

Study Report

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

*Simulations potatoes, oil seed rape, and vegetables (granular
application)*

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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 (granular application)*" 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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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 “**Granular linear incorporated at 4 cm**” means a linear incorporation into the upper 4 cm of the soil.

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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	Granular, linear	4 (default)	260	end of February/ beginning of April
		2nd	Granular, linear	4 (default)	130	mid of May
2	Potatoes	1st	Granular, linear	4 (default)	260	beginning of April
		2nd	Granular, linear	4 (default)	90	mid of May
3	Vegetables (leafy)	1st	Granular, linear	4 (default)	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

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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 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 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.

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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	$4.3 \cdot 10^{-5}$	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 in water (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	36220.4
2	Potatoes, beginning of April, 260kg, mid of May, 90kg	15900.8
3	(Leafy) vegetables, default, 430kg,	16882

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

Scen. ID	Crop/Scenario	Scenario	PEC _{sw} (µg/L)	PEC _{sed} (µg/kg)
1	Oilseed rape (winter), end of February/ begin of April, 260kg, begin/mid of April, 130kg	D2_Ditch	36220.4	8016.9
		D2_Stream	24354.3	4649.7
		D3_Ditch	413	378.6
		D4_Pond	323.6	187.5
		D4_Stream	432.7	204.2
		D5_Pond	42.98	22.18
		D5_Stream	56.57	24.19
		R1_Pond	64.73	17.24
		R1_Stream	2708.9	142.5
		R3_Stream	4478.8	262.6
2	Potatoes, begin of April, 260kg, mid of May, 90kg	D3_Ditch	510.3	459.2
		D4_Pond	302	201.8
		D4_Stream	1061.6	470.3
		D6_Ditch	1752.8	179.4
		D6_Ditch2	1752.8	179.4
		R1_Pond	233.5	44.06
		R1_Stream	3665.9	323
		R2_Stream	2850.4	190.5
		R3_Stream	15900.8	766.7
3	(Leafy) vegetables, default, 430kg,	D3_Ditch	498.2	459.6
		D3_Ditch2	3292.2	2872.8
		D4_Pond	403.8	263.5
		D4_Stream	1318.6	542.3
		D6_Ditch	5614.7	602

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Scen. ID	Crop/Scenario	Scenario	PEC _{sw} (µg/L)	PEC _{sed} (µg/kg)
		R1_Pond	4.263	1.182
		R1_Pond2	0.001203	0.000233
		R1_Stream	1086.5	62.8
		R1_Stream2	0.01917	0.001594
		R2_Stream	4124.1	262
		R2_Stream2	113.6	8.354
		R3_Stream	6961.7	419.8
		R3_Stream2	7104.6	666
		R4_Stream	14276.7	1187.8
		R4_Stream2	16882	1415.4

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 in water (PECmax) of 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	36220.4
2	Potatoes, begin of April, 260kg, mid of May, 90kg	15900.8
3	(Leafy) vegetables, default, 430kg,	16882

