Bugs in FOCUS_TOXSWA 4.3.3, July 2016

This note explains six bugs in the FOCUS_TOXSWA version 4.4.3 (Beltman et al, 2014). The bugs will be repaired in the next version of FOCUS_TOXSWA.

1. TOXSWA run with metabolite(s) may stop for parent *or* metabolite with K_{oc} > 30 000 L/kg

TOXSWA may stop and give the error message "`Positivity condition 5 (rdd >=0) not fulfilled`" in the RunID.ERR file when a simulation is done where metabolites are formed, when the parent or the metabolite sediment K_{oc} value is > 30 000 L/kg and the other value much lower than 30 000 L/kg (e.g. 100 L/kg). Not fulfilling positivity conditions results in negative concentrations. For FOCUS simulations, it is advised to use a finer segmentation of the sediment for substances with K_{oc} > 30 000 L/kg (see section 4.4.3 of Beltman et al., 2014). For step 3 runs the TOXSWA user interface selects the finer FOCUS_highKoc segmentation if the parent has a K_{oc} value > 30 000 L/kg. In the case described here the parent *or* the metabolite needs the finer segmentation to obtain a convergent solution of the mass balance equation for the sediment. However, the combination of the fine segmentation with the low K_{oc} value of either the parent or the metabolite may result in not meeting the positivity conditions and then the TOXSWA run stops.

A work-around is:
- perform a run with the parent only (Step 3, so a suitable sediment segmentation is selected, the standard or the finer segmentation, depending on the K_{oc} value of the parent),
- perform a run with parent and metabolite using the standard segmentation for both the parent and the metabolite by copying the FOCUS Step 3 project (within the TOXSWA user interface); in the copied project automatically the standard sediment segmentation is selected, i.e. not replaced by the finer sediment segmentation as in Step 3 runs).

The results of the first run with the parent only are correct. For the metabolite it depends on the situation:

Metabolite K_{oc} < 30 000 L/kg (so, parent K_{oc} > 30 000 L/kg)
The metabolite concentrations obtained by the second run may differ from a run with the finer sediment segmentation, that is needed to obtain accurate parent concentrations (i.e. concentrations that do not change significantly for mass balance solutions obtained with sediment segments of half or twice the original size). The formation of the metabolite depends on the accuracy of the parent concentrations. So, if the parent concentrations are not accurate (which probably is the case for this second run with a too coarse sediment segmentation for the parent), the metabolite concentrations are inaccurate as well. We advise to compare the parent concentrations of the first and the second. And if their difference is small or negligible, the inaccuracy in the calculated metabolite concentration is probably small as well.

Metabolite K_{oc} > 30 000 L/kg
The metabolite concentrations of the second run may differ from those of a proper run, because in the second run the sediment segmentation is too coarse to obtain accurate metabolite concentrations. Hence the metabolite concentrations will change significantly for other sediment segmentations, indicating that the mass balance for the sediment has not been solved in a convergent way. Possibly, this run will stop. Please, then contact toxswa-swash@wur.nl for further advice. To assess the effect of the sediment segmentation on the accuracy of the metabolite concentrations, simulations can be done with different sediment segmentations of intermediate fineness.

2. Tiny spray drift loadings not transferred exactly into TOXSWA input

Tiny spray drift loadings are not transferred from the TOXSWA user interface into the TOXSWA input file in an exact way. The TOXSWA user interface rounds values to four decimal places in column 3 of table Loadings (in mg/m^2) in Section 7 in the TOXSWA input file, RunID.txw. This is a problem for all spray drift loadings where the fifth decimal value of the loading mass is relevant. This may occur when a Step 4 calculation is done in which a low application rate combined with a low spray drift percentage occurs. The resulting PECs are not exactly correct: if rounding to 4 decimals resulted in smaller loadings (e.g. for a fifth decimal of 4, rounded to 0) the PECs are too low and if rounding to 4 decimals resulted in higher loadings (e.g. for a fifth decimal of 7) the PECs are too high.

This problem can be circumvented by running TOXSWA outside its user interface:
1. Set up the run using SWASH and TOXSWA (with a default spray drift deposition).
2. Execute the run from within the TO
3. Calculate the wished spray drift mass deposition, or take it from SWAN.
4. Open the folder of the TOXSWA run (:\SWASHprojects\Project_name\TOXSWA).
5. Use a text editor to open the TOXSWA input file (RunID.txw). In Section 7 change the Drift deposition value (mg/m^2). Up to 15 decimal places can be read in by the TOXSWA source code.

```
table Loadings
30-Dec-1899 drift 0.0002142 0. 100.
end_table
```

6. Start the run by clicking on the toxswa.bat file, present in the folder.
7. Results of the run can be viewed via the user interface of TOXSWA. Note, do not repeat the run from within the user interface, because then the TOXSWA input file that you just edited will be overwritten and thus, you will not obtain the wished results.

In the next version of FOCUS_TOXSWA more decimal places will be filled by the user interface.

3. Maximum runoff concentration reported in summary file not correct

The maximum concentration in runoff as well as the timing of the peak value reported in the summary output of TOXSWA are not correct. When one needs to know the concentration in the runoff water we suggest to use the output of the PRZM model, i.e. the RunID.p2t output file. Divide the values in the column Runoff flux by the values in the column Runoff volume, this results in the concentrations in the runoff water in mg/L, from which the maximum value and associated timing can be selected.

