

Study Report

Predicted Environmental Concentrations in Surface Water
of Cyanamide and PERLKA after fertilization with PERLKA
based on FOCUS STEP3

*Simulations maize, potatoes, pome and stone fruit, and
vegetables*

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May 7, 2018

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**Report: Predicted Environmental Concentration in Surface Water of
Cyanamide and PERLKA based on FOCUS STEP3**

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GLP-compliance

This study "*Predicted Environmental Concentrations in Surface Water for cyanamide and PERLKA based on FOCUS STEP3 Simulations in maize, potatoes, pome and stone fruit, 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 study does not describe an experimental study, so 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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 Cyanamide and PERLKA based on FOCUS STEP3 **- page 4/22 -**

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1. Simulation models

The program SWASH 5.3 (FOCUS 2001) was used to create 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 was 1 m.

2. Input parameters

2.1 Agricultural use pattern

PERLKA is applied in various crops with different application pattern as summarised in the following table.

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

Crop	App. method	Incorp. Depth (cm)	App. Rate (kg/ha)	Start of the application window
Vegetables leafy	Incorporated	at 15 cm	400	14 days before emergence (= planting)
Maize	Incorporated	at 10 cm	200	14 days before emergence (= planting)
Potatoes	Incorporated	at 15 cm	250	14 days before emergence (= planting)
Pome/Stone fruit	Granular app.	0 cm	200	14 days before leaf emergence

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

Table 2: Application pattern in winter cereals considered for the simulations

Crop	Scenario	application date calculated by FOCUS PAT
Maize	D3 (drainage)	20 April
Maize	D4 (drainage)	26 April
Maize	D5 (drainage)	26 April
Maize	D6 (drainage)	9 April
Maize	R1 (runoff)	26 April
Maize	R2 (runoff)	22 April
Maize	R3 (runoff)	22 April
Maize	R4 (runoff)	7 April
Potatoes	D3 (drainage)	04 May
Potatoes	D4 (drainage)	17 May
Potatoes	D6 1 st season (drainage)	02 April
Potatoes	D6 2 nd season (drainage)	25 July
Potatoes	R1 (runoff)	26 April
Potatoes	R2 (runoff)	01 March
Potatoes	R3 (runoff)	28 March
Pome/stone fruit	D3 (drainage)	04 April
Pome/stone fruit	D4 (drainage)	18 April
Pome/stone fruit	D5 (drainage)	08 April
Pome/stone fruit	R1 (runoff)	26 April
Pome/stone fruit	R2 (runoff)	01 March
Pome/stone fruit	R3 (runoff)	28 March
Pome/stone fruit	R4 (runoff)	05 March
vegetables	D3 1 st season (drainage)	10 April
vegetables	D3 2 nd season (drainage)	25 July
vegetables	D4 (drainage)	16 May
vegetables	D6 (drainage)	04 August
vegetables	R1 1 st season (runoff)	26 April
vegetables	R1 2 nd season (runoff)	28 July
vegetables	R2 1 st season (runoff)	6 March
vegetables	R2 2 nd season (runoff)	08 August
vegetables	R3 1 st season (runoff)	19 February

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Crop	Scenario	application date calculated by FOCUS PAT
vegetables	R3 2 nd season (runoff)	02 June
vegetables	R4 1 st season (runoff)	01 Mar
vegetables	R4 2 nd season (runoff)	01 June

2.2 Substance properties of Calcium Cyanamide (PERLKA) and Cyanamide

PERLKA

PERLKA consists to about 44% of calcium cyanamide. In order to simulate the slow release in soil of cyanamide from PERLKA granules adequately cyanamide was defined as metabolite. According to experimental data within 1 day up to 50% of the cyanamide is released out of the granules at 12 °C and 10% soil moisture (see appendix 1). Consequently, a half life of 1 day under standard conditions was assumed for the formation of cyanamide. The same release (half life of 1 day) was considered for the water phase. This value was used as a minimum number for the simulation model FOCUS TOXSWA.

Cyanamide

According to experimental data cyanamide is further transformed to urea (DegT₅₀ of cyanamide 2.89 days at 12 °C) at 5% and 10% soil moisture.

Furthermore, according to EFSA (2010) the half life of cyanamide in the water-sediment system is 3.5 days (geometric mean of two studies). According to the FOCUS recommendations, this value of 3.5 days must be considered for the transformation of cyanamide in water whereas a default value of 1000 days was considered for the sediment phase. The experimental disappearance time cannot be used for the modelling since it includes not only degradation but also transportation which is considered in the model separately.

