

## Difference in type of concentrations in the FOCUS\_TOXSWA 4.4.3 output files Runid.SUM and Runid.OUT

This note has the intention to clarify existing confusions on the type of concentrations and contents, given in the Runid.SUM and Runid.OUT output files of FOCUS\_TOXSWA version 4.4.3 (Beltman et al, 2014).

### Differences in exposure concentrations

While in former FOCUS\_TOXSWA versions (Beltman et al, 2006) all concentrations and contents were given as momentary values, i.e. occurring at a certain moment in time, unless clearly stated to be average values (i.e. the TWAEC values in the former Runid.SUM file), FOCUS\_TOXSWA 4.4.3 uses two different types of concentrations and contents in its output files:

In the Runid.SUM files:

- a. all concentrations and contents are momentary values occurring at a certain moment in time and allocated to this very moment, i.e. DATE-xxh00.

In the Runid.OUT files:

- a. all concentrations and contents are hourly-averaged values allocated at the centre of the hour, i.e. DATE-xxh30, but
- b. an exception is the variable *ConLiqWatLayCur*, which is a momentary value occurring at a certain moment in time and allocated to this very moment, i.e. DATE-xxh00.

Additionally, in the Runid.SUM file Time Weighted Average Exposure Concentrations (i.e. the TWAEC values) are given, these average values are allocated to the last moment in time of the period over which the average was taken.

### Overview of the exposure concentrations

Details on the PEC values have been summarised in Table 1 below.

Table 1. Predicted Environmental Concentrations (PEC) in surface water and sediment in the Runid.SUM file and corresponding concentrations in the Runid.OUT file for FOCUS\_TOXSWA 4.4.3

Runid.SUM file		Runid.OUT file	
<b>PEC<sub>sw</sub></b>	momentary value at full hour (DATE-xxh00)	variable <i>ConLiqWatLayCur</i> *	time series - momentary values at each full hour (DATE-xxh00)
-	-	variable <i>ConLiqWatLay</i> *	time series - hourly averaged values allocated at the centre of the hour (DATE-xxh30)
<b>PEC<sub>sw</sub> (incl. susp. solids)</b>	momentary value at full hour (DATE-xxh00)	-	-
-	-	variable <i>ConSysWatLay</i> *	time series - hourly averaged values allocated at the centre of the hour (DATE-xxh30)
<b>PEC<sub>sed</sub></b>	momentary value at full hour (DATE-xxh00)	-	-
-	-	variable <i>CntSedTgt</i> *	time series - hourly averaged values allocated at the centre of the hour (DATE-xxh30)

\**ConLiqWatLayCur* - Concentration dissolved in water layer, momentary value (g.m<sup>-3</sup>)  
*ConLiqWatLay* - Concentration dissolved in water layer, hourly-averaged value (g.m<sup>-3</sup>)  
*ConSysWatLay* - Total concentration in water layer, hourly-averaged value (g.m<sup>-3</sup>)  
*CntSedTgt* - Total content in target layer of sediment, hourly-averaged value (g.kg<sup>-1</sup>)

## Calculation of wished exposure concentrations

Below it is indicated how wished exposure concentrations can be calculated from the time-series in the Runid.OUT file

### 1. How to calculate the (momentary) PEC<sub>sw</sub> from the time-series in the Runid.OUT file ?

Momentary concentrations in water are available in the Runid.OUT file as the variable (*ConLiqWatLayCur*).

### 2. How to calculate the (momentary) PEC<sub>sw</sub> (including suspended solids) from the time-series in the Runid.OUT file ?

Momentary total concentrations (including suspended solids, but excluding macrophytes in FOCUS scenarios) can be calculated from the variable *ConSysWatLay* of the Runid.OUT file with Eqs. 4.1 – 4.3 in Adriaanse (1996, p.31). The maximum value of PEC<sub>sw</sub> including suspended solids of the Runid.SUM file is slightly different from the maximum value of the variable *ConSysWatLay* of the Runid.OUT file.

### 3. How to calculate the (momentary) PEC<sub>sed</sub> from the time-series in the Runid.OUT file ?

Momentary contents in the target layer of the sediment are not available, since only hourly-averaged values are available for the variable *CntSedTgt* in the Runid.OUT file. So, the maximum value of PEC<sub>sed</sub> of the Runid.SUM file is slightly different from the maximum value of the variable *CntSedTgt* of the Runid.OUT file

### 4. How to calculate TWAECs from the time-series in the Runid.OUT file ?

TWAEC values for wished time-periods in days can be calculated with the aid of the hourly-averaged values of the Runid.OUT file by taking a backward average. An example is the TWAEC<sub>4days</sub> for the concentration in water, calculated as the average of 96 hourly concentrations *ConLiqWatLay* of the Runid.OUT file from 02-Jan 9:30 to 06-Jan 8:30 and allocated to 06-Jan 9:00 (backward average).

These TWAEC values will correspond exactly with those in the Runid.SUM file, because both the TWAEC values of the Runid.SUM file and the hourly-averaged values of the Runid.OUT file are based upon results of all time steps used in the numerical solution (so, also at time steps within the hour, which are not shown in the output files).

## References

- Adriaanse, P.I., 1996. Fate of pesticides in field ditches: the TOXSWA model. Report 90, DLO Winand Staring Centre, Wageningen, The Netherlands.
- Beltman, W.H.J., M.M.S. Ter Horst, P.I. Adriaanse, A. De Jong, 2006. Manual of FOCUS\_TOXSWA version 2.2.1. Alterra-rapport 586, Alterra, Wageningen, The Netherlands.
- Beltman, W.H.J., M.M.S. ter Horst, P.I. Adriaanse, A. de Jong and J. Deneer, 2014. FOCUS\_TOXSWA manual 4.4.2. User's Guide version 4. Statutory Research Task Unit for Nature and the Environment (WOT Natuur & Milieu), WOT-technical report 14. Wageningen University and Research centre (WUR), Wageningen, The Netherlands.