**Study Report**

Predicted Environmental Concentrations in Surface Water
of Urea based on FOCUS STEP3

*Simulations potatoes, oil seed rape, and vegetables*

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Statement of compliance

This study “*Predicted Environmental Concentrations in Surface Water of Urea based on FOCUS STEP3; Simulations potatoes, oil seed rape, and vegetables*” 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 to the “Codex of Good Modelling Practices” (Görlitz 1993 und Travis 1995).

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# Simulation models

For the STEP3 calculations the computer tool SWASH was used which mainly creates the necessary input data for MACRO 5.5.4, PRZM 4.3.1 and TOXSWA 4.4 which were used for the simulations. All models are described in FOCUS (2001). The standard buffer zone was 1 m.

They represent start-of-the-art PEC-calculations for all type active compounds (pesticides, biocides and veterinary compounds). They are also the most recent versions. The history of versions is summarised at the FOCUS homepage (<https://esdac.jrc.ec.europa.eu/projects/focus-dg-sante>).

# Input parameters

## Agricultural use pattern

Urea is applied in various crops with different application patterns as summarised in the following table.

The term “**Incorporated at 10 cm**” means a uniform incorporation into the upper 10 cm of the soil.

Table 1: Application pattern of urea in various crops considered for the simulations

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Scen. id** | **Crop** | **Nr. of app.** | **App. method** | **Incorp. Depth** | **App. Rate Urea** | **Start of the application window** |
|   |   |   |  | **(cm)** | **(kg/ha)** |  |
| 1 | Oil seed rape | 1st | Incorporated | 10 | 260 | end of February/ beginning of April |
| 2nd | Incorporated | 10 | 130 | mid of May |
| 2 | Potatoes | 1st | Incorporated | 15 | 260 | beginning of April |
| 2nd | Incorporated | 15 | 90 | mid of May |
| 3 | Vegetables (leafy) | 1st | Incorporated | 15 | 430 | default |

Based on the information given in Table 1 the following application dates were automatically calculated for the different crops at the different scenarios.

Table 2: Application date calculated by FOCUS PAT considered for the simulations

| **Scen. ID** | **Crop** | **Scenario** | **application date calculated by FOCUS PAT** |
| --- | --- | --- | --- |
| 1 | Oil seed rape | D2\_Ditch | 01. Apr 82 |
| D2\_Stream | 01. Apr 82 |
| D3\_Ditch | 01. Apr 86 |
| D4\_Pond | 01. Apr 86 |
| D4\_Stream | 04. Apr 92 |
| D5\_Pond | 18. Apr 85 |
| D5\_Stream | 18. Apr 85 |
| R1\_Pond | 08. Apr 78 |
| R1\_Stream | 08. Apr 78 |
| R3\_Stream | 22. Apr 77 |
| 2 | Potatoes | D3\_Ditch | 04. Apr 80 |
| D4\_Pond | 01. Apr 82 |
| D4\_Stream | 01. Apr 82 |
| D6\_Ditch | 01. Apr 86 |
| D6\_Ditch2 | 01. Apr 86 |
| R1\_Pond | 04. Apr 92 |
| R1\_Stream | 18. Apr 85 |
| R2\_Stream | 18. Apr 85 |
| R3\_Stream | 08. Apr 78 |
| 3 | Vegetables (leafy) | D3\_Ditch | 08. Apr 78 |
| D3\_Ditch2 | 22. Apr 77 |
| D4\_Pond | 04. Apr 80 |
| D4\_Stream | 17. Jun 82 |
| D6\_Ditch | 17. Jun 82 |
| R1\_Pond | 02. Jun 86 |
| R1\_Pond2 | 02. Jun 86 |
| R1\_Stream | 14. Jun 92 |
| R1\_Stream2 | 01. Jun 85 |
| R2\_Stream | 01. Jun 85 |
| R2\_Stream2 | 09. Jun 78 |
| R3\_Stream | 09. Jun 78 |
| R3\_Stream2 | 04. Jun 89 |
| R4\_Stream | 02. Jun 75 |
| R4\_Stream2 | 17. Jun 82 |

## Substance properties of urea

According to experimental data cyanamide is further transformed to urea (Vilsmeier et Amberger 1978). The molecular weight was conversed based on EFSA (2010) assuming a 13.4% cyanamide-to-urea conversion rate in water/sediment – corrected for the relative molecular weight of cyanamide and urea.