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 PERLKA and cyanamide

Parameter	PERLKA	Cyanamide
Water	1 (at 12 °C)	2.89 (at 12 °C)
Sediment	1 (at 12 °C)	1000 (at 20 °C)
Soil	1 (at 12 °C)	1.4 (at 20 °C)

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 K_{OC} 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. For PERLKA residues in surface water the same value was considered as for cyanamide.

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 $2.68 \cdot 10^{-5}$ J/mol. However this value cannot be entered directly into the simulation model 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.

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

Table 4: Other input parameters used for the simulations of PERLKA and Cyanamide

Parameter	PERLKA	Cyanamide	remark
Sorption constant KOC in soil (L/kg)	172400	4	EFSA (2010)
Sorption constant KOC in water body (L/kg)	0	4	EFSA (2010)
Freundlich exponent (-)	1	1	EFSA (2010)
vapour pressure (20°C, Pa)	0	0.51 Pa	
Molar mass (g/mol)	80.11	42.04*	
Henry's law constant (J/mol)	-	$2.68 \cdot 10^{-5}$	EFSA (2010)
Water solubility (20°C, mg/L)	800000	800000	EFSA (2010)
molar enthalpy of vaporisation	95000	95000	default
molar enthalpy of dissolution	27000	27000	default
diffusion coefficient in water	$4.3 \cdot 10^{-5}$	$4.3 \cdot 10^{-5}$	default
diffusion coefficient in air	0.43	0.43	default
Plant uptake factor	0	0	default

* hydrogen cyanamide

3. Results

The global maximum concentrations for all scenarios and crops are summarised in the following Table 5. In total 58 FOCUS crop-location combinations were simulated.

The following maximum concentrations were calculated for cyanamide in the simulations:

Maize: 200 kg/ha, Underground fertilisation at 10 cm: **< 0.1 µg/L**

Potatoes: 250 kg/ha, Underground fertilisation at 15 cm: **< 0.1 µg/L**

Pome/stone fruits: 200 kg/ha, granular application: **2.639 µg/L**

Vegetables: 400 kg/ha Underground fertilisation at 15 cm: **<0.1 µg/L**

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Table 5: Global maximum concentrations of PERLKA and Cyanamide at FOCUS Step 3

Crop	Scenario	PERLKA	Cyanamide	
		PEC _{sw} (µg/L)	PEC _{sw} (µg/L)	PEC _{sed} (µg/kg)
Maize	D3_Ditch	0.000	0.001	0.001
	D4_Pond	0.000	0.004	0.002
	D4_Stream	0.000	0.012	0.006
	D5_Pond	0.000	0.000	0.000
	D5_Stream	0.000	0.000	0.000
	D6_Ditch	0.000	0.049	0.021
	R1_Pond	0.000	0.000	0.000
	R1_Stream	0.000	0.000	0.000
	R2_Stream	0.000	0.000	0.000
	R3_Stream	0.000	0.000	0.000
	R4_Stream	0.000	0.000	0.000
Potatoes	D3_Ditch	0.000	0.000	0.000
	D4_Pond	0.000	0.000	0.000
	D4_Stream	0.000	0.002	0.001
	D6_Ditch	0.000	0.065	0.003
	D6_Ditch	0.000	0.012	0.001
	R1_Pond	0.000	0.000	0.000
	R1_Stream	0.000	0.000	0.000
	R2_Stream	0.000	0.000	0.000
	R3_Stream	0.000	0.000	0.000
Pome/stone fruit	D3_Ditch	0.000	0.000	0.000
	D4_Pond	0.000	0.001	0.001
	D4_Stream	0.000	0.004	0.002
	D5_Pond	0.000	0.000	0.000
	D5_Stream	0.000	0.000	0.000
	R1_Pond	0.000	0.001	0.000
	R1_Stream	0.000	0.293	0.005
	R2_Stream	0.000	2.052	0.039
	R3_Stream	0.000	2.639	0.091
	R4_Stream	0.000	0.000	0.000

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Crop	Scenario	PERLKA	Cyanamide	
		PEC _{sw} (µg/L)	PEC _{sw} (µg/L)	PEC _{sed} (µg/kg)
Leafy vegetables (400 kg/ha underground fertilisation at 15 cm)	D3_Ditch	0.000	0.000	0.000
	D3_Ditch	0.000	0.003	0.002
	D4_Pond	0.000	0.001	0.000
	D4_Stream	0.000	0.002	0.001
	D6_Ditch	0.000	0.022	0.002
	R1_Pond	0.000	0.000	0.000
	R1_Pond	0.000	0.000	0.000
	R1_Stream	0.000	0.000	0.000
	R1_Stream	0.000	0.000	0.000
	R2_Stream	0.000	0.000	0.000
	R2_Stream	0.000	0.000	0.000
	R3_Stream	0.000	0.000	0.000
	R3_Stream	0.000	0.000	0.000
	R4_Stream	0.000	0.000	0.000
	R4_Stream	0.000	0.000	0.000

