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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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October 28, 2019

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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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28 October 2019

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Contents **page**

1. 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).

2. Input parameters

2.1 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 (cm)	App. Rate Urea (kg/ha)	Start of the application window
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 (1st)	application date calculated by FOCUS PAT (2nd)
1	Oil seed rape	D2_Ditch	22. Feb 86	09. Apr 86
		D2_Stream	22. Feb 86	09. Apr 86
		D3_Ditch	29. Feb 92	20. Apr 92
		D4_Pond	24. Feb 85	18. Apr 85
		D4_Stream	24. Feb 85	18. Apr 85
		D5_Pond	21. Feb 78	08. Apr 78
		D5_Stream	21. Feb 78	08. Apr 78
		R1_Pond	24. Feb 79	12. Apr 79
		R1_Stream	24. Feb 79	12. Apr 79
		R3_Stream	20. Feb 81	13. Apr 81

2	Potatoes	D3_Ditch	04. Apr 92	24. May 92
		D4_Pond	18. Apr 85	02. Jun 85
		D4_Stream	18. Apr 85	02. Jun 85
		D6_Ditch	02. Apr 86	17. May 86
		D6_Ditch2	02. Apr 86	17. May 86
		R1_Pond	26. Apr 84	13. Jun 84
		R1_Stream	26. Apr 84	13. Jun 84
		R2_Stream	22. Apr 77	14. Jun 77
		R3_Stream	04. Apr 80	01. Jun 80
3	Vegetables (leafy)	D3_Ditch	10. Apr 92	
		D3_Ditch2	25. Jul 92	
		D4_Pond	16. May 85	
		D4_Stream	16. May 85	
		D6_Ditch	04. Aug 86	
		R1_Pond	26. Apr 84	
		R1_Pond2	28. Jul 78	
		R1_Stream	26. Apr 84	
		R1_Stream2	28. Jul 78	
		R2_Stream	06. Mar 78	
		R2_Stream2	05. Aug 89	
		R3_Stream	19. Feb 81	
		R3_Stream2	02. Jun 75	
		R4_Stream	01. Mar 80	
		R4_Stream2	01. Jun 85	

2.2 Substance properties of 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 transfers the half lives at standard temperatures into the actual conditions of the scenarios.

All $DegT_{50}$ values in water, sediment-system and in soil considered in the simulations are presented in Table 3.

Table 3: $DegT_{50}$-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 K_{OC} was set to 7.2 L/kg which was calculated from Hongprayoon (1991). The taken K_{OC} value for urea corresponds to the mean of K_{OC} 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

3. 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,	3268.1

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	254.7	165
		D4_Stream	778.6	357.5
		D6_Ditch	71	6.769
		D6_Ditch2	71	6.769
		R1_Pond	36.29	6.851
		R1_Stream	569.8	50.15
		R2_Stream	433.5	28.97
		R3_Stream	2533.6	122.2
3	(Leafy) vegetables, default, 430kg,	D3_Ditch	498.2	459.6
		D3_Ditch2	3268.1	2864.3
		D4_Pond	337.1	213
		D4_Stream	1005.2	402.5
		D6_Ditch	215.8	28.86

Scen. ID	Crop/Scenario	Scenario	PECsw (µg/L)	PECsed (µg/kg)
		R1_Pond	0.6518	0.1826
		R1_Pond2	0.000174	0.000034
		R1_Stream	173	9.997
		R1_Stream2	0.002776	0.000231
		R2_Stream	631.2	40.1
		R2_Stream2	17.25	1.268
		R3_Stream	1071.2	64.59
		R3_Stream2	1129.5	105.9
		R4_Stream	2247.7	187
		R4_Stream2	2672.2	223.8

4. 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,	3268.1

5. 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.