Explanation:
a mm/h as Runoff volume on 1 m^2 soil surface area corresponds to a L/(m^2.h). If you have b mg a.s. /(m^2.h) as Pesticide mass flux, then the concentration in the runoff flow will be: b/a in mg/L or (b/a)* 1000 in μg/L (because mg/(m^2.h) divided by L/(m^2.h) = mg/L).

4. Unjustified mass balance warning in FOCUS stream scenarios for runs with metabolites that are formed in soil *and* in water

A warning message "`Difference in cumulative fluxes and mass present (%):`" is shown in the DOS-box and in the RunID.WRN file. This occurs in runs of FOCUS stream scenarios where the same metabolite is formed in soil and in water. The warning is unjustified.

The reason for this unjustified warning is that TOXSWA checks the mass balance for the 100-m FOCUS stream by adding up and subtracting all mass components entering and leaving the stream. The mass component for entering the 100-m stream from the upstream catchment for metabolites should consist of (a) the metabolite mass that was already formed in soil and discharged into the upstream catchment water and of (b) metabolite mass formed in the upstream catchment from the parent. However, (a) is not added in the calculation. So, this is a bug. There are no consequences for the simulated parent and metabolite concentrations, because they have been correctly calculated.

5. Graph presenting content in sediment shows concentration of factor 1000 too low

The graph "Content in FOCUS layer in sediment below FOCUS water layer segment of substance" shows concentrations (indicated on the y-axis) that are a factor of 1000 too low. Instead of the unit mg.kg^{-1}, the unit should be µg.kg^{-1}). This bug is only on the outside, i.e. the TOXSWA calculations are correct. You can obtain the correct unit along the y-axis by changing the text along the vertical axis: change the unit from mg into µg. This can be done in the graph: Select Edit in the menu bar of the graph and next, go to Axis -> Title -> Style (see below).
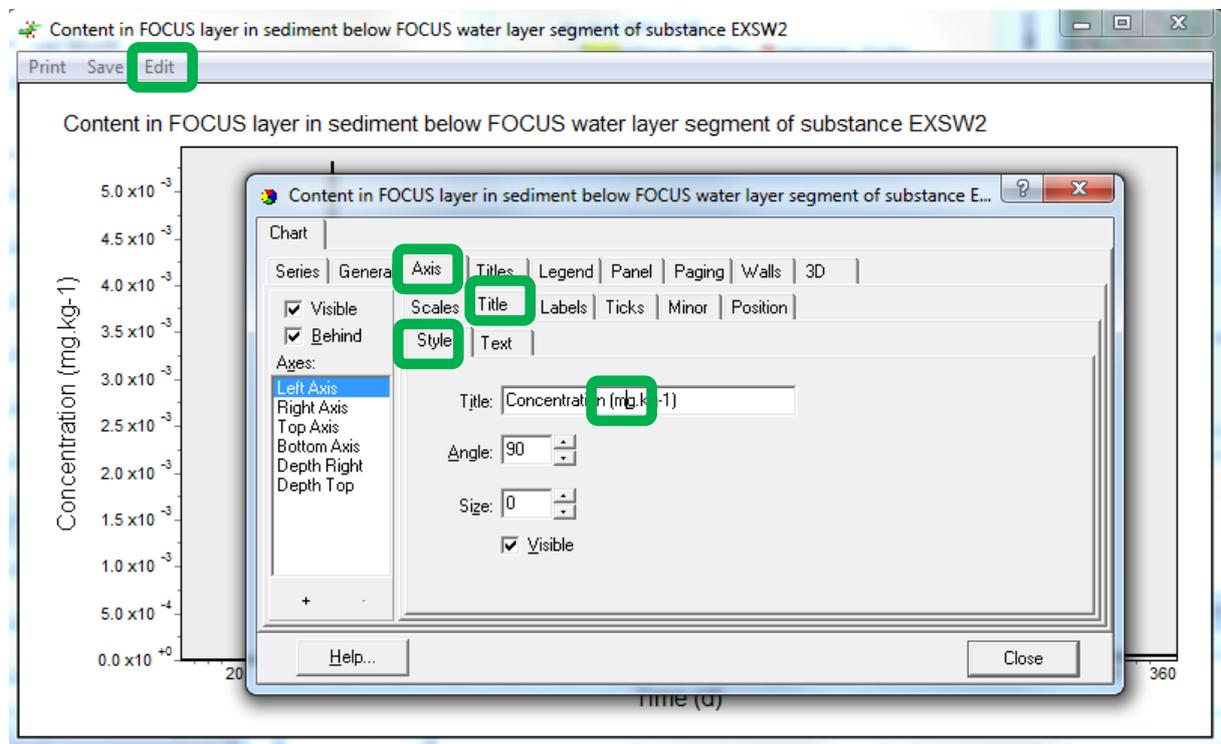
6. Addendum manual FOCUS_TOXSWA 4.4.2 for FOCUS_TOXSWA 4.4.3

The manual of FOCUS_TOXSWA 4.4.2 is available via the user interface of FOCUS_TOXSWA 4.4.3 (via the menu bar, "Help" and select "Help manual"). However the addendum to update this manual for FOCUS_TOXSWA 4.4.3 is not accessible via the menu of the user interface. The addendum is available at:

http://www.pesticidemodels.eu/sites/default/files/downloads/gem/Addendum_to_Manual_%20FOCUS_TOXSWA_4.2.2.pdf

References
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.