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Conclusions

The following maximum concentrations were calculated for cyanamide at step 3 simulations:

Maize: 200 kg/ha, Underground fertilisation at 10 cm: **< 0.1 µg/L**

Potatoes: 250 kg/ha, Underground fertilisation at 15 cm: **< 0.1 µg/L**

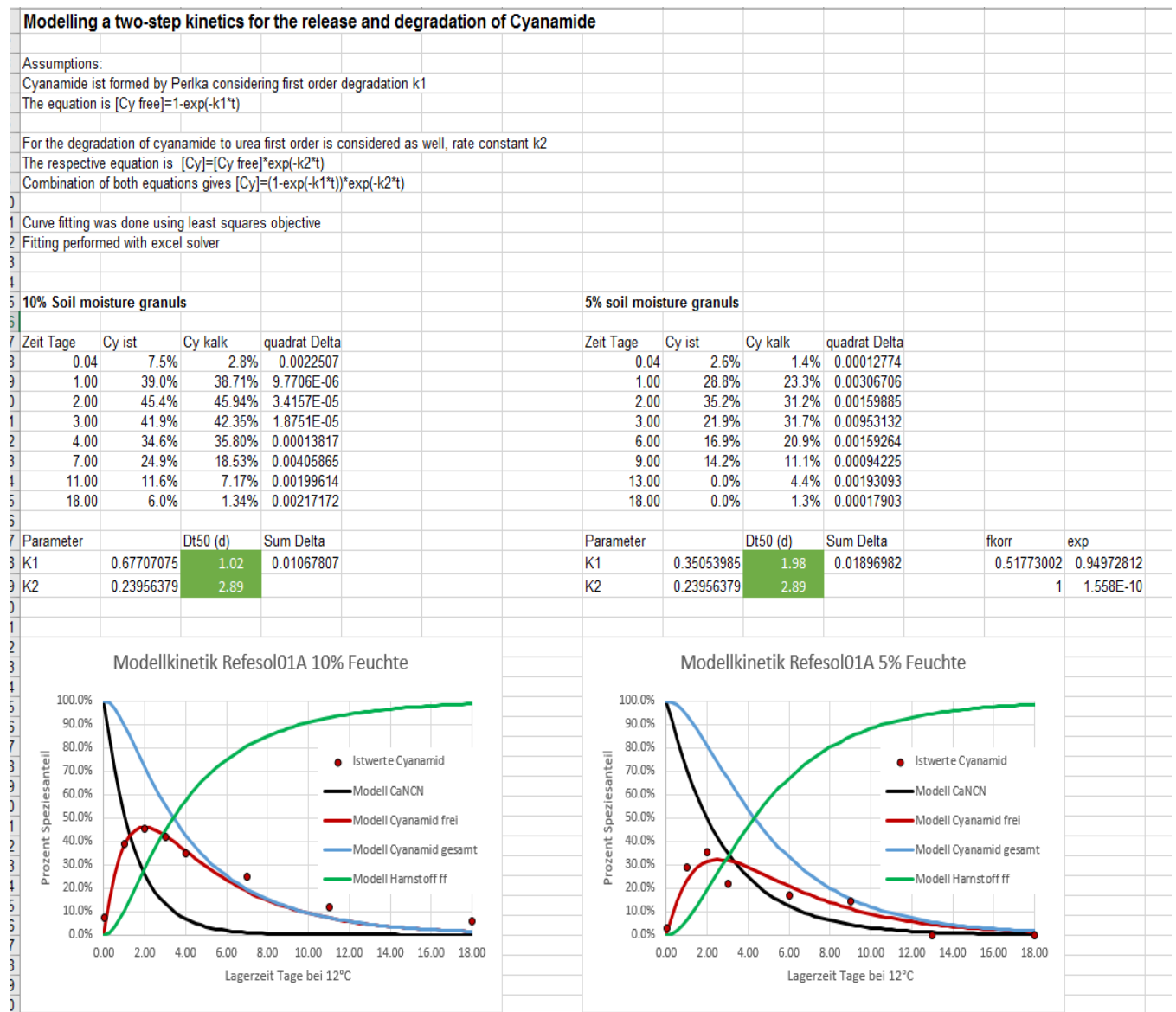
Pome/stone fruits: 200 kg/ha, granular application: **2.639 µg/L**

