Fraunhofer IME

Study Report

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

Comparison of two different half-lives in soil for vegetables

Sponsor

AlzChem Trostberg GmbH
Dr.-Albert-Frank-Str. 32
83308 Trostberg
Germany

Institute
Fraunhofer-Institute for Molecular Biology and Applied Ecology (IME)

Auf dem Aberg 1
57392 Schmallenberg
Germany

Director Applied Ecology
Prof. Dr. Christoph Schäfers

Author
Dr. Michael Klein
Dr. Judith Klein

October 28, 2019

This page was intentionally left blank for statements of the sponsor or submitter.

Statement of compliance

This study "*Predicted Environmental Concentrations in Surface Water of Urea based on FOCUS STEP3; Comparison of two different half-lives in soil for 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).

J. Klein

28 October 2019

Dr. Judith Klein
Statistics and Modelling
Fraunhofer Institute
Auf dem Aberg 1
57392 Schmallenberg
Germany

Tel +49 2972 302 256
Fax +49 2972 302 319
judith.klein@ime.fraunhofer.de

Date

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 15 cm**" means a uniform incorporation into the upper 15 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	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	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. Two scenarios are considered:

- Scenario A: 30 days (at 12 °C)
- Scenario B: 3.9 days (at 20 °C)

For scenario A, the default for a readily biodegradable substance is used, namely 30 days at 12°C for the half-life in soil.
For scenario B, the half-life in soil is estimated according to Vilsmeier and Amberger 1978. It is assumed that under temperature between 20°C and 30°C and suitable moisture after 10 days approximately 83% of urea is formed into nitrate.

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 (scenario A)	30 (at 12 °C)
Soil (scenario B)	3.9 (at 20 °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 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)
1A	(Leafy) vegetables, DT50soil 30 d (12°C)	3268.1
1B	(Leafy) vegetables, DT50soil 3.9 d (20°C)	1608.2

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

Crop	Scenario	PECsw (µg/L)		PECsed (µg/kg)	
		Scenario A - DT50 soil: 30 d at 12 °C	Scenario B - DT50 soil: 3.9 d at 20 °C	Scenario A - DT50 soil: 30 d at 12 °C	Scenario B - DT50 soil: 3.9 d at 20 °C
(Leafy) vegetables, default, 430kg,	D3_Ditch	498.2	0.1768	459.6	0.1438
	D3_Ditch2	3268.1	15.36	2864.3	12.01
	D4_Pond	337.1	0.4878	213	0.2391
	D4_Stream	1005.2	2.271	402.5	0.7825
	D6_Ditch	215.8	22.47	28.86	2.234
	R1_Pond	0.6518	0.296	0.1826	0.09188
	R1_Pond2	0.000174	0.000004	0.000034	0
	R1_Stream	173	109.6	9.997	6.337
	R1_Stream2	0.002776	0.00007	0.000231	0.000006
	R2_Stream	631.2	371.7	40.1	23.61
	R2_Stream2	17.25	0.008551	1.268	0.000629
	R3_Stream	1071.2	838.2	64.59	50.54
	R3_Stream2	1129.5	341.7	105.9	32.04
	R4_Stream	2247.7	1608.2	187	133.8
	R4_Stream2	2672.2	981.8	223.8	82.31

4. Conclusions

The following maximum concentrations were calculated for urea at step 3 simulations (no additional buffer strip to the surface water body): Scenario A using a DT50 in soil of 30 days at 12 °C leads to a PECmax that is twice that high than scenario B using a DT50 in soil of 3.9 days at 20°C.

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

Scen. ID	Scenaro/Crop	PECmax (µg/L)
1A	(Leafy) vegetables, DT50soil 30 d (12°C)	3268.1
1B	(Leafy) vegetables, DT50soil 3.9 d (20°C)	1608.2

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 Vegetables (leafy), default, 430kg, DT50soil 3.9 d (20°C)

```
* 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, 15:54
*
* 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)
*
* 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 **********************************************
```

6.2 Vegetables (leafy), default, 430kg, DT50soil 30 d (12°C)

```
* 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.
*
*
```

```
*************************************************************************************************************************************************
*  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)
*
* 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 **********************************************
```