For the half-life of urea in surface water 4.8 days at 20°C was taken. This is the geometric mean given in EFSA (2010). A default value of 1000 days was considered for the sediment phase. For soil, the default for a readily biodegradable substance is used, namely 30 days at 12°C. The computer automatically transfer the half lives at standard temperatures into the actual conditions of the scenarios.

All DegT50 values in water, sediment-system and in soil considered in the simulations are presented in Table 3.

Table 3: DegT50-values (d) of urea

|  |  |
| --- | --- |
| **Parameter** | **Urea** |
| Water | 4.8 (at 20 °C) |
| Sediment | 1000 (at 20 °C) |
| Soil | 30 (at 12 °C) |

The sorption constant in soil KOC was set to 7.2 L/kg which was calculated from Hongprayoon (1991). The taken KOC value for urea corresponds to the mean of KOC values ranging from 5.3 to 9.1.

Plant uptake via roots was not considered since urea is usually applied before emergence of the crop.

All other input parameters used for the simulations are summarised in Table 4.

Table 4: Other input parameters used for the simulations of urea

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Urea** | **Remark** |
| Sorption constant KOC in soil (L/kg) | 7.2 | EFSA (2010) |
| Sorption constant KOC in water body (L/kg) | 7.2 | EFSA (2010) |
| Freundlich exponent (-) | 1 | EFSA (2010) |
| Vapour pressure (25°C, Pa) | 0.0016 |  |
| Molar mass (g/mol) | 60.06 |  |
| Water solubility (20°C, mg/L) | 624000 | EFSA (2010) |
| Molar enthalpy of vaporisation | 95000 | default |
| Molar enthalpy of dissolution | 27000 | default |
| Diffusion coefficient in water | 4.3 10-5 | default |
| Diffusion coefficient in air | 0.43 | default |
| Plant uptake factor | 0 | default |

# Results

The maximum concentrations for all scenarios and crops are summarised in the following Table 6.

Table 5: Maximum concentrations (PECmax) of urea at FOCUS Step 3

|  |  |  |
| --- | --- | --- |
| **Scen. ID** | **Scenaro/Crop** | **PECmax (µg/L)** |
| 1 | Oilseed rape (winter), end of February/ beginning of April, 260kg, beginning/mid of April, 130kg | 1024.6 |
| 2 | Potatoes, beginning of April, 260kg, mid of May, 90kg | 2533.6 |
| 3 | (Leafy) vegetables, default, 430kg, | 5768.4 |

Table 6: Global maximum concentrations of urea at FOCUS Step 3

| **Scen. ID** | **Crop/Scenario** | **Scenario** | **PECsw (µg/L)** | **PECsed (µg/kg)** |
| --- | --- | --- | --- | --- |
| 1 | Oilseed rape (winter), end of February/ begin of April, 260kg, begin/mid of April, 130kg | D2\_Ditch | 467.9 | 150.1 |
| D2\_Stream | 293.2 | 87.23 |
| D3\_Ditch | 411.9 | 378 |
| D4\_Pond | 305.4 | 176.3 |
| D4\_Stream | 403.9 | 191.5 |
| D5\_Pond | 28.41 | 14.42 |
| D5\_Stream | 31.12 | 14.9 |
| R1\_Pond | 14.61 | 3.889 |
| R1\_Stream | 604.7 | 31.81 |
| R3\_Stream | 1024.6 | 60.08 |
| 2 | Potatoes, begin of April, 260kg, mid of May, 90kg | D3\_Ditch | 510.3 | 459.1 |
| D4\_Pond | 300.7 | 201.8 |
| D4\_Stream | 1191.2 | 468.9 |
| D6\_Ditch | 1752.8 | 183.3 |
| D6\_Ditch2 | 1752.8 | 183.3 |
| R1\_Pond | 44.97 | 12.13 |
| R1\_Stream | 811.5 | 51.64 |
| R2\_Stream | 1074.9 | 30.17 |
| R3\_Stream | 2533.6 | 132.4 |
| 3 | (Leafy) vegetables, default, 430kg,  | D3\_Ditch | 5768.4 | 2812.8 |
| D3\_Ditch2 | 498.2 | 459.6 |
| D4\_Pond | 399 | 261.6 |
| D4\_Stream | 2471.8 | 536.8 |
| D6\_Ditch | 5614.9 | 743.6 |
| R1\_Pond | 94.03 | 20.94 |
| R1\_Pond2 | 94.03 | 15.62 |
| R1\_Stream | 1797.2 | 63.93 |
| R1\_Stream2 | 1781.8 | 56.79 |
| R2\_Stream | 2356.8 | 48.42 |
| R2\_Stream2 | 2417 | 62.55 |
| R3\_Stream | 2541.5 | 122.7 |
| R3\_Stream2 | 2533.7 | 121.2 |
| R4\_Stream | 2247.7 | 190.3 |
| R4\_Stream2 | 2672.2 | 229.7 |