Vegetables: 400 kg/ha Underground fertilisation at 15 cm: **<0.1 µg/L**

4. References

- FOCUS (2000): "FOCUS groundwater scenarios in the EU review of active substances". Report of the FOCUS Groundwater Scenarios Workgroup, EC Doc. Ref. SANCO/321/2000 rev. 2; and "Generic guidance for FOCUS groundwater scenarios". FOCUS Groundwater Scenario Workgroup, May 2001, Version
- 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.- in: 'Leaching Models and EU registration'. Final report of the FOCUS Group. Doc. 4952/VI/95.
- FOCUS (2007). "Landscape And Mitigation Factors In Aquatic Risk Assessment. Volume 1. Extended Summary and Recommendations". Report of the FOCUS Working Group on Landscape and Mitigation Factors in Ecological Risk Assessment, EC Document Reference SANCO/10422/2005 v2.0. 169 pp.

5. Appendix 1: Fitting the release and degradation of cyanamide



6.

6.1

```
* SWASH report file
* made by FOCUS-SWASH UI v. 5 (internal version 5.1.0, 02 April 2015)
*
* File Name      : E:\SwashProjects\CN2_VEG3\CN2_VEG3_report.txt
* Description    : 400 kg 15 cm uniform
* Substance      : CN2Gr
*
* Creation       : 03-May-2018, 15:32
*
* 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.
```

Report:

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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)	
*								
* 1048	Vegetables,	leafy(1st)	D3_Ditch	soil incorp.	11-Apr/11-May/1	1 400.0000	0.000	0.000
*								
* 1049	Vegetables,	leafy(2nd)	D3_Ditch	soil incorp.	22-Jul/21-Aug/1	1 400.0000	0.000	0.000
*								
* 1050	Vegetables,	leafy(1st)	D4_Pond	soil incorp.	26-Apr/26-May/1	1 400.0000	0.000	0.000
*								
* 1051	Vegetables,	leafy(1st)	D4_Stream	soil incorp.	26-Apr/26-May/1	1 400.0000	0.000	0.000
*								
* 1052	Vegetables,	leafy(1st)	D6_Ditch	soil incorp.	1-Aug /31-Aug/1	1 400.0000	0.000	0.000
*								
* 1053	Vegetables,	leafy(1st)	R1_Pond	soil incorp.	6-Apr /6-May /1	1 400.0000	0.000	0.000
*								
* 1054	Vegetables,	leafy(2nd)	R1_Pond	soil incorp.	17-Jul/16-Aug/1	1 400.0000	0.000	0.000
*								
* 1055	Vegetables,	leafy(1st)	R1_Stream	soil incorp.	6-Apr /6-May /1	1 400.0000	0.000	0.000
*								
* 1056	Vegetables,	leafy(2nd)	R1_Stream	soil incorp.	17-Jul/16-Aug/1	1 400.0000	0.000	0.000
*								
* 1057	Vegetables,	leafy(1st)	R2_Stream	soil incorp.	14-Feb/16-Mar/1	1 400.0000	0.000	0.000
*								
* 1058	Vegetables,	leafy(2nd)	R2_Stream	soil incorp.	17-Jul/16-Aug/1	1 400.0000	0.000	0.000
*								
* 1059	Vegetables,	leafy(1st)	R3_Stream	soil incorp.	15-Feb/17-Mar/1	1 400.0000	0.000	0.000
*								
* 1060	Vegetables,	leafy(2nd)	R3_Stream	soil incorp.	1-Jun /1-Jul /1	1 400.0000	0.000	0.000
*								
* 1061	Vegetables,	leafy(1st)	R4_Stream	soil incorp.	15-Feb/17-Mar/1	1 400.0000	0.000	0.000
*								
* 1062	Vegetables,	leafy(2nd)	R4_Stream	soil incorp.	1-Jun /1-Jul /1	1 400.0000	0.000	0.000
*								
***** Surface Water Scenarios Help *****								

6.2 Application in Potatoes (250 kg/ha)

* SWASH report file
* made by FOCUS-SWASH UI v. 5 (internal version 5.1.0, 02 April 2015)
*
* File Name : E:\SwashProjects\CN2_PO1\CN2_PO1_report.txt
* Description : 250 kg at 15 cm
* Substance : CN2Gr
*
* Creation : 25-Apr-2018, 10:44
*
* Remarks : SWASH report helps you to set up the needed runs to calculate the PEC_{sw} and PEC_{sed}, 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.
*



