

Bug: Drainage runs with metabolite formed both in soil and in water layer or sediment

A bug has been found in FOCUS_TOXSWA 4.4.3 for a metabolite that is formed both in soil and in water layer or sediment, and next, forms a sequential metabolite in the water layer or sediment. The bug may occur in the following metabolite schemes:

- a. Metabolite 1 formed in the soil and formed in the water layer may be transformed into metabolite 2 in the water layer:

Soil: parent -> metabolite 1
Water: parent -> metabolite 1
Water: metabolite 1 -> metabolite 2

- b. Metabolite 1 formed in the soil and formed in the water layer may diffuse into the sediment, where it is transformed into metabolite 2:

Soil: parent -> metabolite 1
Water: parent -> metabolite 1
Sediment: metabolite 1 -> metabolite 2

- c. Metabolite 1 formed in soil and parent diffused into the sediment where it is transformed into metabolite 1, may be transformed into metabolite 2 in the sediment:

Soil: parent -> metabolite 1
Sediment: parent -> metabolite 1
Sediment: metabolite 1 -> metabolite 2

- d. Metabolite 1 formed in the soil and parent diffused into the sediment where it is transformed into metabolite 1, may diffuse back to the water layer where it is transformed into metabolite 2:

Soil: parent -> metabolite 1
Sediment: parent -> metabolite 1
Water: metabolite 1 -> metabolite 2

This bug occurs only in drainage runs. The TOXSWA GUI writes an incomplete metabolite scheme to the TOXSWA input file, i.e. omitting the sequential metabolite (metabolite 2) formed in water layer or sediment. A workaround is to do the drainage run outside the GUI. The steps are:

- (1) open the SWASHprojects\projectname\TOXSWA folder,
- (2) replace the compound section (Section 6) of the runID.twx file of the drainage run by the compound section of a runoff file in the same project,
- (3) edit the toxswa.bat file; replace the runID in the file by the runID of the drainage run,
- (4) double-click the toxswa.bat file, and
- (5) the output of the run can be accessed from the GUI.