# Conclusions

The following maximum concentrations were calculated for urea at step 3 simulations (no additional buffer strip to the surface water body):

Table 7: Maximum concentrations (PECmax) urea at FOCUS Step 3

|  |  |  |
| --- | --- | --- |
| **Scen. ID** | **Scenaro/Crop** | **PECmax (µg/L)** |
| 1 | Oilseed rape (winter), end of February/ begin of April, 260kg, begin/mid of April, 130kg | 1024.6 |
| 2 | Potatoes, begin of April, 260kg, mid of May, 90kg | 2533.6 |
| 3 | (Leafy) vegetables, default, 430kg, | 5768.4 |

# References

EFSA (2010): “Conclusion on the peer review of the pesticide risk assessment of the active substance cyanamide”. EFSA Journal 2010;8(11):1873.

FOCUS (2001). “FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC”. Report of the FOCUS Working Group on Surface Water Scenarios, EC

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.”: ‘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: SWASH Report Files

## Oilseed rape (winter), end of February/ begin of April, 260kg, begin/mid of April, 130kg

 \* SWASH report file

 \* made by FOCUS-SWASH UI v. 5 (internal version 5.1.0, 02 April 2015)

 \*

 \* File Name : E:\SwashProjects\HS\_20190925\HS\_OSR\HS\_OSR\_report.txt

 \* Description : Oilseed rape, end of February/ begin of April, 260kg, begin/mid of April, 130kg

 \* Substance : HS

 \*

 \* Creation : 26-Sep-2019, 12:19

 \*

 \* Remarks : SWASH report helps you to set up the needed runs to calculate the PECsw and PECsed, occuring in the EU

 \* for the selected substance, used on the selected crop. The scenario code informs you which models you need to

 \* run for this scenario.

 \* D1-D6: drainage entries calculated by the MACRO model, fate in surface water calculated by the TOXSWA model

 \*

 \* R1-R4: runoff and erosion entries calculated by the PRZM model, fate in surface water calculated by the TOXSWA model

 \*

 \*

 \* For STREAMS the Mean Deposition and Mass Loading, as calculated by the FOCUS Drift Calculator, have been multiplied by a

 \* factor 1.2 to account for pesticide mass incoming from the upstream catchment as decided by the FOCUS Surface Water

 \* Scenarios Working Group.

