	NO3	369525.132	JOKIOINEN	Nitrate_PO	JOKI-SPOTATOES	JOKI-S_Soil	JOKI-M	No
115	Concentration closest to the 80th percentile (ug/L)	NO3	185514.318	KREMSMUENSTER	Nitrate_PO	KREM-SPOTATOES	KREM-S_Soil	KREM-M	No
116	Concentration closest to the 80th percentile (ug/L)	NO3	149220.097	OKEHAMPTON	Nitrate_PO	OKEH-SPOTATOES	OKEH-S_Soil	OKEH-M	No
117	Concentration closest to the 80th percentile (ug/L)	NO3	239289.372	PIACENZA	Nitrate_PO	PIAC-SPOTATOES	PIAC-S_Soil	PIAC-M	FOCUS
118	Concentration closest to the 80th percentile (ug/L)	NO3	121735.34	PORTO	Nitrate_PO	PORT-SPOTATOES	PORT-S_Soil	PORT-M	FOCUS
119	Concentration closest to the 80th percentile (ug/L)	NO3	420744.024	SEVILLA	Nitrate_PO	SEVI-SPOTATOES	SEVI-S_Soil	SEVI-M	FOCUS
120	Concentration closest to the 80th percentile (ug/L)	NO3	539480.048	THIVA	Nitrate_PO	THIV-SPOTATOES	THIV-S_Soil	THIV-M	FOCUS

Cabbage, 262.2 kg/ha in May, 335.7 kg/ha in May/June, in July and in August

RUN_ID	RESULT_TEXT	SUBSTANCE	NO3	LOCATION	APPLICATION_SCHEME	CROP_CALENDAR	SOIL_TYPE	METEO_STATION	IRRIGATION_SCHEME
121	Concentration closest to the 80th percentile (ug/L)	NO3	670070.964	CHATEAUDUN	Nitrate_VEG	CHAT-CABBAGE	CHAT-S_Soil	CHAT-M	FOCUS
122	Concentration closest to the 80th percentile (ug/L)	NO3	648717.868	HAMBURG	Nitrate_VEG	HAMB-CABBAGE	HAMB-S_Soil	HAMB-M	No
123	Concentration closest to the 80th percentile (ug/L)	NO3	886762.517	JOKIOINEN	Nitrate_VEG	JOKI-CABBAGE	JOKI-S_Soil	JOKI-M	No
124	Concentration closest to the 80th percentile (ug/L)	NO3	401065.527	KREMSMUENSTER	Nitrate_VEG	KREM-CABBAGE	KREM-S_Soil	KREM-M	No
125	Concentration closest to the 80th percentile (ug/L)	NO3	262669.438	PORTO	Nitrate_VEG	PORT-CABBAGE	PORT-S_Soil	PORT-M	FOCUS
126	Concentration closest to the 80th percentile (ug/L)	NO3	**********	SEVILLA	Nitrate_VEG	SEVI-CABBAGE	SEVI-S_Soil	SEVI-M	FOCUS
127	Concentration closest to the 80th percentile (ug/L)	NO3	659263.41	THIVA	Nitrate_VEG	THIV-CABBAGE	THIV-S_Soil	THIV-M	FOCUS