

### Test results for FOCUS\_TOXSWA\_4.4.3

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Standard drainage and runoff input files are used to test the new TOXSWA version<sup>1</sup>. These are:

- 6 \*.m2t files and 4 \*.p2t files,
- representing output for 3 applications of 1 kg/ha
- of FOCUS Compound D\_sw
- to winter cereals (maize for R2)
- with the first appln at the day around emergence (appln window for PAT: emergence-5 up to emergence+50 d,
- appln interval 6 d,
- application method: ground spray).

They can be found at the home page of the workgroup. The \*.m2t and \*.p2t file need to be copied into the corresponding SWASHprojects folder for MACRO and PRZM, respectively. Change the runid's of these files to the runid's necessary for running TOXSWA (see the exact path in the corresponding txw input file).

These 'average' drainage and runoff fluxes are coupled to a less and a more persistent compound in water, respectively FOCUS Compound A\_sw and H\_sw.

So create 2 projects in SWASH with:

- compound A\_sw and compound H\_sw
- winter cereals (maize for R2)
- 3 applications of 1 kg/ha
- with the first appln at the day around emergence (appln window for PAT: emergence-5 up to emergence+50 d,
- appln interval 6 d
- application method: ground spray

#### 1. Model output for 3 applications of 1 kg/ha of FOCUS Compound A\_sw to winter cereals (maize for R2) with the first appln at the day around emergence

Scenario	Appln date (not changed)	Water		Sediment
		Global max (µg/L) [Date]	TWAC 28 d (µg/L)	Global max (µg/L) [Date]
D1-Ditch	3-Oct-1982 23-Oct-1982 5-Nov-1982	225.3 22-nov-1982	144.9	57.59 25-nov-1982
D1-Stream	3-Oct-1982 23-Oct-1982 5-Nov-1982	157.5 13-nov-1982	101.0	39.10 25-nov-1982
D2-Ditch	3-Nov-1986 28-Nov-1986 8-Dec-1986	465.3 12-dec-1986	156.6	69.11 15-dec-1986
D2-Stream	3-Nov-1986 28-Nov-1986 8-Dec-1986	329.2 11-dec-1986	102.1	44.05 15-dec-1986

<sup>1</sup> Please note that these runs are intended as a test for the TOXSWA software only. They do not correspond to sensible, consistent step 3 FOCUS runs that can be used for risk assessment purposes. (E.g. because PRZM and MACRO do calculations for a pesticide with D-sw properties, while TOXSWA performs calculations for a pesticide with A-sw or H-sw properties.)

D3-Ditch	22-Nov-1992 28-Nov-1992 10-Dec-1992	29.89 22-nov-1992	25.77	8.797 10-dec-1992
D4-Pond	28-Sep-1985 4-Oct-1985 26-Oct-1985	31.20 21-dec-1985	23.76	9.367 23-dec-1985
D4-Stream	28-Sep-1985 4-Oct-1985 26-Oct-1985	102.2 9-dec-1985	75.33	26.29 21-dec-1985
D5-Pond	27-Nov-1978 18-Dec-1978 01-Jan-1979	42.09 12-feb-1979	18.31	9.965 14-feb-1979
D5-Stream	27-Nov-1978 18-Dec-1978 01-Jan-1979	70.35 11-feb-1979	40.86	17.58 13-feb-1979
D6-Ditch	6-Dec-1986 30-Dec-1986 14-Jan-1987	156.2 19-jan-1987	26.26	15.29 19-jan-1987
R1-Pond	14-Nov-1978 20-Nov-1978 27-Nov-1978	1.100 25-nov-1978	0.2505	0.1626 28-nov-1978
R1-Stream	14-Nov-1978 20-Nov-1978 27-Nov-1978	91.23 25-nov-1978	1.488	5.641 25-nov-1978
R2-Stream	26-Apr-1977 7-May-1977 20-May-1977	35.34 13-may-1977	1.030	2.833 13-may-1977
R3-Stream	5-Dec-1980 11-Dec-1980 20-Dec-1980	157.7 16-dec-1980	4.71	10.52 16-dec-1980
R4-Stream	5-Nov-1979 10-Dec-1979 24-Dec-1979	10.62 21-dec-1979	0.2460	0.7535 21-dec-1979

2. Model output for 3 applications of 1 kg/ha of FOCUS Compound H\_sw to winter cereals (maize for R2) with the first appln at the day around emergence