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\* CREATED RUNS

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 \*

 \* |--------------- APPLICATION -----------------|----- on Water Surface -----|

 \* -ID------Crop(1st/2nd)-------Scenario-WaterbodyType-|-Method--------First/Last/Interval--#---Rate-|-Mean Deposition-Mass Loading

 (d) (kg/ha) (% of Appl. Rate) (mg/m2)

 \*

 \* 41 Oil seed rape, winte(1st) D2\_Ditch soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 42 Oil seed rape, winte(1st) D2\_Stream soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 43 Oil seed rape, winte(1st) D3\_Ditch soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 44 Oil seed rape, winte(1st) D4\_Pond soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 45 Oil seed rape, winte(1st) D4\_Stream soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 46 Oil seed rape, winte(1st) D5\_Pond soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 47 Oil seed rape, winte(1st) D5\_Stream soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 48 Oil seed rape, winte(1st) R1\_Pond soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 49 Oil seed rape, winte(1st) R1\_Stream soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

 \* 50 Oil seed rape, winte(1st) R3\_Stream soil incorp. 20-Feb/6-May /45 1 260.0000 0.000 0.000

 \* 2 130.0000 0.000 0.000

 \*

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## Potatoes, begin of April, 260kg, mid of May, 90kg

 \* SWASH report file

 \* made by FOCUS-SWASH UI v. 5 (internal version 5.1.0, 02 April 2015)

 \*

 \* File Name : E:\SwashProjects\HS\_20190925\HS\_PO\HS\_PO\_report.txt

 \* Description : Potatoes, begin of April, 260kg, mid of May, 90kg

 \* Substance : HS

 \*

 \* Creation : 26-Sep-2019, 12:19

 \*

 \* Remarks : SWASH report helps you to set up the needed runs to calculate the PECsw and PECsed, occuring in the EU

 \* for the selected substance, used on the selected crop. The scenario code informs you which models you need to

 \* run for this scenario.

 \* D1-D6: drainage entries calculated by the MACRO model, fate in surface water calculated by the TOXSWA model

 \*

 \* R1-R4: runoff and erosion entries calculated by the PRZM model, fate in surface water calculated by the TOXSWA model

 \*

 \*

 \* For STREAMS the Mean Deposition and Mass Loading, as calculated by the FOCUS Drift Calculator, have been multiplied by a

 \* factor 1.2 to account for pesticide mass incoming from the upstream catchment as decided by the FOCUS Surface Water

 \* Scenarios Working Group.

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 \* CREATED RUNS

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 \*

 \* |--------------- APPLICATION -----------------|----- on Water Surface -----|

 \* -ID------Crop(1st/2nd)-------Scenario-WaterbodyType-|-Method--------First/Last/Interval--#---Rate-|-Mean Deposition-Mass Loading

 (d) (kg/ha) (% of Appl. Rate) (mg/m2)

 \*

 \* 9 Potatoes(1st) D3\_Ditch soil incorp. 1-Apr /15-Jun/45 1 260.0000 0.000 0.000

 \* 2 90.0000 0.000 0.000

 \*

 \* 10 Potatoes(1st) D4\_Pond ground spray 1-Apr /15-Jun/45 1 260.0000 0.173 45.063

 \* 2 90.0000 0.173 15.599

 \*

 \* 11 Potatoes(1st) D4\_Stream ground spray 1-Apr /15-Jun/45 1 260.0000 1.282 333.321

 \* 2 90.0000 1.282 115.380

 \*

 \* 12 Potatoes(1st) D6\_Ditch ground spray 1-Apr /15-Jun/45 1 260.0000 1.383 359.623

 \* 2 90.0000 1.383 124.485

 \*

 \* 13 Potatoes(2nd) D6\_Ditch ground spray 1-Apr /15-Jun/45 1 260.0000 1.383 359.623

 \* 2 90.0000 1.383 124.485

 \*

 \* 14 Potatoes(1st) R1\_Pond ground spray 1-Apr /15-Jun/45 1 260.0000 0.173 45.063

 \* 2 90.0000 0.173 15.599

 \*

 \* 15 Potatoes(1st) R1\_Stream ground spray 1-Apr /15-Jun/45 1 260.0000 1.282 333.321

 \* 2 90.0000 1.282 115.380

 \*

 \* 16 Potatoes(1st) R2\_Stream ground spray 1-Apr /15-Jun/45 1 260.0000 1.282 333.321

 \* 2 90.0000 1.282 115.380

 \*

 \* 17 Potatoes(1st) R3\_Stream ground spray 1-Apr /15-Jun/45 1 260.0000 1.282 333.321

 \* 2 90.0000 1.282 115.380

 \*

 \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Surface WAter Scenarios Help \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

