**Addendum to update the manual of FOCUS_TOXSWA 4.4.2 for FOCUS_TOXSWA 4.4.3**

This form intends to update the manual of FOCUS_TOXSWA 4.4.2 (Beltman *et al.*, 2014) for FOCUS_TOXSWA 4.4.3. While FOCUS_TOXSWA 4.4.2 could only account for the formation of one metabolite in the water of the upstream catchment of FOCUS stream scenarios, this new FOCUS version of the TOXSWA model can handle the formation of more metabolites in one simulation. FOCUS_TOXSWA 4.4.2 was submitted to the FOCUS Version Control Group ([http://focus.jrc.ec.europa.eu/](http://focus.jrc.ec.europa.eu/)), but never released. By substituting the changes described in this form into the manual of FOCUS_TOXSW 4.4.2 the manual is valid for version 4.4.3.

The correction factors for metabolite formation in the upstream catchment of the FOCUS stream scenarios are substance-specific as well as scenario-specific. They are calculated by FOCUS_SWASH with the aid of the degradation rates of the parent and of the metabolite and a conservative estimate of the residence time in the upstream catchment of the scenario.  They are stored in the database of FOCUS_SWASH, from where they are retrieved in the TOXSWA-GUI

**Updated parts of section 3.3.10 of the FOCUS_TOXSWA 4.4.2 manual:  Section 7 Management**

The updates below refer to (i) the text under the subheading  Metabolite formation in water in upstream catchment and (ii) part of Figure 3.7.

*Metabolite formation in water in upstream catchment*
In the upstream catchment of FOCUS stream scenarios metabolites are formed in molar fractions varying between 0 (no metabolite formation) and 1 (1 mol parent has been transformed into 1 mol metabolite). A factor, $CF_{m,up}$ (FraMetForUps), is needed to account for this. This correction factor is specific for the metabolite, the substance and the scenario (because of the temperature as well as the time spent in the upstream catchment during which the metabolite can be formed). The correction factor accounts both for metabolite mass formed from parent mass deposited by spray drift on the water surface area in the upstream catchment, and for metabolite mass formed from parent mass originated from drainage or runoff in the upstream catchment. See Adriaanse et al. (2014) for the theoretical basis of this correction factor and the procedure to calculate it. Because these correction factors depend on the substance as well as the scenario they have been incorporated in the management section of the input file (see Fig. 3.7).

```
*-----------------------------------------------------------------------------
*
* Section 7: Management section
*-----------------------------------------------------------------------------
*
.


.
* If: CallingProgram = FOCUS and OptWaterSystemType = WaterCourse
Yes          OptUpsInp               ! Switch for upstream catchment treated (Yes, No)
0.           RatAreaUpsApp (-)       ! Ratio of upstream catchment treated [0.0 – 1]
0.774        FraMetForUps_MWP1 (-)   ! Correction Factor primary metabolite upstream catchment
0.957        FraMetForUps_MWP2 (-)   ! Correction Factor primary metabolite upstream catchment
```

*Figure 3.7 Excerpt of the Management section in the TOXSWA input file showing the correction factor for metabolite formation in the upstream catchment of FOCUS stream scenarios, $CF_{m,up}$ (FraMetForUps). In this example two primary metabolites are formed, MWP1 and MWP2.*

**Updated parts of section 4.4.4 of the FOCUS_TOXSWA 4.4.2 manual:  Special cases: metabolite formation in the upstream catchment of FOCUS streams**

The updates below refer to Figure 4.3 and its three-lines description given above this figure. In addition the last two sentences of this section can be deleted: "The entry of this factor for FOCUS Step 3 runs……. , i.e. a conservative estimate."

In the TOXSWA_GUI the correction factors $CF_{m,up}$ can be viewed (FOCUS Step 3 calculations) or entered or changed (FOCUS Step 4 calculations) at the Edit runs form accessed via the Entries tab, in the section Upstream catchment entries (Fig. 4.3a). By clicking the button CF the *CF* form can be accessed (Fig. 4.3b).

Figure 4.3a Entries tab of the Edit runs form. The section Upstream catchment entries contains the button CF; after clicking on it the correction factors for formation of primary water metabolites in the upstream catchment of FOCUS stream scenarios are shown.



Figure 4.3b Browse Correction Factor water metabolites form.