**Study Report**

Predicted Environmental Concentrations in Groundwater

of Cyanamide and PERLKA after fertilization with PERLKA

*using FOCUSPEARL and FOCUSPELMO*

*Simulations in cabbage*

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GLP-compliance

This study “*Predicted Environmental Concentrations in Groundwater of Cyanamide and PERLKA after fertilization with PERLKA using FOCUSPEARL and FOCUSPELMO Simulations in 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 study does not describe an experimental study, so 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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# Simulation model

The simulation models FOCUS-PEARL 4.4.4 and FOCUS PELMO were used for the calculation of the predicted environmental concentrations in groundwater (PECgw) of Sulfamethoxazol. Solute transport is calculated with the Convection-Dispersion-Equation (CDE). Non-linear sorption is 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. 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 simulation a single variation (continuous cropping of cabbage) over a period of 26 years is taken into account according to the recommendations of FOCUS [FOCUS 2000].

# Physico-chemical and Degradation Data

PERLKA

PERLKA consists to about 45% of calcium cyanamide. In order to simulate the slow release in soil of cyanamide from PERLKA granules adequately cyanamide was defined as metabolite. According to experimental data within 1 day up to 50% of the cyanamide is released out of the granules at 12 °C and 10% soil moisture (see appendix 1). Consequtently, a half life of 1 day under standard conditions was assumed for the formation of cyanamide.

PERLKA granules cannot be dissolved in water without being transformed to cyanamide. In order to simulate the fate of PERLKA realistically the sorption constant in soil KOC was set to an artificial, high number (172400 L/kg). That should guarantee that the granules remain at the applied location in soil and are only transformed to cyanamide without leaching to deeper soil layers.

Cyanamide

According to experimental data cyanamide is further transformed to urea (DegT50 of cyanamide 2.89 days at 12 °C) at 5% and 10% soil moisture.

For cyanamide an average (geomean) sorption constant of 4 L/kg was considered which was based on experimental sorption studies. It was considered more reliable than results based on the HPLC methodology.

Cyanamide has a Henry’s law constant of 2.68 10-5 J/mol. However this value cannot be entered directly into FOCUS PEARL but will be internally calculated based on water solubility, vapour pressure and molecular mass. For PELMO no volatilisation was considered since PELMO does not consider this process for metabolites.

Plant uptake was not considered since the granules are usually applied before emergence of the crop.

PERLKA

Molecular Mass: 80.11 g/mol

Vapour pressure: 0

Water solubility: 800 000 mg/L at 20 °C

Adsorption 172400 L/kg (Koc)

 100 000 L/kg (Kom)

Freundlich Exponent. 1 (worst case)

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: 1 d at 12 °C

 Temperature correction:

 Reference temperature T0: 12 °C (FOCUS, 2000)

 Activation energy: 65.4 kJ (FOCUS, 2009)

 Moisture correction:

 Moisture exponent: 0.7 (FOCUS, 2000)

 Reference soil moisture: 100 % FC

Application date: 14 days before emergence to guarantee that the application is done before sowing

Application mode: annual application

Application rates: 500 kg/ha

Incorporation depth: 10 cm

Plant uptake factor: 0.0 (worst case)

Cyanamide

Molecular Mass: 42.04 g/mol

Vapour pressure: 0.51 Pa
(PELMO: 0 since volatilisation is not considered for metabolites)

Water solubility: 800 000 mg/L at 20 °C

Adsorption 4 L/kg (Koc)

 2.32 L/kg (Kom)

Freundlich Exponent. 1 (worst case)

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: 1.4 d at 12 °C

 Temperature correction:

 Reference temperature T0: 12 °C (FOCUS, 2000)

 Activation energy: 65.4 kJ (FOCUS, 2009)

 Moisture correction:

 Moisture exponent: 0.7 (FOCUS, 2000)

 Reference soil moisture: 100 % FC

Formation fraction: 100%

Plant uptake factor: 0.0 (worst case)

# Results

The global maximum concentrations are summarised in the following tables.