## Vegetables (leafy), default, 430kg,

 \* SWASH report file

 \* made by FOCUS-SWASH UI v. 5 (internal version 5.1.0, 02 April 2015)

 \*

 \* File Name : E:\SwashProjects\HS\_20190925\HS\_VEG\HS\_VEG\_report.txt

 \* Description : (Leafy) vegetables, default, 430kg

 \* Substance : HS

 \*

 \* Creation : 26-Sep-2019, 12:19

 \*

 \* Remarks : SWASH report helps you to set up the needed runs to calculate the PECsw and PECsed, occuring in the EU

 \* for the selected substance, used on the selected crop. The scenario code informs you which models you need to

 \* run for this scenario.

 \* D1-D6: drainage entries calculated by the MACRO model, fate in surface water calculated by the TOXSWA model

 \*

 \* R1-R4: runoff and erosion entries calculated by the PRZM model, fate in surface water calculated by the TOXSWA model

 \*

 \*

 \* For STREAMS the Mean Deposition and Mass Loading, as calculated by the FOCUS Drift Calculator, have been multiplied by a

 \* factor 1.2 to account for pesticide mass incoming from the upstream catchment as decided by the FOCUS Surface Water

 \* Scenarios Working Group.

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 \* CREATED RUNS

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 \*

 \* |--------------- APPLICATION -----------------|----- on Water Surface -----|

 \* -ID------Crop(1st/2nd)-------Scenario-WaterbodyType-|-Method--------First/Last/Interval--#---Rate-|-Mean Deposition-Mass Loading

 (d) (kg/ha) (% of Appl. Rate) (mg/m2)

 \*

 \* 26 Vegetables, leafy(1st) D3\_Ditch soil incorp. 11-Apr/11-May/1 1 430.0000 0.000 0.000

 \*

 \* 27 Vegetables, leafy(2nd) D3\_Ditch ground spray 22-Jul/21-Aug/1 1 430.0000 1.927 828.779

 \*

 \* 28 Vegetables, leafy(1st) D4\_Pond ground spray 26-Apr/26-May/1 1 430.0000 0.219 94.196

 \*

 \* 29 Vegetables, leafy(1st) D4\_Stream ground spray 26-Apr/26-May/1 1 430.0000 1.716 738.066

 \*

 \* 30 Vegetables, leafy(1st) D6\_Ditch ground spray 1-Aug /31-Aug/1 1 430.0000 1.927 828.779

 \*

 \* 31 Vegetables, leafy(1st) R1\_Pond ground spray 6-Apr /6-May /1 1 430.0000 0.219 94.196

 \*

 \* 32 Vegetables, leafy(2nd) R1\_Pond ground spray 17-Jul/16-Aug/1 1 430.0000 0.219 94.196

 \*

 \* 33 Vegetables, leafy(1st) R1\_Stream ground spray 6-Apr /6-May /1 1 430.0000 1.716 738.066

 \*

 \* 34 Vegetables, leafy(2nd) R1\_Stream ground spray 17-Jul/16-Aug/1 1 430.0000 1.716 738.066

 \*

 \* 35 Vegetables, leafy(1st) R2\_Stream ground spray 14-Feb/16-Mar/1 1 430.0000 1.716 738.066

 \*

 \* 36 Vegetables, leafy(2nd) R2\_Stream ground spray 17-Jul/16-Aug/1 1 430.0000 1.716 738.066

 \*

 \* 37 Vegetables, leafy(1st) R3\_Stream ground spray 15-Feb/17-Mar/1 1 430.0000 1.716 738.066

 \*

 \* 38 Vegetables, leafy(2nd) R3\_Stream ground spray 1-Jun /1-Jul /1 1 430.0000 1.716 738.066

 \*

 \* 39 Vegetables, leafy(1st) R4\_Stream ground spray 15-Feb/17-Mar/1 1 430.0000 1.716 738.066

 \*

 \* 40 Vegetables, leafy(2nd) R4\_Stream ground spray 1-Jun /1-Jul /1 1 430.0000 1.716 738.066

 \*

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