IME

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* CREATED RUNS								

*								
*								
* -ID-----Crop(1st/2nd)-----Scenario-WaterbodyType-	-----APPLICATION -----		---- on Water Surface ----'					
	-Method-----First/Last/Interval--#---Rate-		-Mean Deposition-Mass Loading					
	(d)	(kg/ha)	(% of Appl. Rate)	(mg/m2)				

* 960	Potatoes(1st)	D3_Ditch	soil incorp.	26-Apr/26-May/1	1	250.0000	0.000	0.000
* 961	Potatoes(1st)	D4_Pond	soil incorp.	8-May /7-Jun /1	1	250.0000	0.000	0.000
* 962	Potatoes(1st)	D4_Stream	soil incorp.	8-May /7-Jun /1	1	250.0000	0.000	0.000
* 963	Potatoes(1st)	D6_Ditch	soil incorp.	27-Mar/26-Apr/1	1	250.0000	0.000	0.000
* 964	Potatoes(2nd)	D6_Ditch	soil incorp.	22-Jul/21-Aug/1	1	250.0000	0.000	0.000
* 965	Potatoes(1st)	R1_Pond	soil incorp.	21-Apr/21-May/1	1	250.0000	0.000	0.000
* 966	Potatoes(1st)	R1_Stream	soil incorp.	21-Apr/21-May/1	1	250.0000	0.000	0.000
* 967	Potatoes(1st)	R2_Stream	soil incorp.	1-Mar /31-Mar/1	1	250.0000	0.000	0.000
* 968	Potatoes(1st)	R3_Stream	soil incorp.	27-Mar/26-Apr/1	1	250.0000	0.000	0.000

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

6.3

```
* SWASH report file
* made by FOCUS-SWASH UI v. 5 (internal version 5.1.0, 02 April 2015)
*
* File Name      : E:\SwashProjects\CN2_POM1\CN2_POM1_report.txt
* Description    : 200 kg at surface
* Substance      : CN2Gr
*
* Creation       : 25-Apr-2018, 10:53
*
* 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)
*
* 978   Pome/stone fruit, ea(1st) D3_Ditch                granular appl. 1-Apr /1-May /1      1 200.0000    0.000    0.000
*
* 979   Pome/stone fruit, ea(1st) D4_Pond                 granular appl. 6-Apr /6-May /1      1 200.0000    0.000    0.000
*
* 980   Pome/stone fruit, ea(1st) D4_Stream              granular appl. 6-Apr /6-May /1      1 200.0000    0.000    0.000
*
* 981   Pome/stone fruit, ea(1st) D5_Pond                 granular appl. 18-Mar/17-Apr/1      1 200.0000    0.000    0.000
*
* 982   Pome/stone fruit, ea(1st) D5_Stream              granular appl. 18-Mar/17-Apr/1      1 200.0000    0.000    0.000
*
* 983   Pome/stone fruit, ea(1st) R1_Pond                 granular appl. 1-Apr /1-May /1      1 200.0000    0.000    0.000
*
* 984   Pome/stone fruit, ea(1st) R1_Stream              granular appl. 1-Apr /1-May /1      1 200.0000    0.000    0.000
*
* 985   Pome/stone fruit, ea(1st) R2_Stream              granular appl. 1-Mar /31-Mar/1      1 200.0000    0.000    0.000
*
* 986   Pome/stone fruit, ea(1st) R3_Stream              granular appl. 18-Mar/17-Apr/1      1 200.0000    0.000    0.000
*
* 987   Pome/stone fruit, ea(1st) R4_Stream              granular appl. 1-Mar /31-Mar/1      1 200.0000    0.000    0.000
*
***** Surface WAter Scenarios Help *****

```

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6.4 Application in Maize (200 kg/ha)

```

* SWASH report file
* made by FOCUS-SWASH UI v. 5 (internal version 5.1.0, 02 April 2015)
*
* File Name   : E:\SwashProjects\CN2_MZ1\CN2_MZ1_report.txt
* Description : 200 kg at 10 cm
* Substance   : CN2Gr
*
* Creation    : 03-May-2018, 15:28
*
* 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)
*
* 1037 Maize(1st)                D3_Ditch                soil incorp.   21-Apr/21-May/1    1  200.0000    0.000    0.000
*
* 1038 Maize(1st)                D4_Pond                soil incorp.   26-Apr/26-May/1    1  200.0000    0.000    0.000

```