6. Appendix: SWASH Report Files

6.1 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

-ID-	Crop(1st/2nd)	Scenario-WaterbodyType-	Method	First/Last/Interval (d)	#	Rate (kg/ha)	Mean Deposition (% of Appl. Rate)	Mass Loading (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

6.2 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    : 07-Oct-2019, 09:53
*
* 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
*****************************************************************************************************************************************
*
*                                                          |--------------- 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               soil incorp.   1-Apr /15-Jun/45     1  260.0000     0.000           0.000
*                                                                                         2  90.0000      0.000           0.000
*
* 11    Potatoes(1st)            D4_Stream             soil incorp.   1-Apr /15-Jun/45     1  260.0000     0.000           0.000
*                                                                                         2  90.0000      0.000           0.000
*
* 12    Potatoes(1st)            D6_Ditch              soil incorp.   1-Apr /15-Jun/45     1  260.0000     0.000           0.000
*                                                                                         2  90.0000      0.000           0.000
*
* 13    Potatoes(2nd)            D6_Ditch              soil incorp.   1-Apr /15-Jun/45     1  260.0000     0.000           0.000
*                                                                                         2  90.0000      0.000           0.000
*
* 14    Potatoes(1st)            R1_Pond               soil incorp.   1-Apr /15-Jun/45     1  260.0000     0.000           0.000
*                                                                                         2  90.0000      0.000           0.000
*
* 15    Potatoes(1st)            R1_Stream             soil incorp.   1-Apr /15-Jun/45     1  260.0000     0.000           0.000
*                                                                                         2  90.0000      0.000           0.000
*
* 16    Potatoes(1st)            R2_Stream             soil incorp.   1-Apr /15-Jun/45     1  260.0000     0.000           0.000
*                                                                                         2  90.0000      0.000           0.000
*
* 17    Potatoes(1st)            R3_Stream             soil incorp.   1-Apr /15-Jun/45     1  260.0000     0.000           0.000
*                                                                                         2  90.0000      0.000           0.000
*
********************************************** Surface WAter Scenarios Help **********************************************
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6.3 Vegetables (leafy), default, 430kg,

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* 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    : 07-Oct-2019, 09:56
*
* 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

ID	Crop (1st/2nd)	Scenario-WaterbodyType	Method	First/Last/Interval (d)	#	Rate (kg/ha)	Mean Deposition (% of Appl. Rate)	Mass Loading on Water Surface (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	soil incorp.	22-Jul/21-Aug/1	1	430.0000	0.000	0.000
28	Vegetables, leafy(1st)	D4_Pond	soil incorp.	26-Apr/26-May/1	1	430.0000	0.000	0.000
29	Vegetables, leafy(1st)	D4_Stream	soil incorp.	26-Apr/26-May/1	1	430.0000	0.000	0.000
30	Vegetables, leafy(1st)	D6_Ditch	soil incorp.	1-Aug /31-Aug/1	1	430.0000	0.000	0.000
31	Vegetables, leafy(1st)	R1_Pond	soil incorp.	6-Apr /6-May /1	1	430.0000	0.000	0.000
32	Vegetables, leafy(2nd)	R1_Pond	soil incorp.	17-Jul/16-Aug/1	1	430.0000	0.000	0.000
33	Vegetables, leafy(1st)	R1_Stream	soil incorp.	6-Apr /6-May /1	1	430.0000	0.000	0.000
34	Vegetables, leafy(2nd)	R1_Stream	soil incorp.	17-Jul/16-Aug/1	1	430.0000	0.000	0.000
35	Vegetables, leafy(1st)	R2_Stream	soil incorp.	14-Feb/16-Mar/1	1	430.0000	0.000	0.000
36	Vegetables, leafy(2nd)	R2_Stream	soil incorp.	17-Jul/16-Aug/1	1	430.0000	0.000	0.000
37	Vegetables, leafy(1st)	R3_Stream	soil incorp.	15-Feb/17-Mar/1	1	430.0000	0.000	0.000
38	Vegetables, leafy(2nd)	R3_Stream	soil incorp.	1-Jun /1-Jul /1	1	430.0000	0.000	0.000
39	Vegetables, leafy(1st)	R4_Stream	soil incorp.	15-Feb/17-Mar/1	1	430.0000	0.000	0.000
40	Vegetables, leafy(2nd)	R4_Stream	soil incorp.	1-Jun /1-Jul /1	1	430.0000	0.000	0.000

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