Scenario	Appln date (not changed)	Water		Sediment
		Global max (µg/L) [Date]	TWAC 28 d (µg/L)	Global max (µg/L) [Date]
D1-Ditch	3-Oct-1982 23-Oct-1982 5-Nov-1982	246.9 20-nov-1982	164.8	222.8 27-nov-1982
D1-Stream	3-Oct-1982 23-Oct-1982 5-Nov-1982	158.3 13-nov-1982	102.2	126.2 27-nov-1982
D2-Ditch	3-Nov-1986 28-Nov-1986 8-Dec-1986	469.1 12-dec-1986	175.3	259.9 31-dec-1986
D2-Stream	3-Nov-1986 28-Nov-1986 8-Dec-1986	329.7 11-dec-1986	102.9	153.3 31-dec-1986
D3-Ditch	22-Nov-1992 28-Nov-1992 10-Dec-1992	33.15 22-nov-1992	30.05	88.79 11-jan-1993
D4-Pond	28-Sep-1985 4-Oct-1985 26-Oct-1985	127.1 31-jan-1986	123.3	286.9 5-apr-1986
D4-Stream	28-Sep-1985 4-Oct-1985 26-Oct-1985	102.3 9-dec-1985	75.58	110.5 30-jan-1986
D5-Pond	27-Nov-1978 18-Dec-1978 01-Jan-1979	110.7 17-feb-1979	106.1	232.2 01-may-1979
D5-Stream	27-Nov-1978 18-Dec-1978 01-Jan-1979	70.42 11-feb-1979	41.03	72.71 11-apr-1979
D6-Ditch	6-Dec-1986 30-Dec-1986 14-Jan-1987	157.2 19-jan-1987	28.96	58.96 20-jan-1987

R1-Pond	14-Nov-1978 20-Nov-1978 27-Nov-1978	1.462 27-nov-1978	1.281	1.845 02-feb-1979
R1-Stream	14-Nov-1978 20-Nov-1978 27-Nov-1978	91.61 25-nov-1978	1.5010	12.26 25-nov-1978
R2-Stream	26-Apr-1977 7-May-1977 20-May-1977	35.72 13-may-1977	1.047	6.492 13-may-1977
R3-Stream	5-Dec-1980 11-Dec-1980 20-Dec-1980	158.4 16-dec-1980	4.806	23.18 16-dec-1980
R4-Stream	5-Nov-1979 10-Dec-1979 24-Dec-1979	10.66 21-dec-1979	0.2489	1.670 21-dec-1979

Table 3 shows the global maximum concentrations in water calculated by v.3.3.1 and by 4.4.3. of compound A from Table 1, and the percentage difference in concentration. Table 4 does the same for compound H from Table 2.

3. Global maximum concentrations calculated by version 3.3.1 and version 4.4.3 of compound A\_sw (from Table 1). The concentraton difference is given as percentage.

Scenario	Global maximum in water (µg/L)		Difference (%)
	v.3.3.1	v.4.4.3	
D1-Ditch	225.322	225.3	0.0
D1-Stream	157.715	157.5	-0.1
D2-Ditch	466.838	465.3	-0.1
D2-Stream	333.303	329.2	-1.2
D3-Ditch	29.885	29.89	0.0
D4-Pond	31.201	31.20	0.0
D4-Stream	102.111	102.2	0.1
D5-Pond	42.088	42.09	0.0
D5-Stream	70.481	70.35	-0.2
D6-Ditch	156.174	156.2	0.0
R1-Pond	1.100	1.100	0.0
R1-Stream	92.865	91.23	-1.8
R2-Stream	35.806	35.34	-1.3
R3-Stream	161.811	157.7	-2.5
R4-Stream	10.770	10.62	-1.4

4. Global maximum concentrations calculated by version 3.3.1 and version 4.4.3 of compound H\_sw (from Table 2). The concentraton difference is given as percentage.

Scenario	Global maximum in water (µg/L)		Difference (%)
	v.3.3.1	v.4.4.3	
D1-Ditch	246.886	246.8	0.0
D1-Stream	158.426	158.3	-0.1
D2-Ditch	470.635	469.0	-0.3
D2-Stream	333.837	329.7	-1.2
D3-Ditch	33.145	33.15	0.0
D4-Pond	127.139	127.1	0.0
D4-Stream	102.289	102.3	0.0
D5-Pond	110.710	110.7	0.0
D5-Stream	70.554	70.42	-0.2
D6-Ditch	157.164	157.2	0.0
R1-Pond	1.462	1.462	0.0
R1-Stream	93.610	91.61	-2.1
R2-Stream	36.198	35.72	-1.3
R3-Stream	163.022	158.4	-2.8
R4-Stream	10.816	10.66	-1.4

The global maximum concentrations in water of compound A (Table 3) and compound H (Table 4) differ maximally 2.8%. The differences in global maximum concentrations are due to a slight difference in the numerical approximations of the water depth of the two versions (see Differences between FOCUS\_TOXSWA v.3.3.1 and FOCUS\_TOXSWA v.4.4.3, item *m4*).

Only the TWA28 of the R3-Stream differs, for both compounds. The differences of 0.6% and of 0.7% are also due to the slight difference in the numerical approximations of the water depth of the two versions (see Differences between FOCUS\_TOXSWA v.3.3.1 and FOCUS\_TOXSWA v.4.4.3, item *m4*).

The global maximum concentration in sediment of compound A found for the D6-Ditch scenario is due to a typo in the Test results of FOCUS\_TOXSWA 3.3.1. Other differences in global maximum concentrations in sediment are less than 1% for all other calculations. These small differences are a consequence of the differences in concentration in water for those runs (see above). The concentration in water determines how much of the substance diffuses between water and sediment.