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       : 02-Oct-2019, 12:50
*
* 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.
*
*****
*   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)

```

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*						
* 41	Oil seed rape, winte(1st) D2_Ditch	granular appl. 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	granular appl. 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	granular appl. 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	granular appl. 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	granular appl. 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	granular appl. 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	granular appl. 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	granular appl. 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	granular appl. 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	granular appl. 20-Feb/6-May /45	1 260.0000	0.000	0.000	
*			2 130.0000	0.000	0.000	
*						

***** Surface Water Scenarios Help *****

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

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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_PO\HS_PO_report.txt
* Description    : Potatoes, begin of April, 260kg, mid of May, 90kg
* Substance      : HS
*
* Creation       : 02-Oct-2019, 12:44
*
* 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.
*
*****
*   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           granular appl. 1-Apr /15-Jun/45      1 260.0000      0.000      0.000

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*				2	90.0000	0.000	0.000
*							
* 10	Potatoes (1st)	D4_Pond	granular appl. 1-Apr /15-Jun/45	1	260.0000	0.000	0.000
*				2	90.0000	0.000	0.000
*							
* 11	Potatoes (1st)	D4_Stream	granular appl. 1-Apr /15-Jun/45	1	260.0000	0.000	0.000
*				2	90.0000	0.000	0.000
*							
* 12	Potatoes (1st)	D6_Ditch	granular appl. 1-Apr /15-Jun/45	1	260.0000	0.000	0.000
*				2	90.0000	0.000	0.000
*							
* 13	Potatoes (2nd)	D6_Ditch	granular appl. 1-Apr /15-Jun/45	1	260.0000	0.000	0.000
*				2	90.0000	0.000	0.000
*							
* 14	Potatoes (1st)	R1_Pond	granular appl. 1-Apr /15-Jun/45	1	260.0000	0.000	0.000
*				2	90.0000	0.000	0.000
*							
* 15	Potatoes (1st)	R1_Stream	granular appl. 1-Apr /15-Jun/45	1	260.0000	0.000	0.000
*				2	90.0000	0.000	0.000
*							
* 16	Potatoes (1st)	R2_Stream	granular appl. 1-Apr /15-Jun/45	1	260.0000	0.000	0.000
*				2	90.0000	0.000	0.000
*							
* 17	Potatoes (1st)	R3_Stream	granular appl. 1-Apr /15-Jun/45	1	260.0000	0.000	0.000
*				2	90.0000	0.000	0.000
*							

***** Surface Water Scenarios Help *****

6.3 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       : 02-Oct-2019, 12:50
*
* Remarks : SWASH report helps you to set up the needed runs to calculate the PECsw and PECsed, occurring 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.
*
*****
*   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)

```

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*							
* 26	Vegetables, leafy(1st)	D3_Ditch	granular appl. 11-Apr/11-May/1	1	430.0000	0.000	0.000
*							
* 27	Vegetables, leafy(2nd)	D3_Ditch	granular appl. 22-Jul/21-Aug/1	1	430.0000	0.000	0.000
*							
* 28	Vegetables, leafy(1st)	D4_Pond	granular appl. 26-Apr/26-May/1	1	430.0000	0.000	0.000
*							
* 29	Vegetables, leafy(1st)	D4_Stream	granular appl. 26-Apr/26-May/1	1	430.0000	0.000	0.000
*							
* 30	Vegetables, leafy(1st)	D6_Ditch	granular appl. 1-Aug /31-Aug/1	1	430.0000	0.000	0.000
*							
* 31	Vegetables, leafy(1st)	R1_Pond	granular appl. 6-Apr /6-May /1	1	430.0000	0.000	0.000
*							
* 32	Vegetables, leafy(2nd)	R1_Pond	granular appl. 17-Jul/16-Aug/1	1	430.0000	0.000	0.000
*							
* 33	Vegetables, leafy(1st)	R1_Stream	granular appl. 6-Apr /6-May /1	1	430.0000	0.000	0.000
*							
* 34	Vegetables, leafy(2nd)	R1_Stream	granular appl. 17-Jul/16-Aug/1	1	430.0000	0.000	0.000
*							
* 35	Vegetables, leafy(1st)	R2_Stream	granular appl. 14-Feb/16-Mar/1	1	430.0000	0.000	0.000
*							
* 36	Vegetables, leafy(2nd)	R2_Stream	granular appl. 17-Jul/16-Aug/1	1	430.0000	0.000	0.000
*							
* 37	Vegetables, leafy(1st)	R3_Stream	granular appl. 15-Feb/17-Mar/1	1	430.0000	0.000	0.000
*							
* 38	Vegetables, leafy(2nd)	R3_Stream	granular appl. 1-Jun /1-Jul /1	1	430.0000	0.000	0.000
*							
* 39	Vegetables, leafy(1st)	R4_Stream	granular appl. 15-Feb/17-Mar/1	1	430.0000	0.000	0.000
*							
* 40	Vegetables, leafy(2nd)	R4_Stream	granular appl. 1-Jun /1-Jul /1	1	430.0000	0.000	0.000
*							

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