Table 2: 80th percentile of annual leaching concentration for PERLKA

|  |  |  |
| --- | --- | --- |
| Computer model | FOCUS PELMO | FOCUS PEARL |
| Location | 80th percentile of concentration in leachate(µg PERLKA/L)  | 80th percentile of concentration in leachate(µg PERLKA/L)  |
| CHATEAUDUN | 0.000000 | 0.000000 |
| HAMBURG | 0.000000 | 0.000000 |
| JOKIOINEN | 0.000000 | 0.000000 |
| KREMSMUENSTER | 0.000000 | 0.000000 |
| PORTO | 0.000000 | 0.000000 |
| SEVILLA | 0.000000 | 0.000000 |
| THIVA | 0.000000 | 0.000000 |

Table 2: 80th percentile of annual leaching concentration for cyanamide

|  |  |  |
| --- | --- | --- |
| Computer model | FOCUS PELMO | FOCUS PEARL |
| Location | 80th percentile of concentration in leachate(µg cyanamide/L)  | 80th percentile of concentration in leachate(µg cyanamide/L)  |
| CHATEAUDUN | 0 | 0 |
| HAMBURG | 0.005 | 0.000018 |
| JOKIOINEN | 0.63 | 0.000161 |
| KREMSMUENSTER | 0.032 | 0.000209 |
| PORTO | 12.595 | 0.201091 |
| SEVILLA | 0.009 | 0 |
| THIVA | 0 | 0 |

Important model output of the simulations can be found in the appendix. Further information and specific model output of the simulations can be made available on request.

# 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

**APPENDIX SUMMARY OUTPUT FILES**

**PELMO**

FOCUS Summary Output File

Model Version: FOCUSPELMO 5.5.3

Date of this simulation: 14/06/2018 15:53:53

Pesticide input file: PERLKA

Simulated crop: Cabbage

Results for ACTIVE SUBSTANCE (PERLKA)

----------------------------------------------------------------------------------

 Location Selected Flux Percolate Conc.

 Period (g/ha) (L/m²) (µg/L)

----------------------------------------------------------------------------------

Châteaudun (C) (4/5) 0.00E+00 654.500 0.000

Hamburg (H) (4/5) 0.00E+00 541.500 0.000

Jokioinen (J) (4/5) 0.00E+00 669.800 0.000

Kremsmünster (K) (4/5) 0.00E+00 979.100 0.000

Porto (O) (4/5) 0.00E+00 2101.00 0.000

Sevilla (S) (4/5) 0.00E+00 519.700 0.000

Thiva (T) (4/5) 0.00E+00 658.900 0.000

Results for METABOLITE A1 (H2CN2)

----------------------------------------------------------------------------------

 Location Selected Flux Percolate Conc.

 Period (g/ha) (L/m²) (µg/L)

----------------------------------------------------------------------------------

Châteaudun (C) (15/1) 6.36E-04 451.600 0.000

Hamburg (H) (18/2) 0.0245190 453.700 0.005

Jokioinen (J) (8/7) 3.2226070 713.900 0.630

Kremsmünster (K) (9/4) 0.1949700 706.700 0.032

Porto (O) (12/17) 203.040 1611.20 12.595

Sevilla (S) (2/17) 0.0512210 388.510 0.009

Thiva (T) (14/15) 4.24E-17 441.040 0.000

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**PEARL FOCUS Summary Output file**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| RUN\_ID | RESULT\_TEXT | SUBSTANCE | PRLKA | CN2 | LOCATION | APPLICATION\_SCHEME | SOIL\_TYPE | METEO\_STATION | IRRIGATION\_SCHEME |
| 2 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0 | CHATEAUDUN | PERLKA\_Cabbage | CHAT-S\_Soil | CHAT-M | FOCUS |
| 3 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000018 | HAMBURG | PERLKA\_Cabbage | HAMB-S\_Soil | HAMB-M | No |
| 4 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000161 | JOKIOINEN | PERLKA\_Cabbage | JOKI-S\_Soil | JOKI-M | No |
| 5 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000209 | KREMSMUENSTER | PERLKA\_Cabbage | KREM-S\_Soil | KREM-M | No |
| 6 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.201091 | PORTO | PERLKA\_Cabbage | PORT-S\_Soil | PORT-M | FOCUS |
| 7 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0 | SEVILLA | PERLKA\_Cabbage | SEVI-S\_Soil | SEVI-M | FOCUS |
| 8 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0 | THIVA | PERLKA\_Cabbage | THIV-S\_Soil | THIV-M | FOCUS |