**Study Report**

Predicted Environmental Concentrations in Groundwater

of Nitrate after fertilization using FOCUSPEARL

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

**Sponsor**

AlzChem Trostberg GmbH

Dr.-Albert-Frank-Str. 32

83308 Trostberg

Germany

**Institute**

Fraunhofer Institute for Molecular  
 Biology and Applied Ecology IME  
 Auf dem Aberg 1

57392 Schmallenberg  
 Germany

**Head of Applied Ecology**

Prof. Dr. Christoph Schäfers

**Author**

Dr. Michael Klein

Dr. Judith Klein

October 16, 2019

This page was intentionally left blank for statements of the sponsor or submitter.

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)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_October 16, 2019\_\_\_\_\_\_

Dr. Judith Klein Date

Modelling and Statistics

Fraunhofer Institute IME

Auf dem Aberg 1

57392 Schmallenberg

Tel +49 2972 302 256

Fax +49 2972 302 319

judith.klein@ime.fraunhofer.de

**Contents page**

[Statement of compliance 3](#_Toc22131161)

[1. Simulation model 5](#_Toc22131162)

[2. Scenarios 5](#_Toc22131163)

[Soil and climate scenarios of the FOCUS simulation models 5](#_Toc22131164)

[Crop scenarios 7](#_Toc22131165)

[3. Physico-chemical and Degradation Data 8](#_Toc22131166)

[4. Results 10](#_Toc22131167)

[5. Conclusion 12](#_Toc22131168)

[6. References 13](#_Toc22131169)

[7. Appendix: PEARL FOCUS Summary Output file 14](#_Toc22131170)

[Oil seed rape (winter), 45 kg/ha in August/September 14](#_Toc22131171)

[Oil seed rape (winter), 215.1 kg/ha in February/March, 258.7 kg/ha in April 15](#_Toc22131172)

[Potatoes, 273.1 kg/ha in begin of April, 279.8 kg/ha in end of June/begin of July 16](#_Toc22131173)

[Cabbage, 262.2 kg/ha in May, 335.7 kg/ha in May/June, in July and in august 17](#_Toc22131174)

# 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).

# 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]** |
| --- | --- | --- | --- | --- |
| audun | silty clay loam | 2.4 | 11.3 | 648 + I\* |
| 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 |

# Physico-chemical and Degradation Data

Nitrate

According to experimental data cyanamide is further transformed via urea to ammonium and nitrate. 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

# Results

The global maximum concentrations are summarised in the following tables. Four simulation 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 | 80th percentile of concentration in leachate | 80th percentile of concentration in leachate |
| (µg NO3 /L) | (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

# 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).

# 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

Vilsmeier, K.; Amberger, A. (1978): Modellversuche zum Umsatz von gemahlenen Kalkstickstoff und Perlkalkstickstoff in Abhängigkeit von Bodenfeuchtigkeit und Applikationsform. In: Z. Acker- und Pflanzenbau 147, S. 68–77.

# 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 |