**Study Report**

Predicted Environmental Concentrations in Groundwater

of Cyanamide and PERLKA after fertilization with PERLKA

*using FOCUSPEARL*

*Simulations in cabbage and potatoes*

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GLP-compliance

This study “*Predicted Environmental Concentrations in Groundwater of Cyanamide and PERLKA after fertilization with PERLKA using FOCUSPEARL- Simulations in cabbage and potatoes*” 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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**Contents page**

[GLP-compliance 3](#_Toc526150255)

[1. Simulation model 7](#_Toc526150256)

[2. Scenarios 7](#_Toc526150257)

[2.1 Soil and climate scenarios of the FOCUS simulation models 7](#_Toc526150258)

[2.2 Crop scenarios 9](#_Toc526150259)

[3. Physico-chemical and Degradation Data 10](#_Toc526150260)

[4. Results 13](#_Toc526150261)

[5. References 15](#_Toc526150262)

[6. Appendix A: PEARL FOCUS Summary Output file 16](#_Toc526150263)

# Simulation model

The simulation models FOCUS-PEARL 4.4.4 was used for the calculation of the predicted environmental concentrations in groundwater (PECgw) of cyanamide after application of PERLKA. 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 simulations a single variation (continuous cropping of cabbage and potatoes) 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 a metabolite. According to experimental data the half life of PERLKA (Ca CN2) in soil was found to be between 0.585 days and 1.21 days. The experimental values were normalised to 20 °C using a Q10 factor of 2.2 as recommended by FOCUS (2000). The experimental half lives were also normalised to pF 2 (field capacity) using an exponent of 0.7 as the model require degradation at optimised moisture conditions. Also the moisture correction was done according to FOCUS (2000). The geometric mean of all normalised half lives was found to be 0.546 days. This value was considered for the modelling.

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. This can be considered a worst case selection of the formation of cyanamide.

Cyanamide

According to experimental data cyanamide is further transformed to urea. Also for cyanamide the experimental half lives were normalised to 20 °C using a Q10-Factor of 2.2 as given by FOCUS (2000). However, for cyanamide no soil moisture normalisation was done since according to the experimental results the degradation of cyanamide does not increase with soil moisture. Consequently, the soil moisture correction in the model FOCUS PEARL model is not suitable and the moisture correction was switched off. For the modelling a half life of 0.755 days was used. The value represents the geometric mean of all experimental data after normalisation to 20 °C but without soil moisture normalisation.

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.

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: 0.546 d at 20 °C

 Temperature correction:

 Reference temperature T0: 20 °C (FOCUS, 2000)

 Activation energy: 54 kJ mol-1 (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 rate: 500 kg/ha (cabbage), 400 kg/ha (potatoes)

Incorporation depth: 15 cm

Plant uptake factor: 0.0 (worst case)

Cyanamide

Molecular Mass: 42.04 g/mol

Vapour pressure: 0.51 Pa
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: 0.766 d at 20 °C

 Temperature correction:

 Reference temperature T0: 20 °C (FOCUS, 2000)

 Activation energy: 54 kJ mol-1 (FOCUS, 2009)

 Moisture correction:

 Moisture exponent: 0 (no correction)

 Reference soil moisture: not applicable

Formation fraction: 45%

Plant uptake factor: 0.0 (worst case)

# Results

The global maximum concentrations are summarised in the following tables. According to the results no concentrations above 0.1 µg/L in the groundwater is expected for both application pattern.

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

|  |  |
| --- | --- |
| Computer model | FOCUS PEARL |
| Scenario | Cabbage, 500 kg/ha, 15 cm uniform incorp. |
| Location | 80th percentile of concentration in leachate | 80th percentile of concentration in leachate |
| (µg PERLKA/L)  | (µg cyanamide/L)  |
| CHATEAUDUN | 0 | 0 |
| HAMBURG | 0 | 0.000002 |
| JOKIOINEN | 0 | 0.000035 |
| KREMSMUENSTER | 0 | 0.000074 |
| PORTO | - | - |
| SEVILLA | - | - |
| THIVA | 0 | 0.08148 |

Table 3: 80th percentile of annual leaching concentration for PERLKA and cyanamide

|  |  |
| --- | --- |
| Computer model | FOCUS PEARL |
| Scenario | Potatoes, 400 kg/ha,15 cm uniform incorp. |
| Location | 80th percentile of concentration in leachate | 80th percentile of concentration in leachate |
| (µg PERLKA/L)  | (µg cyanamide/L)  |
| CHATEAUDUN | 0 | 0 |
| HAMBURG | 0 | 0.000002 |
| JOKIOINEN | 0 | 0.000046 |
| KREMSMUENSTER | 0 | 0.0001 |
| OKEHAMPTON | 0 | 0.001744 |
| PIACENZA | 0 | 0.00006 |
| PORTO | 0 | 0.00167 |
| SEVILLA | 0 | 0.001073 |
| THIVA | 0 | 0.000009 |

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 A: 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-CABBAGE | CHAT-S\_Soil | CHAT-M |
| 3 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000002 | HAMBURG | PERLKA\_Cabbage | HAMB-CABBAGE | HAMB-S\_Soil | HAMB-M |
| 4 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000035 | JOKIOINEN | PERLKA\_Cabbage | JOKI-CABBAGE | JOKI-S\_Soil | JOKI-M |
| 5 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000074 | KREMSMUENSTER | PERLKA\_Cabbage | KREM-CABBAGE | KREM-S\_Soil | KREM-M |
| 6 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.08148 | PORTO | PERLKA\_Cabbage | PORT-CABBAGE | PORT-S\_Soil | PORT-M |
| 7 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0 | SEVILLA | PERLKA\_Cabbage | SEVI-CABBAGE | SEVI-S\_Soil | SEVI-M |
| 8 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0 | THIVA | PERLKA\_Cabbage | THIV-CABBAGE | THIV-S\_Soil | THIV-M |
| 16 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0 | CHATEAUDUN | PERLKA\_Potatoes | CHAT-SPOTATOES | CHAT-S\_Soil | CHAT-M |
| 17 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000002 | HAMBURG | PERLKA\_Potatoes | HAMB-SPOTATOES | HAMB-S\_Soil | HAMB-M |
| 18 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000046 | JOKIOINEN | PERLKA\_Potatoes | JOKI-SPOTATOES | JOKI-S\_Soil | JOKI-M |
| 19 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.0001 | KREMSMUENSTER | PERLKA\_Potatoes | KREM-SPOTATOES | KREM-S\_Soil | KREM-M |
| 20 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.001744 | OKEHAMPTON | PERLKA\_Potatoes | OKEH-SPOTATOES | OKEH-S\_Soil | OKEH-M |
| 21 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.00006 | PIACENZA | PERLKA\_Potatoes | PIAC-SPOTATOES | PIAC-S\_Soil | PIAC-M |
| 22 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.00167 | PORTO | PERLKA\_Potatoes | PORT-SPOTATOES | PORT-S\_Soil | PORT-M |
| 23 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.001073 | SEVILLA | PERLKA\_Potatoes | SEVI-SPOTATOES | SEVI-S\_Soil | SEVI-M |
| 24 | Concentration closest to the 80th percentile (ug/L) | PRLKA | 0 | 0.000009 | THIVA | PERLKA\_Potatoes | THIV-SPOTATOES | THIV-S\_Soil | THIV-M |